Metric properties of large graphs

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Abstract

Large scale *communication networks* are everywhere, ranging from data centers with millions of servers to social networks with billions of users. This thesis is devoted to the fine-grained complexity analysis of combinatorial problems on these networks.

In the first part, we focus on the embeddability of communication networks to tree topologies. This property has been shown to be crucial in the understanding of some aspects of network traffic (such as congestion). More precisely, we study the computational complexity of Gromov hyperbolicity and of tree decomposition parameters in graphs – including treelength and treebreadth. On the way, we give new bounds on these parameters in several graph classes of interest, some of them being used in the design of data center interconnection networks. The main result in this part is a relationship between treelength and *treewidth*: another well-studied graph parameter, that gives a unifying view of treelikeness in graphs and has algorithmic applications. This part borrows from graph theory and recent techniques in complexity theory.

The second part of the thesis is on the modeling of two privacy concerns with social networking services. We aim at analysing information flows in these networks, represented as dynamical processes on graphs. First, a coloring game on graphs is studied as a solution concept for the dynamic of online communities. We give a fine-grained complexity analysis for computing Nash and strong Nash equilibria in this game, thereby answering open questions from the literature. On the way, we propose new directions in algorithmic game theory and parallel complexity, using coloring games as a case example. Finally, we introduce a new learning problem that is motivated by the need for users to uncover any misuse of their personal data online. We give positive and negative results on the tractability of this problem.

Keywords: Graph; Algorithms; Complexity in P; Gromov Hyperbolicity; Treelength; Treebreadth; Treewidth; Coloring games; Nash equilibrium; Boolean function learning.

Résumé

Les grands *réseaux de communication* sont partout, des centres de données avec des millions de serveurs jusqu'aux réseaux sociaux avec plusieurs milliards d'utilisateurs. Cette thèse est dédiée à l'étude fine de la complexité de différents problèmes combinatoires sur ces réseaux.

Dans la première partie, nous nous intéressons aux propriétés des plongements des réseaux de communication dans les arbres. Ces propriétés aident à mieux comprendre divers aspects du trafic dans les réseaux (tels que la congestion). Plus précisément, nous étudions la complexité du calcul de l'hyperbolicité au sens de Gromov et de paramètres des décompositions arborescentes dans les graphes. Ces paramètres incluent la longueur arborescente (treelength) et l'épaisseur arborescente (treebreadth). Au passage, nous démontrons de nouvelles bornes sur ces paramètres dans de nombreuses classes de graphes, certaines d'entre elles ayant été utilisées dans la conception de réseaux d'interconnexion des centres de données. Le résultat principal dans cette partie est une relation entre longueur et largeur arborescentes (*treewidth*), qui est un autre paramètre très étudié des graphes. De ce résultat, nous obtenons une vision unifiée de la ressemblance des graphes avec un arbre, ainsi que différentes applications algorithmiques. Nous utilisons dans cette partie divers outils de la théorie des graphes et des techniques récentes de la théorie de la complexité.

La seconde partie de cette thèse est consacrée à la modélisation de deux problèmes motivés par le respect de la vie privée sur les réseaux sociaux. Notre objectif est d'analyser les flux d'information dans ces réseaux, représentés par des processus dynamiques sur des graphes. Tout d'abord, nous étudions un jeu de coloration sur les graphes, en tant que concept de solution pour la dynamique des communautés en ligne. Nous donnons une analyse fine de la complexité du calcul d'équilibres de Nash dans ce jeu, ce qui nous permet de répondre à des questions ouvertes de la littérature. De plus, nous proposons de nouvelles directions en théorie algorithmique des jeux et en théorie de la complexité parallèle, que nous illustrons à l'aide des jeux de coloration. Finalement, nous proposons un tout nouveau problème d'apprentissage, motivé par le besoin des utilisateurs en ligne d'identifier les mauvais usages de leurs données personnelles. Nous donnons des résultats, positifs comme négatifs, sur la faisabilité de ce problème.

Mots clés: Graphe; Algorithmes; Complexité dans P; Hyperbolicité; Treelength; Treebreadth; Treewidth; Jeux de coloration; Équilibre de Nash; Apprentissage de fonction Booléenne.

Contents

Chapter 1

Introduction

Contents

1.1 Context

Information sharing online has been gaining momentum over the last decades. As examples, as of 2015 there have been 205 billion emails sent on a daily basis [Ema]; Twitter reports on 500 million messages exchanged a day on its social platform [Twi]; more generally, the global Internet traffic has been observed to grow from 100 GB per day in 1992 to 20,235 GBps in 2015 [Cisa]. Accordingly, the volume of data stored also has increased, and it is now expected to exceed 40 zettabytes by 2020 [IDC].

As we now enter into this "zettabyte era" [Cisb], information technologists are confronted to several issues that are regularly covered by the media. Two of them are addressed in this thesis.

- **Scalability** – is defined in [Ten16] as the requirement for the algorithms to run in quasi-linear time in the size of the network. Put in less restrictive terms, there is a need for efficient algorithms in order to process the communication networks. Higher demands for such algorithms emerge from numerous domains, including telecommunications, social networks, bio informatics, computer vision, and economics. However, the rapid expansion of information sharing and data collection has lead these networks to scale up, with now millions of servers in some data centers [DCM], billions of users in social networks [FBN], etc. Textbook methods do not scale well with networks of these sizes, thereby increasing the gap between what we aim at computing and what can be achieved in practice. Hence, there is a need for revisiting what efficient/scalable computation means in this context.

  We will propose advances in this direction based on tools from (algorithmic) graph theory and complexity theory.

- **Privacy** – is defined in [EDP] as "*a right which prevents public authorities [or any other organization or individual] from measures which are [invasive for the respect of private life], unless certain conditions have been met.*" In particular, the agressive collection of data by online companies has started raising alarms as now reports on potential abuses are surfacing on a regular basis [Gou14, Mat12, VDSVS12, The14]. Therefore, there is a need for predictive models in order to detect, on an individual level, when these violations occur, or even better to identify them.

  Our main tools in this task will be computational learning theory and algorithmic game theory.

Before summarizing our contributions in Section 1.2, let us sketch our approach for the thesis. Roughly, this work concentrates on a collection of combinatorial problems on graphs, whose study is motivated by these above two issues in information technology. Since the proposed solutions are aimed at scaling up with large networks, we are particularly interested in obtaining a *fine-grained* complexity analysis for these problems.

In particular, our study in Part I puts the focus on some graph invariants which have been shown in previous works [NS11] to be related with these above two issues in information technology. Studying properties of the "complex networks" and their applications is not new, and this area has been proved successful in finding relevant parameters and properties to study, such as: clustering [LLDM09], power-law degree distribution [BAJ00], navigability [BKC09], (ultra) small world phenomenon [WS98], structural decomposition into a core and peripheries [DGM06], etc. In this work, we emphasize on the *metric tree-likeness* in graphs: a topic that has been receiving growing attention over the last decades and that summarizes at measuring how close the distance distribution of a graph is to a tree metric [Gro87].

We argue that studying the properties of the distance distribution is a natural choice when considering information propagation in the graph. Furthermore, we will detail more in Part I how the advantages and disadvantages of trees (with nice algorithmic applications on the one hand, but vulnerabilities on the other hand) can be translated to the graphs that are (metrically) "tree-like".

This main line of study will be completed with the complexity analysis of two dynamical processes on graphs in Part II, that both cover some aspects of privacy in communication networks. Simply put, the aim of this side line of the thesis is to design scalable tools in order to enforce privacy in these networks.

1.2 Contributions

Our work is presented in two separate parts which can be read independently. We present their content in Sections 1.2.1 and 1.2.2, respectively.

Full papers can be found in the appendix. Indeed, we made the choice not to include all proofs in the body of the chapters, partly for ease of readability as some of them are very long (dozens of pages). We will only give the proofs that, in our opinion, are the best illustrations of our techniques. Sketches of the longest proofs will be also provided.

1.2.1 Part I: Metric tree-likeness in graphs

A main objective of Part I is to obtain a finer-grained analysis for the complexity of computing (metric) tree-likeness parameters and decompositions of graphs. Especially, can these properties be computed on large-scale graphs, with sometimes millions of nodes and billions of edges ? On the way, our analysis will conduce to study the relationships between metric tree-likeness in graphs and other graph properties (structural, topological, algebraic, etc.).

1.2.1.1 Chapter 2: A survey on graph hyperbolicity

This chapter introduces the notion of graph hyperbolicity, that gives lower and upper bounds on the best possible distortion of the distances in a graph when it is embedded into a tree.

First, we show positive and negative results on the complexity of computing this parameter. In particular, on the positive side we propose a preprocessing method for decreasing the size of the input graph by using the well-known clique-decomposition [BPS10], of which we give a fine-grained analysis. However, on a more negative side, we prove that the recognition of graphs with small hyperbolicity (at most $1/2$) is computationally equivalent to the detection of induced squares in a graph. The latter result implies a conditional *cubic* lower-bound on the complexity of computing graph hyperbolicity. This is joint work with Nathann Cohen, David Coudert and Aurélien Lancin [CD14, CCDL17].

Then, we establish new bounds on this parameter in some graph classes that are used in the design of data center interconnection networks. In practice, these bounds can be used in order to sharply estimate the hyperbolicity in these classes of graphs. We complement these results with a fine-grained analysis of the variations of hyperbolicity that may be caused by various graph operations such as line graph, clique graph, etc. This analysis is particularly interesting in some cases where the operation can be efficiently reversed (*e.g.*, the root of a line graph can be computed in linear time [Whi92]), as then it leads to new preprocessing methods for the computation of graph hyperbolicity. This is joint work with David Coudert [CD16a, CD16b].

1.2.1.2 Chapter 3: Tree decompositions with metric constraints on the bags

New results are presented on the complexity of computing *tree decompositions* (decompositions of a graph in a tree-like manner) with metric constraints on their bags (*a.k.a.*, subgraphs resulting from the decomposition).

A finer-grained analysis of the complexity of computing the clique-decomposition is first presented. This problem is proved to be computationally equivalent, under standard complexity assumptions, to the detection of triangles in graphs and the multiplication of two square matrices. On a more positive side, we show that it can be solved in quasi-linear time on some classes of graph where the maximum size of a clique is bounded. This is joint work with David Coudert [DC17].

Second, we answer open questions in the literature on the complexity of computing treebreadth, pathbreadth and pathlength: that are tree-likeness parameters all related to the notion of graph hyperbolicity. Namely, computing any of these parameters is an NP-hard problem. In particular, recognizing the graphs with treebreadth at most one is NP-complete. However, we prove that the latter problem can be solved in polynomial-time for bipartite graphs and planar graphs. This is joint work with Sylvain Legay and Nicolas Nisse [DLN16a].

Finally, we investigate the relationships between another metric tree-likeness parameter, called *treelength*, and a well-known *structural* tree-likeness parameter that is called *treewidth*. Roughly, we establish upper and lower bounds on the treewidth with linear dependency on the treelength in the classes of graph with bounded-length isometric cycle (*i.e.*, with no shortcut) and bounded genus (*i.e.*, that can be drawn with no edge-crossing in a surface of bounded Euler genus). On the scalability point of view, algorithmic applications of these results will be further discussed. This is joint work with David Coudert and Nicolas Nisse [CDN16].

1.2.2 Part II: Privacy at large scale in social graphs

Two problems on privacy are discussed and studied in this part. Our objective is to obtain a finer-grained analysis for the complexity of these two problems.

1.2.2.1 Chapter 4: The computation of equilibria in coloring games

We consider a coloring game played on a graph. This game has been proposed in [KL13] as a solution concept for the dynamics of communities' formation in social networks. Earlier applications of the game have been suggested in [CKPS10] for securing group communications.

We present some new results on the complexity for computing equilibria in this game. More precisely, better-response dynamics can be used in order to compute a stronger notion of Nash equilibrium: that is robust to every coalition of agents of size at most a *fixed k*. On the positive side, we establish the exact convergence time of the dynamic for coalitions of size at most two. However, on the negative side, we prove that this convergence time is *superpolynomial* for coalitions of size at least four, thereby answering negatively to open questions from [EGM12, KL13]. This is joint work with Dorian Mazauric and Augustin Chaintreau [DMC13a, DMC17].

The latter results are complemented with a refined analysis for the complexity of computing a Nash equilibrium in this game (robust to coalitions of size one). This problem will be shown to be PTIME-hard under parallel reductions (and in particular, to logspace reductions), which is strong evidence that it is inherently sequential [Duc16].

Then, the remaining of the chapter is devoted to a natural generalization of coloring games on edge-weighted graphs. We give sufficient conditions for the existence of equilibria in these games depending on the structure of the underlying graph. We also propose surprising constructions of games that do not admit such equilibria. Last, we prove that the recognition of generalized coloring games that admit such equilibria is NP-complete. Extensions of all these results to broader classes of games will be discussed. This is joint work with Dorian Mazauric and Augustin Chaintreau [DMC12, DMC13a, DMC17].

1.2.2.2 Chapter 5: Learning formulas in a noisy model

We next focus on a learning problem whose context can be roughly described as follows. Suppose we are given a fixed ground-set $\mathcal{D}$ (representing keywords) and a graph where each node is labeled with a subset of $\mathcal{D}$ (*i.e.*, a collection of keywords). The nodes are assigned a Boolean under some (black-box) random process, that is correlated with an unknown Boolean function over the labels. Then, the objective is to learn this function. We aim at modeling with this problem the detection of any (mis)use of individual data by online advertisers.

First, we propose an algorithm for learning the function in the simpler case where it depends on at most one input. The latter algorithm will be the cornerstone of more sophisticated methods in order to learn any function – but under more restrictive hypotheses. Additional constraints are proved to be necessary in the general case, as otherwise the function cannot be learnt already if it depends on two inputs. This is joint work with Mathias Lécuyer, Francis Lan, Max Tucker, Riley Sphan, Andrei Papancea, Theofilos Petsios, Augustin Chaintreau and Roxana Geambasu [LDL$^+$14, DLCG15, DTC17, CD17].

1.3 Preliminaries and notations

We borrow from the graph terminology of [BM08, Die10]. All graphs considered will be finite, undirected, unweighted, simple (hence, with neither loops nor multiple edges) and connected. In this situation, for every graph $G = (V, E)$ we can define the distance between every two vertices $u, v \in V$ as the minimum number of edges onto a uv-path of G. This distance is denoted by $\mathrm{d}_G(u, v)$ in what follows, or simply $\mathrm{d}(u, v)$ when there is no ambiguity on the graph G. Our proofs will make use of the notions of subgraphs, induced subgraphs and isometric subgraphs, the latter denoting a subgraph H of a graph G such that the distance between every two vertices in H is the same in H as in G.

Let us introduce additional distance notations. The *eccentricity* of a vertex $v \in V$, denoted by $ecc(v) = \max_{u \in V} \mathrm{d}_G(u, v)$ is the maximum distance in G between v and another vertex. The *diameter* of G, denoted by $diam(G) = \max_{v \in V} ecc(v)$, is the maximum eccentricity of a vertex of G. Furthermore, let $B_G(v, r) = \{u \in V \mid \mathrm{d}(u, v) \leq r\}$ be the ball of radius r centered on vertex v. The *radius* of G, denoted by $rad(G) = \min_{v \in V} ecc(v)$, is the least r such that $B_G(v, r) = V$ for some vertex

v. Finally, let $N_G[v] = B_G(v,1)$ be the closed neighbourhood of a vertex. The open neighbourhood of v is defined as $N_G(v) = N_G[v] \setminus v$. By extension, let us define for every subset $S \subseteq V$ its open neighbourhood $N_G(S) = \left(\bigcup_{v \in S} N_G(v)\right) \setminus S$ and its closed neighbourhood $N_G[S] = N_G(S) \cup S$. We will remove the subscript when no ambiguity occurs.

1.4 List of publications

Journal papers

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International conference papers

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[LDL$^+$14] M. Lécuyer, G. Ducoffe, F. Lan, A. Papancea, T. Petsios, R. Spahn, A. Chaintreau, and R. Geambasu. Xray: Enhancing the web's transparency with differential correlation. In *USENIX Security Symposium*, pages 49–64, 2014. (Cited in pages 5, 159, 160, 161, 162, 163, 165, 166, 168, 169, 170, 176, 188, 189 and 223.)

National conference papers

[CD16] D. Coudert and G. Ducoffe. Liens entre symétries et étirements de routages dans les réseaux d'interconnexion de centres de données. In *ALGOTEL 2016 – 18èmes Rencontres Francophones sur les Aspects Algorithmiques des Télécommunications*, pages 1–4, 2016. (Uncited.)

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[CD17] A. Chaintreau and G. Ducoffe. A theory for ad targeting identification. In preparation, 2017. (Cited in pages 5, 159, 163, 169, 184 and 223.)

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Part I

Metric tree-likeness in graphs

The purpose of the next two chapters is to study geometric and topological properties of graphs. They have been shown to be directly related to some important aspects of communications in large-scale data networks, such as *e.g.*, their performances, reliability and security [NS11]. Hence the need for better understanding and computing these graph properties, in order to better analyse and improve upon these aspects of network communications.

- Chapter 2 is a survey on **graph hyperbolicity**: a parameter that somewhat represents the "curvature" of the network. We are particularly interested in characterizing the graph classes where this parameter is either bounded or unbounded (respectively called hyperbolic and non hyperbolic graph classes), and to improve upon its computation in large-scale graphs.
- Chapter 3 presents new results on **tree decompositions** in graphs. Namely, positive and negative results are obtained on the complexity for computing tree decompositions that are defined via metric constraints on their bags. On the way, a finer-grained study of the relationships between structural and metric graph properties is proposed, that culminates with new relationships between the two graph parameters called *treewidth* and *treelength*.

Chapter 2

A survey on graph hyperbolicity

Summary

This chapter summarizes my work on graph hyperbolicity. It will be presented as a survey. The initial motivation for this work was to improve the practical computation of hyperbolicity on large graphs. In particular, I focused on the following general question: among the graph transformations that can be efficiently computed, which ones do not affect the value of hyperbolicity by more than a moderate term (multiplicative or, preferably, additive) ? I proved it was the case for clique-decomposition (Section 2.6.2.2) and the line graph operation (Section 2.4.3). Furthermore, my work on clique-decomposition has been successfully applied on large co-authorship graphs in order to compute their hyperbolicity [CCDL17].

I also proved new lower-bounds on graph hyperbolicity (using graph endomorphisms) that may further help reducing the complexity for computing the hyperbolicity in some graph classes (Section 2.5.2.4). By doing so, I answered an open question from researchers at the University of Girona (private communication) who aimed at sharply estimating the hyperbolicity of very large underlying topologies that are used for data center interconnection networks. Indeed, these graphs have more than one million nodes each, that overrule the current limitations of the existing algorithms for computing this parameter. By using my lower-bound techniques, I was able to give the exact value of the hyperbolicity for most topologies, and to prove close lower and upper bounds for the hyperbolicity of many other ones [CD16a].

I complemented these results with a conditional lower-bound on the complexity of recognizing graphs with hyperbolicity at most 1/2 (Section 2.6.3). It suggests that there does not exist any truly subcubic *combinatorial* algorithm for computing hyperbolicity on general graphs.

All my papers on graph hyperbolicity [CCDL17, CD16a, CD16b, CD14] are collected in the appendix.

Contents

2.1 Introduction

In this chapter we survey the study on Gromov hyperbolicity in graphs [Gro87, Ben13]. Roughly, it is a parameter which measures how close a given metric space is to a *metric tree* [Ban90, Bun74] (formal definitions are postponed to Section 2.3). In particular, it gives sharp bounds on the least distortion of the distances in a (finite) metric space when its elements are mapped to the nodes of an edge-weighted tree. Trees and bounded diameter graphs (embeddable into any shortest-path tree with constant distortion of their distances) will be shown to be trivially hyperbolic.

Gromov hyperbolicity is a broad concept that can be defined for any metric space. In fact, it has been first investigated for word metric spaces on groups [Gro87]. This notion of hyperbolicity in groups is now regarded as a powerful tool that can be used in order to capture broad classes of groups with precise and important structural properties [GdLH90]. In particular, it has applications in the study of *automatic groups* [Gro87, EPC+92], where informally speaking, elements of the groups are the vertices of some (Cayley) graph and it can be checked with finite-state automata whether two words represent either a same vertex or two adjacent vertices. Automatic groups have nice algorithmic applications. For instance the word problem can be solved in quadratic time for these groups [EPC+92]. These applications transpose to groups with finite hyperbolicity, that are a particular case of automatic groups.

There is now a rich literature on the hyperbolicity of groups as metric spaces [ABC+91, BH11, GdLH90]. In this chapter, built as a survey, we emphasize on some results that are more specific, and relevant, to graph theory.

I will present my contributions on this topic in this chapter. They will be highlighted at various places in what follows. I hope that the organization of this chapter will help the reader to have a good overview of the positioning of my work in the growing literature on graph hyperbolicity.

Foreword

Let us start motivating the study of graph hyperbolicity in computer science. These aspects will be further developed in Sections 2.2 and 2.7.

In what follows, hyperbolicity should be understood as a graph parameter which gives bounds on the least distortion of the distances in a graph when its vertices are mapped to points in some "tree-like" metric space. Namely, such spaces comprise (weighted) trees, Hyperbolic spaces, and more generally speaking spaces with negative curvature. In general, embedding a graph into one of those spaces with minimum distortion is NP-hard [ABF+98]. As we shall see in this chapter, one interest of hyperbolicity is that it provides sharp bounds on this distortion in polynomial time (we will come back to this aspect in Section 2.7.1).

A rough description of hyperbolicity in graphs can be found at the beginning of Section 2.2. It should be noted, however, that there exists a bewildering zoo of "equivalent" definitions for this concept, whose formal presentation is postponed to Section 2.3.

Why studying hyperbolicity ? Depending on its order of magnitude, the value of hyperbolicity has some implications on network properties which, to my mind, motivate the study of this parameter in graphs. Indeed, studies on it have found applications in the analysis of congestion [CDV16], routing schemes [AGCFV, CDE+12, GL05], network security [JL04], bioinformatics [DMT96, MS99] and even in advertising allocation in social networks [MGHB15] — to name a few. I shall detail more about the above in Section 2.2. Most of these applications follow from, and can be better explained by, the close relationship between hyperbolicity and the best possible stretch (or distortion) of the distances in a graph when it is embedded into a Hyperbolic space (see [BS11, VS14]).

Hyperbolicity in graphs has strong geometric interpretations. It allows to extend the mathematical concept of *curvature* to discrete combinatorial structures such as graphs. Further, it can be used to characterize the so-called "underlying hidden geometry" of complex networks [KPK+10]. In this aspect, graph hyperbolicity adds up to other classification critera for networks such as (ultra) small world phenomenon [WS98], power law degree distribution [BAJ00], navigability [BKC09], high clustering coefficients [LLDM09], existence of a core [DGM06], etc. Relationships between hyperbolicity and these more classical features have been investigated, *e.g.*, in [CFHM13, JLB08, DX09, ASM13].

On the algorithmic side, another interest of hyperbolicity is that it helps analyzing, and designing, some graph heuristics on large-scale networks. For instance, the *2-sweep* heuristic for computing the diameter is well-known to provide very good results in practice [MLH08], and such good results can be explained assuming a bounded hyperbolicity [CDE+08]. I shall come back to the algorithmic applications of hyperbolicity in Section 2.7.

We next introduce two general objectives in the study of graph hyperbolicity, that will be the backbone of the main technical sections of this chapter. On the way, the personal contributions in this chapter are summarized and classified with respect to these two general objectives.

Namely, what we aim at obtaining through this study on hyperbolicity is: a better characterization of hyperbolic and non hyperbolic graph classes (Section 2.1.1), and a finer-grained analysis of the complexity of computing this parameter (Section 2.1.2). The outline of the chapter will be detailed in Section 2.1.3.

2.1.1 First objective: characterizing "hyperbolic" and "non hyperbolic" graph classes

The first objective is to derive lower and upper bound techniques for graph hyperbolicity. Indeed, it has become a growing line of research to characterize the classes of "hyperbolic" graphs, *a.k.a.* graphs with "small" hyperbolicity. – We shall make more precise what a hyperbolic graph is in Section 2.3.3 –. Partial results on that topic have been obtained in [BRSV13, HPR14] and the papers cited therein. They often derive from upper and lower bounds on the hyperbolicity of a given graph w.r.t. some other graph parameters and properties.

In Sections 2.4 and 2.5, I shall revisit the known bounds on the hyperbolicity of a given graph. Equipped with these bounds, I shall detail their application to some graph classes.

My main contributions in this area, found in collaboration with David Coudert, are twofold.

2.1.1.1 New lower bounds on the hyperbolicity of graphs

First, based on a game-theoretic definition of hyperbolicity, we provide some new lower-bound techniques on the hyperbolicity of graphs. Altogether combined with the existence of certain type of *symmetries* (graph endomorphisms), these techniques are used in order to estimate the correct order of magnitude for the hyperbolicity in various graph classes. In particular, it follows directly from this work that many classical topologies that are used for the design of the data center interconnection networks [AK89] have their hyperbolicity that is proportional to their diameter.

This part of the contributions has been published in [CD16a]. I will describe these lower-bound techniques in Section 2.5.2, with some new results that are yet to be published.

2.1.1.2 A framework to bound the variations of hyperbolicity

Second, I present a simple framework in order to lower and upper bound the variations of hyperbolicity that may be caused by various graph operations. This framework applies to the line graph [Whi92], clique graph [Ham68] and biclique graph [GS10] operations, among some others, and the bounds so obtained are either new or improving upon the existing ones. Furthermore, the framework is mainly based on a new property of the hyperbolicity of bipartite graphs, that is of independent interest.

This part of the results has been published in [CD16b]. I will expand on it in Section 2.4.

2.1.2 Second objective: computing the hyperbolicity of large graphs

Then, as the second main technical part of this chapter, we will consider the complexity of computing the hyperbolicity of a given graph. That is, we will review the best-known algorithms for computing this parameter (exact and approximate), heuristics, and conditional lower-bounds on the best possible complexity for doing so. We note that an efficient computation of hyperbolicity can help characterizing which graph classes are hyperbolic. Furthermore, computing the hyperbolicity is a prerequesite for some of the above-mentioned applications to network problems [KL06, VS14] (see also Section 2.7).

There is a trivial algorithm to compute the hyperbolicity of a given n-vertex graph in $\mathcal{O}(n^4)$-time and $\mathcal{O}(n^2)$-space. Therefore, the problem is polynomial-time solvable (complexity class P). The latter is often regarded as a synonym for "tractable" [Reu16]. However, with the growing size of real-life networks, ranging from thousands to millions of nodes and billions of edges, we need to revisit the time and space complexity of polynomial problems. This finer-grained complexity of polynomial problems has become a boiling topic of research [Wil16]. In this aspect, we note that it is also of independent interest to study on the complexity of computing the hyperbolicity so as to obtain a better understanding of the hardness in P.

I will present in Section 2.6 the state-of-the-art algorithms for computing the hyperbolicity. I will also present some conditional lower-bounds on the time complexity for this problem.

My main contributions in the area can be summarized as follows:

2.1.2.1 A preprocessing method for the computation of hyperbolicity

On the positive side, relationships between hyperbolicity and *clique-minimal decomposition* [BPS10] are proved and exploited for algorithmic purposes. This is joint work with Nathann Cohen, David Coudert and Aurélien Lancin. See also the PHD thesis of Aurélien Lancin [Lan14] for complementary information on this work.

Precisely, we prove that the hyperbolicity of a graph is at most one unit off from the maximum hyperbolicity from its *atoms* – *a.k.a.* the subgraphs resulting from its decomposition by clique minimal separators. Then, we base on this result in order to design a preprocessing algorithm for the computation of hyperbolicity. It substitutes to a given graph a collection of supergraphs of its atoms.

As a byproduct, we obtain a linear-time algorithm for computing the hyperbolicity of a given *outerplanar graph.*

These results [CCDL17] are to be submitted for publication in a journal. They will be detailed in Section 2.6.2.

2.1.2.2 Conditional lower-bound on the recognition of graphs with small hyperbolicity

Finally, a computational equivalence is proven between the recognition of graphs with hyperbolicity at most 1/2 and the detection of induced cycles of length at most four in graphs. It can be derived from this result a conditional lower-bound on the complexity of computing hyperbolicity, as well as a theoretically better algorithm for the recognition of 1/2-hyperbolic graphs.

These results, found in collaboration with David Coudert, have been published in [CD14]. I shall come back to them in Section 2.6.3.

2.1.3 Outline of the chapter

We start providing concrete applications of hyperbolicity in different fields of computer science (Section 2.2). In our opinion, these applications should better motivate the study of this parameter in graphs, and especially in network analysis. A rough definition of hyperbolicity is also given in Section 2.2, whose only role is to make the applications of this parameter more intuitive.

Then, formal definitions and preliminary results will be given in Section 2.3 (restating properly the informal definition of Section 2.2 with details). This section is the most technical one of the chapter, as it goes deeper in the relationships between hyperbolicity and many other “equivalent” graph properties.

Sections 2.4 and 2.5 are devoted to our first main objective: to find upper and lower bounds on graph hyperbolicity, with the two sections being devoted respectively to upper and lower bound techniques.

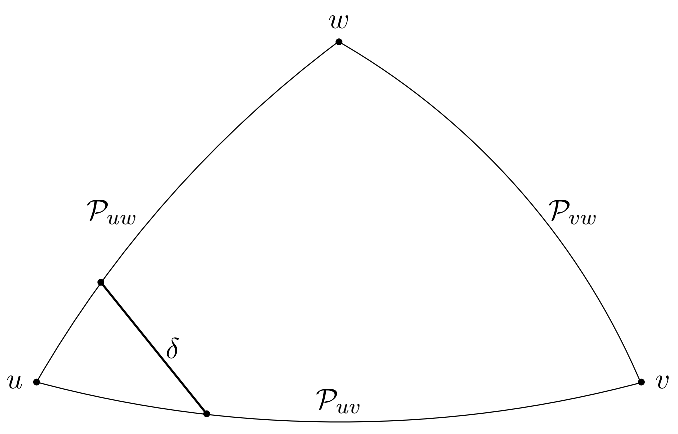


Figure 2.1: a geodesic triangle $\Delta(u, v, w)$.

Finally, the two last technical Sections 2.6 and 2.7 cover the algorithmic aspects of this parameter. In particular, the computational aspects of hyperbolicity are covered in Section 2.6, that is the second main objective in our study.

In Section 2.7 we detail algorithmic applications of hyperbolicity to various graph problems, that can be seen as a technical prolongation of Section 2.2. This section is placed on purpose after all the other sections, so as to give the reader a better overview of the ("hyperbolic") graph classes to which these algorithmic results can be applied. On the way, we mention several interesting open problems that are left for future work.

We finally conclude the chapter in Section 2.8.

2.2 Motivation

In this section, we will outline fields in computer science where the study of graph hyperbolicity plays a role. Our goal in doing so is to motivate the study of this parameter for computer scientists. Before introducing these applications of hyperbolicity, though, we will need to sketch a few graph properties that are related to this notion. They will be used in what follows in order to better intuit the role played by graph hyperbolicity in some applications.

Let us start giving an intuitive definition of hyperbolicity, that is sometimes named Rips condition in the literature [Gro87].

Consider any three vertices u, v, w in a given connected graph $G = (V, E)$. By the triangular inequality, we have $\mathrm{d}_G(u, v) \leq \mathrm{d}_G(u, w) + \mathrm{d}_G(w, v)$, with $\mathrm{d}_G(u, v)$ being the distance (minimum number of edges onto a uv-path) between u and v in G. We can represent this situation with a *geodesic triangle* $\Delta(u, v, w) = \mathcal{P}_{uv} \cup \mathcal{P}_{uw} \cup \mathcal{P}_{vw}$ with its three respective sides being a fixed shortest uv-path $\mathcal{P}_{uv}$, a fixed shortest uw-path $\mathcal{P}_{uw}$ and a fixed shortest vw-path $\mathcal{P}_{vw}$ (cf. Figure 2.1).

Then, one may wonder how far a detour by vertex w can make us go from the shortest uv-path. The graph G is said to have δ-slim triangles if for every geodesic triangle $\Delta(u,v,w)$, any vertex onto the shortest uv-path $\mathcal{P}_{uv}$ is at distance at most δ from $\mathcal{P}_{uw} \cup \mathcal{P}_{vw}$. The hyperbolicity of G is – up to a constant-factor – the smallest δ such that it has δ-slim triangles.

As an example, if G is a tree then since there exists a unique uv-path, any vertex of $\Delta(u,v,w)$ must lie on two sides of the triangle, and so, the triangles in G are 0-slim. We shall come back to formal definitions of hyperbolicity in Section 2.3. For now, let us describe informally a few properties of graphs with δ-slim triangles.

Property 1: Almost shortest-paths stay close from each other. We first sketch a relationship between the value of hyperbolicity and the distance between (almost) shortest-paths in a graph. Let $\lambda \geq 1$ and $\varepsilon \in \mathbb{R}$ be fixed constants. An (λ,ε)-almost shortest-path between u and v is any uv-path with length at most $\lambda \cdot \mathrm{d}_G(u,v) + \varepsilon$. The length of this path thus differs by at most a fixed constant (multiplicatively or additively) from the length of a shortest uv-path. In particular, a shortest-path is an $(1,0)$-almost shortest-path. In Figure 2.2, the path drawn with thicker edges is an $(2,1)$-almost shortest-path.

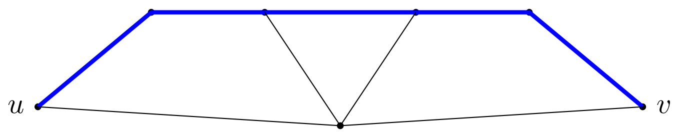


Figure 2.2: a $(2,1)$-almost shortest uv-path.

Graph hyperbolicity measures the closeness of almost shortest-paths, in the following sense. Two paths $\mathcal{P}, \mathcal{Q}$ are at Haussdorf distance [RW09] at most d if every $x \in \mathcal{P}$ is at distance $\mathrm{d}_G(x,\mathcal{Q}) \leq d$ from the path $\mathcal{Q}$, and in the same way every vertex $y \in \mathcal{Q}$ is at distance $\mathrm{d}_G(y,\mathcal{P}) \leq d$ from the path $\mathcal{P}$. A key property of graphs with bounded hyperbolicity is that *any two almost shortest-paths with same endpoints stay close from each other.* That is, their Haussdorf distance is upper-bounded by a linear function of the hyperbolicity of G [Shc13a]

As an instructive example, consider the particular case of two shortest uv-paths. They can be seen as a "flat triangle" $\Delta(u,v,u)$. In particular, in a graph with δ-slim triangles, any two vertices on these shortest-paths that are at same distance from u (or equivalently, to v) in the graph are at distance at most 2δ (*e.g.*, see Figure 2.3). This property is sometimes called the k-fellow traveler property (here, for $k = 2\delta$) [NS95]. The more general Property 1 that almost shortest-paths stay close to each other is sometimes called geodesic stability [Fin15].

Property 2: Existence of a core. The second property that I want to point out can be summarized as a property of concentration for the almost shortest-paths in a graph. Let us fix two arbitrary constants λ and ε. We call a subset S of vertices an α-core if for some fraction α of all possible pairs of vertices in the graph, every

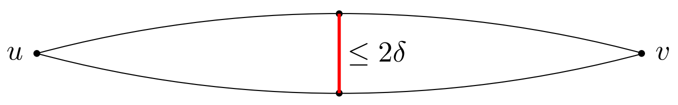


Figure 2.3: Shortest paths stay close in a δ-hyperbolic graph.

(λ, ε)-almost shortest-path with its two ends among these pairs is intersected by S. As an example, the whole vertex-set is trivially a 1-core, and the neighbourhood of a single vertex is an $\frac{n-1}{\binom{n}{2}} = 2/n$-core (it intersects all paths between this vertex and the other $n-1$ vertices). As shown with Figure 2.4, the root of a complete binary rooted tree is an 1/2-core. More generally, every tree has a vertex being an 1/2-core, that is sometimes called a *centroid* [Gol71].

Recall that the hyperbolicity measures the closeness of a graph from a metric tree. The second key property of graphs with bounded hyperbolicity that we focus on in this section is that *there exists a ball of small radius that is an $\frac{1}{2}$-core*. Precisely, the radius of the ball is upper-bounded by a linear function of the hyperbolicity of the graph G [CDV16].

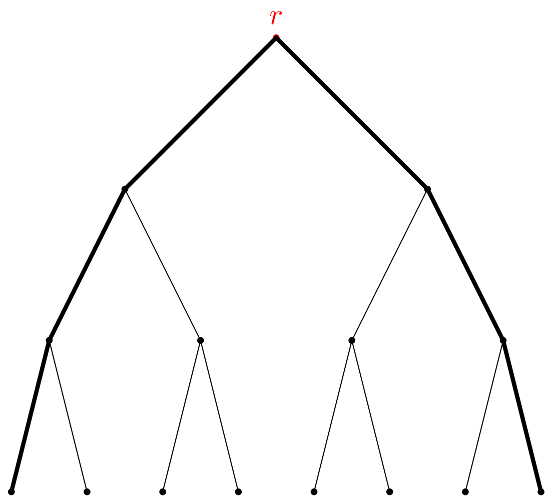


Figure 2.4: all shortest-paths between a vertex in the left subtree and a vertex in the right subtree go through the root.

Altogether, in any graph with bounded hyperbolicity, almost shortest-paths between any pair of vertices stay close to each other and there exists a ball with small radius intersecting almost all of these paths.

Equipped with these two intuitive properties, we will motivate the study of graph hyperbolicity next.

2.2.1 Implications/applications of hyperbolicity

We now list applications and implications of graph hyperbolicity in different fields of computer science. They encompass most of the work on the hyperbolicity in real-life graphs over the last decades. In what follows, these applications are more or less presented from the earliest ones to the newest ones.

Biology

One of the earliest applications of graph hyperbolicity that we are aware of is in biology, where there is a need to obtain some trees reflecting the similarity between a collection of species, *a.k.a.* phylogenetic trees [DMT96, MS99]. Known similarities between the species can be encoded as a graph, whose vertices are the species and whose edge-set corresponds to the pairs of species that are closely similar. Then, the problem summarizes as embedding the species into the leaves of some rooted tree so that the distance between any two species in the tree corresponds to their similarity. However, the available data is biased, and so, such a tree may not always exist. Since, hyperbolicity is a measure of the closeness of a graph to a metric tree, it has been proposed as a natural estimate for the bias of the data. Thus, standard results on graphs with small hyperbolicity (summarized in the later sections) can be applied on the data in order to find an approximate distance-preserving phylogenetic tree [DHH$^+$05].

Geometric routings

Hyperbolicity comes into play in the study of certain *geometric routing schemes*. More precisely, we recall that the hyperbolicity is a measure of the closeness of a graph to a tree. As we shall explain, graph hyperbolicity was shown to provide (lower and upper) bounds on the stretch of the paths obtained with geometric routing schemes in some “tree-like” spaces [AGCFV, VS14].

Roughly, a *routing scheme* is a mapping of each pair of vertices u, v to a uv-path, that is to be followed in order to transit a message between u and v. Usually, we evaluate the quality of a routing scheme on the amount of information that needs to be stored locally at each node in order to retrieve the paths, and on the length of the paths that are used for the transit. That is, on the distributed computing point of view, the aim of *compact routing* schemes is to achieve a good compromise between minimizing the local information to be stored and keeping close to optimal the length of the paths that are used for the mapping.

A geometric routing scheme is one that embeds a given graph into a “simpler” metric space. Then, the paths of the routings are constructed greedily, starting from the source, with each vertex choosing as its successor on the path any of its neighbours that is strictly closer – w.r.t. their coordinates in the metric space – to the destination. In general, routing this way may not allow to reach all possible destinations. For instance, it may lead to infinite loops, and so, additional features are required in order to prevent loss of packet [PR05].

However, in his seminal paper [Kle07], Kleinberg has proved that for *every* graph, there exist embeddings into the *Hyperbolic space* (*i.e.*, canonical space with negative curvature, where the classical Euclidean geometry is replaced by hyperbolic geometry) such that greedy routing is always successful ! This paves the way to an in-depth study of greedy routings in the Hyperbolic space [BPK10, ST08], as well as in other "tree-like" metric spaces such as the word metric space of the free group [CPFV14]. In particular, in some classes of graphs with bounded hyperbolicity, we obtain compact routings with this greedy approach. We also refer to [DDGY07, GL05, KLNS15] for more examples of compact routing schemes in some classes of graphs with bounded hyperbolicity.

Furthermore, it is worth pointing out that embeddings with coordinates of polylogarithmic size in the number of vertices can be computed for those above spaces. In contrast to this positive result, there are graphs for which *greedy routing is always successful* in a given space but that cannot be embedded into the space with coordinates of sublinear size [BL05].

Network congestion

Of importance is also the implications of hyperbolicity on congestion in networks for all-to-all communications. Precisely, consider a unit traffic between each pair of vertices in a network, with the unit flow between any two vertices u, v being equally split among the shortest uv-paths. The *load* of a given vertex is the amount of flow which transits by this vertex. In more graph-theoretic terms, it corresponds to the *betweenness centrality* of the vertex [Bra01]. It is well-known and easy to observe that in trees, there is a a vertex with *quadratic* load $\Theta(n^2)$. What has been observed experimentally in [NS11] is that, more generally, for every graph with small hyperbolicity there is a ball of small radius such that the sum of the loads of the vertices in the ball is also quadratic.

Basing on the above observations, the authors in [JLBB11] have conjectured the existence in hyperbolic graphs of a ball of small radius through which it transits a *constant* proportion of traffic paths. The existence of a 1/2-core with small radius in graphs with bounded hyperbolicity (*i.e.*, Property 2) was shown in order to prove the above conjecture [CDV16]. See also [BT12, LT15, Yan15] for more implications of hyperbolicity on network congestion that take into account different traffic rates on the communications.

Network security

In their survey [JL04] and the papers cited therein, Jonckheere and Lohsoonthorn also have demonstrated the implication of "geometric" graph properties on some aspects of network security. On the way, they classified these geometric properties according to three levels of granularity (small, medium and large scale). At large scale, when considering graphs with a growing diameter, going to infinity (topologies in expansion such as the Internet Service Provider graph), the authors claim the hyperbolicity to be the relevant parameter to study for a better understanding of the geometric aspects of network security.

They support their claim through a case-study of various security attacks. For instance, consider an attempt of "eavesdropping" or "packet sniffing" on the network — unauthorized packet interception along a given link. Due to the limited abilities to reorder the packets with TCP, they are often sent along near-optimal routes, *i.e.*, almost shortest-paths. Hence, since almost shortest-paths stay close to each other in hyperbolic graphs (Property 1), a small hyperbolicity might be detrimental in Information Warfare, causing the routes of the packets to be too close by security standards.

Other attacks and defense strategies where the value of hyperbolicity plays a role are Distributed Denial of Service (DDoS) attacks, and Worm Propagation, to name a few [JL04].

Democracy in complex networks

More recently, a new implication of hyperbolicity was suggested in [BCC15], as a measure of democracy in complex networks, on which we now emphasize. The latter is usually measured through *assortativity*, *i.e.*, the likeliness of vertices that are "similar" in some ways to be adjacent [New02] (see also [ALPT16, Lot15] for other recent approaches). In contrast with this more classical approach, the authors in [BCC15] (see also [ADM14]) consider a set of vertices to be "influencial" if it intersects the (almost shortest) paths between a large number of vertices. With respect to their interpretation, the graph is all the more democratic that it has no influential set of small size.

From this classification, it follows that graphs with small hyperbolicity are "aristocratic" (non democratic). Indeed, we recall that a small hyperbolicity implies the existence of a core with small radius (Property 2), which combined with some properties of real-life graphs (sparse, power-law, etc.) can be shown to be an influential set of small size. Let us point out that it has been experimentally shown that social networks have small hyperbolicity [AAD16]. Therefore, I think that this new notion of "influential set" and its relationships with hyperbolicity could and should be used in the study of *elites* in these networks — *i.e.*, relatively small subsets of vertices that are well-connected and highly connected to the other vertices [ALNP15, ALP11].

The above listing, which of course may be not exhaustive, shows the implications and applications of graph hyperbolicity in various areas. We expect more applications of hyperbolicity to be found.

2.3 Definitions of hyperbolicity

The purpose of this section is to present the formal definitions of graph hyperbolicity and related concepts. The standard definitions for this parameter will be introduced in Section 2.3.1. Then, the focus of Section 2.3.2 will be on "reformulations" of hyperbolicity , *i.e.*, other geometric graph parameters than can be lower and upper bounded by functions of the hyperbolicity. We will end discussing on what should be understood as a "hyperbolic" graph in the remaining of this chapter (Section 2.3.3).

2.3.1 δ-hyperbolic graphs

Let us start introducing the standard definition for graph hyperbolicity. It can be written in two equivalent ways, that will be presented and explained next.

2.3.1.1 Four-point Condition

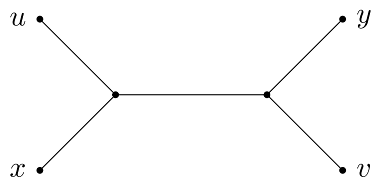
In what follows, the classical definition of hyperbolicity and its interpretation in relation to tree embeddings are given. In the line of many papers [BKM01, BC03, KM02], we define hyperbolicity via the following, rather abstract, four-point condition.

Definition 1 (**4-points Condition, [AJ13, Gro87]**)**.** Let $G = (V, E)$ be a connected graph.

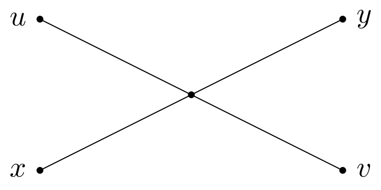
For every 4-tuple u, v, x, y of V, let $\delta(u, v, x, y)$ be defined as half of the difference between the two largest sums amongst:

$$S_1 = \mathrm{d}_G(u, v) + \mathrm{d}_G(x, y),\ S_2 = \mathrm{d}_G(u, x) + \mathrm{d}_G(v, y), \text{ and } S_3 = \mathrm{d}_G(u, y) + \mathrm{d}_G(v, x).$$

The graph hyperbolicity, denoted by $\delta(G)$, is equal to $\max_{u,v,x,y \in V} \delta(u, v, x, y)$. Moreover, we say that G is δ-*hyperbolic* for every $\delta \geq \delta(G)$.



(a) Every vertex on the central path is a centroid of the 4-tuple.



(b) The central vertex is the unique centroid of the 4-tuple.

Figure 2.5: Possible 4-tuples in a tree. Each edge represents a path in the tree.

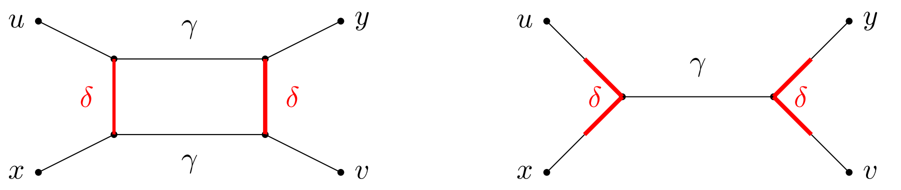
Definition 1 generalizes a well-known four-point characterization of *metric trees*. Indeed, a discrete metric space (and in particular, a graph), can be isometrically embedded into the nodes of an edge-weighted tree if and only if it is 0-hyperbolic [Bun74]. We show one part of this equivalence with Figure 2.5. Indeed, for every 4-tuple u, v, x, y in a tree, it can always be found a centroid such that there is no more than two nodes among u, v, x, y in each branch. Then, it can be checked by the calculation that any such 4-tuple has null hyperbolicity.

Furthermore, for general graphs G (not necessarily metric trees), hyperbolicity can also be interpreted in terms of tree embedding. In order to show that, let us fix any four vertices u, v, x, y of G. Suppose we aim at embedding u, v, x, y in a tree T such that $\mathrm{d}_G(s,t) \leq \mathrm{d}_T(s,t)$ for every $s, t \in \{u, v, x, y\}$ (non contractive embedding) and the additive distortion $\alpha(u, v, x, y) = \min_T \max_{s,t \in \{u,v,x,y\}} \mathrm{d}_T(s,t) - \mathrm{d}_G(s,t)$ is minimized. We claim that $\alpha(u, v, x, y) = \delta(u, v, x, y)$, *i.e.*, the least possible distortion is given by the hyperbolicity of the 4-tuple.

On the one direction, let us fix T minimizing the distortion, and let us write:

$$S_1' = \mathrm{d}_T(u,v) + \mathrm{d}_T(x,y),\ S_2' = \mathrm{d}_T(u,x) + \mathrm{d}_T(v,y),\text{ and } S_3' = \mathrm{d}_T(u,y) + \mathrm{d}_T(v,x).$$

In this situation, for every i we have $S_i \leq S_i' \leq S_i + 2\alpha(u, v, x, y)$, since by the hypothesis $\mathrm{d}_G(s,t) \leq \mathrm{d}_T(s,t) \leq \mathrm{d}_G(s,t) + \alpha(u, v, x, y)$ for every $s, t \in \{u, v, x, y\}$. Two cases need to be distinguished. If $S_1' < \max\{S_2', S_3'\}$ then we have $S_1 \leq S_1' < \max\{S_2', S_3'\} \leq S_2 + 2\alpha(u, v, x, y)$. In this situation, since $S_1 = S_2 + 2\delta(u, v, x, y)$, we get $\delta(u, v, x, y) < \alpha(u, v, x, y)$. Otherwise, $S_1' \geq \max\{S_2', S_3'\}$. In particular, the two largest sums amongst S_1', S_2', S_3' must differ by at least $2(\delta(u, v, x, y) - \alpha(u, v, x, y))$. Since T is a tree, and so, it is 0-hyperbolic, it follows that $\alpha(u, v, x, y) \geq \delta(u, v, x, y)$ also in this case.



(a) Canonical realization of the 4-tuple. Distances in the realization are exactly the distances in the graph.

(b) Non contractive tree embedding with distortion δ that is obtained from the realization.

Figure 2.6: A 4-tuple so that $S_1 = \mathrm{d}(u,v) + \mathrm{d}(x,y) \geq S_2 = \mathrm{d}(u,y) + \mathrm{d}(v,x) \geq S_3 = \mathrm{d}(u,x) + \mathrm{d}(v,y)$. We denote by $\delta = (S_1 - S_2)/2$ and $\gamma = (S_1 - S_3)/2$.

On the other direction, consider in Figure 2.6a the so-called "canonical realization" of the metric space $(\{u, v, x, y\}, \mathrm{d}_G)$ with four elements. Using this representation, it is not difficult to see that u, v, x, y can be mapped to the four leaves of an edge-weighted tree with 6 nodes so that the embedding is non contractive and with distortion $\delta(u, v, x, y)$. Altogether combined, $\alpha(u, v, x, y) = \delta(u, v, x, y)$, and so, the hyperbolicity $\delta(G)$ is the least value δ such that for *every* 4-tuple of G, there exists a non contractive embedding into a tree with distortion at most δ.

In particular, we point out that since distances in an unweighted graph are integer-valued, the hyperbolicity is always a half-integer. This observation is sometimes useful in order to refine the bounds on the hyperbolicity, and in order to simplify some arguments in the proofs.

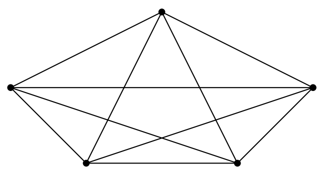
2.3.1.2 Toy examples

In order to give a better intuition of what this parameter represents, let us give the hyperbolicity of a few simple graphs.

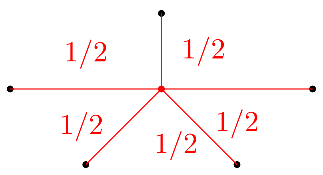
Trees. In a tree, it is trivial that every 4-tuple can be embedded into a tree with null distortion. Therefore, every tree is 0-hyperbolic.

Intuitively, similar arguments should apply to the graphs that are "metrically" tree-like, *i.e.*, embeddable into a tree with constant distortion of their distances. This will be further discussed in Section 2.4.1 (upper-bounds on graph hyperbolicity).

Complete graphs. Perhaps more surprisingly, complete graphs are another example of 0-hyperbolic graphs. Indeed, as shown with Figure 2.7, a complete graph K_n with n vertices can be isometrically embedded into a star with $n+1$ nodes and all its edges weighted $1/2$.



(a) A complete graph K_5 with five vertices.



(b) An isometric embedding of K_5 to the leaves of an edge-weighted star.

Figure 2.7: Complete graphs are 0-hyperbolic.

Cycles. In spite of their simple structure, the cycles are the classical examples of graphs with large hyperbolicity. For instance, let $C_{4n} = (v_0, v_1, \ldots, v_{4n-1}, v_0)$ be a cycle with $4n$ vertices. Then, it follows from the four-point condition that $\delta(v_0, v_n, v_{2n}, v_{3n}) = n$ (see also Figure 2.8). Therefore, the hyperbolicity of a cycle grows linearly with its length. More generally, for every $n \geq 1$ and $\varepsilon \in \{0, 1, 2, 3\}$, we have $\delta(C_{4n+\varepsilon}) = n - 1/2$ if $\varepsilon = 1$ and $\delta(C_{4n+\varepsilon}) = n$ otherwise [WZ11].

Grids. Last, consider a rectangular grid with n columns and m rows. By taking the four corners of the grid, it comes from the 4-point Condition that the hyperbolicity of the grid is at least $\min\{n, m\} - 1$, that turns out to be its exact value [WZ11]. We refer to Figure 2.9 for an illustration.

It might help to observe that for grids and cycles, the shortest paths between the two vertices of any diametral pair do not stay close from each other. In contrast, we mentioned in previous Section 2.2 that in every graph with constant hyperbolicity, almost shortest paths stay close from each other (Property 2).

Furthermore, let us call a subgraph H of a graph G *isometric* if for every two vertices in H, their distance in this subgraph is exactly their distance in G. Since cycles and grids have unbounded hyperbolicity, any graph that contains a large cycle or a large grid as an isometric subgraph also has a large hyperbolicity, that directly follows from Definition 1. This point will be further discussed in Section 2.5.2.1 (lower-bounds on graph hyperbolicity).

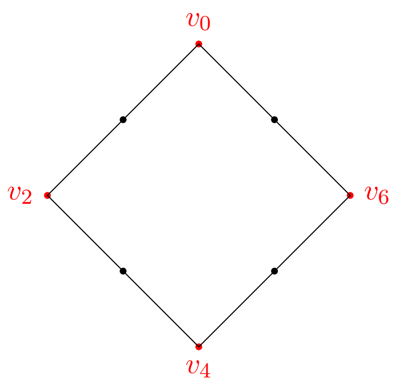


Figure 2.8: A cycle with eight vertices.

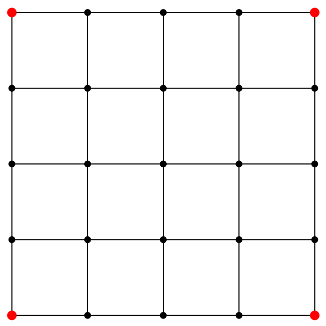


Figure 2.9: A square grid with side length four.

2.3.1.3 Gromov product, Farris transform and ultrametrics

In his seminal paper [Gro87], Gromov defines hyperbolicity via a different (but equivalent) formulation than Definition 1. In what follows, this formulation and its interpretation in terms of ultrametric embedding are stated. Before this, we need to introduce additional notions and terminology that are of independent interest.

Definition 2. Let $G = (V, E)$ be a graph. For every $u, v, w \in V$ the *Gromov product* of u and v with base vertex w is defined as $\langle u, v\rangle_w = (\mathrm{d}_G(u, w) + \mathrm{d}_G(w, v) - \mathrm{d}_G(u, v))/2$.

This notion of Gromov product naturally arises in the above canonical realization of 4-tuples (Figure 2.6a). Indeed, by the calculation we have that the length of the edge between vertex u and the central rectangle in the realization is exactly $\langle x, y\rangle_u$.

Note that $\langle u, v\rangle_w \geq 0$ by the triangular inequality. In particular, $\langle u, v\rangle_w = 0$ if and only if w lies onto a shortest uv-path. Thus, the Gromov product $\langle u, v\rangle_w$ can be seen as a measure of how close w is from a shortest uv-path.

In order to have a better insight of what this product represents, let us consider the particular case where G is a tree rooted at w. Let r be the lowest common ancestor of u and v. In this situation, $\langle u,v\rangle_w = (\mathrm{d}(u,w)+\mathrm{d}(v,w)-\mathrm{d}(u,v))/2 = ((\mathrm{d}(u,r)+\mathrm{d}(r,w))+(\mathrm{d}(v,r)+\mathrm{d}(r,w))-(\mathrm{d}(u,r)+\mathrm{d}(r,v)))/2 = \mathrm{d}(r,w)$. Therefore, in a tree rooted at w, the Gromov product $\langle u,v\rangle_w$ is equal to the depth of the lowest common ancestor of u and v.

Let us also point out that $\langle u,w\rangle_v + \langle w,v\rangle_u = \mathrm{d}_G(u,v)$. In order to exemplify this equality, let us again consider the particular case where G is a tree. Then, $\langle u,w\rangle_v = \mathrm{d}(r,v)$ and $\langle v,w\rangle_u = \mathrm{d}(r,u)$, with r being the lowest common ancestor of u and v when the tree is rooted at w. As a result, $\langle u,w\rangle_v + \langle w,v\rangle_u = \mathrm{d}(r,v)+\mathrm{d}(r,u) = \mathrm{d}(u,v)$, as desired.

Finally, let $D \geq diam(G)$ be any upper-bound on the distances in G. We fix any base vertex x and define:

$$\mathrm{d}^{(x)}(u,v) = \begin{cases} 2D - \langle u,v\rangle_x \text{ if } u \neq v \\ 0 \text{ otherwise.} \end{cases}$$

Then, it can be checked that $\mathrm{d}^{(x)}$ is a distance function, that is sometimes called a *Farris transform* [Far72]. Furthermore, an interesting property of the Farris transform is that for a 0-hyperbolic G, the distance function $\mathrm{d}^{(x)}$ is an *ultrametric*. That is, $\mathrm{d}^{(x)}(u,v) \leq \max\{\mathrm{d}^{(x)}(u,y), \mathrm{d}^{(x)}(y,v)\}$ for every three vertices u,v,y [Ban90]. Put in simpler terms, the above property just says that in a tree rooted at x, if we denote by $r_{s,t}$ the lowest common ancestor between s and t, then for every u,v,y we have that $\mathrm{d}(x,r_{uv}) \geq \min\{\mathrm{d}(x,r_{uy}),\mathrm{d}(x,r_{vy})\}$.

Hyperbolicity of a graph can be seen as a measure of the closeness of its Farris transform to an ultrametric. We can formalize it as follows.

Definition 3 ([Gro87]). A connected graph $G=(V,E)$ is δ-hyperbolic if and only if for every 4-tuple $u,v,x,y \in V$, we have $\langle u,v\rangle_x \geq \min\{\langle u,y\rangle_x, \langle v,y\rangle_x\} - \delta$.

A proof of the equivalence between Definitions 1 and 3 can be found, *e.g.*, in [AJ13]. The two of them use a characterization of metric trees, and they define δ-hyperbolic graphs by relaxing these characterizations. The same can be done with other characterizations of metric trees, but then the corresponding values so obtained may not equal the hyperbolicity of the graph. Nonetheless, as seen in the following Section 2.3.2, they can only differ from the hyperbolicity by a constant-factor.

2.3.2 Reformulation of hyperbolicity

In what follows, we will complete the picture by presenting some of the alternative definitions for graph hyperbolicity. They are useful in order to prove some properties of δ-hyperbolic graphs. On the way, we will report on known relationships between these definitions (Table 2.1). We deem it as an important task. Indeed, the use of multiple definitions quickly lead to large constant-factors in the proofs, with negative consequences on the analysis of some graph algorithms [CCPP14].

Note that except for Section 2.3.2.2, we will not use these alternative definitions in what follows. Therefore, this part can be read independently from the remaining of the chapter. In what follows, some of the reformulations of hyperbolicity will be grouped together when they can be defined in a similar fashion.

2.3.2.1 Definitions with triangles

Let us start from the definition given in previous Section 2.2. First, we recall that a geodesic triangle $\Delta(u,v,w)$ is the union of three shortest-paths $\mathcal{P}_{uv}, \mathcal{P}_{vw}, \mathcal{P}_{wu}$ with respective ends u and v, v and w, w and u. The above shortest-paths are called the sides of the triangle.

Definition 4 (Rips condition, [Gro87, BH11]). A connected graph $G = (V,E)$ has δ_0-slim triangles if and only if for every geodesic triangle $\Delta(u,v,w)$, for every vertex $x \in \mathcal{P}_{uv}$, we have that $\mathrm{d}_G(x, \mathcal{P}_{vw} \cup \mathcal{P}_{wu}) \leq \delta_0$.

In order to see the relationship between Definitions 1 and 4, the following construction was proposed in [SG11].

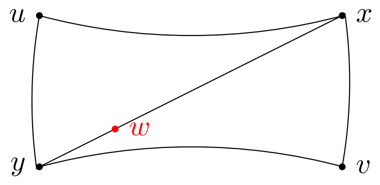


Figure 2.10: Split of a 4-tuple in two triangles. The vertex w is chosen so that $\mathrm{d}(x,w) = \mathrm{d}(v,x) - \lfloor \langle x,y \rangle_v \rfloor$, and so, $\mathrm{d}(y,w) = \mathrm{d}(v,y) - \lceil \langle x,y \rangle_v \rceil$.

Let u,v,x,y be any 4-tuple satisfying $\mathrm{d}(u,v) + \mathrm{d}(x,y) \geq \mathrm{d}(u,x) + \mathrm{d}(v,y) \geq \mathrm{d}(u,y) + \mathrm{d}(v,x)$. We fix a shortest path between every two pairs of vertices in the 4-tuple, and then we use these paths in order to construct the two geodesic triangles $\Delta(u,x,y)$ and $\Delta(v,x,y)$. The gist of the construction is to show that the hyperbolicity of the 4-tuple depends linearly on the slimness of these two triangles. To show that, we choose a vertex $w \in \mathcal{P}_{xy}$ such that $\delta(u,v,x,y) \leq \delta(u,w,x,y) + \delta(w,v,x,y) + 1/2$ (see Figure 2.10 for an illustration). Finally, a clever analysis from [SG11] shows that when the triangles $\Delta(u,x,y)$ and $\Delta(v,x,y)$ are δ-slim, it implies $\delta(u,w,x,y) \leq \delta$, and in the same way $\delta(w,v,x,y) \leq \delta$. Therefore, if G has δ-slim triangles then it is $(2\delta + 1/2)$-hyperbolic and the bound is sharp, as shown in [SG11].

We refer to [BH11] for a proof that conversely, every δ-hyperbolic graph has 3δ-slim triangles.

Other definitions of hyperbolicity than Definition 4 can be stated in terms of geodesic triangles. We summarize some of them below.

In order to get a better intuition of the following definitions, we recall that hyperbolicity measures the closeness of a graph to a metric tree. Let us fix any geodesic triangle $\Delta(u,v,w)$. The three vertices u,v,w can be isometrically embedded into a tree as follows. We map them to the three leaves u',v',w' of a star with center node $s \notin V$ so that the edges $\{s,u'\},\{s,v'\},\{s,w'\}$ have respective length $\langle v,w\rangle_u, \langle u,w\rangle_v, \langle u,v\rangle_w$. We refer to Figure 2.11 for an illustration.

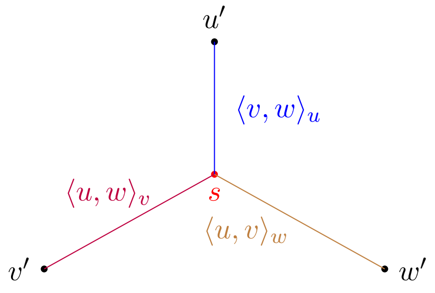


Figure 2.11: Isometric embedding of a 3-tuple to the leaves of a star (*a.k.a.*, tripod). We recall that $\langle v,w\rangle_u + \langle u,w\rangle_v = \mathrm{d}(u,v)$.

Then, by an appropriate subdivision of the three edges of the star, it can be obtained a tree T so that the shortest path $\mathcal{P}_{uv}$ (resp., $\mathcal{P}_{vw}$, resp., $\mathcal{P}_{wu}$) can be isometrically embedded to the unique $u'v'$-path in T (resp., $v'w'$-path, resp., $w'u'$-path). However, by doing so, some vertices in different sides of the triangle are mapped to the same node of T, and so, we aim at keeping small the distance in G between any two such vertices.

Definition 5 ([ABC$^+$91, BH11, Gro87, GdLH90]). For every graph $G = (V,E)$ (with hyperbolicity $\delta(G)$), the following properties hold true:

- There exists $\delta_1(G) = \Theta(\delta(G))$ such that G has $\delta_1(G)$-*thin triangles*: for every triangle $\Delta(u,v,w)$ and for every $x \in \mathcal{P}_{uv}$, $y \in \mathcal{P}_{uw}$ such that $\mathrm{d}(u,x) = \mathrm{d}(u,y) \leq \langle v,w\rangle_u$, we have that $\mathrm{d}(x,y) \leq \delta_1(G)$.
- There exists $\delta_2(G) = \Theta(\delta(G))$ such that G has triangles with *insize* at most $\delta_2(G)$: for every triangle $\Delta(u,v,w)$ and for every $x \in \mathcal{P}_{uv}$, $y \in \mathcal{P}_{uw}$ such that $\mathrm{d}(u,x) = \mathrm{d}(u,y) = \lfloor \langle v,w\rangle_u \rfloor$[1], we have that $\mathrm{d}(x,y) \leq \delta_2(G)$.
- There exists $\delta_3(G) = \Theta(\delta(G))$ such that G has triangles with *girth* at most $\delta_3(G)$: for every triangle $\Delta(u,v,w)$, there exist $x \in \mathcal{P}_{uv}, y \in \mathcal{P}_{uw}, z \in \mathcal{P}_{vw}$ such that $\max\{\mathrm{d}(x,y),\mathrm{d}(x,z),\mathrm{d}(y,z)\} \leq \delta_3(G)$.
- There exists $\delta_4(G) = \Theta(\delta(G))$ such that: for every triangle $\Delta(u,v,w)$, there is some vertex $m \in V$ such that $\max\{\mathrm{d}(m,\mathcal{P}_{uv}),\mathrm{d}(m,\mathcal{P}_{uw}),\mathrm{d}(m,\mathcal{P}_{vw})\} \leq \delta_4(G)$.

Further geometric interpretation of the above definitions of hyperbolicity can be found, *e.g.*, in [BH11]. Interestingly, not all geodesic triangles need to be considered. In fact, we can constrain ourselves to “flat” triangles, *a.k.a.* bigons, and define hyperbolicity as follows:

[1]The ceiling ensures the distances to be integer values.

Definition 6. A graph $G = (V, E)$ has ε-thin bigons if for every $u, v, x, y \in V$ such that all of the following hold:

$$\mathrm{d}(u, v) = \mathrm{d}(u, x) + \mathrm{d}(x, v) = \mathrm{d}(u, y) + \mathrm{d}(y, v) \text{ and } \mathrm{d}(u, x) = \mathrm{d}(u, y)$$

we have $\mathrm{d}(x, y) \leq \varepsilon$.

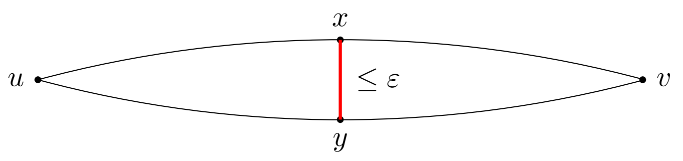


Figure 2.12: An ε-thin bigon.

We refer to Figure 2.12 for an illustration. Notice that when we take u, v, x, y as in the above Definition 6 then we obtain by the calculation $\delta(u, v, x, y) = \mathrm{d}(x, y)/2 \leq \varepsilon/2$. Therefore, a δ-hyperbolic graph has 2δ-thin bigons (see also Figure 2.3 and Property 1 in Section 2.2). Surprisingly, a converse relationship holds: if we subdivide once every edge in a graph G and the subdivided graph has ε-thin bigons, then G is $f(\varepsilon)$-hyperbolic for some (doubly exponential) function f [Pap95]. It is open whether f can be chosen as a linear function.

2.3.2.2 Cop and Robber games with different speeds

More recently, a game-theoretic characterization of hyperbolicity was proved.

A *Cop and Robber game* is a well-known two-player game that is played on a graph $G = (V, E)$. Classically, the two players are named the Cop and the Robber. At first, the Cop chooses any vertex $v_0 \in V$ as her position in the graph, then the Robber also chooses her initial position $u_0 \in V$. Then, the two players move sequentially, with the Cop playing first. At each turn $t \geq 1$, a player can either stay on her current position or move on an adjacent vertex.

The graph G is called *Cop-win* if whatever the Robber does, the Cop can end up on the same position as the Robber within a finite number of moves. Cop-win graphs have been characterized early in [NW83, Qui83]. Since then, several extensions of Cop and Robber games have been studied [Nis14]. One of them has a relationship with hyperbolicity.

Precisely, in this variant the Cop and the Robber move at different speeds s' (for the Cop) and s (for the Robber), with $s' \leq s$, where the speed of a player denotes the maximum distance in the graph between any two of its consecutive positions [CCNV11]. The graph G is called (s, s')-Cop-win if it is Cop-win in this variant. In particular, Cop-win graphs in the classical Cop and Robber game are exactly the $(1, 1)$-Cop-win graphs. Perhaps surprisingly, the values of s and s' for which a given graph G is (s, s')-Cop-win are related with its hyperbolicity. We first need to introduce the following dismantling orderings. We recall that throughout this thesis, we will denote by $B_G(v,r)$ the ball of radius r centered on the vertex v in a given graph G.

Definition 7. An $(s,s')^*$-dismantling ordering of $G=(V,E)$ is a total ordering $(v_1,v_2,\ldots,v_n)$ of V such that for every $i<n$, we have $B_G(v_i,s)\cap\{v_i,v_{i+1},\ldots,v_n\}\subseteq B_G(v_j,s')$ for some $j>i$.

It can be shown that every graph with an $(s,s')^*$-dismantling ordering is (s,s')-Cop-win. Conversely, if a graph is (s,s')-Cop-win, for some $s'<s$, then it has an $(s,s-1)^*$-dismantling ordering [CCPP14].

Lemma 8 ([CCPP14]). *Let $G=(V,E)$ be a graph.*

If G is δ-hyperbolic then it has a $(2r,r+2\delta)^*$-dismantling ordering for every positive integer $r\geq 2\delta$.

Conversely, if G has a $(s,s')^*$-dismantling ordering, for some $s'<s$, then it has hyperbolicity at most $16(s+s')\left\lceil\frac{s+s'}{s-s'}\right\rceil+1/2$.

One important byproduct of Lemma 8 is that every δ-hyperbolic graph G admits a $(4\delta,4\delta)^*$-dismantling ordering, that is a classical dismantling ordering for its *graph power* $G^{4\delta}$ — obtained from G by adding an edge between every two distinct vertices that are at distance no more than 4δ in G. Simply put, if G is δ-hyperbolic then $G^{4\delta}$ is Cop-win. As we will show in Section 2.5.2, this original characterization of hyperbolicity is helpful in order to obtain new lower-bounds on this parameter.

2.3.2.3 Other definitions

In an attempt to make this part as exhaustive as possible, some other reformulations for graph hyperbolicity are now mentioned. These alternative definitions are not detailed, as it would require to introduce new technical notions that I feel to be unnecessary for the understanding of what follows. Below, the interested reader will be referred to some papers that are related with these alternative definitions.

Definition 9. The hyperbolicity of a graph G can be defined via the smallest parameters defining:

- its asymptotic upper curvature, denoted by κ (curvature) and c (an adjustment variable) [BF06];
- or a divergence function on its shortest-paths that is superlinear, denoted by $e(0)$ (initial value) and α (rate of divergence) [BH11] ;
- or a linear isoperimetric inequality, denoted by N (filling) and K [CCPP14].

Reformulations of hyperbolicity and their relationships with the standard definition are summarized in Table 2.1. In what follows, we name δ the hyperbolicity of the graph (w.r.t. Definition 1). The symbols that are used for each reformulation correspond to the ones that are given in the above definitions.

δ_0-slim triangles	$\delta_0 \leq 3\delta$	[AJ13]	$\delta \leq 2\delta_0 + 1/2$	[SG11]
δ_1-thin triangles	$\delta_1 \leq 4\delta$	[ABC+91]	$\delta \leq \delta_1$	[BH11]
insize δ_2	$\delta_2 \leq 12\delta$	[BH11]	$\delta \leq \delta_2$	[BH11]
δ_3	$\delta_3 \leq 12\delta$	[BH11]	$\delta \leq 3\delta_3$	[BH11]
δ_4	$\delta_4 \leq 12\delta + 1$	[BH11]	$\delta \leq 6\delta_4$	[BH11]
ε-thin bigons	$\varepsilon \leq 2\delta$	[Gro87]	$\delta = 2^{2^{\mathcal{O}(\varepsilon)}}$	[CN04]
$(s,s')^*$-dismantlable	$s \leq 2s' - 4\delta$	[CCNV11]	$\delta \leq 16(s+s')\left\lceil \frac{s+s'}{s-s'} \right\rceil + 1/2$	[CCPP14]
asymptotic upper curvature "κ, c"	$\kappa \leq -1/(4\delta^2)$	[BF06]	$\delta \leq \log 2/\sqrt{-\kappa} + c$	[BF06]
divergence function e	$e(0) \leq 4\delta,\ e(r) \geq 2^{\frac{r-4\delta-1}{12\delta}}$	[BH11]	$\delta \leq 6e(0) + 9\alpha$	[BH11]
(N,K)-filling	$N \leq 16\delta$	[ABC+91]	$\delta \leq 32KN^2 + 1/2$	[CCPP14]

Table 2.1: Comparison between the definitions of hyperbolicity. The first column is for the upper-bounds that are implied by δ for each reformulation. Conversely, the second column is for the upper-bounds on δ that are implied by each reformulation.

2.3.3 What is a “hyperbolic” graph ?

In the seminal work of Gromov [Gro87], hyperbolic graphs simply refer to the graphs with finite hyperbolicity. This definition makes sense since he studies on the hyperbolicity of Cayley graphs of finitely generated groups, that may and will be infinite. However according to the above definition, finite graphs are trivially hyperbolic in the sense that for every graph G, there exists a finite δ such that G is δ-hyperbolic. Thus, we shoud call the cycle C_n “hyperbolic” whereas it has hyperbolicity $\Omega(n)$!

In order to override this limitation, we can transpose the notion of hyperbolicity to *graph classes*. As a first attempt, let us define the hyperbolicity of a given graph class $\mathcal{G}$ as $\delta(\mathcal{G}) = \sup_{G \in \mathcal{G}} \delta(G)$. Then, we call $\mathcal{G}$ hyperbolic if $\delta(\mathcal{G}) < +\infty$. As expected, we have that the class of trees is hyperbolic, but the class of cycles is non hyperbolic. By abuse of notation, we refer by “hyperbolic graphs” for the graphs in a hyperbolic graph class.

In the literature [Ben98], a broader concept of hyperbolic graph class is preferred. It is based on the property that the hyperbolicity of a given graph is upper-bounded by its diameter (we shall come back to this relationship later on in Section 2.4) [WZ11]. The latter means that any graph G with diameter D_G is trivially D_G-hyperbolic, that does not really look satisfying. Indeed, we would prefer to call it hyperbolic only if $\delta(G) \ll D_G$.

Formally, let $\mathcal{G}$ be any class of graphs and let $\mathcal{G}_n = \{G_n \in \mathcal{G} \mid diam(G_n) = n\}$. Since graphs in $\mathcal{G}_n$ are trivially n-hyperbolic, the hyperbolicity $\delta(\mathcal{G}_n)$ is finite (by convention, $\delta(\emptyset) = 0$). Then, the graph class $\mathcal{G}$ is called hyperbolic if and only if $\lim\limits_{n \to +\infty} \frac{\delta(\mathcal{G}_n)}{n} = 0$.

Further refinements of the concept have been suggested, *e.g.*, in [CFHM13]. They are listed in what follows.

Definition 10 ([CFHM13])**.** A given graph class $\mathcal{G}$ is called:

- *constantly hyperbolic* if $\delta(\mathcal{G}_n) = \mathcal{O}(1)$ (that corresponds to the case where $\delta(\mathcal{G})$ is finite);
- *(poly)logarithmically hyperbolic* if $\delta(\mathcal{G}_n) = \mathcal{O}(\log n)$ or $\delta(\mathcal{G}_n) = \log^{\mathcal{O}(1)} n$;
- *weakly hyperbolic* if $\delta(\mathcal{G}_n) = o(n)$;
- and *non hyperbolic* otherwise.

A shorter classification is adopted in [AD15]. Namely, a graph class is called hyperbolic in [AD15] only if it is logarithmically hyperbolic (w.r.t. Definition 10), and non hyperbolic otherwise. Furthermore, a graph class is called *strongly hyperbolic* in [AD15] if $\delta(\mathcal{G}_n) = \mathcal{O}(\log\log n)$.

Finally, we note that in [DKMY15], the authors consider a graph class to be hyperbolic only if it has the additional requirement that the graphs in the class have their maximum degree Δ that is constantly upper-bounded. By doing so, since the diameter of an n-vertex graph must be $\Omega(\log n / \log \Delta)$, there can be no constant upper-bound on the diameter in an infinite graph class, and so, we can dismiss all the classes of bounded diameter graphs (that are trivially hyperbolic). As we will discuss next in Section 2.7, this choice presents algorithmic advantages.

2.4 Hyperbolic graph classes

The next two sections are devoted to the first objective in this study of hyperbolicity, *i.e.*, the characterization of hyperbolic and non hyperbolic graph classes. In particular, this section covers known upper-bound techniques on graph hyperbolicity. We list *sufficient* conditions for a graph class to be constantly hyperbolic. Examples of (hyperbolic) graph classes for which these conditions hold are given. We also provide examples of hyperbolic graphs that do *not* satisfy these conditions. The latter will show the limitations of these upper-bound techniques.

Outline of the section. In Section 2.4.1, we present upper-bounds depending on the best distortion of the distances in a graph when it is embedded in a tree. We also discuss about relationships between hyperbolicity and tree decompositions. Then in Section 2.4.2, we present two more upper-bounds on the hyperbolicity depending on the diameter and the chordality properties of the graph. We end up in Section 2.4.3 on personal contributions, showing upper and lower bounds on the variations of hyperbolicity that may be caused by various graph operations. The latter result is joint work with David Coudert.

2.4.1 Tree-likeness in graphs and hyperbolicity

We start presenting upper-bounds on the hyperbolicity that depend on the best possible distortion of the distances in a graph when it is embedded into a tree.

Indeed, we recall that hyperbolicity measures how close a given graph is to a metric tree. Unsurprisingly, there exists a strong relationship between this parameter and the (NP-hard) problem of embedding a given graph into a tree with minimum distortion (additive or multiplicative). In particular, as we showed in Section 2.3 the hyperbolicity $\delta(G)$ of a given graph G is the minimum possible δ such that every 4-tuple of vertices in G can be (non contractively) embedded into a tree with additive distortion at most δ. Therefore, $\delta(G)$ is a *lower bound* on the parameters:

- *tree-distortion* (minimum multiplicative distortion in a tree embedding);
- and *tree-stretch* (minimum t such that G admits a *tree t-spanner*, *i.e.*, a spanning tree with multiplicative distortion at most t).

These above relationships are described in the survey [AAD16] and the papers cited therein. Summarizing, we get the following upper-bounds on hyperbolicity:

Theorem 11 ([AAD16]). *Every graph with tree-distortion at most d is d-hyperbolic. Similarly, for every $t \geq 1$, every graph with a tree t-spanner is t-hyperbolic.*

2.4.1.1 Application: hyperbolic graph classes

Below, we give examples of graph classes that are (metrically) “tree-like”, and so, hyperbolic.

Graphs with a tree t-spanner. By Theorem 11, for any fixed $t \geq 1$, the class of graphs with a tree t-spanner is constantly hyperbolic. The latter includes well-known classes such as: trees (trivially), interval graphs [LB62], split graphs [FH76], convex bipartite graphs [Glo67] and chordal bipartite graphs (*a.k.a.*, bipartite graphs with no induced cycle of length at least six) [GG78], etc.

Graphs with bounded tree distortion. Similarly, by Theorem 11 any class of graphs with bounded tree distortion is constantly hyperbolic. In particular, the classes of chordal graphs (graphs with no induced cycles of length at least four) and dually chordal graphs (*a.k.a.*, $(2,1)$-Cop win graphs, see Section 2.3.2.2) are constantly hyperbolic [Dir61, BDCV98]. It can be intuited (and, with slightly more work, formally proved) from the existence of their respective tree-representations, sometimes called the clique-tree (for chordal graphs) [Gav74] and the compatible tree (for dually chordal graphs) [DCG14].

2.4.1.2 Examples of hyperbolic graphs that are not “tree-like”

However, a converse of Theorem 11 does not hold : not all hyperbolic graphs have a constant tree-distortion or tree-stretch. In fact, these two parameters can differ from $\delta(G)$ by at most a logarithmic or polylogarithmic factor [AAD16], and this is sharp. We illustrate this fact with the following construction in Figure 2.13, sometimes called a *ringed tree* [CFHM13].

The ringed tree $RT(k)$ is obtained from a rooted complete binary tree with k levels by connecting the vertices at the same level with a circle, that is constructed under rules that we now detail. Formally, we start from a complete binary tree, then we label the vertices as follows. The root is labeled 0, and the two children of a vertex labeled i are labeled $2i+1$ and $2i+2$. Finally, at each level $l \geq 0$, nodes are labeled from $2^l - 1$ to $2^{l+1} - 2$, and we add edges in order to obtain the cycle $(2^l - 1, 2^l + 1, \ldots, 2^l + i, \ldots, 2^{l+1} - 2)$.

As a side contribution of this thesis (not published elsewhere), we improve upon the best-known upper-bound on the hyperbolicity of ringed trees:

Lemma 12. $\delta(RT(k)) \leq 3$.

Proof. For every vertex v, let $\ell(v)$ be its level in the underlying rooted tree (its distance to the root). Suppose for the sake of contradiction that $\delta(RT(k)) > 3$. Let u, v, x, y be such that $\delta(u, v, x, y) > 3$ and $\ell(u) + \ell(v) + \ell(x) + \ell(y)$ is minimized. W.l.o.g., vertex u is on the lowest level, *i.e.*, $\ell(u) \geq \max\{\ell(v), \ell(x), \ell(y)\}$. As proved in [CFHM13], it implies that for every vertex w in a upper level $\ell(w) \leq \ell(u)$, there exists a shortest uw-path which first goes up for some time, then stays on the same

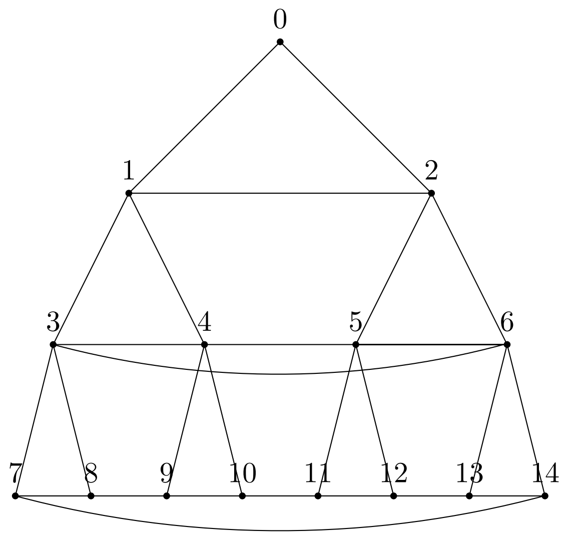


Figure 2.13: a ringed tree $RT(3)$.

level for at most three hops, and finally goes down. Indeed, this construction can be intuited by noticing that the two ends s and t of a "horizontal" st-path of length $p \geq 4$, staying on the same level $\ell(s) = \ell(t)$, can be connected via a path of length $\leq 2 + \lceil p/2 \rceil \leq p$ which first goes up for one hop, then stays at the same level $\ell(s) - 1$ and finally goes down for one hop. We call it a canonical shortest path.

Let us use the above property in order to prove the existence of some vertex of v, x, y that is at distance at most three from u. Indeed, let u' be the parent node of u in the underlying rooted tree. Since $\ell(u') = \ell(u) - 1$, we have by the minimality of $\ell(u) + \ell(v) + \ell(x) + \ell(y)$ that $\delta(u', v, x, y) \leq 3$. In this situation, we note that if it were the case that for any of v, x, y, there is a shortest path between this vertex and u passing by u', then it would follow from the 4-point Condition (Definition 1) that $\delta(u, v, x, y) = \delta(u', v, x, y) \leq 3$, that is a contradiction. So, let us assume w.l.o.g. that u' does not lie on any shortest uv-path. In particular, the canonical shortest uv-path does not go up, and so, $\ell(v) = \ell(u)$. Furthermore, since this path stays at most three hops on the same level, we get $\mathrm{d}(u, v) \leq 3$.

However, in this situation $\delta(u, v, x, y) \leq \mathrm{d}(u, v) \leq 3$ [SG11], that is a contradiction. Indeed, the upper-bound $\delta(u, v, x, y) \leq \mathrm{d}(u, v)$ can be seen as follows. As we observed earlier (Figure 2.11), the three vertices u, x, y can be embedded to the three leaves u', x', y' of an edge-weighted star S with null distortion. If we add a new leaf node v' that we make adjacent to u' in S, then by weighting $\mathrm{d}(u, v)$ the edge $\{u', v'\}$, one obtains a tree embedding of the 4-tuple with distortion at most $\mathrm{d}(u, v)$, and so, $\delta(u, v, x, y) \leq \mathrm{d}(u, v)$.

Altogether, $\delta(RT(k)) \leq 3$. □

Lemma 12 improves on [CFHM13], where they proved that $\delta(RT(k)) \leq 40$. It proves that we have a constant upper-bound on the hyperbolicity of any ringed tree.

In contrast, the following lemma shows that the tree distortion of a ringed tree can be arbitrarily large.

Lemma 13 ([Yan15]). *Any tree embedding of $RT(k)$ has distortion $\Omega(k)$.*

To have a better intuition of Lemma 13, we first observe that the underlying rooted tree of $RT(k)$ is a shortest-path tree. In a rooted tree T, the path between two vertices at same distance from the root r must pass by their lowest common ancestor, that is strictly closer from r. In contrast, all vertices at the same layer ℓ in $RT(k)$ can be connected via a circle, with only vertices at same distance ℓ from the root. Intuitively, it implies that in a (non expansive) tree embedding of $RT(k)$, the circles in each layer should be contracted to a single node [2]. Hence, the distortion of any tree embedding of $RT(k)$ should be at least the maximum distance between any two vertices at the same level, that is $\Omega(k)$ for the lowest level.

2.4.1.3 Relationship with tree decompositions

We complement Section 2.4.1 with relationships between hyperbolicity and tree decompositions [RS86], that are a more common way to measure tree-likeness in graphs. Formally, a *tree decomposition* $(T, \mathcal{X})$ of G is a pair consisting of a tree T and of a family $\mathcal{X} = (X_t)_{t \in V(T)}$ of subsets of V indexed by the nodes of T and satisfying:

- $\bigcup_{t \in V(T)} X_t = V$;
- for any edge $e = \{u, v\} \in E$, there exists $t \in V(T)$ such that $u, v \in X_t$;
- for any $v \in V$, $\{t \in V(T) \mid v \in X_t\}$ induces a subtree, denoted by T_v, of T.

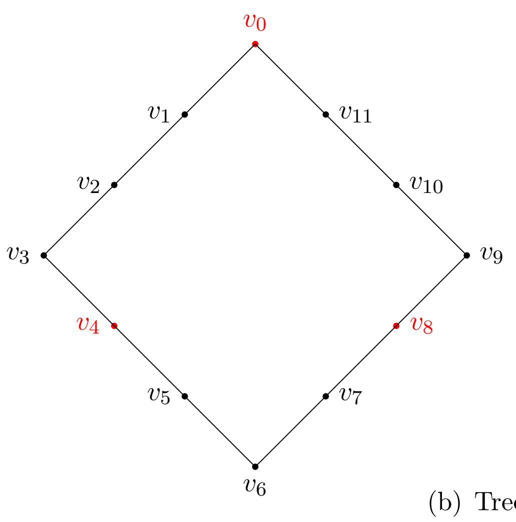
The sets X_t are called *the bags* of the decomposition. As an example, we give a tree decomposition of a cycle in Figure 2.14b.

A graph has *treewidth* at most k if it has a tree decompositions with bags of size at most $k + 1$. As an example, trees are exactly the graphs with treewidth 1.

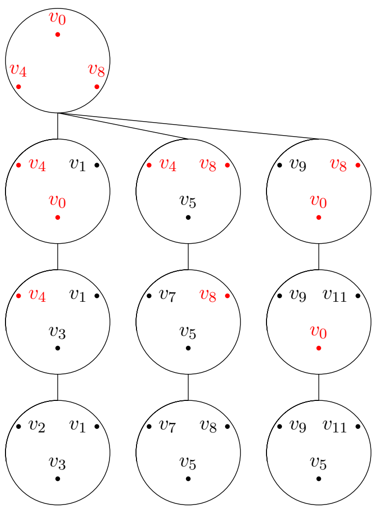
Treewidth is a well-studied parameter [Bod06], and is generally accepted as a good measure of the structural tree-likeness in graph. In contrast, hyperbolicity is a measure of the metric tree-likeness in graphs, and as such it is uncomparable with treewidth. Indeed, as shown with Figure 2.14b, cycles have treewidth at most 2, whereas we proved in Section 2.3.1.2 that the hyperbolicity of cycles grows linearly with their size. Conversely, it is well-known that the complete graph K_n with n vertices has treewidth $n - 1$, whereas we proved in Section 2.3.1.2 that it has null hyperbolicity.

On the other hand, we can compare graph hyperbolicity with *treelength* [DG07] and *treebreadth* [DK14], that can also be defined in terms of tree decompositions. A graph has treelength at most l if it has a tree decomposition where the distance in the graph between any two vertices in a same bag is at most l. It has treebreadth

[2]This intuition can be formalized through the notion of *layering tree* [CD00], that will be further discussed in the next Section 2.7.



(a) Cycle C_{12} with twelve vertices.



(b) Tree-decomposition of C_{12} of width two and length four.

Figure 2.14: Cycles have treewidth two and treelength $\lceil n/3 \rceil$.

at most r if it has a tree decomposition whose every bag is contained in a ball of radius at most r (the center of the ball may not be in the bag). Treelength and treebreadth differ from tree distortion by at most a constant-factor, and so, they can be compared with hyperbolicity the same way [AAD16].

I will expand more on treelength and treebreadth in the next chapter on tree decompositions. In particular, I will show that in some cases where there is no large clique-minor and no long isometric cycle in the graph, treewidth can be compared with treelength (and so, with hyperbolicity) [CDN16].

2.4.2 Classical upper-bounds on hyperbolicity

In this subsection, we now survey two classical techniques in order to upper-bound graph hyperbolicity. Section 2.4.2.1 is devoted to the relationship between diameter and hyperbolicity. In Section 2.4.2.2, relationships between hyperbolicity and chordality properties of the graph are presented.

2.4.2.1 Diameter

As stated earlier, there is a standard upper-bound of graph hyperbolicity using the diameter of the graph.

Lemma 14 ([KM02, MP14, WZ11]). *For every graph $G = (V, E)$, we have $\delta(G) \leq \lfloor diam(G)/2 \rfloor$.*

A simple proof of Lemma 14 can be easily derived from the 4-point condition (Definition 1). Furthermore, we point out that since any graph G can be embedded in a shortest-path tree with distortion $\mathcal{O}(diam(G))$, Lemma 14 is not that surprising. Of course, the converse of the lemma holds false, as easily seen with any path.

It follows that any class of graphs with constant upper-bound on the diameter is (trivially) constantly hyperbolic. Since the domination number and other domination-like parameters are themselves upper-bounds on the diameter, the authors in [HPR14] notice that the class of graphs with bounded domination number is also constantly hyperbolic.

We note that in [BCCM15, CCL15], it can be found variations of Lemma 14 (some of them using the eccentricity of the vertices, *i.e.*, the maximum distance in the graph between a given vertex and any other vertex).

2.4.2.2 Chordality

Much stronger upper-bounds on the hyperbolicity can be derived from the *chordality* of the graph. Namely, a k-chordal graph is a graph with no induced cycle of length at least $k+1$ [Ueh99]. In particular, 3-chordal graphs are exactly the usual chordal graphs. We recall that the class of chordal graphs is constantly hyperbolic [BKM01]. The result extends to the class of k-chordal graphs:

Theorem 15 ([CD00, WZ11]). *For every $k \geq 4$, every k-chordal graph G is $\lfloor k/2 \rfloor /2$-hyperbolic, and the bound is sharp.*

The converse of Theorem 15 holds false. As an example, consider a wheel W_n (obtained from the cycle C_n with n vertices by adding a universal vertex). On the one hand, it has diameter at most two and so, it has hyperbolicity at most 1 by Lemma 14. On the other hand, it is n-chordal.

Application: even more hyperbolic graph classes. By Theorem 15, the class of k-chordal graphs is constantly hyperbolic for every fixed $k \geq 4$. The latter encompass well-studied graph classes such as: chordal graphs (trivially), with well-known subclasses such as strongly chordal graphs [Far83]; weakly chordal graphs [Hay85]; AT-free graphs [COS97], and so, cocomparability graphs [GMT84] and permutation graphs [EPL72]; distance-hereditary graphs [BM86] and cographs [Sei74].

More recently, a result of the same flavour as Theorem 15 was proved in [MP15] with a different (and more technical) notion of chordality. Given $G = (V,E)$ and a cycle C in G, a *bridge* (or shortcut) of C is any shortest uv-path between two vertices $u, v \in C$ such that $\mathrm{d}_C(u,v) > \mathrm{d}_G(u,v)$. The bridge is called strict when it intersects the cycle C only in its two endvertices. Let $D_m(C) \subseteq V(C)$ contain the ends of all strict bridges of C of length at most m.

Then, a graph G is called *ε-densely (k,m)-path chordal* if for every cycle C with length at least k, every vertex in C is at distance at most ε from a vertex in $D_m(C)$ (see Figure 2.15 for an example). In particular, k-chordal graphs are $\lfloor k/2 \rfloor$-densely $(k, \lfloor k/2 \rfloor)$-path chordal [MP15].

Theorem 16 ([MP15]). *Every ε-densely (k,m)-path chordal graph has $(\max\{k/4, \varepsilon + m\})$-slim triangles.*

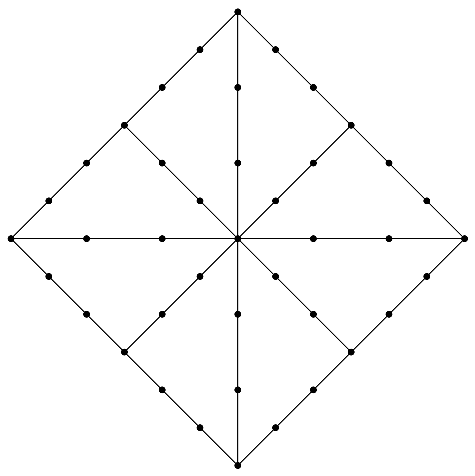


Figure 2.15: The uniform subdivision of the wheel is 3-densely $(9, 3)$-path chordal.

I confess that the impact of this result, compared to Theorem 15, is unclear to me.

2.4.3 Contribution: Graph operations and hyperbolicity

Finally, a generic framework is presented in order to prove that some graph operations preserve the hyperbolicity up to an additive term. In particular, this can be used in order to construct new hyperbolic graph classes from existing ones. Although we concentrate more on how to use this framework in order to prove that some graph classes are hyperbolic, it gives precise information on the variations of hyperbolicity that can be useful in a broader context (*e.g.*, in preprocessing and approximation algorithms for computing this parameter).

More precisely, new classes of hyperbolic graphs can be obtained from classes already known to be hyperbolic, by applying some graph operations such as line graphs [Whi92], clique graphs [Ham68], etc. In [CD16b], we designed a unifying framework in order to prove that these graph operations preserve hyperbolicity up to an additive term. The purpose of this work was to make simpler the computation of the sharp distortion of the hyperbolicity constant under these operations. It is based on two ingredients. The first is that the hyperbolicity of a given *bipartite graph* can be closely approximated (up to an additive term) by considering only one side of its bipartition.

Lemma 17. *Let $B = (V_0 \cup V_1, E)$ be a bipartite graph. For every $i \in \{0, 1\}$, let $G_i = (V_i, \{\{u, v\} \mid \mathrm{d}_B(u, v) = 2\})$.*

Then, $2\delta(G_i) \leq \delta(B) \leq 2\delta(G_i) + 2$ and the bounds are sharp.

It can be observed that since V_i is a dominating set of the bipartite graph G, we can relate every 4-tuple in G with a 4-tuple in G_i by substituting every vertex in V_{1-i} of the 4-tuple with any one of its neighbours. By doing so, we can use the 4-point Condition directly (Definition 1) in order to prove a weaker version of Lemma 17. This weaker relationship between dominating set and hyperbolicity was already known and used in some algorithms for computing this parameter [CCL15]. In the case of bipartite graphs, the main technical difficulty was to obtain the sharp upper-bound on the distortion of hyperbolicity, which has required us a finer-grained analysis of the 4-tuples with maximum hyperbolicity in G.

The second property used in the framework is that for every $G = (V, E)$, since the distances in its j^{th} graph power are roughly divided by j, the hyperbolicity of this power is roughly $\delta(G)/j$.

Lemma 18. *For every graph $G = (V, E)$ and $j \geq 1$, we have $\frac{\delta(G)+1}{j} - 1 \leq \delta(G^j) \leq \frac{\delta(G)-1}{j} + 1$ and the bounds are sharp.*

Finally, we recall that an intersection graph over a ground-set S has for vertices a family of subsets in S together with an edge between every two intersecting subsets. It can be naturally represented as a bipartite graph, with vertices of the graph on one side and the elements of S on the other side. Combining the two above lemmas, we obtain our main result in [CD16b]:

Theorem 19. *For every graph $G = (V, E)$ and $j \geq 1$, let $\mathcal{S} = \{S_1, S_2, \ldots, S_k\}$ be a clique edge cover of G^j (a collection of cliques of G^j covering all its edges). Then the intersection graph $I_{\mathcal{S}}$, constructed from the subsets in $\mathcal{S}$ satisfies:*

$$\frac{\delta(G)+1}{j} - 2 \leq \delta(I_{\mathcal{S}}) \leq \frac{\delta(G)-1}{j} + 2.$$

Proof. We recall that every $S_i \in \mathcal{S}$ is a subset of V. Let $B_{\mathcal{S}}$ be the bipartite graph with sides V and $\mathcal{S}$, and with edge-set $\{\{v, S_i\} \mid v \in S_i\}$. By construction, two subsets $S_i, S_j \in \mathcal{S}$ are at distance two in $B_{\mathcal{S}}$ if and only if they intersect, that is if and only if $\{S_i, S_j\}$ is an edge of $I_{\mathcal{S}}$. Furthermore, since by the hypothesis $\mathcal{S}$ is a clique edge cover of G^j, two vertices $u, v \in V$ are at distance two in $B_{\mathcal{S}}$ if and only if $\{u, v\}$ is an edge of G^j. It follows by applying twice Lemma 17:

$$2\delta(I_{\mathcal{S}}) \leq \delta(B_{\mathcal{S}}) \leq 2\delta(I_{\mathcal{S}}) + 2,$$

$$2\delta(G^j) \leq \delta(B_{\mathcal{S}}) \leq 2\delta(G^j) + 2.$$

By mixing up the two chains of inequalities, one obtains $\delta(G^j) - 1 \leq \delta(I_{\mathcal{S}}) \leq \delta(G^j) + 1$. Then, by Lemma 18, it implies $\frac{\delta(G)+1}{j} - 2 \leq \delta(I_{\mathcal{S}}) \leq \frac{\delta(G)-1}{j} + 2$, as desired. □

The line graph and the clique graph of $G = (V, E)$, respectively denoted by $L(G)$ and $K(G)$, are respectively the intersection graph of its edges and of its maximal cliques. Therefore, Theorem 19 applies to these two typical graph operations by taking $j = 1$, which gives $\delta(G) - 1 \leq \delta(L(G)) \leq \delta(G) + 1$ and $\delta(G) - 1 \leq \delta(K(G)) \leq \delta(G) + 1$ for every graph G. These bounds are proved to be sharp in [CD16b]. In fact, we show in [CD16b] that for every possible $i \in \{-1, -1/2, 0, 1/2, 1\}$, there are graphs G_i and H_i such that $\delta(L(G_i)) - \delta(G_i) = i$ and similarly, $\delta(K(H_i)) - \delta(H_i) = i$.

Other graph operations to which the theorem applies are: the k-edge graph (intersection graph of the cliques of size k and the maximal cliques of size at most $k-1$ [Pri94]) with $j = 1$, the middle graph (intersection graph of the cliques of size at most two [Pri95]) with $j = 1$, the biclique graph (intersection graph of the maximal induced complete bipartite subgraphs [GS10]) with $j = 2$, etc. Furthermore, for all these above operations (except for line graph) these are the first bounds proved on the variations for hyperbolicity.

2.4.3.1 New classes of hyperbolic graphs

Finally, some new graph classes are proved to be constantly hyperbolic by using Theorem 19. A *clique-chordal graph* is a graph whose clique graph is chordal [BDCV98]. Since chordal graphs are 1-hyperbolic [BKM01], by Theorem 19 clique-chordal graphs are 2-hyperbolic.

Another example is the class of *n-convergent* graphs: $G = (V, E)$ is n-convergent if its n^{th} iterated clique-graph is a complete graph [LdMS98]. By iterating Theorem 19, we obtain that if G is n-convergent then $\delta(G) \leq \delta(K_{|V|}) + n = n$. Therefore, every n-convergent graph is n-hyperbolic.

2.4.4 Conclusion and open perspectives

Some classical graph parameters are shown to give upper-bounds on hyperbolicity in Sections 2.4.1 and 2.4.2. It would be very interesting to enrich this list. Similarly, it is now a growing topic to provide bounds on the variations for hyperbolicity that may be caused by various graph operations [MRSV10, CRS15]. In this aspect, it would be interesting to prove some new results in the spirit of Theorem 19.

2.5 Obstructions to hyperbolicity

In the continuity of Section 2.4, we now cover some known lower-bound techniques on graph hyperbolicity. The latter results will complete our first objective in the study of this parameter by giving characterizations for non hyperbolic graph classes, or equivalently *necessary* conditions for a graph to be hyperbolic. Like we did in Section 2.4, we will also provide examples of non hyperbolic graph classes that do *not* satisfy these characterizations, thereby showing the limitations of the lower-bound techniques.

Outline of the section. The rest of the section is divided as follows. First, I survey some results on the hyperbolicity of random graphs in Section 2.5.1. They show that, in some sense, most graphs are non hyperbolic. Then I present in Section 2.5.2 the typical obstructions that are used to show that a given graph class is non hyperbolic. These tools comprise: forbidden isometric subgraphs (Section 2.5.2.1), quasi-cycles (Section 2.5.2.2) and graph powers with some given properties (Section 2.5.2.4). Finally, some open problems are mentioned in Section 2.5.3.

My personal contributions: two new techniques using graph powers in order to lower-bound hyperbolicity, are presented in Section 2.5.2.4. This is joint work with David Coudert. Furthermore, as a side contribution of this thesis, I answer an open question from [VS14] on the relationship between hyperbolicity and quasi-cycles (Section 2.5.2.2).

2.5.1 Related work: random graphs are non hyperbolic

It is natural to ask for hyperbolicity, as for any graph parameter, what its typical value is on graphs. Put in other terms, the question is whether classes of random graphs are hyperbolic. The tendency is that, for a large spectrum of random graph models [CFHM13, NST15, Sha11, Sha12, Sha13, FGL$^+$15, Tuc13, MP14, BHO$^+$11], the graphs so obtained are non hyperbolic. The following results could be used in probabilistic methods in order to give lower-bounds on graph hyperbolicity.

In Sections 2.5.1.1 and 2.5.1.2, we emphasize on the results obtained on the hyperbolicity of the (classical) Erdös-Rény random graphs and the random regular graphs. We briefly mention the techniques used in the proofs of these results, that will be further detailed in Section 2.5.2. Then, Section 2.5.1.3 covers the known results on the hyperbolicity for other types of random graphs, and some open questions.

2.5.1.1 Erdös-Rényi random graphs

In particular, the most common model of random graphs is the Erdös-Rényi model $\mathcal{G}_{n,p}$, sometimes called the binomial random graph model. In a binomial random graph $G_n \in \mathcal{G}_{n,p}$, each possible edge exists with probability p. Note that p may, and usually does, depend on the number n of vertices in the graph.

It turns out that, for most regimes of p, the binomial random graphs are *non hyperbolic* with high probability. Precisely, the authors in [NST15] proved that in the sparse case $p = \mathcal{O}(1/n)$, binomial random graphs are non constantly hyperbolic. The latter result follows from the existence of arbitrarily long isometric cycles with positive probability (see Section 2.5.2.1). In a denser case where $p = 1 - \omega(1/n^2)$, Mitsche and Hell proved in [MP14] that binomial random graphs are non hyperbolic in the strong sense, *i.e.*, diameter-hyperbolic.

2.5.1.2 Random d-regular graphs

Similar results are obtained in [BHO$^+$11, Tuc13] for the class $\mathcal{G}_{n,d}$ of random d-regular graphs with the uniform probability distribution, that are proved to be non hyperbolic in the strong sense (diameter-hyperbolic). In order to prove that these random graphs are non hyperbolic, the authors in [BHO$^+$11] show the existence with high probability of large *quasi-cycles*. I shall come back in details on the notion of quasi-cycles when I present the known lower-bounds on graph hyperbolicity in Section 2.5.2.2.

2.5.1.3 Other random models of complex networks

Finally, since the above-mentioned models do not reflect well the structure of real-life graphs [BAJ00], it is interesting to ask whether random models of complex networks exhibit the same behaviour. Unfortunately, that seems to be the case.

In particular, it is proved in [CFHM13] that in most regimes, the random graphs that are obtained with the small-world model of Kleinberg are either non hyperbolic or non polylogarithmically hyperbolic. Some range of random graphs that are obtained with the Chung-Lu model are proved to be non constantly hyperbolic in [Sha13].

Perspectives. Surprisingly, we are not aware of any lower-bound on the hyperbolicity of Barabási-Albert random graphs (this problem has been studied only through experimentations [JLB08]). Furthermore, to find a pertinent class of random graphs that is hyperbolic – reflecting the properties of real-life networks such as the graph of the Autonomous of the Internet, that has a small hyperbolicity [CCL15, dMSV11] – is to my mind an important open question. In particular, the HOT model [FKP02] may be worth studying since it has been first defined to generate random trees.

2.5.2 Lower-bounds on the hyperbolicity

The remaining of the section will be devoted to a detailed presentation of the known lower-bound techniques on graph hyperbolicity, some of them have been briefly mentioned in our survey on the hyperbolicity of random graphs in Section 2.5.1. In Section 2.5.2.1, we present a basic technique in order to lower-bound hyperbolicity using isometric subgraphs. Next, we introduce quasi-cyclicity in Section 2.5.2.2, and as a side contribution of this thesis, we answer an open question from [VS14] on its relationship with graph hyperbolicity. Other personal lower-bound techniques, that are based on a game-theoretic characterization of hyperbolicity in [CCNV11], are finally presented in Section 2.5.2.4. The results in this last section are joint work with David Coudert.

2.5.2.1 Forbidden isometric subgraphs

We say that a graph parameter Π is closed under taking subgraphs if for every graph G and for every subgraph H of G, $\Pi(H) \leq \Pi(G)$. We now discuss on the stability of hyperbolicity under taking subgraphs.

Unlike many graph properties, hyperbolicity is not closed under taking subgraphs. That can be easily seen with the complete graph K_n, that is 0-hyperbolic and contains all possible n-vertex graphs as a subgraph. It is not closed under taking *induced* subgraphs either. Indeed, every graph G is the induced subgraph of a 1-hyperbolic graph G' with diameter two, obtained from G by adding a universal vertex u (the shortest-path tree of G' rooted at u is a star with additive distortion of the distances in G' at most one). However, we recall that a subgraph H

of $G = (V, E)$ is called *isometric* if it is distance-preserving, *i.e.*, the distance between every two vertices in H is the same in H as in G. By the 4-point Condition (Definition 1), it implies that $\delta(H) \leq \delta(G)$ for any isometric subgraph H of G. Hence, a classical technique in order to lower-bound the hyperbolicity is to exhibit an isometric subgraph from a well-known non hyperbolic graph class, such as *e.g.*, cycles and grids.

As an example, recall that the *girth* of a given graph G, denoted by $g(G)$ in what follows, is a well-known parameter that is the minimum length of a cycle in G. By minimality of its length, any cycle with length $g(G)$ is isometric, and so, the hyperbolicity can be lower-bounded using the girth:

Lemma 20 ([WZ11]). *For every $G = (V, E)$, we have $\delta(G) \geq \lfloor g(G)/4 \rfloor - 1/2$ if $g(G) \equiv 1 \mod 4$, and $\delta(G) \geq \lfloor g(G)/4 \rfloor$ otherwise.*

It follows that in order for a graph class to be constantly hyperbolic, the graphs must have a girth that is constantly upper-bounded. Actually, the length of *any* isometric cycle in the graphs must be constantly upper-bounded. This is a strictly stronger condition since there are graphs with bounded girth and arbitrarily large isometric cycles. I illustrate this fact with the construction of Figure 2.16, that is a side contribution of this thesis. Namely, the construction shows examples of planar graphs G_ℓ that are $(1,1)$-*dismantlable* (see Section 2.3.2.2), and so, with girth tree, but with an isometric cycle of length ℓ.

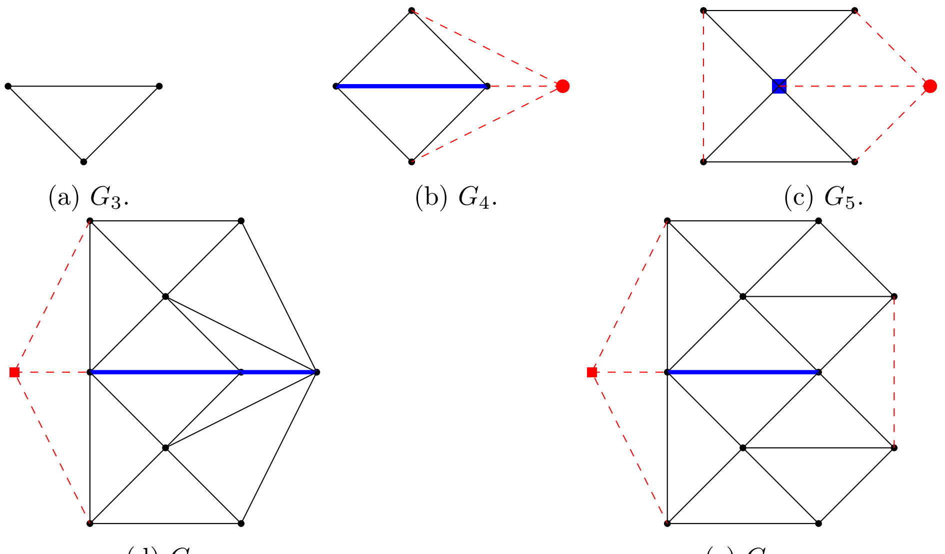


Figure 2.16: Examples of plane cop-win graphs G_ℓ such that their outerface is an isometric cycle of length ℓ. The graph G_ℓ is obtained from two copies of $G_{2\lfloor \ell/2 \rfloor - 1}$ by identifying a path on their respective outerface (drawn in thick blue), then adding a new dominated vertex on its outerface and additional edges (drawn in dashed red).

The graph G_ℓ of the construction satisfies a stronger property, that is, it admits a planar embedding where the outerface is an isometric cycle of length ℓ. For every $i \geq 2$, G_{2i} and G_{2i+1} are obtained from two copies of G_{2i-1} as follows. We start identifying a path $\mathcal{P}_i$ on their outerface with length $i-1$ (for the even case $\ell = 2i$) or $i-2$ (for the odd case $\ell = 2i+1$). Then, let us fix one end v_i of $\mathcal{P}_i$. In each of the two copies of G_{2i-1}, v_i has one neighbour on the outerface that is not part of $\mathcal{P}_i$. We add a new vertex of degree three that is made adjacent to v_i and to its two neighbours $u_i, u_i' \notin \mathcal{P}_i$ on the outerface in each copy. Note that the closed neighbourhood of this new vertex is dominated by v_i by construction. Furthermore, in doing so, we obtain in the even case $\ell = 2i$ an outerface which is an isometric cycle of length $2(2i-1) - 2|\mathcal{P}_i| + 1 = 2i = \ell$. Finally, in order to complete the construction in the odd case $\ell = 2i+1$, we consider the second end of $\mathcal{P}_i$ and we make adjacent its two neighbours $x_i, x_i' \notin \mathcal{P}_i$ on the outerface in each copy.

Note that on the other hand, not every graph with bounded-length isometric cycle has small hyperbolicity. For instance, the hexagonal grid with n columns and m rows (cf. Figure 2.17) is a *bridged graph* – *i.e.*, with no isometric cycle of length at least four – yet it is $(\min\{n,m\}-1)/2$-hyperbolic [CD16a].

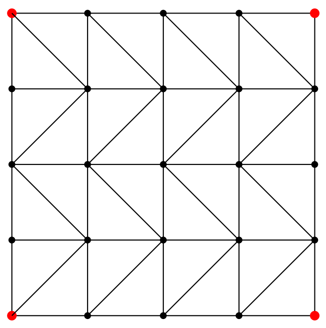


Figure 2.17: Hexagonal grid.

2.5.2.2 Quasi-cycles

We now describe quasi-cyclicity and its relationship with hyperbolicity. A lower bound technique is derived from the relationship, that is successful in some cases where we fail exhibiting an isometric cycle (e.g., grid-like graphs). Namely, in [VS14], Verbeek and Suri relax the notion of isometric cycles to the one of (weak) quasi-cycles. Given $G = (V, E)$, a cycle C of length n is an (α, β)-quasi-cycle if for every $u, v \in C$ such that $d_C(u,v) \geq \beta n$ we have that $d_G(u,v) \geq \alpha\, d_C(u,v)$. Verbeek and Suri have proved in [VS14] that every graph G has an $(\alpha, 1/3)$-quasi-cycle of length $\Omega(\delta(G))$, for some constant α independent from $\delta(G)$. Therefore, the existence of large quasi-cycles is a necessary condition for a graph to have a large hyperbolicity.

They proved the condition to be sufficient when $\alpha > 1/2$. Indeed, an easy application of the 4-point Condition (Definition 1) shows that in this situation, the graph has hyperbolicity at least $\Omega((\alpha - 1/2)n)$ [VS14].

Answering an open question from [VS14], we now prove more cases where the existence of large quasi-cycles implies a large hyperbolicity. The latter result is a side contribution of this thesis that has not been published elsewhere.

Lemma 21. *For every $\alpha \le 1, \beta \le 1/3$, if $G = (V,E)$ has an (α,β)-quasi-cycle of length n then $\delta(G) = \Omega\left(\alpha^2 n\right)$.*

Proof. We give an illustration of the proof with Figure 2.18. For simplicity, we will ignore the ceilings in the proof.

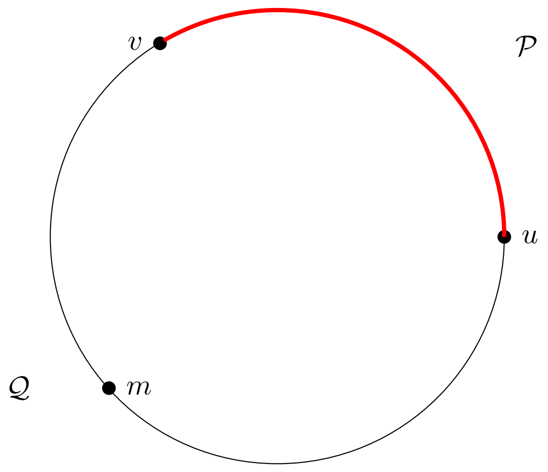


Figure 2.18: Proof of Lemma 21.

Let C be an (α,β)-quasi-cycle of length n, which exists by the hypothesis. Let us pick $u, v \in C$ such that $d_C(u,v) = n/3$. We can partition the cycle C into two uv-paths $\mathcal{P}, \mathcal{Q}$ of respective length $n/3$ and $2n/3$. In this situation, since C is assumed to be an (α,β)-quasi-cycle and $\beta \le 1/3$, we have $d_G(u,v) \ge \alpha n/3$, and so, $\mathcal{P}$ and $\mathcal{Q}$ are $(\frac{2}{\alpha},0)$-almost shortest uv-paths. Then, let $m \in \mathcal{Q}$ be a middle-vertex, *i.e.*, chosen such that $d_C(m,u) = |\mathcal{Q}|/2$. By the choice of m, $d_C(m,\mathcal{P}) = d_C(m,u) = n/3$. Furthermore, since $\beta \le 1/3$, it implies $d_G(m,\mathcal{P}) \ge \alpha n/3$. However, recall that in a hyperbolic graph, almost shortest-paths stay close to each other. Precisely, the Hausdorff distance between $\mathcal{P}$ and $\mathcal{Q}$ is an $\mathcal{O}\left(\delta(G)/\alpha\right)$ [Shc13b, GdLH90]. In particular, we have $\alpha n/3 \le d_C(m,\mathcal{P}) = \mathcal{O}\left(\delta(G)/\alpha\right)$. Altogether, $\delta(G) = \Omega\left(\alpha^2 n\right)$. □

2.5.2.3 Graph expansion

Other lower-bounds can be deduced from the existence of a core in graphs with small hyperbolicity[3]. Namely, we now present lower-bound techniques for hyperbolicity that are based on graph expansion (defined below). Lower-bounds are more complex to derive with this technique than with isometric subgraphs and quasi-cycles.

[3]The following result can also be intuited with another property of hyperbolic graphs, that is called the exponential divergence of shortest-paths [BH11].

The expansion of $G = (V, E)$, sometimes called the Cheeger constant, is the largest h such that for every subset S with at most $|V|/2$ vertices, there are at least $h|S|$ edges of G with one end in S and the other end in $V \setminus S$. The graphs in a class $\mathcal{G}$ are *expander* if there exist constants h, Δ such that every $G \in \mathcal{G}$ has maximum degree at most Δ and expansion at least h [HLW06]. The authors in [Ben98, Mal15] proved that expander graphs are non hyperbolic.

Theorem 22 ([Mal15]). *For every h, Δ, there exists a constant $C_{\Delta,h}$ such that every $G = (V, E)$ with maximum degree at most Δ and expansion at least h has hyperbolicity at least $C_{\Delta,h} \cdot \log(|V|)$.*

Intuitively, Theorem 22 can be explained as follows. In an expander graph with diameter D, since the number of vertices is exponential in D, removing a ball of radius $\Theta(D)$ will only remove a sublinear number of vertices, that does not affect too much the expansion. In particular, the order of magnitude of the diameter stays $\Theta(D)$, and so, the removal of the ball can only increase the distances by at most a constant-factor. In contrast, in a δ-hyperbolic graph there must be a core, *i.e.*, a ball of radius $\mathcal{O}(\delta)$ intersecting the (almost) shortest-paths between half of the pairs of vertices [CDV16]. By removing a core, one could increase the distances by more than any fixed constant-factor. This forces the core to have radius $\Omega(D)$, and so, the hyperbolicity of a given expander graph must scale with its diameter.

2.5.2.4 Contribution: Using dismantlable graph powers

Finally, we show how to use the game-theoretic characterization for hyperbolicity that has been proved in [CCPP14] in order to obtain new non-trivial lower-bounds on this parameter. New examples of non hyperbolic graph classes will be derived from these techniques. The results in what follows are joint work with David Coudert.

We refer to Section 2.3.2.2 for the game-theoretic characterization of hyperbolicity. Recall that for every $j \geq 1$, the j^{th} power of $G = (V, E)$ is the graph G^j that is obtained from G by adding an edge between every two distinct vertices u, v such that $d_G(u, v) \leq j$. If G is δ-hyperbolic for some $\delta > 0$, then by Lemma 8 G has a $(4\delta, 4\delta)$-dismantlable ordering [CCNV11]. The latter is a (classical) dismantling ordering for its power $G^{4\delta}$, hence $G^{4\delta}$ is a Cop-win graph. Conversely, disproving that G^j is Cop-win, for some range of j, will give lower-bounds on $\delta(G)$. This approach is used in [CD16a] in order to prove that most underlying graphs of the data center interconnection networks are non hyperbolic.

We start this section with additional properties of Cop-win graphs. They will be used in what follows.

Required background. Let us recall that an endomorphism of $G = (V, E)$ is an edge-preserving mapping $\sigma : V \to V$.

Lemma 23 ([AF84]). *If $G = (V, E)$ is a connected dismantlable graph that is regular then G is a complete graph.*

Lemma 24 ([BCF94]). *If $G = (V, E)$ is a connected dismantlable graph then it has the clique invariant property: for every endomorphism σ of G, there is a nonempty clique C of G such that $\sigma(C) = C$.*

Next, we present our lower-bound techniques.

New lower-bound techniques. Our contributions are summarized in Propositions 26 and 25. Given an endomorphism σ of $G = (V, E)$, let the mobility of σ be defined as $\min_v \mathrm{d}_G(v, \sigma(v))$. Then, generalizing the terminology of [DRB99], the *weak mobility* of G is the largest l such that G has an endomorphism with mobility l. Note that by Lemma 24, any tree (and more generally, any Cop-win graph) satisfies the clique-invariant property. Since a clique has diameter one, it follows that any tree (and more generally, any Cop-win graph) has weak mobility at most one. Based on this observation, we prove in [CD16a] that a large weak mobility implies a large hyperbolicity. Indeed, a weak mobility at least l can be shown to imply that no graph power $G^{l'}$, for $l' = \mathcal{O}(l)$, can satisfy the clique-invariant property. As a result, no such power can be a Cop-win graph by Lemma 24, and so, since $G^{4\delta(G)}$ must be Cop-win by Lemma 8, the latter implies that G must have hyperbolicity $\delta(G) = \Omega(l)$. Below, we formalize this intuition.

Proposition 25. *If $G = (V, E)$ has weak mobility $l \geq 2$ then $\delta(G) \geq \lceil l/2 \rceil / 2$.*

Proof. We prove that $G^{l'}$ is not dismantlable for every $1 \leq l' \leq l - 1$. It implies by Lemma 8 that G is not δ-hyperbolic for any $\delta < l/4$, and so, since $\delta(G)$ is a half-integer, $\delta(G) \geq \lceil l/2 \rceil / 2$. Indeed, since G has weak mobility l and every endomorphism of G is also an endomorphism of $G^{l'}$, the graph power $G^{l'}$ has weak mobility at least $\lceil l/l' \rceil \geq 2$. Therefore, $G^{l'}$ falsifies the clique invariant property, hence it is not dismantlable by Lemma 24. $\square$

Then, we recall that in a tree, there exists a leaf ℓ, *i.e.*, a vertex of degree one. In this situation, let p be its unique neighbour. Clearly, every node at distance $d > 1$ from ℓ is at distance $d - 1$ from p. The latter means that for every tree T with diameter $D > 1$, its powers T^j are not regular for every $j < D$ (because for any ℓ on a diametral path, its parent p has at least one more neighbour than ℓ). Following this intuition, if a given graph G with diameter D has small hyperbolicity δ then there should exist a small constant $j_0 = \mathcal{O}(\delta)$ such that: for every $j_0 \leq j \leq D-1$, its graph power G^j is not regular. We formalize this intuition below, using Lemma 23.

Proposition 26. *Let $G = (V, E)$ and $2 \leq r \leq diam(G)$ be such that G^{r-1} is a regular graph. Then, $\delta(G) \geq \lceil r/2 \rceil / 2$.*

Proof. Suppose for the sake of contradiction that $4\delta(G) < r$. In particular, G is $\lfloor (r-1)/2 \rfloor / 2$-hyperbolic, and so, by Lemma 8, it has a $(2 \lceil (r-1)/2 \rceil, r-1)^*$-dismantling ordering. The latter ordering is also a $(r-1, r-1)^*$-dismantling ordering, hence G^{r-1} is Cop-win. However, since G^{r-1} is assumed to be regular, it must be a complete graph by Lemma 23. The latter contradicts that $r - 1 < diam(G)$. As a result, $4\delta(G) \geq r$, as desired. $\square$

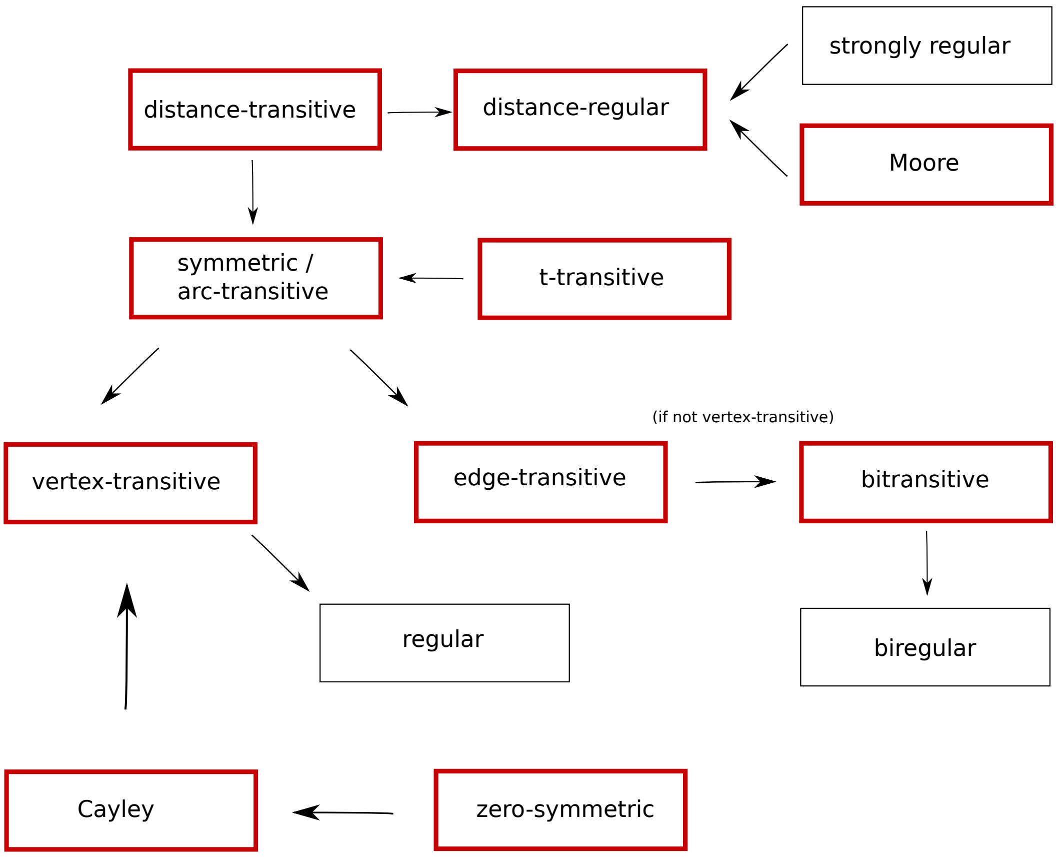


Figure 2.19: Relationships of inclusion between some graph classes. The rectangles for non hyperbolic graph classes (in red) are drawn thicker.

Application: non hyperbolic graph classes. We finally present some graph classes that can be proved to be non hyperbolic by using Propositions 26 and 25. To the best of our knowledge, these results are new, except for vertex-transitive graphs (defined below), of which we give a simpler proof they are non hyperbolic than in [BS12]. Furthermore, relationships of inclusion between the following graph classes are presented in Figure 2.19.

- We recall that an automorphism is a one-to-one endomorphism, and $G = (V, E)$ is *vertex-transitive* if for every $u, v \in V$, there is an automorphism mapping u to v.

  Note that most underlying graphs of data center interconnection networks that are proposed in the literature are vertex-transitive [AK89].
- A graph G is said to be *distance-regular* if it is a regular graph such that for every $i, j, k \geq 0$, there is some constant $c_{i,j,k}$ with the property that for every two vertices u and v at distance i in G, the number of vertices that are simultaneously at distance j from u and distance k from v in G is exactly $c_{i,j,k}$ [BH12].
- *Moore graphs* [Dam73] are a particular case of distance-regular graphs: namely,

an n-vertex d-regular graph is a Moore graph if $n = 1 + d \cdot \sum_{k=0}^{D-1}(d-1)^k$, with D being the diameter of the graph.

Theorem 27. *If a graph is vertex-transitive, distance-regular or Moore then it is non hyperbolic.*

Proof. Let G be a vertex-transitive graph. Since an endomorphism of G is also an endomorphism for every of its powers, it implies that if G is vertex-transitive then so are all its powers. Hence all the powers of G are regular graphs. Altogether, by Proposition 26 the hyperbolicity of G is constantly proportional to its diameter.

Similar arguments apply to distance-regular graphs and Moore graphs. Indeed, if a graph belongs to these classes then all its powers are regular [BH12]. Therefore, its hyperbolicity is constantly proportional to its diameter. $\square$

A *bitransitive graph* is a bipartite graph such that for every two vertices u, v that are in the same side of the bipartition, there exists an automorphism mapping u to v. In the spirit of what is done for the framework presented in Section 2.4.3 (Lemma 17), let us pick one side of the bipartition and add an edge between every two vertices in this side that are at distance two. Then, the graph so obtained is vertex-transitive. This observation allows to prove that the class of bitransitive graphs, and so, the related classes of edge-transitive and nonedge-transitive graphs [GR13] are also non hyperbolic.

Refinements of Proposition 26 can lead to sharper lower-bounds on the hyperbolicity (but under stronger assomptions). In Table 2.2, we report on some results obtained with our lower-bound techniques (detailed in [CD16a]). For every graph in the table, the values of the diameter and the hyperbolicity are compared, with the two values only differing by at most a constant-factor in most cases. All these results are mainly obtained with Propositions 25 and 26, or some of their variations that are proved in [CD16a]. However, we also report on the hyperbolicity of grid-like graphs, on which these lower-bound techniques do not apply. We managed to obtain the *exact* value for the hyperbolicity of these graphs through a deeper analysis of their shortest-path distribution.

2.5.3 Open problems

So far, there are few reported lower-bounds on graph hyperbolicity. Finding new lower-bounds is an important open problem, that would improve our understanding of this parameter and could also help improving its computation. A related open problem is to prove some new lower-bounds on the hyperbolicity of random graph classes, such as Barabási-Albert random graphs and random geometric graphs in the Hyperbolic plane [KPK+10][4].

[4]Note that there exist duality results between these two random models [FCM14].

Name	Degree max.	Diameter	Order	δ
de Bruijn graph, $UB(d,D)$	$2d$	D	d^D	$\frac{1}{2}\left\lfloor\frac{D}{2}\right\rfloor \leq \delta \leq \left\lfloor\frac{D}{2}\right\rfloor$
Kautz graph, $UK(d,D)$	$2d$	D	$d^D(d+1)$	$\left\lfloor\frac{D}{4}\right\rfloor + \varepsilon \leq \delta \leq \left\lfloor\frac{D}{2}\right\rfloor, \varepsilon \in \{0,1\}$
Shuffle exchange, $SE(n)$	3	$2n-1$	2^n	$\frac{1}{2}\left\lfloor\frac{n}{2}\right\rfloor \leq \delta \leq n-1$
(n,m)-grid	4	$n+m-2$	nm	$\min\{n,m\}-1$
d-dimensional grid of size s	$2d$	$d(s-1)$	s^d	$(s-1)\left\lfloor\frac{d}{2}\right\rfloor$
Triangular (n,m)-grid	6	$n+m-2$	nm	$\frac{\min\{n,m\}-1}{2}$
Hexagonal (n,m)-grid	6	$\begin{cases} n-1+\left\lceil\frac{m-1}{2}\right\rceil & \text{when } m \leq 2n-1 \\ m-1 & \text{otherwise}\end{cases}$	nm	$\frac{\min\{n,m\}-1}{2}$
Torus (n,m)-grid	4	$\left\lfloor\frac{n}{2}\right\rfloor + \left\lfloor\frac{m}{2}\right\rfloor$	nm	$\left\lfloor\frac{1}{2}\left(\left\lfloor\frac{n}{2}\right\rfloor + \left\lfloor\frac{m}{2}\right\rfloor\right)\right\rfloor - 1 \leq \delta \leq \left\lfloor\frac{1}{2}\left(\left\lfloor\frac{n}{2}\right\rfloor + \left\lfloor\frac{m}{2}\right\rfloor\right)\right\rfloor$
Gen. hypercube, $G(m_1,\ldots,m_r)$	$\sum_{i=1}^r m_i - r$	r	$\prod_{i=1}^r m_i$	$\left\lfloor\frac{r}{2}\right\rfloor$
Cube Connected Cycle, $CCC(n)$	3	$2n-2+\max\left\{2,\left\lfloor\frac{n}{2}\right\rfloor\right\}$	$n2^n$	$n \leq \delta \leq n-1+\left\lfloor\frac{\max\{2,\lfloor\frac{n}{2}\rfloor\}}{2}\right\rfloor$
BCube$_k(n)$	$\max\{n,k+1\}$	$2(k+1)$	$n^k(n+k+1)$	$k+1$
Fat-Tree$_k$	k	6	$\frac{k^2}{4}(k+5)$	2
Butterfly graph, $BF(n)$	4	$2n$	$2^n(n+1)$	n
k-ary n-fly	$2k$	$2n$	$k^n(n+1)$	n
k-ary n-tree	$3k$	$2n$	$k^{n-1}(n+k)$	$n-1$
Bubble-sort graph, $BS(n)$	$n-1$	$\binom{n}{2}$	$n!$	$\left\lfloor\frac{n(n-1)}{4}\right\rfloor$
Transposition graph, $T(n)$	$\binom{n}{2}$	$n-1$	$n!$	$\frac{1}{2}\left\lfloor\frac{n-1}{2}\right\rfloor \leq \delta \leq \left\lfloor\frac{n-1}{2}\right\rfloor$
Star graph, $S(n)$	$n-1$	$\left\lfloor\frac{3(n-1)}{2}\right\rfloor$	$n!$	$\left\lfloor\frac{1}{2}\left\lfloor\frac{3(n-1)}{2}\right\rfloor - \frac{1}{2}\right\rfloor \leq \delta \leq \left\lfloor\frac{1}{2}\left\lfloor\frac{3(n-1)}{2}\right\rfloor\right\rfloor$

Table 2.2: Bounds and exact value of the hyperbolicity of some graph classes [CD16a].

2.6 On computing the hyperbolicity of graphs

The remaining of this chapter is devoted to algorithmic and complexity problems. In particular, computational aspects of hyperbolicity will be covered in this section, thereby fulfilling our second main objective in the study of this parameter.

Motivations for an efficient computation of hyperbolicity are: to help characterizing the hyperbolic graph classes, or to measure the quality of approximations obtained with some graph heuristics (the latter will be further dicussed in Section 2.7) [VS14, CDE$^+$08, CE07, EKS16, KL06, DKMY15].

By using the 4-point Condition (Definition 1), it is easy to see that the hyperbolicity of a given n-vertex graph can be computed in $\Theta(n^4)$-time. However, this too simple approach is prohibitive on large graphs, even when we use massively parallelization [ASHM13]. In what follows, improved algorithms for computing or approximating graph hyperbolicity will be sketched, with an emphasis on my personal contribution in this topic.

Note that we will only consider *finite* graphs in this section. Computing the hyperbolicity of *infinite* graphs is highly nontrivial. However, surprisingly, there exists a simple (approximation) partial algorithm for computing the hyperbolicity of the graph representations of finitely generated groups [Pap96].

Outline of the section. The best known algorithms for computing graph hyperbolicity are collected in Section 2.6.1. We sketch their basic principles and their limitations. Then, the next two Sections 2.6.2 and 2.6.3 are mostly centered on the contributions of this thesis.

In particular, the design and the analysis of some preprocessing methods for the computation of hyperbolicity are presented in Section 2.6.2. This part is largely devoted to personal contributions on the study of the relationships between the hyperbolicity of a graph and the maximum hyperbolicity from its *atoms* — *a.k.a.*, the subgraphs resulting from its decomposition by clique-minimal separators [BPS10] (Section 2.6.2.2). As a side contribution, I will also present a short analysis of the heuristic from [KNS13] (Section 2.6.2.1). Finally, conditional lower-bounds on the time complexity for computing graph hyperbolicity will be also mentioned in Section 2.6.3, including one of my own invention.

This is joint work with Nathann Cohen, David Coudert and Aurélien Lancin.

2.6.1 Related work

In this subsection, a state of the art on exact and approximate algorithms for computing the hyperbolicity of a graph is presented. We also comment on the limitations of these algorithms. In what follows, exact algorithms will be presented first (Section 2.6.1.1), then the approximation algorithms will be introduced by increasing approximation factor (Section 2.6.1.2).

2.6.1.1 Exact algorithms

Best known algorithm. The best known algorithm for computing the hyperbolicity runs in $\mathcal{O}(n^{3.69})$-time [FIV15]. It relates the computation of graph hyperbolicity with a variation of matrix multiplication.

Indeed, recall (Definition 3) that $G = (V, E)$ is δ-hyperbolic if and only if we have for every u, v, x, y that $\langle u, v\rangle_x \geq \min\{\langle u, y\rangle_x, \langle y, v\rangle_x\} - \delta$, where $\langle \cdot, \cdot\rangle_x$ denotes the Gromov product with base vertex x. In particular, let M_x be the $n \times n$ matrix such that $M_x[u, v] = \langle u, v\rangle_x$ for every $u, v \in V$. The $(\max, \min)$-product of M_x with itself is an $n \times n$ matrix denoted by $M_x \otimes M_x$ such that for every $u, v \in V$,

$$(M_x \otimes M_x)[u, v] = \max_{y \in V} \min\{M_x[u, y], M_x[y, v]\} = \max_{y \in V} \min\{\langle u, y\rangle_x, \langle y, v\rangle_x\}.$$

By Definition 3, G is δ-hyperbolic if and only if for every $x \in V$, all entries in $M_x \otimes M_x - M_x$ are lower than or equal to δ. Therefore, $\delta(G)$ can be computed with n computations of $(\max, \min)$-products.

Combinatorial algorithms. One drawback of the above algorithm is that it uses as a subroutine the best known algorithm for computing the (classical) matrix multiplication [DP09]. This algorithm requires quadratic-space and its time complexity $\mathcal{O}(n^{2.3729})$ hides a large constant-factor [LG14]. So, in order to compute hyperbolicity in practice on real-life graphs, *combinatorial algorithms* should be preferred.

In [CCL15], Cohen et al. base on the following simple, but elegant observation.

Lemma 28 ([CCL15]). *Let $G = (V, E)$ and $u, v, x, y \in V$ be such that $\mathrm{d}(u, v) + \mathrm{d}(x, y) \geq \max\{\mathrm{d}(u, x) + \mathrm{d}(v, y), \mathrm{d}(u, y) + \mathrm{d}(v, x)\}$. Then, $\delta(u, v, x, y) \leq \min\{\mathrm{d}(u, v), \mathrm{d}(x, y)\}/2$.*

The latter lemma gives a simple "cut-rule" in order to avoid considering all possible 4-tuples. Indeed, let us consider the 4-tuples u, v, x, y of $G = (V, E)$ by non increasing value of $\mathrm{d}(u, v) + \mathrm{d}(x, y)$. A lower-bound δ^* on the hyperbolicity $\delta(G)$ is maintained. By Lemma 28, every time the lower-bound improves, all 4-tuples such that $\min\{\mathrm{d}(u, v), \mathrm{d}(x, y)\} \leq 2\delta^*$ can be discarded. While this algorithm still runs in $\mathcal{O}(n^4)$-time, experiments have shown that it is much faster in practice.

Since then, additional cut-rules have been introduced in [BCCM15], which further speed-up the practical computation of hyperbolicity. So far, the hyperbolicity of graphs with tens of thousands of nodes can be computed within a reasonable amount of time. The true limitation of the algorithm comes from the storage in quadratic space of the distance matrix.

2.6.1.2 Approximation algorithms

Then, we report on the few existing approximation algorithms for computing hyperbolicity. The main message here is that these algorithms either have a large approximation factor (sometimes non constant) or they require the challenging best-known algorithm for computing matrix multiplication as a subroutine.

Using $(\max, \min)$**-product.** The simplest of these approximation algorithms reduces to the problem HYPERBOLICITY WITH FIXED BASE VERTEX: given $G = (V, E)$ and $x \in V$, compute $\delta_x(G) = \max_{u,v,y \in V} (\min\{\langle u, y\rangle_x, \langle y, v\rangle_x\} - \langle u, v\rangle_x)$. Note that $\delta(G) = \max_{x \in V} \delta_x(G)$. Furthermore, it can be proved using the triangular inequality that for every fixed $x \in V$, we have $\delta_x(G) \geq \delta(G)/2$ [Gro87]. As a result, solving the problem HYPERBOLICITY WITH FIXED BASE VERTEX gives a 2-approximation for computing hyperbolicity, and it can be done in $\mathcal{O}(n^{2.69})$-time by using the above-mentioned relationship with $(\max, \min)$-product [FIV15].

More recently, Duan has proved that the $(\max, \min)$-product can be computed faster when all entries in the matrices are bounded. Based on this result, he has described $(1 + \varepsilon)$-approximation algorithms for computing graph hyperbolicity, for every $\varepsilon \geq 0$ [Dua14].

Using Cop and Robber games. Another constant-factor approximation algorithm for computing this parameter was proposed in [CCPP14]. Roughly, given the distance-matrix of the graph (it can be precomputed in $\mathcal{O}(\min\{nm, n^{2.3729}\})$-time) this algorithm computes in $\mathcal{O}(n^2)$-time the smallest r such that the input graph has a $(4r, 3r)^*$-dismantling ordering. Altogether combined with the game-theoretic definition of hyperbolicity (Definition 7), the value gotten for r differs from the hyperbolicity by at most an (unfortunately large) constant-factor.

Using Tree embeddings. Finally, another approach for approximating the hyperbolicity is based on the relationships between this parameter and tree embeddings. Precisely, every δ-hyperbolic graph can be embedded into a tree with additive distortion of the distances at most $2\delta \log n$ [Gro87] (that will be further discussed in Section 2.7). In [FIV15], Fournier et al. notice that computing this tree embedding does not require the knowledge of the hyperbolicity. Therefore, an $\mathcal{O}(\log n)$-approximation algorithm for computing the hyperbolicity of a graph can be obtained in $\tilde{O}(n^2)$-time by computing this tree embedding, and then the resulting distortion of the distances in the tree[5].

2.6.2 Contribution of this thesis: Preprocessing

In order to overcome the current limitations for computing graph hyperbolicity (sketched above), it looks natural to seek for *preprocessing methods*, that aim at decreasing the size of the input and, possibly, at simplifying its structure. My main contribution in the field is the design and the analysis of some of these methods. I will first sketch a short analysis of the heuristic from [KNS13], before presenting my work on graph decompositions.

[5]The time complexity of this algorithm was proved in [FIV15]. However, the authors in [FIV15] assume that the distance matrix is given as input. We explain in [CD14] how to obtain the same time complexity for graphs encoded as adjacency lists.

2.6.2.1 Reducing the size of the graph by contracting matchings

In order to make tractable the approximate computation of hyperbolicity on large graphs, the authors in [KNS13] present a simple renormalization process. Put in more graph-theoretic terms, their process pick a maximal matching of the graph and then contract its edges. By doing so, the number of vertices is decreased by half. They repeat the process until the size of the graph is judged small enough in order to compute its hyperbolicity.

In what follows, we analyze the quality of this above heuristic for computing hyperbolicity. In order to do so, the hyperbolicity of a given graph G is compared with the hyperbolicity of its contraction minors (graphs obtained by contracting some edges of G), that is a study of independent interest.

Contraction minors and hyperbolicity. Although the distances in a graph cannot increase when we contract an edge, it turns out that, surprisingly, the hyperbolicity can do so. For instance, a cycle C_5 of length five is 1/2-hyperbolic, but contracting any one of its edges results in a cycle C_4 of length four, that is an 1-hyperbolic graph.

More generally, the following result is a side contribution of this thesis.

Lemma 29. *For every δ-hyperbolic n-vertex graph G, every contraction minor of G is $\mathcal{O}(\delta \log n)$-hyperbolic and this upper-bound is sharp.*

Proof. The upper-bound can be established by using the relationships between hyperbolicity and another tree-likeness parameter called *treelength* (see Section 2.4.1). Indeed, if G is a δ-hyperbolic n-vertex graph then it has treelength at least δ and at most $2\delta \log n + 1$ [AAD16]. The treelength is a contraction closed parameter. Therefore, every contraction minor of G must have hyperbolicity $\mathcal{O}(\delta \log n)$. The main difficulty is to prove the sharpness of the upper-bound.

In Figure 2.20, we illustrate this worst-case scenario with a ringed tree $RT(k)$ (previously introduced in Section 2.4.1). Note that this graph has $n = 2^{\mathcal{O}(k)}$ vertices, and in addition we have $\delta(RT(k)) \leq 3$ by Lemma 12[6]. So, every contraction minor of this ringed tree is $\mathcal{O}(k)$-hyperbolic. We aim at proving the existence of a contraction minor of $RT(k)$ with hyperbolicity $\Omega(k)$. the gist of the construction is to show that $RT(k)$ has a contraction minor H with a large *induced* (cylindrical) grid of dimensions $\Omega(k) \times \Omega(k)$. It can be constructed by fixing some level $\ell = \Theta(k)$ and then contracting on the cycles in each lower level the consecutive nodes with a common ancestor at level ℓ (*i.e.*, see Figure 2.20). Furthermore, since the graph is planar, it can be obtained an *isometric* (square) grid of comparable dimensions $\Omega(k) \times \Omega(k)$ by removing one third of the rows and one third of the columns on the borders. We recall that a grid of dimensions $\Omega(k) \times \Omega(k)$ has hyperbolicity $\Omega(k)$ [WZ11]. Altogether combined, this contraction minor H has hyperbolicity $\Omega(k)$, as desired. □

[6]This value of the hyperbolicity can be increased to some constant $\Theta(\delta)$ for every $\delta > 0$ by taking a uniform subdivision of $RT(k)$.

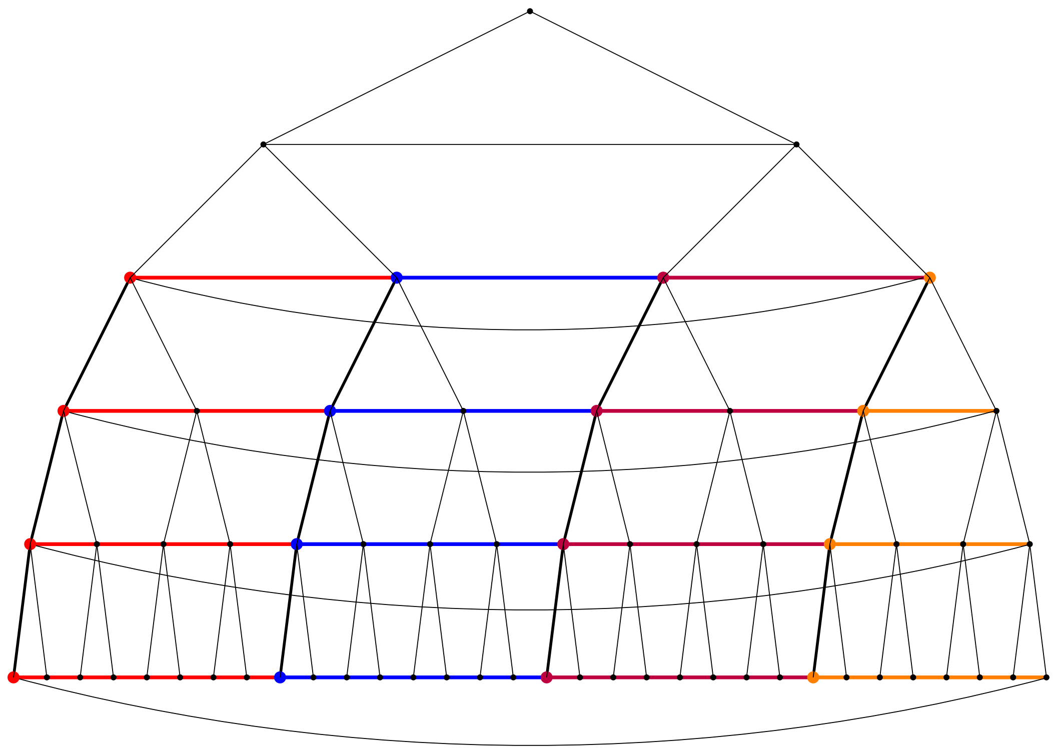


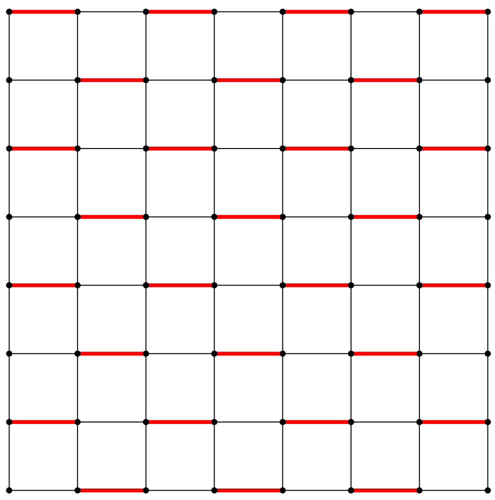
Figure 2.20: Construction of a cylindrical grid in $RT(k)$. We fix some level $\ell = \Theta(k)$ and then we contract on each lower level the nodes with a common ancestor at level ℓ. Paths contracted to a single node are delimited with thicker nodes.

Variations of hyperbolicity under one renormalization. The edge contractions in the renormalization process of [KNS13] are more controlled. Indeed, they must induce a matching. In this situation, let $\varphi : V(G) \to V(\hat{G})$ map every vertex of G to the corresponding vertex to which it has been contracted in the renormalized graph $\hat{G}$. We have that $\lfloor d_G(u,v)/2 \rfloor \leq d_{\hat{G}}(\varphi(u), \varphi(v)) \leq d_G(u,v)$ for every $u, v \in V(G)$. So, it follows from the preservation of hyperbolicity under quasi-isometry [Shc13b, GdLH90] that $\delta(\hat{G}) = \Theta(\delta(G))$. The above Θ notation hides a large constant-factor that may be improved with a more in-depth analysis. Nonetheless, what can be shown is that there exist infinitely many graphs G such that $\delta(G) \geq 4\delta(\hat{G})$. We illustrate this fact with Figure 2.21.

To summarize, it is my opinion that the confidence interval that is provided by the renormalization process is too large to give good estimates of graph hyperbolicity.

2.6.2.2 Relationship between clique-decomposition and hyperbolicity

Contrary to Section 2.6.2.1, the approach in this part rather consists in bounding the hyperbolicity of a given graph from the computation of the hyperbolicity of some of its subgraphs. Equivalently, given a decomposition of $G = (V, E)$ into some of its subgraphs, it is studied whether we can upper and lower bound $\delta(G)$ by using


(a) The square grid with side length n is $(n-1)$-hyperbolic.

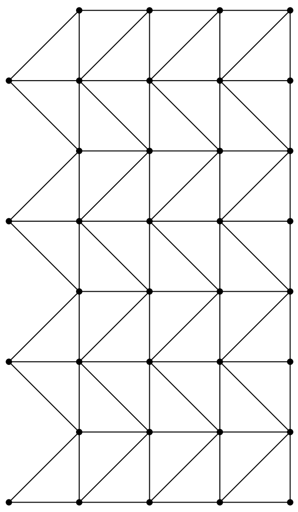

(b) The renormalized square grid is $(n-1)/4$-hyperbolic.

Figure 2.21: Renormalization process on a Square grid. The edges contracted are drawn in thick red. Roughly, it gives a Hexagonal grid with twice less columns. Since the hyperbolicity of a Rectangular grid is twice larger than the hyperbolicity of a Hexagonal grid with same dimensions [CD16a], it shows that the renormalization process divides the hyperbolicity of a square grid by four.

the maximum hyperbolicity from the subgraphs. Let us motivate this approach and present existing results.

On the one hand, when G is "prime" (undecomposable w.r.t. the decomposition process), the input cannot be split, and so, we don't decrease the size of the input either. On the other hand, it happens that many interesting classes of real-life graphs are *not* prime. Furthermore, in all cases we gain more insights on the structure of the input.

Let us outline interesting byproducts of this decomposition approach:

- when every graph in a given class can be decomposed in "trivial" subgraphs, the class is proved to be constantly hyperbolic;
- for some other graph classes, the decomposition is a first step toward an efficient computation of the hyperbolicity in this class of graphs.

Related work. Of course, we need some structure on the graph decomposition in order to be able to prove something. Soto [SG11] has proved that two well-known graph decompositions can be used as a preprocessing step for computing graph hyperbolicity. Namely, these are the modular decomposition [Gal67] and its generalization the split-decomposition [Cun82] where informally, the graph is disconnected by using some edge-cutsets inducing a complete bipartite subgraph. More precisely, the hyperbolicity of a given graph is equal to the maximum hyperbolicity taken from the subgraphs output by these decompositions.

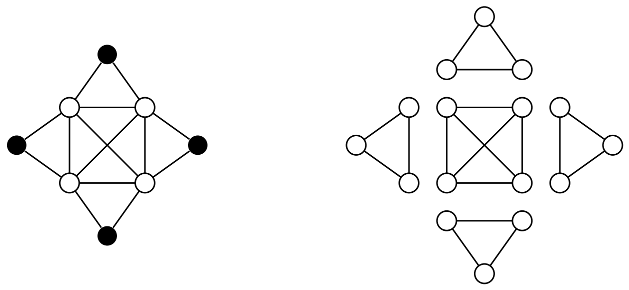


Figure 2.22: Clique-decomposition of a graph in five atoms. A 4-tuple with hyperbolicity 1 is drawn in bold.

Our main result. In a joint work with Nathann Cohen, David Coudert and Aurélien Lancin [CCDL17], we have proved similar results for the clique-decomposition [BPS10]. Given $G = (V, E)$, an atom of G is any subset $A \subseteq V$ such that there is no clique-separator in $G[A]$ and A is inclusion wise maximal w.r.t. this property. The clique-decomposition of G is the collection of its atoms. See Figure 2.22 for an example. It can be computed in $\mathcal{O}(|V||E|)$-time.

Theorem 30. *Given $G = (V, E)$, let $A_1, \ldots, A_k$ be its atoms. Then, $\max_i \delta(G[A_i]) \leq \delta(G) \leq \max_i \delta(G[A_i]) + 1$ and the bounds are sharp.*

Below, we detail further the proof of Theorem 30. It is based on two ingredients. The first is that disconnecting the graph with a separator of small diameter D can change the value of the hyperbolicity by at most an additive term $D/2$. This part requires a tedious analysis of the different types of 4-tuples in the graph in order to be proved.

Lemma 31 ([SG11])**.** *Given $G = (V, E)$, let $X \subseteq V$ be such that $G[X]$ is isometric and has diameter at most D. Then, let $C_1, \ldots, C_k$ be the connected components of $G \setminus X$, we have:*

$$\max_{1 \leq i \leq k} \delta(G[C_i \cup X]) \leq \delta(G) \leq \max\{D/2, \max_{1 \leq i \leq k} \delta(G[C_i \cup X])\} + D/2.$$

In [CCDL17], we give a proof of this result in the case of clique-separator ($D \leq 1$). Note that $G[X]$ must be isometric in order to ensure that the resulting subgraphs $G[C_i \cup X]$ are also isometric. Indeed, we recall that the hyperbolicity is not stable under taking induced subgraphs. However, we observe that when X is a clique-separator, the requirement for $G[X]$ to be isometric is always satisfied.

By Lemma 31, if we disconnect the graph with a small diameter separator then we can approximate the hyperbolicity up to an additive term. Unfortunately, these additive errors can add up when we further decompose the graph. We prove it is the case even for separators of diameter at most two [CCDL17]. However, in the special case of clique-separators, we can bound the final additive error with the following lemma.

Lemma 32. *Given $G = (V, E)$, let $u, v, x, y \in V$ satisfy $\delta(u, v, x, y) \geq 3/2$. There exists an atom A_0 intersecting all the paths between any two vertices of the 4-tuple.*

Proof. Let $(T, \mathcal{X})$ be a tree decomposition of G whose bags are the atoms of G. Such a tree decomposition was proved to exist in [BPS14]. In order to prove the lemma, it suffices to find an atom A_0 such that there is no more than one vertex of the 4-tuple u, v, x, y in each component of $G \setminus A_0$. We shall find an atom A_0 with the weaker property that no more than two vertices among $\{u, v, x, y\} \setminus A_0$ are in the same connected component of $G \setminus A_0$. Then, we will prove that in fact, there is no more than one vertex of the 4-tuple in each component, by elaborating on the property that $\delta(u, v, x, y) \geq 3/2$. First, in order to find the desired atom, we will weight the bags of $\mathcal{X}$ (we will then choose the atom A_0 in the *weighted centroid* of T).

Precisely, for every of u, v, x, y we pick an atom which contains it and we define the weight of an atom as the number of times it has been picked. In particular, an atom has weight between 0 and 4, and the sum of weight of the atoms is equal to $\mathcal{W} = 4$. It is well-known that for any node-weighted tree with sum of weights $\mathcal{W}$, there is a node whose removal splits the tree into connected components where the sum of weight of the nodes is at most $\mathcal{W}/2$ [Gol71]. So, let A_0 be an atom of G such that no component of $T \setminus \{A_0\}$ has the sum of weight of its bags greater than 2. We claim that $\forall s \in \{u, v, x, y\} \setminus A_0$, there is a clique-separator $X_s \subseteq A_0$ which separates s from $\{u, v, x, y\} \setminus \{s\}$, that will prove the lemma.

Indeed, let $s \in \{u, v, x, y\} \setminus A_0$ be arbitrary. By the properties of a tree decomposition, T_s (induced by the atoms containing s) is the subtree of a component C_s of $T \setminus \{A_0\}$. Let $V_s \subseteq V$ be the subset of vertices that are contained in an atom in C_s, and let $A_s \in C_s$ be the atom that is adjacent to A_0 in T. Since A_s and A_0 are atoms of G, their intersection, denoted by $X_s = A_s \cap A_0$, is a clique [BPS10]. Furthermore, by the properties of a tree decomposition, X_s is a is a separator of G that disconnects V_s from $V \setminus V_s$. Therefore, we are left to prove that no vertex of $\{u, v, x, y\} \setminus \{s\}$ is in V_s, for the latter will prove that X_s is a clique-separator which separates s from $\{u, v, x, y\} \setminus \{s\}$. Assume for the sake of contradiction the existence of a vertex $t \in \{u, v, x, y\} \setminus \{s\}$ that is contained in V_s. We distinguish between two cases.

- Suppose that $t \notin X_s$. In this situation, T_s, T_t are subtrees of C_s. It implies that the sum of weight of the atoms in C_s is at least 2, and so, by the choice of atom A_0, it is equal to 2. In particular, s and t are the only two vertices of the 4-tuple that are in $V_s \setminus X_s$ (else, the sum of weight of the atoms in C_s should be at least 3). However, we prove in [CCDL17] that in this situation, $\delta(u, v, x, y) \leq 1$, that contradicts the hypothesis that $\delta(u, v, x, y) \geq 3/2$. This part of the analysis makes use of our proof of Lemma 31 for the case of clique-separators.
- Else, $t \in X_s$ and we can assume w.l.o.g. that no vertex of $\{u, v, x, y\} \setminus \{s\}$ is in $V_s \setminus X_s$ (else, we go back to the previous case). However, we prove in [CCDL17], as before, that in this situation, $\delta(u, v, x, y) \leq 1$, that again contradicts the hypothesis that $\delta(u, v, x, y) \geq 3/2$.

As a result, no vertex of $\{u, v, x, y\} \setminus \{s\}$ is in V_s, and so, X_s is a clique-separator which separates s from $\{u, v, x, y\} \setminus \{s\}$. Since $X_s \subseteq A_0$, the latter proves the claim on A_0, hence the lemma. □

The gist of Lemma 32 is that the atoms of $G = (V, E)$ are the bags of a tree decomposition of G (this will be further discussed in the next chapter on tree decompositions). We use it in [CCDL17] in order to prove that the hyperbolicity of any 4-tuple with large hyperbolicity is at most one unit off from the hyperbolicity of a given atom, and so, Theorem 30 holds.

Further applications of clique-decompositions. On the way to prove Theorem 30, we were able to (partly) characterize the cases where the hyperbolicity of a graph cannot be deduced from its clique-decomposition directly. We leverage from this characterization the following result:

Theorem 33. *Given $G = (V, E)$, let $A_1, A_2, \ldots A_k$ be its atoms. In $\mathcal{O}(|V||E|)$-time, we can compute $G_1^*, \ldots, G_k^*$ such that:*

- *each G_i^* is obtained from $G[A_i]$ by adding simplicial vertices;*
- *and if $\delta(G) \geq 1$ then $\delta(G) = \max\{1\} \cup \{\delta(G_i^*) \mid 1 \leq i \leq k\}$.*

The above preprocessing method has been successfully applied on large co-authorship graph in order to compute their hyperbolicity. On a more theoretical side, we have used it in order to improve the computation of hyperbolicity for outerplanar graphs, *a.k.a.* the graphs whose atoms are cycles [Sys79]:

Theorem 34. *If $G = (V, E)$ is outerplanar then $\delta(G)$ can be computed in $\mathcal{O}(|V|)$-time.*

In order to prove Theorem 34, we have established a simple characterization of outerplanar graphs with hyperbolicity strictly less than one. More precisely, this characterization is based on the property that every induced cycle in an outerplanar graph is isometric [Sys79]. In particular, since every cycle of length at least six has hyperbolicity at least one [WZ11], every outerplanar 1/2-hyperbolic graph is 5-chordal. So, we obtain our characterization of outerplanar 1/2-hyperbolic graphs as a particular case of the characterization in [WZ11] of 1/2-hyperbolic 5-chordal graphs.

Then, for outerplanar graphs with hyperbolicity at least one, we have refined the results of Theorem 33. In particular, since the atoms of outerplanar graphs are cycles, the graphs $G_1^*, \ldots, G_k^*$ output by the preprocessing method have a very simple structure (they are obtained from a cycle by adding, for every edge e in the cycle, at most one simplicial vertex that is adjacent to the two ends of e). So, their hyperbolicity can be derived from the hyperbolicity of cycles and additional parity conditions. Details can be found in our report [CCDL17].

Final remark: combining many decompositions. It may be the case that the atoms can be further split or reduced, using another graph decomposition. For instance, a graph is EPT if it is the edge intersection graph of paths in a tree [GJ85]. The atoms of an EPT graph are line graphs [Tar85]. So, we can replace each atom with its root (the graph of which it is the line graph), and we have by Theorem 19 that it does not affect their hyperbolicity by more than an additive term. Furthermore, computing the root of each atom can be done in linear time [Leh74].

Then, the roots of the atoms may be further decomposable using modular, split or clique decomposition, etc. If the root is prime under all these decompositions but it is a bipartite graph, we may still decrease its size by half as follows. We take the smaller side of its bipartition and we add an edge between every two vertices at distance two in the root. By Lemma 17, the hyperbolicity of the gotten graph is roughly half of the hyperbolicity of the root.

2.6.3 Hardness results

In the previous Section 2.6.2, we show that the computation of hyperbolicity (exact or approximate) can be sped up on certain graph classes by using graph decompositions. This approach does not extend to general graphs. So, a complementary approach is to prove, or show strong evidence of, lower-bounds on the complexity of computing this parameter. In this section, conditional lower-bounds on this complexity are presented, with an emphasis on a reduction from the QUADRANGLE DETECTION problem, that is part of my contributions.

2.6.3.1 Related work

As a warm-up, we recall that the problem HYPERBOLICITY WITH FIXED BASE VERTEX can be reduced in quadratic-time to the computation of a $(\max, \min)$-product between two matrices. In [FIV15], the authors prove that a converse reduction also holds true: if HYPERBOLICITY WITH FIXED BASE VERTEX can be solved in $\mathcal{O}(n^{\upsilon})$-time on n-vertex graphs then the $(\max, \min)$-product of two $n \times n$ matrices can be computed in $\mathcal{O}(n^{2+\upsilon/3} \log n)$-time. In particular, any $\mathcal{O}(n^{2.05})$-time algorithm for solving HYPERBOLICITY WITH FIXED BASE VERTEX would immediately improve the best-known algorithms for $(\max, \min)$-product. These relationships suggest a strong equivalence between the computation of hyperbolicity and the $(\max, \min)$-product, that resembles the existing ones between all-pairs-shortest-paths and $(\min, +)$-product [FM71].

SETH-hardness. More recently, several authors have proved conditional lower-bounds on the complexity of polynomial-time problems on graphs under the Strong Exponential Time Hypothesis (SETH) [Wil16]. Roughly, the hypothesis says that SAT cannot be solved in $2^{(1-\varepsilon)n}$-time for any $\varepsilon > 0$ [IPZ98]. Under SETH it has been proved that computing the diameter of a graph cannot be done in truly subquadratic-time, even on sparse graphs; that is, it cannot be computed in $\mathcal{O}(n^{2-\varepsilon})$-time for any

$\varepsilon > 0$ [BCH16]. The authors in [BCH16] have used this result in order to prove conditional lower-bounds on the complexity of computing the hyperbolicity of a graph:

Theorem 35 ([BCH16]). *Under SETH, none of the following problems can be solved in truly subquadratic time, even on sparse graphs:*

- *computing the hyperbolicity of a given graph;*
- *deciding whether a given graph has hyperbolicity at most one.*

A similar but weaker result was proved by Fang in [Fan11].

2.6.3.2 Contribution of this thesis: Truly subcubic reduction to Quadrangle Detection

The concept of q-reduction was introduced by Williams and Vassilevska Williams in [VWW10]. Informally, if there is a q-reduction from a problem A to a problem B, and B can be solved in $\tilde{\mathcal{O}}(n^{q-\eta})$-time[7] for some $\eta > 0$, then problem A can be solved in $\tilde{\mathcal{O}}(n^{q-\varepsilon})$-time for some other $\varepsilon > 0$. More formally, a Turing reduction from a problem A to a problem B is an algorithm to solve A using an oracle to solve B as a soubroutine. It is called a q-reduction if for every $\eta > 0$ there exists ε such that the following holds for every input of size n:

- the reduction runs in $\tilde{\mathcal{O}}(n^{q-\varepsilon})$-time;
- and if the oracle to solve problem B is called on instances with respective sizes $n_1, n_2, \ldots, n_k$ then $\sum_{i=1}^k \tilde{\mathcal{O}}(n_i^{q-\eta}) = \tilde{\mathcal{O}}(n^{q-\varepsilon})$.

This concept formalizes prior work from, *e.g.*, [GO95, KS06a].

Two problems are called subcubic equivalent if every of the two problems can be 3-reduced to the other. In this situation, either both problems are solvable in truly subcubic time, or none of them is. My main contribution in [CD14], found with David Coudert, can be stated as follows.

Theorem 36. *The two following problems are subcubic equivalent:*

- *deciding whether a graph has hyperbolicity equal to $1/2$;*
- *deciding whether a graph contains an induced cycle of length four.*

Furthermore, both problems can be solved in deterministic $\mathcal{O}(n^{3.26})$-time and in randomized $\tilde{\mathcal{O}}(n^{2.3729})$-time.

Theorem 36 shows a surprising gap in the complexity of recognizing graphs with small hyperbolicity. Indeed, it has been proved in [How79] that the 0-hyperbolic graphs can be recognized in linear time. In contrast, recognizing 1/2-hyperbolic graphs in (deterministic) truly subcubic time seems to be a much harder task.

A reduction from Quadrangle detection to the recognition of 1/2-hyperbolic graphs has been sketched in earlier papers [KM02, WZ11]. So, the main difficulty was to show the converse reduction. Our proof for Theorem 36 makes use

[7]The $\tilde{\mathcal{O}}$ notation suppresses the polylog factors.

of a (non algorithmic) characterization of 1/2-hyperbolic graphs from Bandelt and Chepoi [BC03]. On the way to prove our result, we have established the following simpler characterization for these graphs. We recall that for every $G = (V, E)$ and $j \geq 1$, the graph power G^j is obtained from G by adding an edge between every two distinct vertices that are at distance at most j in G.

Definition 37. For every $G = (V, E)$, the graph $G^{[2]} = (V^{[2]}, E^{[2]})$ is defined as follows:

- $V^{[2]} \simeq V \times \{0, 1\}$;
- $G[V \times \{0\}] \simeq G$;
- $G[V \times \{1\}] \simeq G^3$;
- and for every $u, v \in V$, the vertices $(u, 0)$ and $(v, 1)$ are adjacent in $G^{[2]}$ if and only if $\mathrm{d}_G(u, v) \leq 2$. In particular, for every $u \in V$, there is an edge between $(u, 0)$ and $(u, 1)$ in $G^{[2]}$.

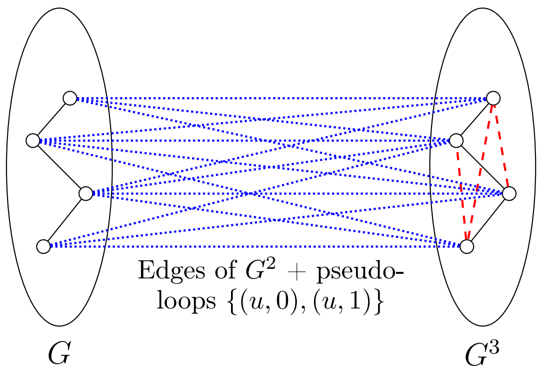


Figure 2.23: The graph $G^{[2]}$.

We refer to Figure 2.23 for an illustration. Intuitively, the graph $G^{[2]}$ can be seen as an intermediate power between the square and the cube of G. Our characterization of 1/2-hyperbolic graphs can now be stated as follows.

Theorem 38. *$G = (V, E)$ is 1/2-hyperbolic if and only if none of the graphs $G^j, j \geq 1$ and $G^{[2]}$ contain an induced cycle of length four.*

By Theorem 38, it can be decided whether $G = (V, E)$ is 1/2-hyperbolic with $diam(G)$ calls to an oracle solving Quadrangle detection – given as inputs $G^{[2]}$ and $G, G^2, G^3, \ldots, G^{diam(G)-1}$. If we precompute, in truly subcubic time, a polylogarithmic-factor approximation for hyperbolicity then this number of calls can be reduced to $\log^{\mathcal{O}(1)}(|V| + |E|)$ (because some powers of G can be discarded), and we so obtain a subcubic reduction from the recognition of 1/2-hyperbolic graphs to Quadrangle detection.

Discussion. As said earlier in this subsection, the authors in [BCH16] show that under SETH, graph hyperbolicity cannot be computed in truly subquadratic time. In contrast, it is proved with Theorem 36 that the weaker task of recognizing 1/2-hyperbolic graphs is equivalent to the QUADRANGLE DETECTION problem. The latter problem can be solved in $\mathcal{O}(m^2)$-time on m-edge graphs, and so, in quadratic time on sparse graphs. However, no truly subquadratic *deterministic* algorithm is known to exist, even for sparse graphs. In [VWWWY15], Vassilevska Williams et al. describe an $\mathcal{O}(m^{1.41})$-time *randomized* algorithm for QUADRANGLE DETECTION, but it is not combinatorial (*i.e.*, it calls matrix multiplication as a subroutine). In order to reinforce this view, we note that there is a linear time reduction from TRIANGLE DETECTION to QUADRANGLE DETECTION [FKLL15], and so, to the problem of computing graph hyperbolicity. It is conjectured that there does not exist any truly subcubic combinatorial algorithm for TRIANGLE DETECTION on general graphs [Wil16].

2.7 Algorithmic applications

Finally, this section covers more technical applications of hyperbolicity, in the field of graph algorithms. The previous sections can help the reader to have better insights on the (hyperbolic) graph classes on which these algorithmic results apply, and the (non hyperbolic) graph classes on which they do not apply. Note that this section is *not* part of the contributions of this thesis. However, I will highlight on the way some open questions on which I am interested to work.

The hyperbolicity has been used recently for the analysis of graph algorithms. Indeed, it is the idea that when the hyperbolicity is small, there are some hard problems on graphs that can be efficiently approximated. In what follows, we outline some interesting algorithmic properties that are enjoyed by constantly hyperbolic graphs. Note that in some cases, the algorithms that are presented in this section keep some interest even for more general hyperbolic graph classes (say, polylogarithmically hyperbolic).

Outline of the section. The first parts of this section (Sections 2.7.1 and 2.7.2) cover distance-related problems in graphs. In Section 2.7.1, we survey applications of hyperbolicity in the analysis of approximate distance oracles. These results are mainly based on the relationships between hyperbolicity and the best possible distortion of the distances in a graph when it is embedded into a “tree-like” metric space. Perspectives for improving upon these relationships, and for refining the proposed constructions, will be discussed. Then, in the continuity of Section 2.7.1, we will cover in Section 2.7.2 some applications of hyperbolicity to graph clustering problems. The techniques presented leave space for promising extensions to a broader family of graph problems, that will be further examined. Finally, we will end the section with algorithmic applications of hyperbolicity to some problems in structural graph theory (Sections 2.7.3 and 2.7.4). Section 2.7.3 is devoted to a PTAS for the

Traveling Salesman Problem in hyperbolic graphs with bounded degree. This algorithm is based on new separability results in hyperbolic graphs, that I think could be useful in other graph problems. Last, constructive relationships between hyperbolicity and vertex expansion are presented in Section 2.7.4. I think that these relationships can be helpful in the design of approximation algorithms for computing the treewidth in hyperbolic graphs with bounded degree.

2.7.1 Distance approximations

This section surveys the known results on the relationship between hyperbolicity and the best-possible stretch for the distances in a graph when it is embedded in a “tree-like" space. Indeed, the basic use of hyperbolicity is for the analysis of approximate distance oracles. Computing the all-pairs-shortest-paths in a graph can be done in polynomial time and space, but in practice this is often too costly on large graphs and there is a need for subquadratic approximations. Some of them consist in embedding the graph into a “simpler” combinatorial or geometrical structure. When the structure is a “tree-like” metric space, the hyperbolicity of the graph comes into play in the distortion.

Note that these results have useful applications in compact routing [GL05].

2.7.1.1 Hyperbolic embedding

As an example, Verbeek and Suri proved in [VS14] that for any embedding of $G = (V, E)$ into a hyperbolic space the multiplicative distortion of the distances is $\Omega(\delta(G)/\log \delta(G))$, and if G has bounded degree then there exists a linear-time computable embedding of G in a Hyperbolic space with additive distortion $\mathcal{O}(\delta(G))$.

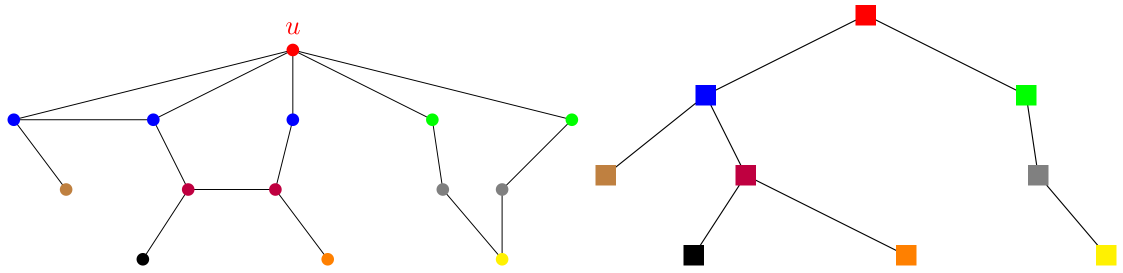
As noted in [ACHK16], every $G = (V, E)$ with maximum degree Δ can be embedded into a graph G' with maximum degree three, up to a multiplicative distortion of the distances $\mathcal{O}(\log \Delta)$. In this situation, $\delta(G') = \mathcal{O}(\delta(G) \log \Delta)$ (we refer to [Shc13b, GdLH90] for a proof of the preservation of hyperbolicity under quasi-isometry). Therefore, every $G = (V, E)$ can be embedded into a Hyperbolic space in linear-time with multiplicative distortion $\mathcal{O}(\delta(G) \log \Delta)$.

2.7.1.2 Tree embedding

In what follows, we survey the relationships between hyperbolicity and the distortions of the distances in a graph that are obtained with different algorithms for embedding a graph into a tree. Some interesting open questions will be also mentioned. Most notably, Gromov has proved the following result on tree embeddings:

Theorem 39 ([Gro87]). *Every $G = (V, E)$ can be embedded into a tree in quadratic-time, up to an additive distortion of the distances at most $2\delta(G) \log |V|$.*

In order to prove Theorem 39, the main contribution of Gromov was to exhibit a pseudo-distance on graphs, and then to upper-bound the additive distortion resulting from the pseudo-distance by $2\delta(G) \log(|V|)$. By construction, every graph equipped with the Gromov pseudo-distance is 0-hyperbolic, and there exist efficient constructions in order to embed 0-hyperbolic spaces into a tree with null distortion. One of them is due to Buneman, and it can be implemented to run in quadratic-time [Bun74, Gro87].



(a) Graph G (b) Layering tree $\mathcal{LC}(u)$.

Figure 2.24: Example of a layering tree.

Relationship with other constructions. Recently, Yancey [Yan15] has proved a close relationship between the construction of Gromov and the so-called *layering trees* [CD00]. Given $G = (V, E)$ and $u \in V$, the layering tree $\mathcal{LC}_G(u)$ is obtained from the shortest-path tree rooted at u as follows: we merge into one node all vertices v, w such that $\mathrm{d}(u, v) = \mathrm{d}(u, w)$ and there exists a vw-path $\mathcal{P}$ such that $\mathrm{d}(u, x) \geq \mathrm{d}(u, v)$ for every $x \in \mathcal{P}$ (see Figure 2.24 for an illustration).

It was already proved that embedding G into one of its layering trees causes a distortion of the distances $\mathcal{O}(\delta(G) \log(|V|))$ [CDE+08]. However, what Yancey proves is that the Gromov distance approximating tree is essentially a layering tree with Steiner points (additional nodes in the tree such that all the edges incident to that node have weight zero). On the algorithmic side, since a layering tree can be computed in linear time [CD00], it gives a simpler and more efficient construction for Theorem 39.

The Gromov distance approximating tree is also equivalent to another construction in the litterature, that is called an Anchored Buneman tree [BFÖ+03].

Perspectives. There exists a “refined Buneman tree” [BFÖ+03], that has been observed to give a lower distortion of the distances in a graph than an Anchored Buneman tree. It can be computed in cubic time. I think that it would be interesting to analyse the distortion caused by an embedding into this tree (w.r.t. graph hyperbolicity), and to improve on its computation (possibly, by using the relationship between Anchored Buneman trees and layering trees).

Another interesting question on tree embeddings was asked by the authors in [ASM16]. Indeed, they notice that for real-life graphs with diameter $\mathcal{O}(\log(|V|))$, a shortest-path tree is enough in order to approximate the distances up to an additive term $\mathcal{O}(\log(|V|))$. Therefore, the tree embedding of Theorem 39 does not look that appealing in that case. Under which conditions can a δ-hyperbolic graph with diameter D be embedded into a tree with distortion $\mathcal{O}(\delta \log D)$? Let us point out that by Lemma 13 the ringed tree $RT(k)$ (defined in Section 2.4.1) has diameter $\Theta(k)$ and hyperbolicity 3 but cannot be embedded into a tree width additive distortion $o(k)$.

2.7.1.3 Approximate extremal distances.

Finally, before concluding this subsection, we point out that if we relax our goal and we only want to approximate the *extremal distances* in $G = (V, E)$ (*i.e.*, the eccentricities, where the eccentricity of a vertex is defined as its largest distance to another vertex in G), then it can be done up to a better additive term $\mathcal{O}(\delta(G))$. In particular, there is a simple algorithm in order to approximate the diameter, that is named Two-Sweep in the literature [MLH08]. Suppose that we compute a breadth-first search from any vertex of the graph $G = (V, E)$, and that it ends on some vertex v. Then, we compute a second breadth-first search from v, and it can be proved that v has eccentricity at least $diam(G) - 2\delta$. The latter generalizes an algorithm of Jordan in order to compute the diameter of trees in linear time [Jor69]. The radius of the graph can be approximated in a similar fashion. We refer to [CDE+08] for details.

2.7.2 p-centers

Next, we present a more refined algorithmic application of hyperbolic graphs to graph clustering problems, that was proposed in [CE07]. This application requires prior results on the relationships between hyperbolicity and tree embeddings (Theorem 39). Precisely, the *p-radius* of $G = (V, E)$ is the smallest radius $r_p(G)$ such that $V = \bigcup_{v \in S} B_G(v, r_p(G))$ for some subset $S \subseteq V$ with $|S| \leq p$ vertices. In particular, the 1-radius of G is simply its *radius*, *a.k.a.*, the minimum eccentricity of a vertex in G. A dual invariant is the *p-diameter* of $G = (V, E)$, that is the largest $d_p(G)$ so that there are at least p vertices of G that are pairwise at distance at least $d_p(G)$. In particular, the 2-diameter of G is simply its diameter, *a.k.a.*, the largest distance between two vertices in G. Furthermore, any subset minimizing $r_p(G)$, resp. maximizing $d_p(G)$, is called a *p-center*, resp. a *p-packing*.

Shier has proved that for any tree T, we have $d_{p+1}(T)/2 \leq r_p(T) \leq d_{p+1}(T)/2 + 1$ [Shi77]. In [CE07], Chepoi and Estellon propose the following generalization to δ-hyperbolic graphs:

Lemma 40 ([CE07]). *For every $G = (V, E)$, it holds $d_{p+1}(G)/2 \leq r_p(G) \leq d_{p+1}(G)/2 + 4\delta(G) + 1$.*

From Lemma 40, they obtain an $\mathcal{O}(n^3)$-algorithm for computing an approximate p-center of graphs [CE07]. It gives an approximation algorithm for computing the p-radius of a given δ-hyperbolic graph up to an additive term $\mathcal{O}(\delta)$. This was recently improved in [EKS16], where Edwards et al. detail an algorithm with the same performances as above, running in $\mathcal{O}(p\delta(n + m) \log n)$-time on δ-hyperbolic graphs.

The gist of these algorithms is to compute an approximate $(p+1)$-packing and then to elaborate on it. It can be done by embedding the graph into a tree with additive distortion of the distances $\mathcal{O}(\delta \log n)$, then to compute an optimal packing for this tree.

Perspectives. Proper generalizations of Lemma 40 to the transversal and the packing numbers of given set families in δ-hyperbolic graphs can be found in [CDV16]. These results are obtained from a primal-dual approach using a linear programming formulation of these parameters. Can it be derived from the relationships in [CDV16] efficient (quasi-linear time) approximation algorithms for computing transversals of these set families ? In particular, can the techniques applied in [EKS16] be useful in the design of such algorithms ?

2.7.3 Traveling Salesman Problem

So far, the problems mentioned in Sections 2.7.1 and 2.7.2 were purely metric. The two last applications (Sections 2.7.3 and 2.7.4) combine some metric aspects of graphs (distances) with structural properties. In particular, we present in this part results on "balanced" separators in hyperbolic graphs, with applications to the Traveling Salesman Problem.

In [KL06], Krauthgamer and Lee initiated a more general study of approximate algorithms on negatively curved spaces. Their algorithms apply to constantly hyperbolic graphs with bounded maximum degree. Their main technical tools are separability properties of hyperbolic graphs, that extend those of trees. As an example, in a rooted tree T with maximum degree Δ, there exists a node z whose subtree comprises between $|T|/(2\Delta) - 1$ and $|T|/2$ nodes. It can be extended to hyperbolic graphs as follows:

Lemma 41 ([KL06]). *Let $G = (V, E)$ be a δ-hyperbolic graph with maximum degree Δ and let $w \in V$. For every $v \in V$ and $t \geq 0$, let us define $X_v^t = \{u \in V \mid \langle u, v\rangle_w \geq d_G(u, w) - t\}$. Then, for every $S \subseteq V$ such that the vertices in S are pairwise at distance at least 20δ, there exists $c \in V$ such that:*

$$|S|/\Delta^{\mathcal{O}(\delta^2)} \leq |S \cap X_c^{\delta}| \leq |S \cap X_c^{3\delta}| \leq |S|/2.$$

Using Lemma 41, Krauthgamer and Lee are able to design a hierarchical data structure for approximate nearest neighbour search [KL06] [KL06].

Their second contribution is a randomized polynomial-time approximation scheme (PTAS) for the well-known Traveling Salesman Problem (TSP). It is based on the existence, for bounded degree hyperbolic graphs, of some *padded probabilistic decompositions*. Roughly, the graph can be decomposed into small diameter subsets in a way that every ball with small radius is contained in one of the subsets with high probability. Assuming the graph has bounded maximum degree, it is the idea that hard problems such as TSP can be solved by brute-force on the subsets (or at least sharply approximated). Then, a global solution for the graph can be computed from the partial solutions by using dynamic programming.

Open questions. Lemma 41 extends a separability property of trees to hyperbolic graphs. What other separability properties of trees can be generalized to hyperbolic graphs in a similar fashion ? Can we use such properties in order to design approximation algorithms on hyperbolic graphs with bounded maximum degree, using dynamic programming, for other problems such as MAXIMUM CLIQUE or MAXIMUM INDEPENDENT SET ?

2.7.4 Cut problems

We end the section with some algorithmic consequences on the relationships between hyperbolicity and graph expansion (Section 2.5.2.3). Unlike the other problems mentioned in the section, the following algorithms also apply to non constantly hyperbolic graph classes. More precisely, although the above algorithmic work on hyperbolicity can sometimes apply to non constantly hyperbolic graph, the authors in [DKMY15] have been the first, to the best of my knowledge, to design algorithms for more general hyperbolic graphs (with non constant hyperbolicity).

We recall the results in [Ben98, Mal15] where they prove that expander graphs are non hyperbolic. In [DKMY15], the authors give constructive proofs on the relationship between graph expansion, maximum degree and hyperbolicity. Precisely, they obtain improved algorithms for the following graph problems. Given an n-vertex graph with maximum degree Δ and hyperbolicity at most δ, the following can be computed in polynomial-time:

- Upper-bounds on the vertex-expansion depending on δ and Δ. The algorithm also outputs a large family of subsets satisfying these bounds, with limited overlap;
- Large st-cuts with $\Delta^{\mathcal{O}(\delta)}$ edges.

The authors also propose an improved algorithm for minimizing the number of bottleneck edges that arises in network design applications. It works in the case where $\delta = o(\log n / \log \Delta)$;

Finally, the authors in [DKMY15] have considered the SMALL-SET EXPANSION problem on hyperbolic graphs, that is a promise problem defined as follows: given a graph $G = (V, E)$ and two constants c and η, distinguish whether `(i)` there exists a subset of V with size $c \cdot |V|$ and vertex-expansion at most η, or `(ii)` every such a subset has vertex-expansion at least $1 - \eta$ [RS10]. It is conjectured that for every fixed η, there exists some constant c such that the corresponding SMALL-SET EXPANSION problem is NP-complete for general graphs [RS10]. In contrast, the authors in [DKMY15] proved that for every constants η and c the SMALL-SET EXPANSION problem can be solved in polynomial time for n-vertex graphs with bounded maximum degree and hyperbolicity $\delta = o(\log n)$.

Conclusion and open perspectives. The SMALL-SET EXPANSION problem implies the UNIQUE GAME conjecture, that is related to the complexity of a label assignment problem on graphs and that has been shown to imply tight inapproximability results for many classic graph problems [Kho02]. Furthermore, the SMALL-SET

EXPANSION problem also implies the nonexistence of constant-factor approximations for treewidth [APW12].

Therefore, the result of [DKMY15] raises the following open problem: can the treewidth of hyperbolic graphs with bounded degree be approximated up to a constant-factor ? Note that computing the treewidth is NP-hard on bounded-degree graphs and on hyperbolic graphs [BT97].

2.8 Conclusion

In Sections 2.4 and 2.5, we presented bounds on graph hyperbolicity. Enriching these results with new lower and upper bound techniques is an important open problem, with potential implications for a faster computation of this parameter in practice. In particular, I believe that new results in the spirit of Section 2.4.3: on the preservation of hyperbolicity under some graph operations, would give a better insight on the structure of hyperbolic graphs. Similarly, new lower-bounds could help the computer scientists in better distinguishing complex networks that are hyperbolic or strongly hyperbolic (*e.g.*, biological and social networks) from those that are non hyperbolic (such as road networks). We refer to [AAD16, AD15, BCCM15, CCL15, ASM13, KNS13] for experiments on the hyperbolicity in complex networks.

On the complexity point of view, it is proved in Section 2.6.3 that the recognition of $1/2$-hyperbolic graphs is subcubic equivalent to the detection of induced cycles of length four in graphs, and so, that no truly subcubic *combinatorial* algorithm for computing the hyperbolicity is likely to exist. It is worth pointing out that in practice, hard instances for the above problem are indeed graphs with small hyperbolicity. I thus conjecture that graphs with large hyperbolicity (say, proportional to their size) can be recognized more efficiently. Results of this fashion have been proved recently for the related problem of computing graph diameter [Dam16].

Open perspectives

As pointed out in Section 2.2, it can be inferred interesting network properties when the graph is δ-hyperbolic. Before we finish this chapter, it is worth mentioning that some other geometric graph parameters have been explored with the same goal in mind as above. Most of them are close in spirit from hyperbolicity, and they can often be defined via a suitable variation of the 4-point Condition (Definition 1) or another reformulation of hyperbolicity. We refer, *e.g.*, to [ABK$^+$07, ADM14, JLB08, LT15, Yan15] for partial relationship between these properties and graph hyperbolicity.

Let us put a focus on two of these competitors to graph hyperbolicity. The first one is the average hyperbolicity, defined as $\frac{1}{\binom{n}{4}} \sum_{u,v,x,y \in V} \delta(u,v,x,y)$ [ADM14]. The second one is the notion of (p,δ)-hyperbolic graphs, that are graphs with at least a fraction p of their geodesic triangles that are δ-slim [LT15]. I think that both concepts should deserve more attention in the future, given that the maximum value for the hyperbolicity is reached by an extremely small fraction of 4-tuples in real-life graphs (*e.g.*, less than 3% in social graphs [AAD16]).

Finally, let us point out that in some cases, complex networks have a meaningful orientation on the edges, *i.e.*, they are directed graph. So far, graph hyperbolicity has been defined and studied only in the undirected case. Thus, it would be very interesting to extend the notion of hyperbolicity (and of Gromov product, see Definition 2) to digraphs. Partial attempts in this direction can be found in [GK14, PRST13]. I let this topic as a future work.

Chapter 3

Tree decompositions with metric constraints on the bags

Summary

We make a complexity study for computing tree decompositions in graphs. The tree decompositions considered are defined via metric constraints on their bags. We aim at obtaining a finer-grained complexity for computing these decompositions in general graphs and in some graph classes with structural properties. To do so, we will prove conditional lower-bounds through reductions.

In Section 3.3, we prove that Triangle Detection reduces in quadratic time to the computation of clique-decomposition. This is a hint that there does not exist any truly subcubic *combinatorial* algorithm for this problem. Furthermore, we prove that computing the clique-decomposition can be reduced to Matrix Multiplication, which combined with the relationships between Matrix Multiplication and Triangle Detection, suggests a computational equivalence between these two problems and computing the clique-decomposition. On the parameterized point of view, we conjecture that clique-decomposition can be computed in quasi-linear time on graphs with bounded *clique-number*, that is formally proved for triangle-free graphs and other special graph classes.

Then, in Section 3.4 we answer open questions of Dragan et al. on the complexity of computing treebreadth, pathlength and pathbreadth in graphs. Namely, we prove that all these problems are NP-hard. More precisely, we prove that the recognition of graphs with treebreadth one is already NP-complete, and the same holds true for the recognition of graphs with pathbreadth one and the recognition of graphs with pathlength at most two. On a more positive side, we prove that deciding whether a bipartite or planar graph has treebreadth one is polynomial-time solvable. The algorithm for planar graphs and its analysis are surprisingly intricate.

Finally, we prove in Section 3.5 new relationships between treelength and treewidth. Precisely, we prove a nontrivial upper-bound on the diameter of minimal separators in a graph by using an algebraic tool called the *cycle basis*. We deduce from this result that the treelength is linearly upper-bounded by the treewidth in the class of graphs with bounded-length isometric cycles. Conversely, we prove that the treewidth is linearly upper-bounded by the treelength in the class of *apex-minor free* graphs, thereby generalizing a result from Dieng and Gavoille on planar graphs [DG09].

All my papers on tree decompositions [CDN16, DLN16a, DC17] are collected in the appendix.

Contents

3.1 Introduction

In the previous chapter, we studied on graph hyperbolicity and its algorithmic applications. Hyperbolicity is a measure of the closeness of a graph metric to a tree metric. Yet, it is not related to a structural decomposition of a graph directly[1]. On the algorithmic point of view, graph decompositions can be useful in order to design divide-and-conquer algorithms on large graphs. In particular, tree decompositions [RS86] aim at decomposing graphs into pieces, called *bags*, organized in a tree-like manner (formal definitions are postponed to Section 3.2). They have been proved to be useful in order to extend some efficient algorithms on trees to larger classes of graphs.

The purpose of this chapter is to describe my work on these decompositions.

3.1.1 Context

The general idea is that when the bags have a "simple enough" structure, there are hard problems on general graphs which can be solved efficiently by using dynamic programming on the tree decomposition. There is now a rich literature on

[1]There does exist a relationship between graph hyperbolicity and some decompositions of graphs with dismantling orderings (Definition 7).

tree decompositions with algorithmic applications, such as *e.g.*, algorithmic meta-theorems (for solving hard problems on graphs with a specified tree decomposition) [Cou90, DH08, FG01], and the well-known biconnected decomposition [Tar72], triconnected decomposition [HT73], clique-decomposition [BPS10], etc.

Furthermore, with the growing size of real-life graphs, tree decompositions have been found useful in order to identify the key aspects of the structure of complex networks, such as *e.g.*, core and periphery [ASM16].

Treewidth is a classical measure for studying tree decompositions. Roughly, the *width* of a tree-decomposition is the maximum size of its bags. The treewidth of a graph is the minimum width among all its tree-decompositions. A lot of work has been dedicated to compute tree-decompositions with small width since such decompositions can be efficiently exploited for algorithmic purposes [Bod06]. However, computing the treewidth of a graph is NP-hard [ACP87] and no constant-approximation algorithm is likely to exist [WAPL14]. Furthermore, real-life networks generally have a large treewidth [dMSV11]. These drawbacks motivated the study of other optimization criteria for tree-decompositions [DG07, KLNS15, Sey16].

Metric tree-likeness in graphs. In this chapter, we mainly focus on optimizing the metric properties of the bags. One first example is an *atom tree* [BPS10], where the bags are maximal subgraphs with no clique-separators. The bags in an atom tree are isometric subgraphs. An atom tree has already nice algorithmic applications, however it may be sometimes more interesting to further decompose the graph. Roughly, the *length* and the *breadth* of a tree-decomposition are the maximum diameter and radius of its bags respectively. The corresponding graph parameters are the *treelength* [DG07] and the *treebreadth* [DK14] respectively. As I mentioned it in Section 2.4.1 (p. 36), these two parameters are closely related to hyperbolicity, and to the best possible distortion of the distances in a graph when it is embedded into a tree. Algorithmic applications of hyperbolic graphs (Section 2.7, p. 67) thus transpose to bounded treelength graphs. See also [DDGY07] for some other applications of treelength in graph algorithms. We point out that recent studies suggest that some classes of real-life networks – including biological networks and social networks – have bounded treelength and treebreadth [AAD16].

3.1.2 General objective: efficient computation of tree decompositions

In the continuity of my work on computing graph hyperbolicity (Section 2.6), I have been interested in computing efficiently tree decompositions with bags of small diameter or radius. To a lesser extent, my results also apply to the computation of other tree-likeness parameters such as, *e.g.*, treewidth.

In what follows, I shall introduce my main contributions to the field.

3.1.2.1 Finer-grained complexity of clique-decomposition

The decomposition of a graph by its clique-separators is sometimes called "clique-decomposition" in the litterature [BPS10]. Its output is an atom tree (mentioned above), that is a tree decomposition whose bags induce subgraphs with no clique-separators, *a.k.a.* atoms. One interest of clique-decomposition is that it can be used for preprocessing the graph in the computation of many other parameters (exact or approximate). In particular, the treewidth of a graph is the maximum treewidth of its atoms, and the same holds true for treelength and treebreadth. In Section 2.6.2, I also detailed a novel application of clique-decomposition for computing the hyperbolicity of large graphs.

My purpose in Section 3.3 is to improve our understanding of the complexity of computing this decomposition. Clique-decomposition can be computed in polynomial-time [Tar85]. However, the best-known algorithms for the problem run in $\mathcal{O}(nm)$-time on n-vertex m-edge graphs, that is prohibitive for large graphs.

In [DC17], we show how to reduce the TRIANGLE DETECTION problem to clique-decomposition, that is strong evidence that the state-of-the-art algorithm for clique-decomposition is essentially optimal. Furthermore, we describe an improved algorithm for computing the clique-separators of a graph, that suggests an interesting relationship between the complexity of computing clique-decomposition and the *clique-number* of a graph (size of a maximum clique).

These results are in revision for *SIAM Journal of Discrete Mathematics.* They are joint work with my supervisor David Coudert. I will detail them in Section 3.3.

3.1.2.2 The (NP-)hardness of computing treebreadth

The remaining of this chapter (Sections 3.4 and 3.5) is devoted to the length and the breadth of tree decompositions. On the complexity point of view, it has been proved by Lokshtanov in [Lok10] that deciding whether a graph has treelength at most k is NP-complete for every fixed $k \geq 2$. However, this was left open for treebreadth [DK14].

We answer to this open problem in [DLN16a]. Precisely, it is proved in the paper that deciding whether a graph has treebreadth at most k is NP-complete for every fixed $k \geq 1$. Similar results are obtained for the "path counterparts" of treelength and treebreadth, that are named pathlength and pathbreadth [DKL14].

On a more positive side, we initiate the study of the complexity of computing treebreadth on certain graph classes. This approach has been well explored for treewidth [BKK95, KK95, Klo96, BKKM98, BM93]. However it has been so far underexplored for treelength and treebreadth. Precisely, it is proved in [DLN16a] that bipartite graphs and planar graphs of treebreadth one can be recognized in polynomial time.

I will expand on this joint work with Nicolas Nisse and Sylvain Legay in Section 3.4.

3.1.2.3 Relationships between treewidth and treelength

Finally, the last Section 3.5 is devoted to new relationships between treelength and treewidth. We obtain this way a unifying view of tree-likeness in graphs. Further motivations to find such relationships are to derive improved algorithms for solving hard problems on certain classes of bounded-treelength graphs, improved approximation algorithms for computing the treewidth on certain graph classes, etc.

In order to better depict the results in this section, found in collaboration with David Coudert and Nicolas Nisse, let it be said that complete graphs are the classical example of graphs with large treewidth but bounded treelength, whereas on the other hand the cycles have bounded treewidth but unbounded treelength [DG07]. These two graph families thus can be used in order to show that treewidth and treelength cannot be compared on general graphs. We prove in [CDN16] that removing these obstructions allows one to upper and lower bound treewidth with functions of the treelength. More formally, what we prove in [CDN16] is that on *apex-minor free* graphs with bounded-length isometric cycles, treelength and treewidth can only differ by at most a constant-factor (full definition for this class of graphs is postponed to Section 3.5).

Definitions and preliminary results are presented in Section 3.2. The technical sections are structured as follows. We start with a short summary of the topic, then, we list our main contributions and we discuss about their implications. We end the sections with sketch proofs of the main results.

3.2 Some basics on tree decompositions

The notion of tree decomposition was briefly introduced in the previous chapter (Section 2.4.1). We restate the definition here for convenience of the reader. A *tree decomposition* $(T, \mathcal{X})$ of $G = (V, E)$ is a pair consisting of a tree T and of a family $\mathcal{X} = (X_t)_{t \in V(T)}$ of subsets of V indexed by the nodes of T and satisfying:

- $\bigcup_{t \in V(T)} X_t = V$;
- for any edge $e = \{u, v\} \in E$, there exists $t \in V(T)$ such that $u, v \in X_t$;
- for any $v \in V$, the set of nodes $\{t \in V(T) \mid v \in X_t\}$ induces a subtree, denoted by T_v, of T.

The sets X_t are called *the bags* of the decomposition. Its *adhesion sets* are the intersections $X_t \cap X_{t'}$ for every edge $\{t, t'\} \in E(T)$. As an example, we show a tree decomposition of the wheel in Figure 3.1. In this case, the tree T is a path, so, we call it a *path decomposition*.

We point out that any graph admits a tree decomposition, resp. a path decomposition. Indeed, the single node tree with bag V satisfies the three above conditions. However, this trivial tree decomposition is not that interesting, so, we aim at imposing additional constraints on the bags or on the adhesion sets.

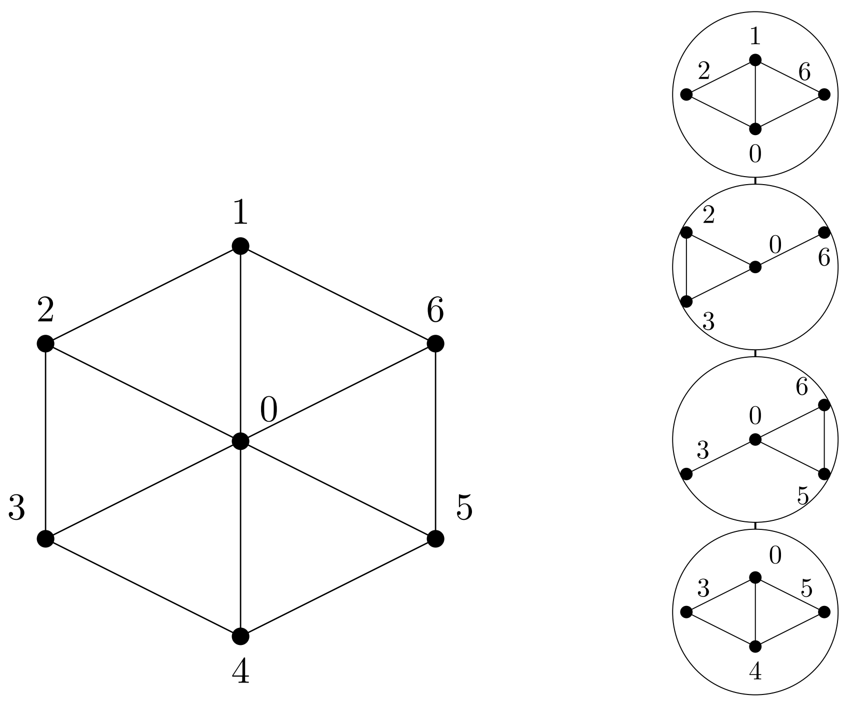


Figure 3.1: A path decomposition of the wheel W_6.

3.2.1 Tree-likeness parameters

Treewidth

The *width* of a tree decomposition is the size of a largest bag minus one. The *treewidth*, resp. the *pathwidth* of a graph G is the least possible width over its tree decompositions, resp. over its path decompositions. In what follows, we denote these two parameters by $tw(G)$ and $pw(G)$, respectively.

Example: graphs with small treewidth. Graphs with treewidth one are exactly the trees (hence, the minus one in the definition).

Furthermore, cycles have treewidth two. It can be shown as follows. When we remove any vertex from a cycle, that will leave a path. This path is a tree, so, it has a tree decomposition of unit width. Then, by adding in every bag the removed vertex, we obtain a tree decomposition of the cycle of width two.

Examples of graphs with large treewidth are the complete graphs and the grids.

Precisely, a complete graph K_n with n vertices has treewidth $n-1$. This well-known result derives from the Helly property: every collection of pairwise intersecting subtrees in a tree have a nonempty intersection. We detail this a bit more below as it is a useful technique in the study of tree decompositions.

Let us fix $(T, \mathcal{X})$ a tree decomposition of K_n. We have for every $u, v \in V(K_n)$

that since u and v are adjacent they must be contained in a common bag. As a result, the subtrees T_v, $v \in V(K_n)$ are pairwise intersecting. By the Helly property, it implies that there must be a bag of $(T, \mathcal{X})$ with all the n vertices in K_n, hence $tw(K_n) \geq n - 1$. The bound is reached by the trivial tree decomposition with one node.

Observe that more generally, we have with the same proof as above that for every G, and every tree decomposition $(T, \mathcal{X})$ of G, every clique of G must be fully contained in one bag of $(T, \mathcal{X})$ [Bod06]. Therefore, the treewidth is lower-bounded by the clique-number (size of a largest clique).

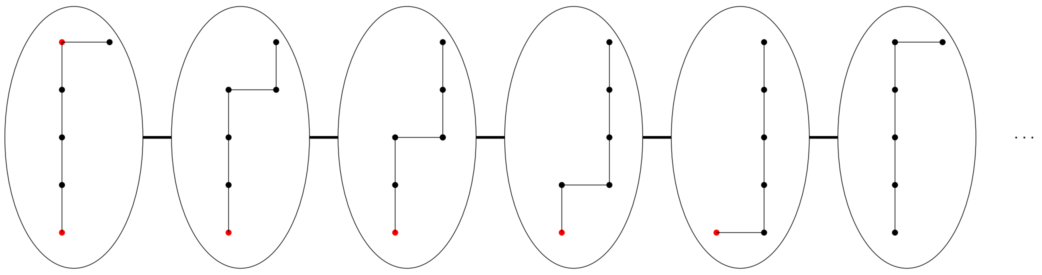


Figure 3.2: Bags in a path decomposition of the grid with side length four (partial view).

Last, given a grid with dimensions m and n, with $n \leq m$, it is not difficult to construct a tree decomposition of width n (see Figure 3.2). This construction is optimal [Die10] but it is technically challenging to prove it.

I will study treewidth in Section 3.5.

3.2.1.1 Treelength and treebreadth

The *length* of a tree decomposition is the maximum distance in the graph between every two vertices in a same bag. The *treelength*, resp. the *pathlength* of a graph G is the least possible length over its tree decompositions, resp. over its path decompositions. In what follows, we denote these two parameters by $tl(G)$ and $pl(G)$, respectively. Note that they are trivially upper-bounded by the diameter $diam(G)$ (that is the length of the trivial tree decomposition with one node).

Close to its length, the *breadth* of a tree decomposition is the minimum r such that every bag is contained in a ball of radius r in the graph (the center of the ball may not be in the bag). The *treebreadth*, resp. the *pathbreadth* of a graph G is the least possible breadth over its tree decompositions, resp. over its path decompositions. In what follows, we denote these two parameters by $tb(G)$ and $pb(G)$, respectively. As an example, the wheel in Figure 3.1 has treebreadth one and treelength two.

Treelength and treebreadth can be seen as a particular case of acyclic (R, D)-clustering, *a.k.a.* tree decompositions with breadth at most R and length at most D [DL07]. The two parameters are closely related. Precisely, $tb(G) \leq tl(G) \leq$

$2 \cdot tb(G)$ and the bounds are sharp [DK14]. The same relationship holds true between pathlength and pathbreadth.

Examples of graphs with small treelength. It turns out that many interesting graph classes with unbounded treewidth have small treelength. As an example, the chordal graphs are a strict generalization of complete graphs. They can be characterized as those graphs admitting a *clique-tree*, that is a tree decompositions whose bags are cliques [Gav74]. Thus, chordal graphs are exactly the graphs with unit treelength. More generally, every k-chordal graph (graph with no induced cycle of length at least $k+1$) has treelength at most $\lfloor k/2 \rfloor$ [DG07].

Related to chordal graphs, the *dually chordal graphs* are the clique-graphs (*i.e.*, intersection graphs of the maximal cliques) of chordal graphs [BDCV98]. We claim that dually chordal graphs have treebreadth one, and so, treelength at most two. Indeed, for every dually chordal graph G, there exists a one-to-one mapping φ from the maximal cliques of some chordal graph H to the vertices of G. Let $(T, \mathcal{X})$ be a clique-tree of H. Since bags of this tree decomposition are maximal cliques of H, we can define, for every node $t \in V(T)$, $Y_t = N_G[\varphi(X_t)]$. Then, it can be checked that $(T', \mathcal{Y}) = (T, (Y_t)_{t \in V(T)})$ is a tree decomposition of G of breadth one. In particular, for every vertex $v \in V(G)$ we have that $T'_v = \bigcup_{u \in \varphi^{-1}(v)} T_u$. It follows, as claimed, that dually chordal graphs have treebreadth one, but this inclusion is proper. To see that, it suffices to notice that every chordal graph also has treebreadth one, while not all chordal graphs are dually chordal [BDCV98].

Another interesting fact is that every graph with diameter at most D also has treelength at most D (trivially). In particular, adding a universal vertex to any graph G with treewidth k will result in a graph G' with $tw(G') = k+1$ and $tl(G') \leq diam(G') \leq 2$. This simple observation will be useful in order to better intuit our results in Section 3.5.

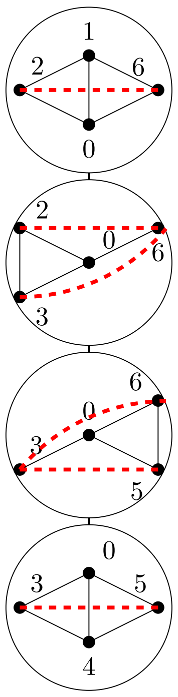
On the other way around, **examples of graphs with large treelength** include cycles and grids [DG07]. Intuitively, this can be explained by the Balanced separation property in tree decompositions: in any tree decomposition $(T, \mathcal{X})$ of G, there must exist a bag $B \in \mathcal{X}$ so that every component of $G \setminus B$ contains no more than $|V|/2$ vertices (it generalizes the existence of a centroid in a tree [Gol71]). It is not hard to see that on a cycle C_n with n vertices, any balanced separator has diameter $\Omega(n)$ (see also Fig. 2.14b). Similar arguments apply to the case of grids.

Finally, it should be noticed that complete graphs have unbounded treewidth and unit treelength, whereas n-vertex cycles have treewidth two and unbounded treelength $\lceil n/3 \rceil$ [DG07]. Altogether combined, it shows that treewidth and treelength are uncomparable on general graphs. We shall discuss when they can be compared in Section 3.5.

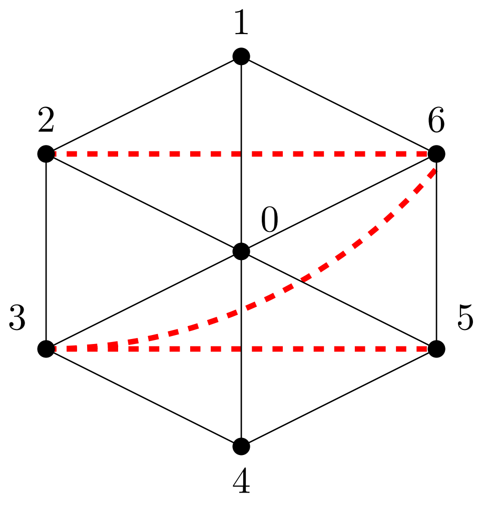
3.2.2 Relationship with triangulations

Tree decompositions can be defined equivalently in terms of graph triangulations. As we will show throughout this chapter, this reformulation is very convenient to use in the proofs.

A triangulation of $G = (V, E)$, sometimes called a fill-in of G, is any chordal supergraph $H = (V, E \cup F)$ of G. Recall that chordal graphs are exactly those graphs with a clique tree, *a.k.a.* tree decomposition whose bags are cliques [Gav74]. If H is a triangulation of G, then any of its clique tree is clearly a tree decomposition for G. Conversely, given a tree decomposition $(T, \mathcal{X})$ of G, we can define a triangulation of G by adding an edge between every two vertices that are in a same bag of the decomposition (*e.g.*, see Figure 3.3 for an illustration).



(a) A tree decomposition of W_6



(b) The corresponding triangulation.

Figure 3.3: Triangulation of the wheel W_6.

Altogether combined, the tree decompositions of G can be defined as the clique trees of its triangulations H. In particular:

- $tw(G) \leq k$ if and only if there exists a triangulation H of G with no clique of size greater than $k + 1$ (sometimes called a k-tree) [Bod06];
- $tl(G) \leq l$ if and only if there exists a triangulation H of G so that $E(H) \subseteq E(G^l)$, where $G^l = (V, \{\{u, v\} \mid 0 < d_G(u, v) \leq l\})$ is the l^{th} power of G [Lok10][2].

[2]I am not aware of any "natural" reformulation of treebreadth in terms of triangulation. It is my opinion that the hypergraph terminology from [BDCV98] would be best suited to reach the

Minimal triangulation and minimal separators. Let $G = (V, E)$ be a graph. A triangulation $H = (V, E \cup F)$ of G is *minimal* if for every strict subset $F' \subset F$, we have that $H' = (V, E \cup F')$ is not chordal. Similarly, a minimal tree decomposition of G is a clique tree of some minimal triangulation of G.

Every triangulation $H = (V, E \cup F)$ of G can be transformed into a minimal one by removing a subset of edges $F' \subseteq F$. Note that it does not make increase the width, length and breadth of the corresponding tree decompositions of G. As a result, it can always be found a minimal tree decomposition of minimum width, resp. of minimum length or of minimum breadth. This observation has motivated an in-depth study of minimal triangulations and their characterizations [Heg06].

In particular, the following characterization is due to Parra and Scheffler [PS97]. Before we can state it properly, we need to introduce standard notions on graph separators.

A *separator* of $G = (V, E)$ is any subset $S \subseteq V$ satisfying that $G \setminus S$ is disconnected. If a, b are two vertices in different components of $G \setminus S$ then we call S an ab-separator. A *minimal separator* is an inclusion wise minimal ab-separator S for some pair of vertices $a, b \in V \setminus S$. Equivalently, a separator S is called minimal if there exist two components A, B of $G \setminus S$ such that $N(A) = N(B) = S$. We note that inclusion wise minimal separators are also minimal separators, but the converse holds false.

Two minimal separators S_1, S_2 of G *cross* if S_1 intersects two connected components of $G \setminus S_2$ (this is an equivalence relation on minimal separators [PS97]). If S_1, S_2 do not cross then they are called *parallel*.

Theorem 42 ([PS97]). *H is a minimal triangulation of a graph G if and only if it is obtained by transforming into cliques all sets in a maximal family of pairwise parallel minimal separators of G.*

3.2.3 Tree decompositions with constrained adhesion sets

The dominant approach in the study of tree decompositions is to try to optimize some properties on the bags. This is the approach presented in Section 3.2.1. Another approach is to impose more structures on the adhesion sets (intersections of adjacent bags). Many graph decompositions can be defined this way. We present some of them below, with an emphasis on clique-decomposition.

First examples. The *biconnected decomposition* of $G = (V, E)$ is the collection of its maximal sets of vertices with no separator of size one (also called cut-vertex). These sets are called biconnected components. It is well-known that the biconnected components are the bags of a tree decomposition of G, sometimes called a *block-cut*

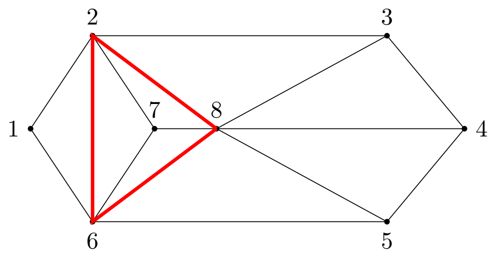
goal. Namely, define for every graph G the hypergraphs $\mathcal{C}(G)$ and $\mathcal{N}(G)$ whose hyperedges are, respectively, the maximal cliques and the closed neighbourhoods in G. Furthermore, given two hypergraphs $\mathcal{H}_1$ and $\mathcal{H}_2$ with same vertex-set, let us write $\mathcal{H}_1 \subseteq \mathcal{H}_2$ if every hyperedge of $\mathcal{H}_1$ is a subhyperedge of $\mathcal{H}_2$. Then, $tb(G) \leq j$ if and only if there exists a chordal supergraph H of G such that $\mathcal{C}(G) \subseteq \mathcal{C}(H) \subseteq \mathcal{N}(G^j)$

tree [Tar72]. In particular, we observe that the adhesion sets of a block-cut-tree are exactly the cut-vertices of G.

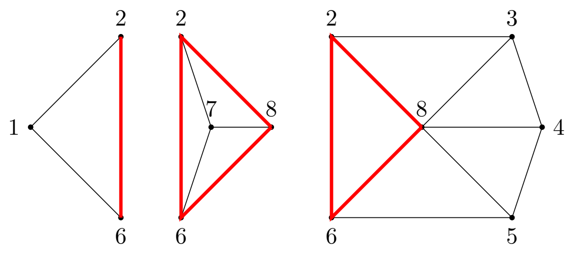
Similarly, the so-called *triconnected components* [HT73] are the bags of a tree decomposition of G, sometimes called a *SPQR-tree* [GM00]. The adhesion sets of a SPQR-tree are pairwise parallel minimal separators of size two. Generalizations to tree decompositions with adhesion sets of size at most k are discussed in [CDHH16, Gro16].

3.2.3.1 Clique-decomposition

Instead of bounding the size of the adhesion sets, we can bound their diameter. A clique-minimal separator of $G = (V, E)$ is a minimal separator inducing a clique of G. The atoms of G are the maximal sets of vertices with no clique separator. Finally, the *clique-decomposition* of G is the collection of its atoms (see Figure 3.4 for an illustration).



(a) A graph G.



(b) The clique-decomposition of G.

Figure 3.4: Example of clique-decomposition.

In the same way as above, the atoms of G are the bags of a tree decomposition, sometimes called an *atom tree* [BPS14]. The atom trees of G are exactly the clique-trees of some triangulation H^+ of G [BPS10]. In general, H^+ is not a minimal triangulation of G. However, we have that H^+ is a supergraph of *any* minimal triangulation of G. More precisely:

Proposition 43 ([BPS10]). *For every minimal triangulation H of $G = (V, E)$, the clique-minimal separators of G are exactly the minimal separators of H that induce a clique of G.*

What Proposition 43 implies is that in order to compute a minimal triangulation of G, it suffices to do so for each atom separately [Tar85]. In particular, it follows that treewidth, treelength and treebreadth can be computed on each atom separately (we obtain their value for G by taking the maximum value over the atoms). This motivates us to study the complexity of computing clique-decomposition in Section 3.3.

3.3 Computational aspects of clique-decomposition

This section is devoted to my work on the time complexity for computing clique-decomposition. We refer the reader to [DC17] for the full version.

3.3.1 State of the art

The clique-decomposition is well-known to be computable in polynomial $\mathcal{O}(nm)$-time on n-vertex m-edge graphs [Lei93, Tar85]. For dense graphs, it can be improved to $\mathcal{O}(n^{2.69})$ [KS06b], but the algorithm is non combinatorial (*i.e.*, it uses matrix multiplication as a routine). Faster combinatorial algorithms have been proposed on certain graph classes such as subclasses of hole-free graphs and claw-free graphs [BBGM15, BW12]. Still, the best-known combinatorial algorithms have $\mathcal{O}(nm)$-time complexity, that is cubic for dense graphs and quadratic for sparse graphs.

As shown with Proposition 43, clique-decomposition is strongly related with minimal triangulations. However, Kratsch and Spinrad proved in [KS06a] that finding a clique-separator is at least as hard as finding a simplicial vertex, *even if a minimal triangulation is given as part of the input.* The latter result implies that computing a minimal triangulation is not the only complexity bottleneck of clique-decomposition algorithms.

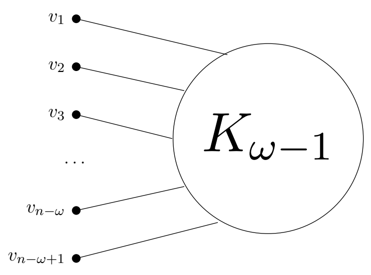


Figure 3.5: An n-vertex split graph with clique-number ω. The vertices are bipartitioned in a clique $K_{\omega-1}$ with $\omega-1$ vertices and an independent set with $n-\omega+1$ vertices. Furthermore, each vertex in the independent set is adjacent to all vertices in the clique. The atoms of the graph are exactly the closed neighbourhoods $N[v_i]$, $1 \leq i \leq n-\omega+1$. Therefore, there are $\omega(\omega-1)(n-\omega+1)/2$ edges in total in the subgraphs induced by the atoms.

Overview. Our results – presented below – suggest that another difficulty comes from the *clique-number* of the graph (size of a largest clique). In order to support our claim, we illustrate with Figure 3.5 that there are n-vertex graphs with clique-number ω such that the total number of edges cumulated on the subgraphs that are induced by their atoms is $\Omega(\omega^2 n)$. It implies that when a clique-decomposition algorithm not only computes the atoms, but also the subgraphs that are induced by them, its time complexity must be $\Omega(\omega^2 n)$.

3.3.2 Contributions

The following is joint work with my supervisor David Coudert.

3.3.2.1 Time complexity lower bound

In the spirit of what has been presented for graph hyperbolicity (Section 2.6.3, p. 64), it is proved in this section a *conditional lower-bound* on the time complexity for computing clique-decomposition. Precisely, computing the clique-decomposition is at least as hard as detecting a triangle in a graph.

We prove the following result in our paper [DC17].

Theorem 44. *The problem of detecting a triangle in an n-vertex graph reduces in quadratic time to the problem of computing the clique-decomposition of a graph with $3n+2$ vertices.*

It is conjectured that no combinatorial truly subcubic algorithm for TRIANGLE DETECTION exists [Wil16]. So, altogether combined, this is hint that the $\mathcal{O}(nm)$-time state-of-the-art algorithm for computing clique-decomposition is essentially optimal.

3.3.2.2 Matching upper bound

In order to better understand the hardness of computing clique-decomposition, we next turn our attention on the *non combinatorial* algorithms. On a more theoretical side, it is proved in our paper [DC17] that clique-decomposition can be computed in $\mathcal{O}(n^\alpha \log n) = \mathcal{O}(n^{2.3729} \log n)$-time by using fast matrix multiplication.

Theorem 45. *For every n-vertex graph $G = (V, E)$, its clique-decomposition can be computed in $\mathcal{O}(n^{2.3729} \log n)$-time.*

Under well-established complexity hypotheses, the latter result matches the lower-bound obtained with TRIANGLE DETECTION for the non combinatorial algorithms. Indeed, we refer to [VWW10] for computational equivalences between TRIANGLE DETECTION AND MATRIX MULTIPLICATION[3]. Hence, these results are hint that (up to logarithmic factors), the time complexity for computing clique decomposition is in $\tilde{\mathcal{O}}(n^{2.3729})$.

3.3.2.3 The role of clique-number

Finally, we consider the seemingly simpler problem of computing the clique-decomposition when a minimal triangulation is given as part of the input. Let us call it the CLIQUE-DECOMPOSITION WITH MINIMAL TRIANGULATION problem.

[3]More explicitly, if MATRIX MULTIPLICATION can be solved in $\mathcal{O}(M(n))$-time then TRIANGLE DETECTION can be solved in $\mathcal{O}(M(n))$-time, and conversely if TRIANGLE DETECTION can be solved in $\mathcal{O}(T(n))$-time then MATRIX MULTIPLICATION can be solved in $\tilde{\mathcal{O}}(n^2 \cdot T(n^{1/3}))$-time.

We shall seek for efficient *parameterized* algorithms for the problem, where the parameter is the clique-number of the graph.

A new paradigm has emerged in Fixed-Parameter Tractability, sometimes called P-FPT (polynomial FPT), where the dependency in the fixed parameter k is required to be polynomial. There have been recent revisitings of polynomial-time graph problems in this polynomial parameterized setting [AVWW16, FLP+15, GMN15]. Our result, that can be found in our paper [DC17], is that CLIQUE-DECOMPOSITION WITH MINIMAL TRIANGULATION can be solved in linear time when the clique-number of the graph is assumed to be a constant.

Theorem 46. *For every $G = (V, E)$ with clique-number ω, and $H = (V, E \cup F)$ any minimal triangulation of G with $f = |F|$ fill edges, the* CLIQUE-DECOMPOSITION WITH MINIMAL TRIANGULATION *problem can be solved in time $\mathcal{O}(m + f + \omega^2 n)$.*

It is open whether more generally, the clique-decomposition can be computed in quasi-linear time on graphs with bounded clique-number. I conjecture that it is the case and this is left as an interesting open question. Furthermore, in order to support my conjecture, I will prove at the end of this section that it holds true for triangle-free graphs ($\omega = 2$).

3.3.3 Summarizing the proofs

3.3.3.1 Reduction from a counting problem

The proof for the lower bound is based on the following result on counting the number of simplicial vertices in a graph.

Lemma 47 ([KS06a])**.** *Counting the number of simplicial vertices in a graph with $3n + 2$ vertices is at least as hard as detecting a triangle in an n-vertex graph.*

I prove that a vertex is simplicial if and only if it is contained in a unique atom and this atom is a clique [DC17]. Based on this characterization, it can be shown that counting the number of simplicial vertices can be done in linear time if the clique-decomposition is given. Theorem 44 follows from this result directly.

Proof of Theorem 44. Let $G = (V, E)$ be any graph with $3n+2$ vertices. In order to prove the theorem, by Lemma 47 it is sufficient to prove that counting the number of simplicial vertices in G can be done in $\mathcal{O}(n+m)$-time if the clique-decomposition of G is given.

We claim that for every simplicial vertex $v \in V$, its closed neighbourhood $N[v]$ is an atom, and in particular it is the unique atom containing v. Indeed, suppose for the sake of contradiction that there exists $u \notin N[v]$ such that u and v lie on a same atom A. Then, $N(v) \cap A$ is an uv-separator in the subgraph $G[A]$. Since $N(v) \cap A$ is a clique, the latter contradicts that $G[A]$ has no clique-separator. Therefore, every atom containing v is a subset of $N[v]$. Finally, since $G[N[v]]$ is complete, we have that $G[N[v]]$ has no clique-separator, and so, by inclusion wise maximality of the atoms, $N[v]$ is the unique atom containing v, that proves the claim.

In particular, it follows from this above claim that a vertex is simplicial if and only if it is contained in a unique atom and this atom is a clique. Indeed, if a vertex is simplicial then by the above claim it satisfies the desired property. Conversely, if a vertex v is uniquely contained in an atom A and A is a clique then v is trivially simplicial with its neighbourhood being equal to $N[v] = A$.

Let us take advantage of this above characterization of simplicial vertices in order to count them in G. Let $A_1, A_2, \ldots, A_k$ be the atoms of G. We will use in the following analysis that $\sum_{i=1}^{k} |A_i| = \mathcal{O}(n+m)$ [BPS10].

We first compute an atom tree of G. In order to do so, we recall that a *dual hypertree* is a hypergraph whose hyperegdes are the maximal cliques of some chordal graph (obtained by adding an edge between every two vertices that are contained in a same hyperedge). Tarjan et al. prove in [TY84] that dual hypertrees can be recognized in linear-time, and that for every dual hypertree, a clique-tree of its underlying chordal graph can be computed within the same amount of time. Therefore, we can use this algorithm from [TY84] in order to compute an atom tree in $\mathcal{O}(\sum_{i=1}^{k} |A_i|) = \mathcal{O}(n+m)$-time.

Then, let A_i be any leaf-bag in the atom tree (a bag whose corresponding node in the tree has degree at most one). Since the intersection of two atoms is a clique [BPS10], we have that A_i is a clique if and only if every vertex that is uniquely contained in A_i has degree $|A_i| - 1$. Furthermore, by removing the set C_i of vertices that are uniquely contained in A_i then discarding A_i from the atom tree, one obtains an atom tree of $G \setminus C_i$. Therefore, we can repeat the above process in order to list all the atoms of G that are cliques. Overall, it takes time $\mathcal{O}(\sum_{v \in V} |N(v)| + \sum_{i=1}^{k} |A_i|) = \mathcal{O}(n+m)$.

Finally, let $A_{i_1}, \ldots, A_{i_l}$ be the atoms of G that are cliques. We can count all the vertices that are only contained in A_{i_j}, for some $1 \leq j \leq l$, simply by scanning all the atoms in $\mathcal{O}(\sum_{i=1}^{k} |A_i|) = \mathcal{O}(n+m)$-time. Since we proved that these are exactly the simplicial vertices of G, the latter achieves proving that counting the number of simplicial vertices can be done in $\mathcal{O}(n+m)$-time if the atoms are given. □

3.3.3.2 Computing the clique-minimal separators

Berry et al. have proved the following result in [BPS14]. Given an n-vertex m-edge graph $G = (V, E)$, suppose we are given $H = (V, E \cup F)$ a minimal triangulation of G with $f = |F|$ fill edges, *and the collection of the clique-minimal separators* of G. Then, the clique-decomposition of G can be computed in time $\mathcal{O}(m+f)$. So, we focused on the problem of computing the clique-minimal separators, given G and H as inputs.

Outline of the method. The gist of the approach for doing so is to use Proposition 43. Indeed, since H is chordal, its minimal separators can be computed in linear $\mathcal{O}(m+f)$-time [Gav72]. In order to extract from these the clique-minimal separators of G, by Proposition 43 it suffices to decide which are cliques of G.

- We prove in [DC17] that it can be done by using the incidence matrix of G and fast matrix multiplication. More precisely, we compute the clique-matrix of the triangulation H, where the minimal separators of H are listed, and then we multiply this matrix with the incidence matrix of G in order to determine which of those are cliques of G. Since in addition, a minimal triangulation H of G can be computed in $\mathcal{O}(n^\alpha \log n)$-time [HTV05], Theorem 45 follows.
- In order to do the same in a combinatorial way, we propose the following algorithm. Let us consider the vertices in G sequentially. At each step i, and for every minimal separator S of H which contains the current vertex v_i, we check whether v_i is adjacent to all the previous vertices $v_j \in S$ with $j < i$. When that is not the case, S cannot be a clique of G and so, we can discard it from the collection of (potential) clique-minimal separators of G. The central idea of the analysis is that since G has clique-number ω, we shall detect whether a minimal separator S of H is not a clique of G by considering no more than $\omega+1$ vertices in S. — Note that we needn't compute ω for the algorithm. — Theorem 46 now follows.

Discussion. The reason why we don't have an algorithm in time $\omega^{\mathcal{O}(1)}(n+m)$ for computing the clique-decomposition is that we don't know how to compute a minimal triangulation within these time bounds. However, there exist quasi-linear time algorithms for computing a minimal triangulation in some classes such as, *e.g.*, planar graphs [Dah98], bounded degree graphs [Dah02] and bounded-treewidth graphs [FLP+15]. Furthermore, we prove that in the special case of triangle-free graphs ($\omega = 2$), a minimal triangulation is not needed in order to compute the clique-decomposition. The latter result generalizes a remark from [BPS11], where Berry et al. notice without giving too much details that computing the clique-decomposition of a given bipartite graph can be done in linear time.

Lemma 48. *If $G = (V, E)$ is triangle-free then an atom tree of G can be computed in $\mathcal{O}(|V| + |E|)$-time.*

Proof. First, we compute a block-cut-tree of G (*a.k.a.* a tree decomposition whose bags are exactly the biconnected components of G, see Section 3.2). It can be done in linear time [Tar72]. We observe that since a cut-vertex is a clique-separator, the atoms of G are exactly the atoms of its biconnected components. In particular, an atom tree of G can be obtained by substituting each biconnected component G_i, in the block-cut-tree, by an atom tree of G_i. So, we can process the biconnected components separately and we now assume that G is biconnected for the remaining of the proof.

Then, we compute the SPQR-tree of G, that can also be done in linear time [GM00]. In [GM00] Gutwenger and Mutzel prove the following result using a different terminology than Parra and Scheffler. We have that up to further splitting the cycles among the triconnected components (using nonedge separators), the collection $\mathcal{F}_2$ of the adhesion sets in the SPQR-tree is a maximal family of pairwise parallel minimal 2-separators of G. In this situation, we observe that since the two ends of an edge cannot be disconnected by any separator of G, an edge-separator is trivially parallel with any other minimal 2-separator of G, and so, it must be contained in $\mathcal{F}_2$. In particular, we can compute all the edge-separators of G by computing $\mathcal{F}_2 \cap E$, that can be done in $\mathcal{O}(|E| + |\mathcal{F}_2|) = \mathcal{O}(|V| + |E|)$-time.

Finally, since G is assumed to be biconnected and triangle-free, its edge-separators are exactly its clique-minimal separators. Therefore, we can compute the atoms of G as follows. We compute the maximal subtrees T_i of T so that for every $\{t, t'\} \in E(T_i)$, the minimal 2-separator $X_t \cap X_{t'}$ is not an edge. It can be done in $\mathcal{O}(\sum_{t \in V(T)} |X_t|) = \mathcal{O}(|V| + |E|)$-time. Then, the atoms of G are exactly the unions of bags in the subtrees, *i.e.*, $\bigcup_{t \in V(T_i)} X_t$ for every i. $\square$

Finally, it would be interesting to determine whether more generally, a graph can be decomposed by its clique-minimal separators of size at most k in $k^{\mathcal{O}(1)}(n+m)$-time. By Lemma 48, it is the case if $k \leq 2$. Furthermore, a positive answer for every k would directly imply that computing the clique-decomposition can be done in $\omega^{\mathcal{O}(1)}(n+m)$-time — given the clique-number ω as part of the input.

3.4 On the complexity of computing treebreadth and its relatives

Computing an atom tree is a first step toward computing more interesting tree decompositions, *e.g.* with optimal width, length or breadth. In this section, we now answer open questions from [DK14] and [DKL14] on the complexity of computing treebreadth, pathlength and pathbreadth. Full results are presented in [DLN16a, DLN16b].

3.4.0.3 Motivations and related work

Treelength and treebreadth. The complexity of computing *treelength* on general graphs is now well understood. Graphs with unit treelength are exactly the chordal graphs [DG07], and they can be recognized in linear time. In contrast, recognizing graphs with treelength at most k is NP-complete for every fixed $k \geq 2$ [Lok10]. However on a more positive side, there exist 3-approximation algorithms for computing this parameter [DG07].

In [Lok10], the reduction used for treelength goes through edge-weighted graphs, and then goes back to unweighted graphs using rather elegant gadgets. It is not clear how to adapt this proof for treebreadth. Since the value for this parameter is a 2-approximation for treelength [DK14], any polynomial-time algorithm for computing treebreadth, or even an α-approximation algorithm for some $\alpha < 3/2$, would improve the best-known approximation algorithms for treelength. Our results (presented below) suggest that no such algorithm is likely to exist.

Pathlength and pathbreadth. As for pathlength (resp., pathbreadth), a 2-approximation (resp., a 3-approximation) algorithm is given for computing this parameter but the computational complexity of both problems is left open in [DKL14]. In the same paper, pathlength and pathbreadth have been shown to be useful in the design of approximation algorithms for bandwidth and line-distortion.

We note that recently, the MINIMUM ECCENTRICITY SHORTEST-PATH problem has been proved NP-hard [DL15]. The latter is a minimization problem where given a graph $G = (V, E)$, it is aimed at computing a shortest-path $\mathcal{P}$ with minimum *eccentricity* $\max_{v \in V} \mathrm{d}_G(v, \mathcal{P})$. Furthermore, it has been proved in [DKL14] that the minimum eccentricity of a shortest-path in G is an $\Theta(pl(G))$ with $pl(G)$ being the pathlength of G. Let us point out that for every fixed k, it can be decided in polynomial time whether a graph admits a shortest-path with eccentricity at most k [DL15]. The following results will show that the situation is different for pathlength and pathbreadth.

3.4.1 Summarize of our contributions

The main contributions in this section are to answer the open questions from [DK14, DKL14] on the complexity of computing treebreadth, pathlength and pathbreadth. Namely, the main results in our paper [DLN16a] can be stated as follows.

Theorem 49. *Recognizing the graphs with pathbreadth at most one is NP-complete.*

Theorem 50. *Recognizing the graphs with pathlength at most two is NP-complete.*

Theorem 51. *Recognizing the graphs with treebreadth at most k is NP-complete for every fixed $k \geq 1$.*

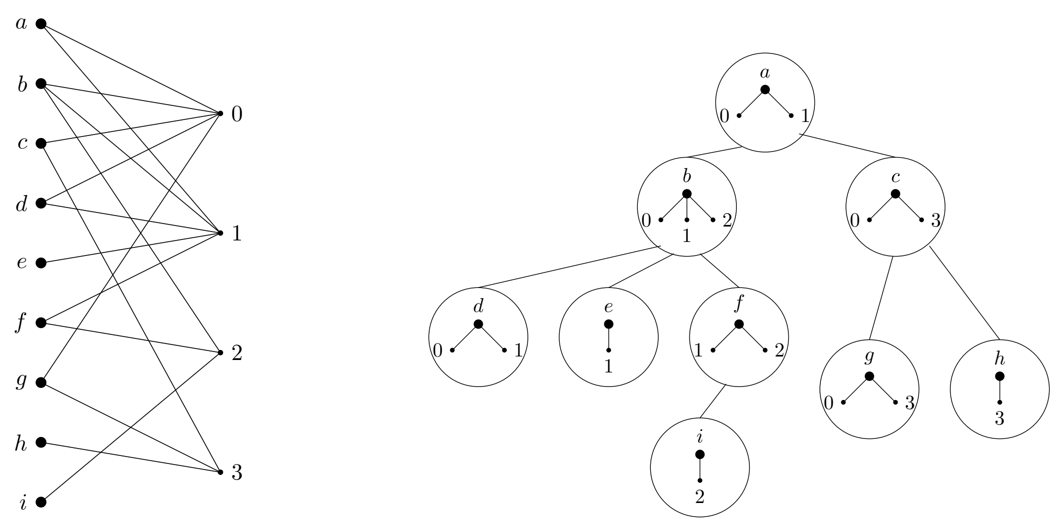
It is likely that recognizing graphs with pathbreadth at most k, resp. pathlength at most $k + 1$, is NP-complete for every fixed $k \geq 1$. This is left open in [DLN16a].

3.4.1.1 Graphs with treebreadth one

We now concentrate on the recognition of graphs with treebreadth at most one. This class of graphs already encompasses well-studied subclasses such as chordal graphs and dually chordal graphs. As it is stated in Theorem 51, recognizing graphs with treebreadth one is NP-complete. However, we prove in [DLN16a] that it can be done in polynomial time for bipartite graphs and planar graphs.

Case of bipartite graphs. Precisely, we obtain in our paper [DLN16a] a simple characterization of bipartite graphs with treebreadth one. Let us call a bipartite graph *tree-convex* if it admits a tree decomposition whose bags are exactly the closed neighbourhoods of the vertices in one side of its bipartition [WLJX12]. We refer to Figure 3.6 for an illustration.

Theorem 52. *A bipartite graph has treebreadth at most one if and only if every of its atoms is tree-convex. It can be verified in linear time.*



(a) A tree-convex graph G. (b) A star-decomposition of G.

Figure 3.6: Tree-convex graphs have treebreadth one.

In contrast, recognizing bipartite graphs with treebreadth at most two is NP-complete. We observe that bipartite graphs with treebreadth one already encompass well-known graph classes such as convex bipartite graphs and chordal bipartite graphs (*a.k.a.*, bipartite graphs with no induced cycle of length at least six).

Case of planar graphs. We don't have a full characterization of planar graphs with treebreadth one. As proved in [DLN16a], a planar graph has treebreadth one only if it has treewidth at most four (more general relationships between treebreadth and treewidth will be discussed in the next Section 3.5). However, this condition is not sufficient, since any cycle of length at most five has treewidth two but treebreadth greater than one. Nonetheless, we have designed an algorithm in order to recognize planar graphs with treebreadth one in polynomial time.

Theorem 53. *Recognizing planar graphs with treebreadth one can be done in quadratic time. Furthermore, given a planar graph with treebreadth one, a tree decomposition with breadth one can be computed in cubic time.*

The algorithm for planar graphs is rather involved and it will be only sketched in what follows. We refer to our research report [DLN16b] for full details.

This part of my contributions is joint work with Nicolas Nisse and Sylvain Legay.

3.4.2 Approach and the techniques used in the proofs

3.4.2.1 A central lemma for graphs of treebreadth one

We start with a structural lemma that is used throughout all the proofs. We name *star-decomposition* a tree decomposition such that for every node $t \in V(T)$, there exists a vertex $u \in X_t$ such that $X_t \subseteq N[u]$. That is, star-decompositions are similar to decompositions of breadth one, but the dominator of each bag has to belong to the bag itself. We prove with the following Lemma 54 that a graph has treebreadth one if and only if it has a star-decomposition.

In what follows, a tree decomposition is called *reduced* if no bag is included in another one. Starting from any tree decomposition, a reduced tree decomposition can be obtained in polynomial time by contracting any two adjacent bags with one contained in the other until it is no more possible to do that. Note that such a process does not modify the width, the length nor the breadth of the decomposition.

Lemma 54. *For any graph G with $tb(G) \leq 1$, every* reduced *tree decomposition of G of breadth one is a star-decomposition.*

The proof of Lemma 54 is an application of the Helly property: if B is a bag of a tree decomposition $(T, \mathcal{X})$ of G and there exists a vertex u dominating this bag, then by the properties of a tree decomposition, the subtrees T_u and T_v, $v \in B$, are pairwise intersecting, and so, by the Helly property there must be a bag with $B \cup \{u\}$. If the tree decomposition is reduced then it implies that $u \in B$.

3.4.2.2 Hardness of treebreadth, pathlength and pathbreadth

On the complexity point of view, the main result in [DLN16a] is the NP-completeness of deciding whether $tb(G) \leq k$, for every fixed $k \geq 1$. We first prove that the problem is NP-complete for $k = 1$, that will be our focus in this section. Then, we show that the problem of computing the treebreadth of a graph is polynomially equivalent to the problem of recognizing graphs with treebreadth one. Using similar techniques, we can prove that computing pathlength, resp., pathbreadth, is NP-hard [DLN16b].

Theorem 51 is proved by reducing a variation of the Chordal Sandwich problem to the recognition of graphs with treebreadth one. The Chordal Sandwich problem takes as input two graphs $G_1 = (V, E_1), G_2 = (V, E_2)$ with $E_1 \subseteq E_2$, and it asks whether there exists a chordal graph $H = (V, E)$ such that $E_1 \subseteq E \subseteq E_2$. This problem is NP-complete [GKS95]. In [Lok10], the author also proposed a reduction from Chordal Sandwich in order to prove that computing treelength is NP-hard. However, we need different gadgets than in [Lok10], and the arguments to prove correctness of the reduction are completely different.

Let us give a flavour of our reduction with Figure 3.7. Suppose we are given an instance $\langle G_1, G_2 \rangle$ of Chordal Sandwich. We aim at computing a supergraph G of G_1 such that in any tree decomposition of G of breadth one, there can be no two nonadjacent vertices in G_2 that are in the same bag. This way, any tree decomposition of G of breadth one can be transformed into a clique-tree for a chordal sandwich between G_1 and G_2. In order to reach this goal, for every nonedge $\{u, v\} \notin E(G_2)$ we add a copy of the gadget in Figure 3.7 and we make both u and v adjacent to both s_{uv}, t_{uv}. By construction, the four vertices (u, s_{uv}, v, t_{uv}) induce a cycle of length four. If we were studying treelength, then this would not give us that much information; indeed, in a tree decomposition of length at least two, all four vertices

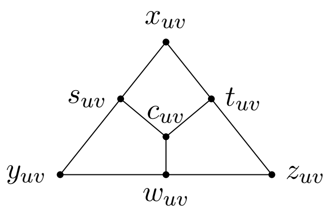


Figure 3.7: Gadget graph F_{uv}. The two vertices x_{uv}, w_{uv} are on disjoint $s_{uv}t_{uv}$-paths. Since they have no common neighbour, it ensures that s_{uv}, t_{uv} must be contained in a same bag in any star-decomposition of F_{uv}.

could be placed in a same bag without violating any constraint. However, this is no more the case for a tree decomposition with unit *breadth.* Indeed, since no vertex dominates the four vertices of the cycle, they cannot be part of a common bag. Hence, the gist of the construction is to ensure that s_{uv}, t_{uv} must be in a common bag in *any* tree decomposition of G of breadth one. Then, one can prove by elaborating on the Helly property that it implies that u and v cannot be in a same bag in any tree decomposition of G of breadth one.

On the technical point of view, the most difficult part of the reduction is to ensure that conversely, if $\langle G_1, G_2 \rangle$ is a yes-instance of Chordal Sandwich then the resulting graph G has treebreadth one. Ideally, we would like to transform some tree decomposition of G_1, with all vertices in a same bag being adjacent in G_2, to a star-decomposition of G. We tried to do so by adapting a technique from Lokshtanov [Lok10] that consists in adding a dominating clique in the graph. However, vertices from the gadgets in Figure 3.7 need to be inserted in the bags as well, thereby complicating the picture. In order to overcome the difficulties that are posed by these gadgets, we aim at better controlling in which bags their vertices need to be inserted, but then we need to impose additional constraints on the tree decomposition of G_1. In general, we are not able to prove that a tree decomposition with the desired constraints always exists. That is why we need to consider a variation of Chordal Sandwich where we impose more structure on the input.

Theorem 55. *The problem of deciding whether a graph has treebreadth one is NP-complete.*

Proof. The problem is in NP. To prove the NP-hardness, we will reduce from a variation of Chordal Sandwich that we name Chordal Sandwich with $\overline{nK_2}$. In this variation, we constrain ourselves to the instances $\langle G_1, G_2 \rangle$ so that the complementary $\bar{G}_2$ of G_2 induces a perfect matching. The problem Chordal Sandwich with $\overline{nK_2}$ is NP-complete [BFW92, GKS95]. Furthermore, perhaps surprisingly, the restriction on the structure of $\bar{G}_2$ will be shown to be a key element in our reduction.

Let $\langle G_1, G_2 \rangle$ be any instance of Chordal Sandwich with $\overline{nK_2}$. Let G' be the graph constructed from G_1 as follows. First, a clique V' of $2n = |V|$ vertices is added to G_1. Vertices $v \in V$ are in one-to-one correspondance with vertices $v' \in V'$.

Then, for every $\{u,v\} \notin E_2$, u and v are respectively made adjacent to all vertices in $V' \setminus v'$ and $V' \setminus u'$. Finally, we add a copy of the gadget F_{uv}, depicted in Figure 3.8a, and the vertices s_{uv} and t_{uv} are made adjacent to the four vertices u, v, u', v'.

We will prove that $tb(G') = 1$ if and only if $\langle G_1, G_2 \rangle$ is a yes-instance of CHORDAL SANDWICH WITH $\overline{nK_2}$.

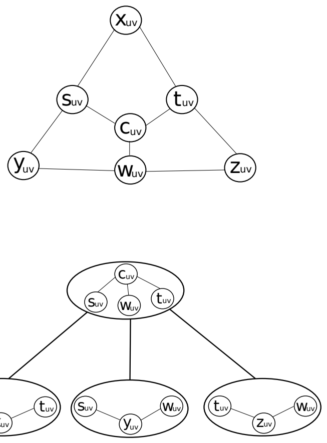
In one direction, assume $tb(G') = 1$, let $(T, \mathcal{X})$ be a star-decomposition of G' (which exists by Lemma 54). We prove that the triangulation of G_1 obtained from this star-decomposition is the desired chordal sandwich. Let $H = (V, \{\{u,v\} \mid T_u \cap T_v \neq \emptyset\})$. H is a chordal graph such that $E_1 \subseteq E(H)$. To prove that $\langle G_1, G_2 \rangle$ is a yes-instance of CHORDAL SANDWICH WITH $\overline{nK_2}$, it suffices to prove that $T_u \cap T_v = \emptyset$ for every $\{u,v\} \notin E_2$. We claim that it is implied by $T_{s_{uv}} \cap T_{t_{uv}} \neq \emptyset$. Indeed, assume $T_{s_{uv}} \cap T_{t_{uv}} \neq \emptyset$ and $T_u \cap T_v \neq \emptyset$. Since $s_{uv}, t_{uv} \in N(u) \cap N(v)$, $T_u, T_v, T_{s_{uv}}, T_{t_{uv}}$ pairwise intersect, there is a bag with u, v, s_{uv}, t_{uv} by the Helly property. The latter contradicts that $(T, \mathcal{X})$ is a star-decomposition because no vertex dominates the four vertices. Hence the claim is proved. So, let us prove that $T_{s_{uv}} \cap T_{t_{uv}} \neq \emptyset$. By contradiction, if $T_{s_{uv}} \cap T_{t_{uv}} = \emptyset$ then every bag B onto the path between $T_{s_{uv}}$ and $T_{t_{uv}}$ must contain c_{uv}, x_{uv}. Since $N[c_{uv}] \cap N[x_{uv}] = \{s_{uv}, t_{uv}\}$ and $(T, \mathcal{X})$ is a star-decomposition, it implies either $s_{uv} \in B$ and $B \subseteq N[s_{uv}]$ or $t_{uv} \in B$ and $B \subseteq N[t_{uv}]$. So, there are two adjacent bags $B_s \in T_{s_{uv}}, B_t \in T_{t_{uv}}$ such that $B_s \subseteq N[s_{uv}]$ and $B_t \subseteq N[t_{uv}]$. In particular, $B_s \cap B_t$ must intersect the path (y_{uv}, w_{uv}, z_{uv}) because $y_{uv} \in N(s_{uv})$ and $z_{uv} \in N(t_{uv})$. However, $N[s_{uv}] \cap N[t_{uv}] \cap \{y_{uv}, w_{uv}, z_{uv}\} = \emptyset$, that is a contradiction. As a result, $T_{s_{uv}} \cap T_{t_{uv}} \neq \emptyset$ and so, $T_u \cap T_v = \emptyset$ for any $\{u,v\} \notin E_2$.

Conversely, assume that $\langle G_1, G_2 \rangle$ is a yes-instance of CHORDAL SANDWICH WITH $\overline{nK_2}$. Let H be any chordal supergraph of G_1 such that $E(H) \subseteq E(G_2)$ and H is edge-maximal w.r.t. this property. We prove in [DLN16b] that every clique-tree of H is a tree decomposition $(T, \mathcal{X})$ of G_1 with $|\mathcal{X}| = |V|/2 + 1$ bags such that for every $\{u,v\} \notin E_2$, $T_u \cap T_v = \emptyset$ and there are two adjacent bags $B_u \in T_u$ and $B_v \in T_v$ such that $B_u \setminus u = B_v \setminus v$. The latter is proved by elaborating on the hypothesis that $\bar{G}_2$ is a perfect matching.

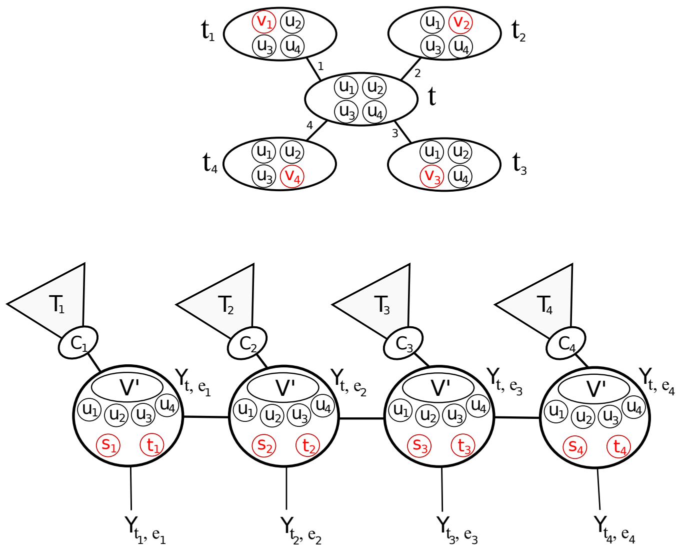
In what follows, we will modify $(T, \mathcal{X})$ in order to obtain a star-decomposition of G'. To do so, we will use the fact that there are $|V|/2 = n$ edges in $E(T)$ and that for every $\{u,v\} \notin E_2$, there are two adjacent bags $B_u \in T_u$ and $B_v \in T_v$ such that $B_u \setminus u = B_v \setminus v$. Indeed, this implies that there is a one-to-one mapping $\alpha : E(T) \to E(\bar{G}_2)$ between the edges of T and the non-edges of G_2. Precisely, for any edge $e = \{t,s\} \in E(T)$, let $\alpha(e) = \{u,v\} \in E(\bar{G}_2)$ be the non-edge of G_2 such that $u \in X_t, v \in X_s$ and $X_t \setminus u = X_s \setminus v$.

Intuitively, the star-decomposition $(T', \mathcal{X}')$ of G' is obtained as follows. For any $t \in V(T)$ with incident edges $e_1, \cdots, e_d$, we first replace X_t by a path decomposition $(Y_{t,e_1}, \cdots, Y_{t,e_d})$. Then, for any edge $e = \{t,s\} \in E(T)$, an edge is added between $Y_{t,e}$ and $Y_{s,e}$. Finally, the center-bag of some star-decomposition of the gadget $F_{\alpha(e)}$ is made adjacent to $Y_{t,e}$ (see Figure 3.8b for an illustration).

More formally, let $t \in V(T)$ and $e \in E(T)$ incident to t, and let $\{u,v\} = \alpha(e)$.



(a) Gadget F_{uv} (top) with a star-decomposition of F_{uv} (bottom).



(b) A subtree of the star-decomposition of G' (bottom) obtained from an internal bag with degree four of $(T, \mathcal{X})$ (top). Subtrees T_i are star-decompositions of the gadgets $F_{u_i v_i}$.

Figure 3.8

Let $Y_{t,e} = V' \cup X_t \cup \{s_{uv}, t_{uv}\}$ (note that $Y_{t,e}$ is dominated by $u' \in V'$). Let $e_1, \cdots, e_d$ be the edges incident to t in T, in any order. For $1 \leq i < d$, add an edge between Y_{t,e_i} and $Y_{t,e_{i+1}}$. For any edge $e = \{t, s\} \in E(T)$, add an edge between $Y_{t,e}$ and $Y_{s,e}$. Finally, add the star-decomposition $(T^e, \mathcal{X}^e)$ for the gadget $F_{\alpha(e)}$ as depicted in Figure 3.8a and add an edge between its center and $Y_{t,e}$.

The resulting $(T', \mathcal{X}')$ is a star-decomposition of G', so, $tb(G') = 1$. □

3.4.2.3 Polynomial cases

Our polynomial-time algorithms are based on a divide and conquer approach. We recall that a separator S of G is minimal if there exist two connected components A, B of $G \setminus S$ such that $N(A) = N(B) = S$. Furthermore, A and B are called *full components* for S, and a *block* is the union of a minimal separator with one of its full components. A remarkable property of graphs with treebreadth one, whose proof is deferred to our research report [DLN16b], is that they are stable under taking blocks.

Lemma 56. *Let $G = (V, E)$, S be a separator and W be the union of some connected components of $G \setminus S$. If $tb(G) = 1$ and W contains a full component for S, then $tb(G[W \cup S]) = 1$.*

Proof. Let $(T, \mathcal{X})$ be a star-decomposition of G. We remove vertices in $V \setminus (W \cup S)$ from bags in $\mathcal{X}$, that yields a tree decomposition $(T, \mathcal{X}')$ of $G[W \cup S]$. We will prove

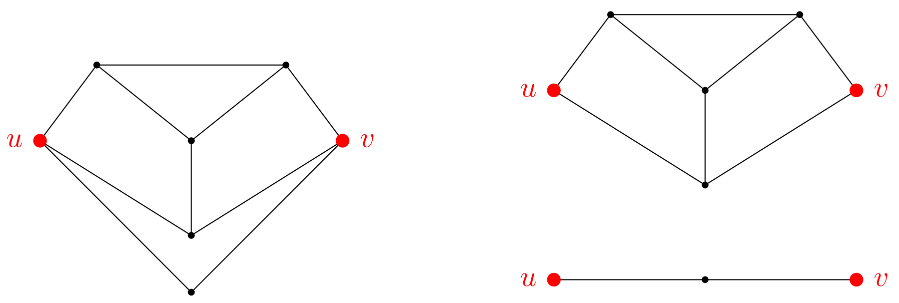


Figure 3.9: The 2-separator $\{u, v\}$ disconnects the graph G (left) in two blocks with treebreadth one (right). However, $tb(G) = 2$.

that $(T, \mathcal{X}')$ has breadth one (but is not necessarily a star-decomposition). Indeed, let $X'_t \in \mathcal{X}'$. By construction, $X'_t \subseteq X_t$ with $X_t \in \mathcal{X}$. Let $v \in X_t$ satisfy $X_t \subseteq N_G[v]$. If $v \in X'_t$, then we are done. Else, since for all $x \notin S \cup W, N(x) \cap (S \cup W) \subseteq S$ (because S is a separator by the hypothesis), we must have that $X_t \subseteq S$. Let $A \subseteq W$ be a full component for S, that exists by the hypothesis, let T_A be induced by the bags intersecting A. Since T_A and the subtrees $T_x, x \in X_t$ pairwise intersect — because for all $x \in X_t$, $x \in S$ and so, x has a neighbour in A —, then by the Helly property there is a bag in $\mathcal{X}$ containing X_t and intersecting A. Furthermore, any $u \in V$ dominating this bag must be either in S or in A, so, in particular there is $u \in A \cup S$ such that $X_t \subseteq N[u]$. □

The converse of Lemma 56 does not hold in general (see Fig. 3.9), yet there are interesting cases where it does. In fact, all our algorithms in what follows are based on particular cases where the converse of Lemma 56 also holds true. One of them is the case where S is a *clique-minimal separator*. In particular, a graph has treebreadth one if and only if every of its atoms have treebreadth one [DLN16a], and so, we may further constrain our studies to graphs without a clique-separator, *a.k.a. prime graphs.*

Case of bipartite graphs. For prime bipartite graphs, it is almost immediate that in any star-decomposition (tree decomposition with a dominator in each bag, see Sec. 3.4.2.1), every two adjacent bags must be dominated by vertices that are on the same side of the bipartition. Indeed, otherwise the adhesion set between these two bags would be either a cut-vertex or an edge-separator. The latter implies that a prime bipartite graph must be tree-convex and so, Theorem 52 follows.

Now, given a bipartite graph G, we can check whether it has treebreadth one as follows. We compute its atoms, that can be done in linear time by Lemma 48. Then, we check whether each of its atoms is tree-convex, that can also be done in linear time[4] [WLJX12]. Finally, by Theorem 52 we output $tb(G) = 1$ if and only if

[4]This problem can be reduced to dual hypertree recognition. See the proof of Theorem 44 for similar techniques.

all its atoms are tree-convex.

Case of planar graphs. Much more work was needed for the recognition of planar graphs with treebreadth one. Perhaps surprisingly, this part was arguably the most difficult one in our work on treebreadth.

The algorithm for planar graphs is recursive. Given $G = (V, E)$, we search for a specific vertex, called a *leaf-vertex*, whose closed neighborhood must be a leaf-bag of a star-decomposition if $tb(G) = 1$ (bag whose corresponding node in the tree has degree at most one). Basing on Lemma 56 and a delicate case-by-case analysis of the structure of star-decompositions, we define three types of leaf-vertices (*e.g.*, see Figure 3.10). A vertex v is a *leaf-vertex* if one of the following conditions hold.

Type 1. $N(v)$ induces an $a_v b_v$-path for some $a_v, b_v \in V \setminus \{v\}$, denoted by Π_v, of length at least 3 and there is $d_v \in V \setminus \{v\}$ such that $N(v) \subseteq N(d_v)$.

Type 2. $N(v)$ induces a path, denoted by $\Pi_v = (a_v, b_v, c_v)$, of length 2.

Type 3. $N(v)$ consists of two non adjacent vertices a_v and c_v, and there is $b_v \in (N(a_v) \cap N(c_v)) \setminus \{v\}$.

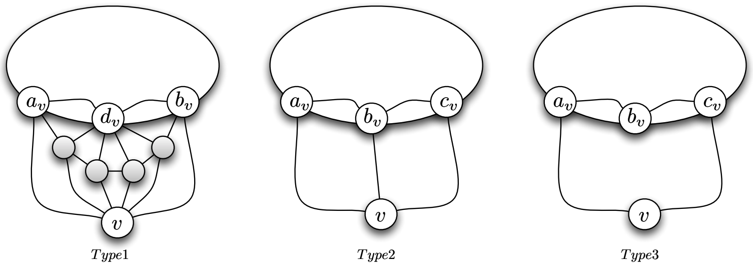


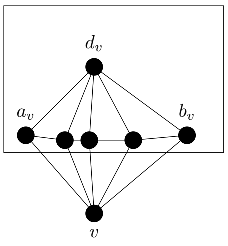
Figure 3.10: The three types of leaf vertices.

Ideally, we would like to remove v from G and apply recursively our algorithm on $G \setminus v$. However, in some case $tb(G \setminus v) = 1$ while $tb(G) > 1$ (see Fig. 3.9). So, we must also add edges between vertices that must be in a common bag of a star-decomposition of G if $tb(G) = 1$[5]. The choice of the edges to add is made more difficult by the need for the resulting graph G' to stay prime and planar in order to apply our algorithm recursively on G'. To show that $tb(G) = 1$ if and only if the resulting graph has treebreadth one also requires tedious lemmas.

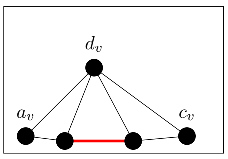
Sketch Proof of Theorem 53. Let $G = (V, E)$ be a prime planar graph. We can assume $|V| \geq 8$ and G has no star-decomposition with two bags (both cases are treated separately by exhaustive search). In such case, $tb(G) = 1$ implies there exists a leaf-vertex v, that can be found in linear time.

We first consider the case where $G \setminus v$ is prime. In this situation, we aim at removing v and applying the algorithm recursively on $G \setminus v$ (*e.g.*, see Figures 3.11a

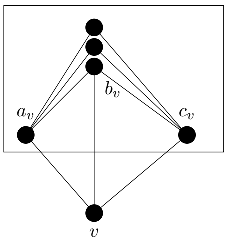
[5]We aim at turning the separator $N(v)$ into a clique. However, we cannot do that directly since it would break the distances in G, and the graph needs to stay planar.



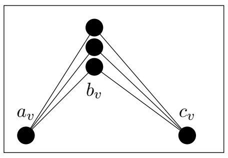
(a) v is of Type 1



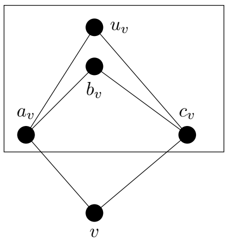
(b) G'



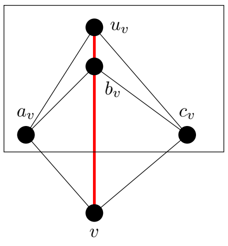
(c) $|(N(a_v) \cap N(c_v)) \setminus v| \geq 3$



(d) $G \setminus v$



(e) $(N(a_v) \cap N(c_v)) \setminus v = \{u_v, b_v\}$



(f) G'

Figure 3.11: Cases where $G \setminus v$ is prime. In every subcase, we apply the algorithm recursively on the graph to the right, that is either smaller or denser than G.

and 3.11b). However, we can do that only if it can be ensured that when $tb(G \setminus v) = 1$, there is a star-decomposition of the subgraph that can be transformed into a star-decomposition of G. Precisely, if v is of Type 1 then we seek for a star-decomposition $(T', \mathcal{X}')$ of $G \setminus v$ such that all the vertices in $N(v)$ are contained into a bag. If v is of Type 2 or 3 then we seek for a star-decomposition $(T', \mathcal{X}')$ of $G \setminus v$ such that either $T'_{a_v} \cap T'_{c_v} \neq \emptyset$, or there are two adjacent bags $B'_{a_v} \in T_{a_v}, B'_{c_v} \in T'_{c_v}$ that are respectively dominated by a_v and c_v. What we prove is that if $tb(G \setminus v) = 1$ and $G \setminus v$ is prime, then a star-decomposition as above always exists, unless we fall in the special case where v is of Type 2 or 3 and $|(N(a_v) \cap N(c_v)) \setminus v| \leq 2$. We do so by proving that it were not the case, there would exist a K_5-minor or a $K_{3,3}$-minor of G. By Kuratowski theorem, it would contradict our assumption that G is planar.

Furthermore, we prove for the latter subcase that a_v, c_v must have two common neighbours u_v, b_v in $G \setminus v$ (else, $tb(G) > 1$). In this situation, the graph G', obtained from G by adding the edges $\{v, u_v\}, \{v, b_v\}$, is planar and prime, and it satisfies $tb(G) = 1$ if and only if $tb(G') = 1$. See Figures 3.11e and 3.11f for an illustration.

So, we call the algorithm either on G' or on $G \setminus v$[6]. We refer to Figure 3.11 for an illustration.

We note that it is conceivable this first part of the analysis could apply to larger classes of H-minor free graphs. This is less clear for what follows.

Indeed, the most difficult situation is when $G \setminus v$ contains a clique-separator. Roughly, in this case we need to test the leaf-vertex v for certain properties. If it satisfies some of them then we can either remove vertices or add new edges in the graph and we call the algorithm recursively on the resulting graph G'. However, in some situations the leaf-vertex v does not satisfy *any* of the desired properties, and then we need to find a better leaf-vertex in its neighbourhood.

First, based on a fine-grained analysis of clique-separators in the subgraph $G \setminus v$, this case is reduced to the one where:

- v is of Type 2;
- there is an edge-separator (b_v, u_v) of $G \setminus v$;
- and $\{a_v, u_v\} \notin E$.

In this situation, our first idea was to add an edge between a_v and c_v in order to force these two vertices to be contained in a common bag in *any* star-decomposition of G', obtained from $G \setminus v$ by adding the edge $\{a_v, c_v\}$. Then, we aim at applying the algorithm recursively on G'. However, $tb(G') = 1$ does not imply $tb(G) = 1$ in general. We prove it is the case if u_v, c_v are nonadjacent or $N(u_v) \cap N(a_v)$ does not disconnect a_v from u_v in $G \setminus (c_v, v)$.

Else, we compute a plane embedding of G, and a vertex $x \in N(a_v) \cap N(u_v)$ such that: v, c_v and all other common neighbours of a_v, u_v are in a same region $\mathcal{R}$, bounded by (a_v, x, u_v, b_v). As illustrated with Figure 3.12, we wish to create an $a_v u_v$-path in $V \setminus \mathcal{R}$ by adding edges in $N(b_v) \cap N(x)$. In doing so, we go back to the previous subcase as now $N(a_v) \cap N(u_v)$ is no more a $a_v u_v$-separator of $G \setminus (c_v, v)$. However, we have to ensure that it is possible to add such a path in $V \setminus \mathcal{R}$, and that its addition does not affect the value of treebreadth for the graph. We prove it is the case unless $V \subseteq \mathcal{R}$ (in which case we apply the algorithm recursively on G', obtained from G by identifying b_v with x), or if there is a leaf-vertex $\ell \in N(b_v) \cap N(x)$. Furthermore, in the latter case we replace v with ℓ in the above analysis, *i.e.*, ℓ becomes the actual leaf-vertex to be considered. It can be shown that $G \setminus \ell$ is prime, so, we can prove that the algorithm always terminates.

Finally, we observe that in the above algorithm, we delete a vertex or add an edge before each recursive call. Moreover, the number of edges removed at each step can be linearly upper-bounded by the number of deleted vertices. Since planar graphs are sparse, we can elaborate on this property in order to upper-bound the number of recursive calls on n-vertex m-edge planar graphs by a linear function $\Theta(n) - m = \Theta(n)$. Each step of the algorithm can be done in linear time, so, altogether combined, it shows that the algorithm runs in quadratic time. $\square$

[6]When v is of Type 1 we call the algorithm on G', obtained from $G \setminus v$ by contracting the internal nodes of Π_v to an edge, in order to obtain a quadratic complexity. We refer to Figures 3.11c and 3.11f for an illustration of that case.

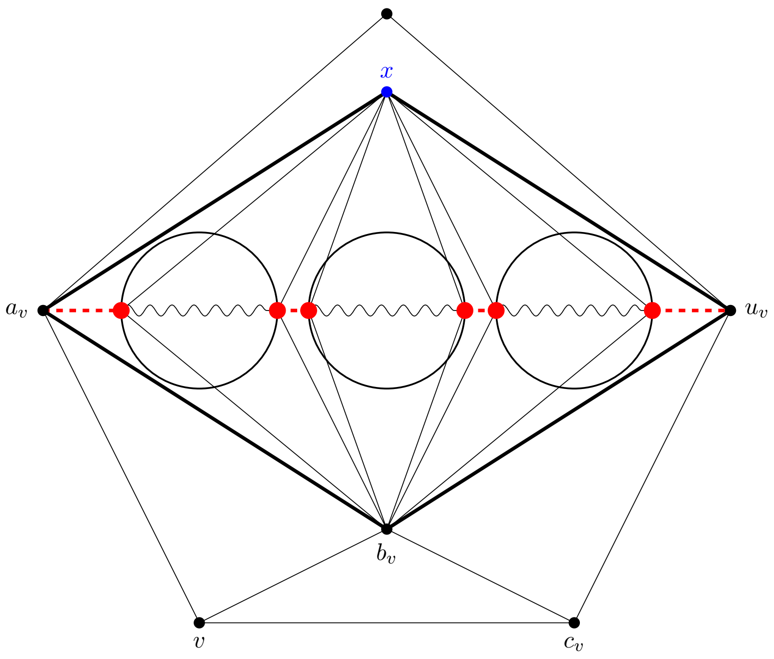


Figure 3.12: Addition of an a_vu_v-path in $V \setminus \mathcal{R}$. Each ball is a connected component of $G[V \setminus \mathcal{R}]$. The edges that are added in order to obtain the a_vu_v-path are drawn in dashed red.

3.4.3 Open problems and future work

We conclude this complexity study by some questions that remain open. First, it would be interesting to know the complexity of computing the treebreadth and the treelength of planar graphs. We did a first step in this direction with Theorem 53. Note that the complexity of computing the treewidth of planar graphs is still open. Second, all the reductions presented in this paper rely on constructions containing large clique or clique-minor. We left open the problem of recognizing graphs with treebreadth one in the class of graphs with bounded treewidth or bounded clique-number. More generally, is the problem of computing the treebreadth Fixed-Parameter Tractable when it is parameterized by the treewidth or by the size of a largest clique-minor? It is part of my ongoing work to answer these questions.

Last, I point out that in this work on star-decompositions, one important tool has been "breadth-maximal" triangulations. Precisely, for any G with $tb(G) = 1$, we call a triangulation H of G breadth-maximal if it has a clique-tree that is a star-decomposition of G and H is edge-maximal w.r.t. this property. Breadth-maximal triangulations have many nice properties which greatly simplify the analysis for the hardness reduction and the polynomial-time algorithms. So, I think this notion of "maximal" triangulation is worth being more investigated in the future, as well as for treebreadth as for treelength, treewidth, etc. The reader may refer to [BK06, BHV06] for related work, where they give sufficient conditions for edges to be always present in a triangulation of minimum width.

3.5 Treewidth versus treelength!

Finally, I present in this section new relationships between treewidth and treelength, that were obtained in collaboration with David Coudert and Nicolas Nisse. On the algorithmic side, we aim at finding such relationships in order to combine the best of both worlds (structural and metric tree-likeness in graphs).

That is, on the one hand treelength and treewidth are both NP-hard to compute [ACP87, Lok10], however treelength is much easier to approximate than treewidth. In particular, there exists a 3-approximation algorithm for computing treelength that only relies on a few breadth-first search [DG07]. In contrast, under the SMALL SET EXPANSION Hypothesis (that implies the UNIQUE GAMES CONJECTURE) there does not exist a constant-factor polynomial-time approximation algorithm for treewidth [APW12]. On the other hand, there are more algorithmic applications for treewidth than for treelength [Cou90], which comes from the fact that several hard problems on graphs remain so even on bounded diameter graphs, thereby preventing the design of dynamic programming algorithms on tree decompositions with bounded length. Thus, by using relationships between treelength and treewidth, we wish to extend the algorithmic applications for bounded treewidth graphs to a large class of bounded treelength graphs. Furthermore, we also wish to compute efficiently (and practically) tree decompositions with bounded width on certain graph classes.

3.5.1 State of the art

As said earlier (*e.g.*, Sec. 3.2.1) the two parameters treewidth and treelength are uncomparable on general graphs. This fact prevents us from expecting simple relations between them.

On the one direction, the cycles have bounded treewidth but unbounded treelength. This suggests that having a large treelength relies on the existence of long cycles in the graph. The authors in [DG07] supported this intuition, proving that the treelength of a graph G is upper-bounded by half of the maximum length of a chordless cycle in G (the latter generalizes a similar Theorem 15 on the relationship between chordality and hyperbolicity). However, not all bounded treelength graphs have bounded chordality, as seen with the case of the wheel W_n which contains an induced C_n while it has treelength ≤ 2. Therefore, it is natural to constrain ourselves to the subcase of *isometric* cycles in graphs. We remind that a subgraph H of G is isometric if for any two vertices of H, the distance between them is the same in H as in G. Unfortunately, there are graphs such as grids with bounded-length isometric cycles and arbitrarily large treelength. As shown below, our results imply that in such a case, we always have that $tl(G) = \mathcal{O}(tw(G))$.

On the other direction, the complete graphs have unbounded treewidth but bounded treelength. Another interesting example is the graph H obtained by adding a universal vertex to a square-grid with n^2 vertices, for which it holds $tw(H) = n+1$ and $tl(H) = 2$. We observed in Section 3.2.1 that more generally, adding a universal vertex to a graph G with arbitrarily large treewidth k will result in a graph G' with large treewidth $k+1$ and treelength at most two. One common trait of these graphs is that they have a large *genus* (they cannot be drawn with no edge-crossings onto a surface with small oriented Euler genus). That is, they are in a sense arbitrarily far from planar graphs. In contrast, it has been proved in [DG09] that $tw(G) < 12 \cdot tl(G)$ for planar graphs. Consequently, it is quite natural to ask whether a treewidth arbitrarily larger than treelength requires a large genus. In what follows, we will prove it is the case, *i.e.*, $tw(G) = \mathcal{O}(tl(G))$ for bounded-genus graphs.

Finally, and independently from this work, Belmonte et al. [BFGR15] proved that $tw(G) = \mathcal{O}(\Delta^{tl(G)})$ for any graph G with *maximum degree* Δ. On the algorithmic point of view, the authors in [BFGR15] built upon their relation in order to design a fixed-parameter-tractable algorithm to compute the metric dimension on bounded treelength graphs.

This upper-bound shows that in a way, our pathological construction which adds a universal vertex in the graph is the only one that prevents from comparing treewidth with treelength. However, it has to be noted that on the converse direction, treelength *cannot* be upper-bounded by any function $f(tw(G), \Delta)$ of the treewidth and the maximum degree, as it can be observed with cycles.

In this section, I will use different techniques in order to upper-bound the treewidth with linear dependency on the treelength.

3.5.2 Contributions: upper and lower bounds for treewidth by using treelength

3.5.2.1 Lower bound

The first result in this section is that treewidth can be lower-bounded by treelength on certain graph classes.

In what follows, a *distance-preserving elimination ordering* of $G = (V, E)$ is a total ordering of its vertex-set V such that every suffix induces an isometric subgraph of G. In particular, it is a *dismantlable ordering* if for every suffix, the closed neighbourhood of the starting vertex is dominated in the subgraph that is induced by this suffix. The latter type of ordering has been introduced in the previous chapter (Definition 7, p. 33). We also refer to the previous chapter for a definition of hyperbolicity, and especially Definition 1 (p. 25).

Theorem 57 ([CDN16]). *For every $G = (V, E)$ we have $tl(G) \leq c \cdot tw(G)$ where:*

- $c \leq \lfloor \ell(G)/2 \rfloor$ *if G has no isometric cycle of length greater than $\ell(G)$;*
- $c \leq 2\delta(G) + 1$ *with $\delta(G)$ being the hyperbolicity of G;*
- $c \leq 2$ *if G admits a distance-preserving elimination ordering.*
- $c \leq 1$ *if G admits a dismantlable ordering.*

Sharper estimates of the constant c will be discussed in what follows. One interesting consequence of this result is that every bounded-treewidth graph G can be embedded into a tree with additive distortion $\Theta(\delta(G))$. Furthermore, it tells us that the hyperbolicity is upper-bounded by the treewidth on graph classes with a dismantlable ordering. These remarks complement Section 2.4.1 in the previous chapter on graph hyperbolicity.

3.5.2.2 Upper bound

On the other hand, treewidth can be upper-bounded by treelength on certain topological graph classes.

Let us introduce the terminology for those classes. We refer to [MT01] for details. We recall that a planar graph is a graph that can be drawn in the Euclidean plane so that edges may only intersect at their endpoints. More generally, a graph has *genus* at most g if it can be drawn in an oriented surface with Euler genus g so that edges may only intersect at their endpoints. Planar graphs are exactly the null-genus graphs. An *apex graph* is obtained from a planar graph by adding a new vertex with arbitrary neighbourhood. Finally, a class of graphs is *apex-minor free* if there is no graph in the class with a H-minor for some fixed apex graph H. Planar graphs and bounded-genus graphs are apex-minor free.

Theorem 58 ([CDN16]). *Let H be an apex graph. There exists a constant c_H that only depends on H and such that for every H-minor free graph G, we have $tw(G) \leq c_H \cdot tl(G)$.*

In particular if G has genus at most g then $tw(G) \leq 72\sqrt{2}(g+1)^{3/2} \cdot tl(G) + \mathcal{O}(g^2)$.

One unexpected consequence of this above result is that on some cases where the treewidth can be efficiently approximated, nontrivial bounds on the genus of the graph can be computed. The exact and approximate computation of graph genus are notoriously hard problems [Tho89, CKK97, KS15].

Our study paves the way to a better understanding on the relationship between structural and metric tree-likeness in graphs, and on its algorithmic consequences. Unfortunately, similar relationships for *path-likeness* in graphs look more challenging to obtain, even for trees. In particular, there are n-node trees with pathlength $\Omega(n)$ [DG07] whereas the pathwidth of an n-node tree is $\mathcal{O}(\log n)$ [Sch92].

So far, the main drawback of Theorem 58 is that it is non *constructive*. That is, when we compute a tree decomposition with bounded length $\mathcal{O}(tl(G))$, we obtain a bound on the treewidth $tw(G) = \mathcal{O}(tl(G))$, but we do not obtain a tree decomposition with bounded *width* $\mathcal{O}(tl(G))$. It is part of my ongoing work to make Theorem 58 constructive, possibly by using the graph minor decomposition from Robertson and Seymour [GKR13, DH04].

3.5.3 Proving the bounds

3.5.3.1 A detour through the diameter of minimal separators in graphs

We recall that there always exists a minimal tree decomposition (clique-tree of some minimal triangulation) with optimal width. See Section 3.2.2. Our results in what follows provide a relationship between the width and the length in any minimal tree decomposition.

More precisely, by Theorem 42, a corresponding minimal triangulation results from the completion of all sets in a maximal family of pairwise parallel minimal separators of the graph G. In this situation, we observe that for every edge in the triangulation, either it is an edge of G or its two ends are in a same separator in the family. Note that in the latter case, the distance in G between the two ends is at most the maximum diameter in the graph over the separators in the family. Therefore, we observe that the length of the tree decomposition ($\geq tl(G)$) is exactly the maximum diameter in the graph over the separators in the family. Furthermore, since each minimal separator of the family induces a clique in the triangulation, it has size upper-bounded by the width of the tree decomposition — that is $tw(G)$ for a minimal tree decomposition with optimal width.

As a result, we are left to upper-bound the diameter of minimal separators in graphs as a function of their size.

Connectivity properties of the minimal separators. Before going into the details of the proof, let us describe the main intuition behind it and the difficulties we had to face on. Let us consider a minimal separator S for G. If it is connected, then it has diameter $\mathcal{O}(|S|)$, and so, we are done. Hence, we may assume that S consists of several connected components. The idea is to find a set of isometric cycles, each of length at most $\ell(G)$ (by definition of $\ell(G)$), such that any of these cycles intersects two components and the subgraph induced by S and these cycles is connected.

For this purpose, let us consider a minimum-length cycle crossing two components of S (such a cycle surely exists because there are at least two full components in $G \setminus S$). If this cycle is isometric, then we are done. Otherwise, it means that there is a shortcut between two nodes of the cycle. However, this shortcut could intersect S more than once which does not help our purpose.

The key point is that, using the shortcut, the initial cycle can be viewed as the sum (symmetric difference) of two smaller cycles. This kind of local view can be generalized to a global one using our main tool, namely the cycle basis (defined below). Indeed, the initial cycle is actually the symmetric difference of a set of isometric cycles [Hor87]. Using this set, we can then prove our upper bound on the diameter of minimal separators in graphs.

The set $\mathcal{C}(G)$ of Eulerian subgraphs of G is called the *cycle space* of G. It is well-known that every Eulerian subgraph can be obtained from the symmetric difference (on the edges) of cycles in G. In fact, the set $\mathcal{C}(G)$ with the symmetric difference is a vector space of dimension $m - n + 1$ if G is connected [Die10, Theorem 1.9.6]. We will call the symmetric difference of two subgraphs H_1, H_2, denoted $H_1 \oplus H_2$, the *sum* of H_1 with H_2. A cycle basis is an inclusion wise minimal set of cycles generating the whole cycle space

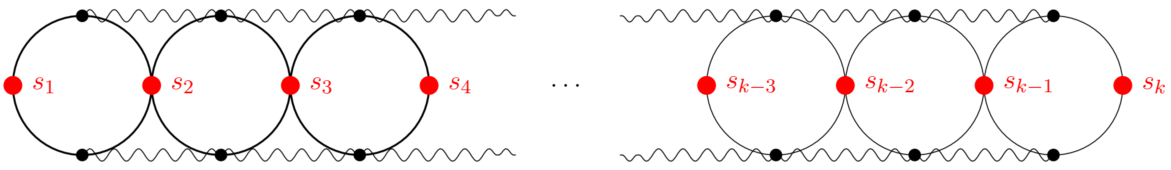


Figure 3.13: A minimal k-separator S for $G \in \mathcal{G}_\ell$ with diameter $\lfloor \ell/2 \rfloor \cdot (k-1)$. Vertices in S are ordered so that any two consecutive vertices s_i and s_{i+1} are diametrically opposed in an isometric cycle of length ℓ. Furthermore, the removal of S disconnects G in two parts, respectively containing the upper and lower sections of these cycles.

The use of the cycle space. For every $\ell \geq 3$, a graph G belongs to the class $\mathcal{G}_\ell$ if any of its cycles can be obtained from the symmetric difference on the edges of cycles of length at most ℓ. More formally, its cycle space admits a cycle basis with only cycles of length at most ℓ. As an example, by Mac Lane's Theorem the inner faces of a plane graph generate its cycle space, and so, a planar graph with inner faces of length at most ℓ is in $\mathcal{G}_\ell$. Furthermore, trees are a trivial example of graphs in $\mathcal{G}_3$ (they have no cycle). Chordal graphs are also in $\mathcal{G}_3$. More generally, every ℓ-chordal graph is in the class $\mathcal{G}_\ell$. Indeed, every chord in a cycle C can be used in order to write C as the sum of two smaller cycles, thereby proving that the induced cycles in a graph can generate its cycle space.

In [CDN16], we prove that $\mathcal{G}_\ell$ is stable under edge-contraction and addition of an edge between two vertices that are at distance at most $\lfloor \ell/2 \rfloor$. The dimension of the cycle space plays an important role in these proofs, as it often provides elegant shortenings of our technical reasonings. In order to illustrate the techniques we used, we prove below the stability of $\mathcal{G}_\ell$ under edge-contractions.

Lemma 59. *Let $\ell \geq 3$, the class $\mathcal{G}_\ell$ is stable under edge-contraction.*

Proof. Let $G \in \mathcal{G}_\ell$ with n vertices and m edges. W.l.o.g., G is connected. The dimension $dim(\mathcal{C}(G))$ of the cycle space $\mathcal{C}(G)$ is $s = m-n+1$ [Die10, Theorem 1.9.6]. Let $e \in E(G)$ such that e lies on $k \geq 0$ triangles in G. By contracting e, we loose one vertex and $k+1$ edges, the edge e and for each triangle which contains e we have to remove one of the resulting multi-edges. Hence, $dim(\mathcal{C}(G/e)) = dim(\mathcal{C}(G)) - k$. Let $\{C_1 \cdots, C_s\}$ be a basis of $\mathcal{C}(G)$ such that each C_i has length at most ℓ. Let $\{C_1', \cdots, C_t'\}$ be the set of cycles in G/e which are obtained by contracting e on each C_i and by removing triangles that contain e from the list. Then, $t \geq dim(\mathcal{C}(G/e)) = s-k$ (since at most k triangles have been removed) and each C_i' has length at most ℓ. We show that $C_1', \cdots, C_t'$ are linearly independent in $\mathcal{C}(G/e)$, which proves that they form a basis of $\mathcal{C}(G/e)$. For purpose of contradiction, let us assume that $C_{i_1}' \oplus \cdots \oplus C_{i_r}' = 0_{G/e}$ for $1 \leq i_1 < \cdots < i_r \leq s$ and $r > 0$, with $0_{G/e}$ being the trivial Eulerian subgraph of G/e with no edges (*a.k.a.*, the neutral element of the cycle space). Then $C_{i_1} \oplus \cdots \oplus C_{i_r}$ is either 0_G or e, with 0_G being the trivial Eulerian subgraph of G with no edges. Therefore, the sum equals e since the C_{i_j}'s are linearly independent in $\mathcal{C}(G)$. This is a contradiction as $(V(G), \{e\})$ is not Eulerian. Hence, since all cycles in the basis $\{C'_1, \cdots, C'_t\}$ have length at most ℓ, it implies that $G/e \in \mathcal{G}_\ell$. □

Furthermore, by combining these two above properties (stability under contraction or addition of some edges), we obtain in our paper [CDN16] the following lemma:

Lemma 60. *For every $G \in \mathcal{G}_\ell$, any minimal separator S for G induces a connected subset in its power $G^{\lfloor \ell/2 \rfloor}$. In particular, the diameter of S in G is at most $\lfloor \ell/2 \rfloor \cdot (|S| - 1)$.*

Proof. By contradiction, let $G \in \mathcal{G}_\ell$, and let S be a minimal separator in G that does not satisfy the property. We first make adjacent every two vertices in S that are at distance at most $\lfloor \ell/2 \rfloor$ in G. We claim that the resulting graph still belongs to $\mathcal{G}_\ell$. Indeed, we proved in [CDN16] that $\mathcal{G}_\ell$ is stable under addition of an edge between two vertices that are at distance at most $\lfloor \ell/2 \rfloor$. Furthermore, adding an edge cannot make the distances increase in the graph, so, we can use this stability result for every edge added by the construction. Consequently, the resulting graph is still in $\mathcal{G}_\ell$. Finally, we contract each connected component of the subgraph induced by S in a single node, thus contracting S to obtain a stable set S', and since $\mathcal{G}_\ell$ is proved to be stable under edge-contractions in Lemma 59, the resulting graph G' still belongs to the class. Furthermore, the stable set S' is a minimal separator in G' by construction. Since S does not satisfy the property of the theorem, we have that all nodes in S' are pairwise at distance at least $\lfloor l/2 \rfloor + 1$ in G'. However, we proved in [CDN16, Lemma 3.3] that for every graph in $\mathcal{G}_\ell$, minimal separators are either cut-vertices or they contain two distinct vertices at distance at most $\lfloor \ell/2 \rfloor$. In particular, since the vertices in S' are pairwise at distance at least $\lfloor l/2 \rfloor + 1$ in G' by construction, it contradicts that $G' \in \mathcal{G}_\ell$. □

The above result improves upon [ASM16] and [DM15]. It is sharp, in the sense that for every size k and for every $\ell \geq 3$, there exists a graph $G \in \mathcal{G}_\ell$ with a minimal separator of size k and diameter $\lfloor \ell/2 \rfloor \cdot (k-1)$ (*e.g.*, see Figure 3.13).

Finally, Theorem 57 follows from our additional proofs in [CDN16] that all graphs with isometric cycles of length at most ℓ belong to the class $\mathcal{G}_\ell$, and in the same way all δ-hyperbolic graphs belong to $\mathcal{G}_{4\delta+3}$, all graphs with a distance-preserving ordering (resp., with a dismantling ordering) belong to $\mathcal{G}_4$ (resp., to $\mathcal{G}_3$).

Discussion. The main idea in this section is that for every G, $tl(G) \leq j \cdot tw(G)$, with j being the minimum index such that all minimal separators for G induce connected subsets in its power G^j. This index satisfies $j \leq \lfloor \ell/2 \rfloor$ for the graphs in $\mathcal{G}_\ell$. In particular, the minimal separators for a graph $G \in \mathcal{G}_3$ induce connected subsets of G, but not all graphs with this property belong to $\mathcal{G}_3$ [DLVM86]. The latter result raises the following open question: does there exist a universal constant ℓ such that the class $\mathcal{G}_\ell$ contains all graphs with connected minimal separators ?

3.5.3.2 Using the bidimensionality theory

For the upper bound, we sketch our approach and its limitations. First we observe that treelength and treewidth are stable under edge-contractions. The *bidimensionality theory* [DH08] offers meta-theorems which, for maximization problems whose solutions cannot increase under edge-contractions[7], are the cornerstone of FPT algorithms with *subexponential dependency* on the treewidth. On the theoretical point of view, these meta-theorems are based on the property that a graph with large treewidth can be edge-contracted to either a large complete graph or a large grid-like minor. The latter result is a refinement of the well-known Excluded Grid Minor Theorem from Robertson and Seymour [RST94].

We will use the same tools for proving our result on the relationship between treelength and treewidth on bounded genus graphs. Precisely, we seek for a subclass of graphs where this large obstruction to treewidth can also be shown to have a large treelength, that will imply the desired upper-bound.

Discarding complete graphs. Complete graphs are the classical examples of graphs with unbounded treewidth but bounded treelength. So, in order to get rid of this first obstruction, it is natural to constrain ourselves to H-minor free graphs, for some fixed graph H. Unfortunately, this is still not enough. Indeed, Fomin et al. proved in [FGT11] that for every fixed H, an H-minor free graph with large treewidth can be contracted either to some canonical partial triangulation of a large square grid[8], or to the same graph augmented with a universal vertex. We illustrate these two cases with Figure 3.14. In the latter case, the obstruction has unbounded treewidth and bounded treelength, which does not help our purposes.

Discarding grid-like obstructions with a universal vertex. The key observation is that this augmented partial triangulation of the grid (Figure 3.14b) is an *apex graph*. We recall that every planar graph is the minor of a grid with large enough dimensions [RS84]. Therefore, in the special case where H is a fixed apex-graph, Fomin et al. were able to refine their results. Precisely, they proved in [FGT11] that every apex-minor free graph with large treewidth can be contracted to the partial planar triangulation of a large grid, that is depicted in Figure 3.14a.

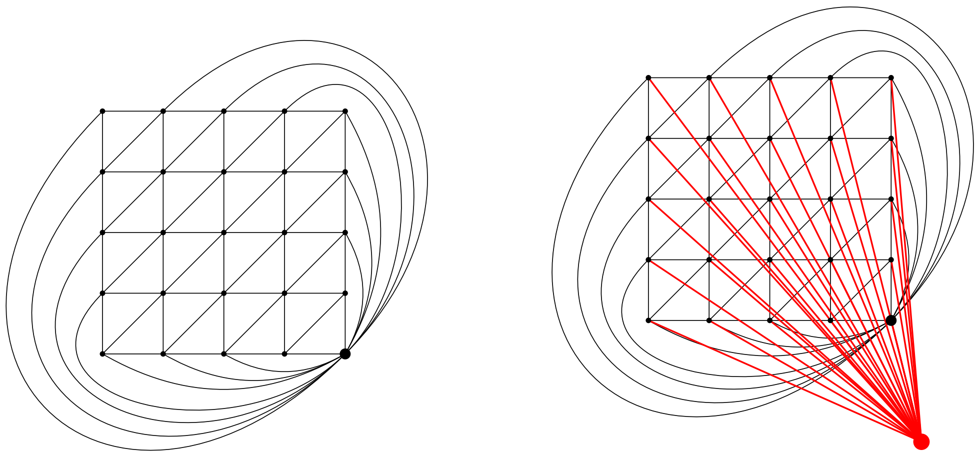
Our contributions in [CDN16] is to prove that any such a partial triangulation must have a large treelength. We do so by adapting some of the lower-bound techniques for the treelength of grids in [DG07].

Lemma 61 ([CDN16]). *Let G be a partially triangulated $(r \times r)$-grid, then $tl(G) \geq \lfloor r/3 \rfloor - 1$.*

Proof. The result holds if $r \leq 3$ because in such a case $tl(G) \geq 1 \geq \lfloor r/3 \rfloor - 1$. Else, let G' be the $(r \times r)$-grid from which G is obtained by planar triangulation.

[7]Some results also have been obtained under different stability assumptions.

[8]A triangulation of a planar graph is a planar supergraph where all the faces are triangles. Despite they share the same terminology, planar triangulations should not be confused with the triangulations from Section 3.2.2 (chordal supergraphs).


(a) Canonical partial triangulation of a grid.

(b) Triangulation augmented with one universal vertex.

Figure 3.14: Contraction obstructions to bounded treewidth.

Let V' be the set of vertices that are at distance at least $\left\lfloor \frac{r-1}{3} \right\rfloor$ from the external face of G'. The vertices of V' induce a partially triangulated $(r' \times r')$-grid F in G, $r = 2\left\lfloor \frac{r-1}{3} \right\rfloor + r'$, such that the external face has not been triangulated. Moreover, F is isometric in G. Hence, $tl(G) \geq tl(F)$. We show that $tl(F) \geq \lfloor r/3 \rfloor - 1$.

Our proof adapts from the lower-bound techniques in [DG07, Sec. 2.3]. Let $(T, \mathcal{X})$ be any tree-decomposition of F. Consider the two subsets of vertices A, B that contain the first and the last row of F respectively. Since A induces a connected subgraph of F, by the properties of tree decompositions the bags in $\mathcal{X}$ that intersect A form a subtree T_A of T. Similarly, the bags in $\mathcal{X}$ that intersect B form a subtree T_B of T. Furthermore, either $T_A \cap T_B \neq \emptyset$ (in which case, the diameter of every bag in $T_A \cap T_B$ is at least $r'-1$), or by [DG07, Lemma 5] there exists a bag which intersects all paths between A and B in F. In the latter case, such bag must intersect the first and last column of F, and so, it has diameter at least $r'-1$. Therefore, $(T, \mathcal{X})$ has length at least $r'-1$ in both cases, that proves that $tl(F) \geq r'-1 \geq \lfloor r/3 \rfloor - 1$. □

Theorem 58 now follows.

We note that in [Epp00], Eppstein has proved that the apex-minor free graphs are exactly the minor-closed families of graphs with treewidth upper-bounded by a function of their diameter. Since treelength is upper-bounded by the diameter, our result can be seen as a strict generalization of his.

3.6 Conclusion

I have been mainly interested in characterizing the complexity of computing tree decompositions with metric constraints on their bags. On the parameterized point of view, my results suggest that the hard instances for this family of problems are graphs with a large clique-number or a large Hadwiger number (size of a largest clique-minor). I insisted on this aspect when I discussed on the complexity of computing the clique-decomposition in Section 3.3. Other examples from metric graph properties studied in the literature support this observation. As an example, under the STRONG EXPONENTIAL TIME Hypothesis the diameter of a graph cannot be computed in truly subquadratic time (see also Section 2.6.3). Hard instances for the diameter computation problem are *split graphs*, *a.k.a.* graphs who vertex-set can be bipartitioned into a clique and an independent set [BCH16].

Intuitively, the existence of a large clique makes the diameter lower in the graph, with a shortest-path between most pairs of vertices passing by the clique. In a way, it thus forces the distance distribution in the graph to be very simple. But at the same time, it gives a larger degree of freedom on the adjacency relations for the vertices out of the clique, in the sense that the edges incident to these vertices shall not affect too much the distances in the graph. Since tree decompositions must span the edge-set of the graph, it may be the case that complicated adjacency relationships for the peripheral vertices render their computation intractable.

This above intuition has guided the hardness reductions in [DLN16a, DC17]. Hence, all the graphs resulting from the hardness reductions for treebreadth, pathlength and pathbreadth have a large clique-number or Hadwiger number. The graphs resulting from the hardness reduction for treelength also satisfy this property [Lok10]. What remains to explore in more details is whether large cliques and clique-minors represent the only obstructions for an efficient computation of these above parameters. Throughout my work, partial results have been obtained in this direction. In particular, planar graphs and bipartite graphs with treebreadth one can be recognized in polynomial time. I conjecture that more generally, graphs of treebreadth one with bounded *clique-number* can be recognized in polynomial time.

However, the above example of bipartite graphs shows that a similar conjecture does not hold true for the more general problem of computing the treebreadth. Indeed, we prove in [DLN16a] that the NP-complete problem of recognizing general graphs with treebreadth one can be reduced to the problem of recognizing bipartite graphs with treebreadth at most two. The latter result suggests that the existence of a large clique-*minor* suffices to render the problem intractable.

Planar graphs are K_5-minor free, and we are currently exploring whether computing the treelength is fixed-parameter-tractable on this class of graphs. Precisely, we are investigating whether we can adapt the algorithm from Bodlaender and Kloks [BK96] to our needs. This work has been started recently during the internship of Simon Nivelle with Nicolas Nisse. I conjecture that computing the treelength of a graph G is FPT when it is parameterized by $tl(G) + tw(G)$. Moreover, it is my opinion that we may be helped in proving this with the relationships between treelength and treewidth in Section 3.5. Similar ideas can be found in [DFG11]. However, I conjecture that the problem of computing the treelength remains NP-complete on planar graphs. This conjecture is motivated by a hardness result on the problem of deciding on the existence of tree t-spanners in these graphs [FK01]. Proving or disproving this conjecture would make advance our understanding on the structure of bounded treelength graphs.

Part II

Privacy at large scale in social graphs

Unlike the previous part, the focus in the next two chapters is on *dynamic* processes on networks. The rules of these dynamics cause certain paths between the vertices to appear or to disappear, hence they impact on the information propagation in the graph. Our general purpose is to predict the outcome of these dynamics.

- Chapter 4 presents new results on the computation of equilibria for a large family of graphical games, that are exemplified by **coloring games**. Note that equilibria for these games have been proposed in [KL13] as a solution concept for the dynamics of communities in social graphs.
- Chapter 5 introduces a new model in order to detect the **targeting** of (potentially sensitive) data by an online advertiser, and to learn which data causes the reception of a given ad. Targeting can be regarded as a dynamic process on an “adgraph” [AMM10]: built from the data inputs and the ad allocation protocols.

Chapter 4

The computation of equilibria in coloring games

Summary

We establish new complexity results for computing k-strong Nash equilibria in coloring games. These results are partly generalized to some other graphical games.

In Section 4.3, we prove that for every fixed $k \geq 1$, it can be computed a k-strong Nash equilibrium for every coloring game with a better-response dynamic. We give the exact worst-case (polynomial) time of convergence for $k \leq 2$, that we prove through an original connection between the executions of the better-response dynamics and the chains (directed paths) in a DAG called the *Dominance lattice*. However, for every $k \geq 4$, we prove that the better-response dynamic converges in *superpolynomial* time in the worst-case. The latter result disproves a conjecture from [KL13, EGM12] that for every $k \geq 1$, this dynamic converges in polynomial time.

Then, in Section 4.4, we establish new results on the parallel and space complexity of computing a Nash equilibrium in coloring games. Precisely, we prove that this problem (that is polynomial-time solvable) is PTIME-hard under NC-reductions. This is hint that computing a Nash equilibrium in these games is a problem inherently sequential, that cannot be solved within limited (logarithmic) workspace, neither with an “efficient” distributed algorithm: with low local computational time and communication complexity.

In Section 4.5, we put the focus on a generalization of coloring games to edge-weighted graphs, sometimes called the additively separable symmetric Hedonic games. We give sufficient conditions for these games to admit a k-strong Nash equilibrium. Then, we prove that for every $k \geq 2$, and for every fixed set of edge-weights $\mathcal{W}$, the following dichotomy results holds true: either all the games played on a graph with edge-weights in $\mathcal{W}$ admit a k-strong Nash equilibrium, or the corresponding decision problem is NP-complete.

Finally, a broader set of graphical games, generalizing coloring games in their own way, is introduced in Section 4.6. For each of those, we discuss on the extent to which our results for coloring games still apply.

My papers on coloring games and their generalizations [DMC12, DMC13a, DMC17, Duc16] are collected in the appendix.

Contents

4.1 Introduction

In this chapter, we aim at better understanding how the rules of the dynamics affect the *privacy* of the users'information in social graphs, that is defined in [EDP] as "*a right which prevents public authorities from measures which are [invasive for the respect of private life], unless certain conditions have been met.*" Formal definitions of this notion of privacy, in game-theoretic terms, can be found, *e.g.*, in [Dwo08]. Note that if we consider a communication network such as a social graph, private information flows through the edges of the graphs. Hence, one important aspect in the study of privacy in these networks can be informally summarized at detecting where the information can be accessed to in the graph over time. As a partial answer to this question, we will study *coloring games* on graphs in this chapter.

Precisely, our aim is to compute equilibria for those games, that have been proposed in [KL13] as a solution concept for the outcome of the communities formation process in social networks. Coloring games and some basic definitions for this chapter will be presented in Section 4.1.1. Then, the content of this chapter will be described in Section 4.1.2. In particular, in what follows, full definitions are given in Section 4.2, while the technical sections range from Sections 4.3 to 4.6.

4.1.1 Presentation of coloring games

A coloring game is played on an undirected graph with each vertex being an agent (formal definitions will be restated with details in Section 4.2). Agents must choose a color in order to construct a proper coloring of the graph, and the individual goal of each agent is to maximize the number of agents with the same color as hers. On a more theoretical side, coloring games have been introduced in [PS08] as a game-theoretic setting for studying the chromatic number in graphs. Precisely, the authors in [PS08] have shown that for every coloring game, there exists a Nash equilibrium where the number of colors is exactly the chromatic number of the graph. Since then, these games have been rediscovered many times, attracting attention on the way in the study of information sharing and propagation in graphs [CKPS10, EGM12, KL13].

4.1.1.1 Some applications of coloring games

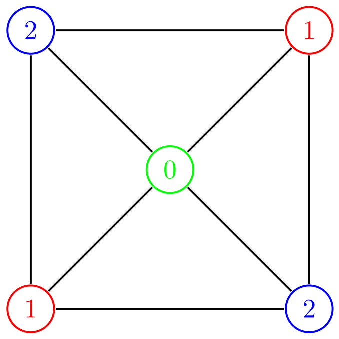
Distributed coloring in graphs. In particular, the authors in [CKPS10] base on coloring games in order to design distributed algorithms for coloring a graph, with applications to the frequency assignment problem and the design of sleep/awake protocols in Wireless Sensor Networks. The latter protocols are the cornerstone of energy saving methods in these networks, and they also serve as a routine for securing group communications.

Later on, in part motivated by the above applications, the authors in [MW13] presented a unifying framework for the so-called "distributed" welfare games. The goal with these games is to encode the solutions of a distributed resource allocation problem as the Nash equilibria of a given graph game. They are specified by assigning each agent an admissible utility function to optimize. Coloring games have been shown to fit in this generic framework.

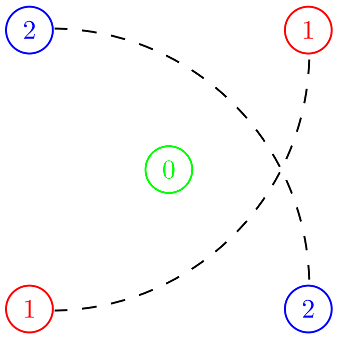
Modeling of community formation in social networks. More recently, coloring games have been proposed in order to model community formation in social networks [KL13]. Indeed, let us assume that each community results from a group of users sharing about some information topic. Let us also assume for simplicity that each user shares about a given topic in only one community[1]. Therefore, given a *fixed* topic, communities partition the users. The dynamics of these communities is modeled with a coloring game, that is played on a "conflict graph" where each edge represents a conflicting opinion between two users.

[1]Note that by doing so, existing correlations between communities that are related to different topics are neglected [KBSP16].

This representation may be confusing because the communities are densely connected subsets in the social graph, whereas here in the coloring game they correspond to color classes, and so, to independent sets of the conflict graph. In this context, it may be more natural to define the game on the *complement* of the conflict graph: agents must construct a clique partition of this graph, and the individual goal of each agent is to maximize the size of her clique (see Figure 4.1 for an illustration).



(a) A coloring game played on a graph G. Agent are labeled with their colour.



(b) The corresponding clique partition in the complement of G.

Figure 4.1: Dual representations for coloring games.

Generalizations of coloring games have been proposed in the literature [ABK$^+$16, BZ03, MW13]. In this chapter, we are particularly interested in a subclass of Hedonic games [Bal04], sometimes called the additively separable symmetric Hedonic games [BZ03]. We will call them *generalized coloring games* because, as shown below, they are a proper extension of the classical coloring games. A generalized coloring game is played on an *edge-weighted* graph, with each vertex being an agent. As before agents must choose a color, and the individual goal of each agent is now to maximize the sum of the weights of the edges that are incident to herself and to another agent with the same color as her.

Formally, let $G = (V, E, w)$ be an edge-weighted graph with $w : E \to \mathbb{Q} \cup \{-\infty\}$ be its weight function. A coloring $c : V \to \mathbb{N}$ of G is a partition of its vertex-set with each class (or group) being assigned a distinct integer, and for every vertex $v \in V$ we denote by $c(v)$ the integer corresponding to her group, also known as her color. Then, in the generalized coloring game that is played on G, the vertices of G are the agents of the game, and the strategy of an agent is her color. Every agent $v \in V$ aims at maximizing her utility function $\sum_{u \in N_G(v) | c(u) = c(v)} w_{uv}$. We refer to Figure 4.2 for an illustration.

Note that every coloring game that is played on an unweighted graph G^- can be transformed into a generalized coloring game, by creating an edge-weighted complete graph with vertex-set $V(G^-)$ where the edges of G^- have weight $-\infty$ and the nonedges of G^- have unit weight.

$\Longrightarrow$ From now on, we will assume the classical coloring games to be defined this way, and all the definitions will be directly given for generalized coloring games.

4.1.2 Contributions

Our main purpose is to characterize the complexity of computing stable partitions for generalized coloring games. Those are configurations where no small subset of agents have an incentive to change their current strategy for the same new color. On a social network point of view, stable partitions ensure that no small coalition of users have an incentive to leave their current community for another one, thus preventing information leakage from a community to another.

More precisely, we carefully control the maximum size k of such a subset, and we aim at computing k-stable partitions, *a.k.a.* configurations of the game where no k-subset of agents have an incentive to deviate from their current strategy (*e.g.*, see Figure 4.3 for an illustration). Note that 1-stable partitions are exactly the Nash equilibria of the game.

Formally, for any $G = (V, E, w)$ and $c : V \to \mathbb{N}$, a k-deviation w.r.t. c is any subset $S \subseteq V$ with $|S| \leq k$ that satisfies the following property: there exists some color $i \in \mathbb{N}$ so that, for every $v \in S$, we have $c(v) \neq i$ and:

$$\sum_{u \in N_G(v) | c(u) = c(v)} w_{uv} < \sum_{u \in N_G(v) | u \in S} w_{uv} + \sum_{u \in N_G(v) | c(u) = i} w_{uv}.$$

The coloring c represents a k-stable partition if there is no k-deviation w.r.t. c[2].

We now describe our contributions in more details. Positive and negative results are obtained on the complexity of computing k-stable partitions for the classical (non generalized) coloring games with better-response dynamics (Section 4.1.2.1) and parallel or space efficient algorithms (Section 4.1.2.2). Our results on the existence of k-stable partitions in generalized coloring games are summarized in Section 4.1.2.3. Extensions of all these results to broader classes of games are finally announced in Section 4.1.2.4.

4.1.2.1 Convergence of better-response dynamics for coloring games

The first two technical sections (Sections 4.3 and 4.4) are devoted to (non generalized) coloring games. In particular, Section 4.3 is devoted to the computation of k-stable partitions for these games.

In [KL13], Kleinberg and Ligett prove that every coloring game with n agents admits a partition that is k-stable for every $k \leq n$, but that it is NP-hard to compute one (this result was also proved independently by Escoffier et al. [EGM12]). Indeed, a largest group in such a partition must be a maximum independent set of the underlying graph. In contrast, it can be computed a k-stable partition in polynomial

[2]There is a more general notion of k-deviations where the agents deviating from their current strategies are not imposed to choose the same color i. However, as shown in [EGM12] for any (non generalized) coloring game, there exists such a k-deviation if and only there is one where the at most k agents deviating choose the same color i.

time for every fixed $k \leq 3$, by using simple *better-response dynamics* [PS08, EGM12, KL13] that we will describe next. The latter results question the role of the value of k in the complexity of computing stable partitions.

Formally, a better-response dynamic proceeds as follows. We start from a trivial coloring of the graph where all the vertices have a different color and then, as long as there exists a k-deviation w.r.t. the current coloring, we pick any one of these k-deviations S and we assign a same new color i to all the vertices in S so that they strictly increase their respective utility function.

We prove in Section 4.3 that better-response dynamics can be used for computing a k-stable partition *for every fixed* $k \geq 1$ (but not necessarily in polynomial time). It shows already that for every fixed $k \geq 1$, the problem of computing a k-stable partition is in the complexity class PLS (Polynomial Local Search), that is conjectured to lie strictly between P and NP [JPY88].

Then, we relate the time of convergence of better-response dynamics with a combinatorial object that is called the *Dominance lattice* [Bry73], thereby obtaining a closed formula for the worst-case time of convergence of the better-response dynamics for $k \leq 2$. Finally, we will show how lower-bounds on the time of convergence for the better-response dynamics can be obtained for larger values of k. These bounds are obtained with a new representation of the Dominance lattice, that I will briefly sketch. In particular, the main result in this section is that for every fixed $k \geq 4$, better-response dynamics converge in *superpolynomial time* $\Omega(n^{\Theta(\log n)})$ in the worst-case. The latter result disproves conjectures of Kleinberg and Ligett [KL13] and Escoffier et al. [EGM12] that better-response dynamics always converge in polynomial time for every fixed k.

This is joint work with Dorian Mazauric and Augustin Chaintreau.

4.1.2.2 The parallel complexity of coloring games

The negative results of Section 4.3 do not preclude the possibility that a k-stable partition can be computed in polynomial time for every fixed $k \geq 4$. For instance, this could be achieved by using a different dynamic. In order to better understand the complexity of this problem, I gave a closer look at the simpler (polynomial-time solvable) problem of computing a Nash equilibrium in coloring games.

More precisely, I investigate in Section 4.4 on the parallel and space complexity of computing a Nash equilibrium in these games. This aspect is also important when considering the applications of coloring games: to serve as a basis for distributed algorithms or to model the social behaviour of users with limited memory and computing power.

I prove in Section 4.4 that the problem of computing a Nash equilibrium in coloring games is PTIME-hard under logspace reductions. The latter result suggests that this problem is inherently sequential, and that it cannot be solved within limited (logarithmic) workspace under the well-established complexity assumption $PTIME \neq LOGSPACE$.

4.1.2.3 Existence of stable partitions for generalized coloring games

We also study in Section 4.5 the existence of k-stable partitions in generalized coloring games, and on the complexity of the related decision problem. So far, it has been proved in [BZ03] that every generalized coloring game admits a Nash equilibrium. However, computing one is a PLS-complete problem. This complexity comes from the fact that edge-weights may be arbitrary. In Section 4.5, we fix in advance a set of admissible edge-weights $\mathcal{W}$. We investigate on how the choice of $\mathcal{W}$ impacts on the existence of stable partitions.

The main result in this section, found in collaboration with Dorian Mazauric and Augustin Chaintreau, is that for every fixed $\mathcal{W}$, there exists a sharp threshold $k(\mathcal{W})$ (possibly, $k(\mathcal{W}) = +\infty$) such that the following dichotomy result holds true:

- every coloring game that is played on a graph with edge-weights in $\mathcal{W}$ admits a k-stable partition for every fixed $k \leq k(\mathcal{W})$;
- however, for every fixed $k > k(\mathcal{W})$, deciding on the existence of a k-stable partition for these games is an NP-complete problem.

This sharp threshold is explicitly given for most sets $\mathcal{W}$. We complement this result with preliminary relationships between the existence of stable partitions and the structure of the underlying graph on which the game is played.

4.1.2.4 Generalization to other games

Finally, in Section 4.6 we discuss on more general games that also extend the coloring games, some of them have been already defined and studied in the literature with a slightly different terminology [KL13, DP94, BZ03]. We show that most of our results from the two previous Sections 4.3 and 4.5 can be extended to those games.

The results that are presented in Sections 4.3, 4.5 and 4.6 are grouped in a paper [DMC17] that has been submitted to *SIAM Journal of Discrete Mathematics* (see also [DMC13a, DMC13b]). Results summarized in Section 4.4 have been published independently in [Duc16].

4.2 Definitions

We refer to [OR94, Mye13] for the basics of game theory. In what follows, we restate the formal notions given in the introduction with more details.

Let $G = (V, E, w)$ be an edge-weighted graph, with $w : E \to \mathbb{Q} \cup \{-\infty\}$ be its weight function. We may assume that G is a clique by replacing the nonedges with null-weight edges, and so, we will write $G = (V, w)$ in what follows. An arbitrary partition of the vertices in G is named a *coloring*. Each group of the partition defines a color.

Every graph G defines a *generalized coloring game* whose agents are its vertices. Configurations of this game are the colorings of G. In particular, the strategy of an agent is her color. Furthermore, given a configuration of the game, every agent

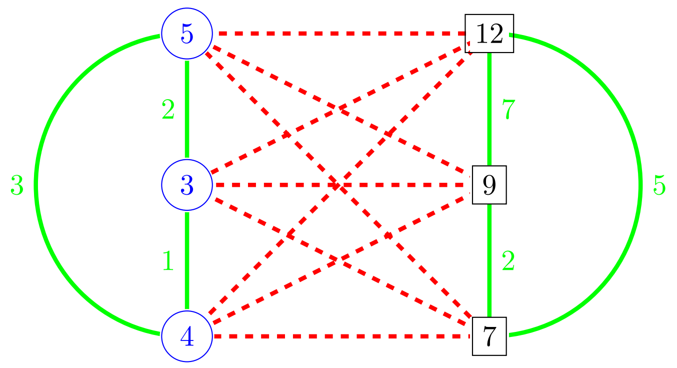


Figure 4.2: A bicoloring of a graph $G = (V, w)$. Agents that are represented by a circle (resp., by a square) have the same color. Red dashed edges have negative weight $-\infty$, while green continuous edges are labeled with their (positive) weight. Furthermore, each agent is labeled with her payoff.

$v \in V(G)$ receives payoff $\sum_{u \in V \setminus v | c(u) = c(v)} w_{uv}$, with $c(u)$ being the color of u. We refer to Figure 4.2 for an illustration.

Let us point out that classically, the non generalized coloring games are defined on an *unweighted* graph that is obtained from G by removing all edges with positive weight. We shall come back to this point later on in the section.

4.2.1 Stable partitions and better-response dynamics

Let us fix a configuration of the (generalized) coloring game that is played on G. A subset $S \subseteq V(G)$ with $|S| \leq k$ is a *k-deviation* if it can be assigned a same color to all the agents in S (different from their current color) so that their respective payoff is increased. Examples of 2-deviations are provided with Figure 4.3. When no k-deviation exists, we call the configuration a *k-stable partition*. The k-stable partitions correspond to the notion of *k-strong* Nash equilibria. In particular, 1-stable partitions correspond to the classical notion of Nash equilibria. Note that a k-stable partition might fail to exist, as shown with Figure 4.3.

The following *better response dynamics* are a classical approach in order to compute stable partitions. They are used in [KL13] in order to model the social choices of users in the community formation process.

Let $k \geq 1$ be fixed. We start from a trivial configuration where each agent has a different color. Then, as long as there exists a k-deviation, we pick any existing k-deviation S and we assign a same color c to all the agents in S so that they increase their respective payoff. Let us point out that c can be either a new colour (we make of S a new color class) or a color already assigned to some other agents not in S (we make the agents in S part of an existing color class). Furthermore, if this above dynamic converges then it stops on a k-stable partition.

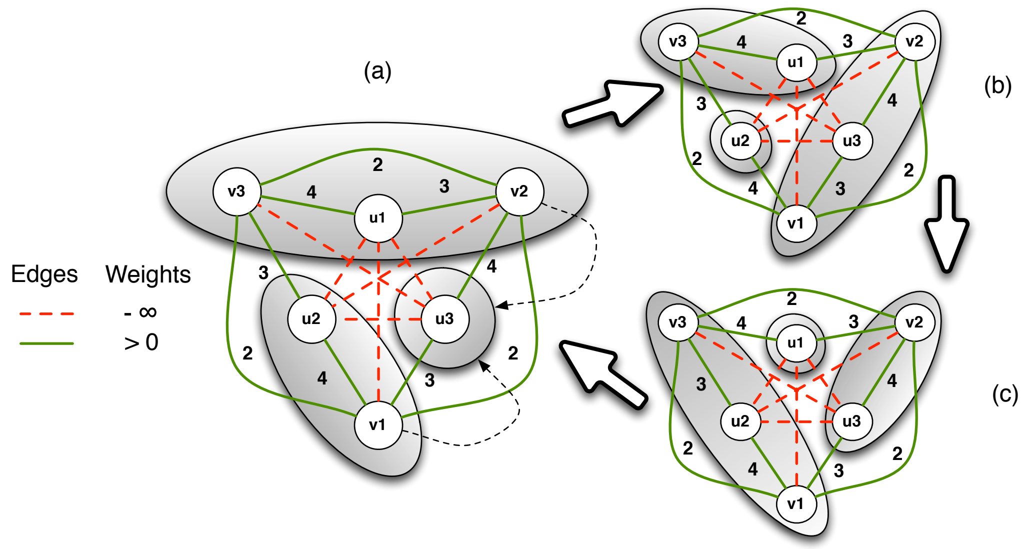


Figure 4.3: A graph $G = (V, w)$ with set of edge-weights $\mathcal{W} = \{-\infty, 2, 3, 4\}$. The coloring game played on G does not admit any 2-stable partition. Indeed, we here represent its 1-stable partitions, none of which is a 2-stable partition.

4.2.2 Friendship and conflict graphs

Finally, given an edge-weighted graph G, we define two unweighted graphs whose properties will be shown to be related to the properties of the generalized coloring game that is played on G.

- The *friendship graph* G^+ has for vertex-set $V(G)$ and for edge-set the edges of G with positive weight;
- Similarly, the *conflict graph* G^- has for vertex-set $V(G)$ and for edge-set the edges of G with negative weight.

As an example, given $G = (V, w)$ in Figure 4.2, the friendship graph G^+ is a disjoint union of two triangles, and the conflict graph G^- is a complete bipartite graph $K_{3,3}$.

Let us consider the particular case where the edges of G have weight either 1 or $-\infty$. In this situation, stable partitions for the coloring game that is played on G are *proper colorings* of the conflict graph G^-, *a.k.a.* colorings where no two adjacent vertices are assigned the same color. This justifies the terminology of coloring games.

4.3 Unweighted games: the time of convergence for better-response dynamics

The next two sections are devoted to the particular case of (non generalized) coloring games, *i.e.*, when the edge-weights of the underlying graph belong to $\{-\infty, 1\}$.

Classically [PS08, CKPS10, KL13, EGM12], these games are assumed to be played on the conflict graph G^- that is induced by the edges weighted $-\infty$. In particular, the goal of each agent is to construct a proper coloring of G^- while maximizing the number of agents with the same color as herself. Since the conflict graph is unweighted, we will sometimes call these games the unweighted coloring games in what follows.

Our purpose in this section is to (partly) characterize the complexity of computing a k-stable partition for these games, for every fixed k. Indeed, Kleinberg and Ligett [KL13] proved that for every k, every unweighted game admits a k-stable partition. However, finding a coloring that is a k-stable partition for every k is an NP-hard problem. In what follows, we will subdivide our contributions in three parts. Each part is devoted to the proofs of upper and lower bounds on the time of convergence for better-response dynamics.

- We first prove in Section 4.3.1 that for every fixed $k \geq 1$, better-response dynamics always converge to a k-stable partition. We discuss on the consequences of this result on the complexity of computing k-stable partitions.
- Then, we obtain in Section 4.3.2 the *exact* worst-case time of convergence for $k \leq 2$.
- Finally, we prove in Section 4.3.3 that better-response dynamics converge in *superpolynomial time* as soon as $k \geq 4$. The latter result answers negatively to an open question from [KL13, EGM12].

4.3.1 A finer-grained complexity for the problem of computing k-stable partitions

First, we prove that when applied to unweighted games, better-response dynamics always converge. Then, we discuss about the implications of this result on the complexity of computing a k-stable partition.

The following proof makes use of a *partition vector*, first introduced in [CKPS10].

Definition 62. Given a proper coloring of G^-, let λ_i be the number of colors c_i so that exactly i agents are colored by c_i. We denote by $\overrightarrow{\Lambda} = (\lambda_n, \ldots, \lambda_1)$ the partition vector of the coloring.

As an example, suppose that G^- is a complete bipartite graph with two sides of respective size n_1 and n_2, and we color all vertices on a same side with the same color. If $n_1 = n_2$ then $\lambda_{n_1} = 2$ and for every $i \neq n_1$, $\lambda_i = 0$. Otherwise, $\lambda_{n_1} = \lambda_{n_2} = 1$, and for every $i \notin \{n_1, n_2\}$, $\lambda_i = 0$.

Lemma 63. *For any (conflict) graph G^-, let us consider the unweighted game that is played on G^-. Then, for every $k \geq 1$, the better-response dynamic applied to this game converges to a k-stable partition.*

Proof. At each time we modify the current coloring of G^-, we also modify the corresponding partition vector $\overrightarrow{\Lambda}$. So, in order to prove that the better-response dynamic converges, it suffices to prove that $\overrightarrow{\Lambda'}$, obtained after the coloring has changed, is lexicographically greater than $\overrightarrow{\Lambda}$. Let us prove this by fixing a k-deviation S (w.r.t. the current coloring). After the coloring has been changed – with respect to S –, all vertices in S have strictly increased their payoff. For unweighted games, this is equivalent to have all vertices in S increase the number of agents with the same color as theirs. In particular, let c be the color assigned to all the agents in S, and let j be the number of agents colored c before the coloring has been changed. By the hypothesis, the change of coloring results in $j + |S|$ vertices colored c. So, we get $\overrightarrow{\Lambda'} - \overrightarrow{\Lambda} = (0, \ldots, 0, \lambda'_{j+|S|} - \lambda_{j+|S|} = 1, \ldots)$, and so, $\overrightarrow{\Lambda} <_{Lex} \overrightarrow{\Lambda'}$. Finally, as the number of possible vectors is finite, we obtain the convergence of the better-response dynamic. □

Next, we discuss on the consequences of Lemma 63 on the complexity of computing k-stable partitions for unweighted games. Informally, an optimization problem is in PLS (Polynomial Local Search) if an optimal solution can be computed with a local-search algorithm, *i.e.*, an algorithm converging to an optimal solution by repeatedly improving a current solution with a slight pertubation of it[3]. Lemma 63 proves that for every fixed k, the problem of computing a k-stable partition for unweighted games is in PLS. This complexity class is strictly included in NP unless NP=coNP [JPY88].

Hence, to summarize this subsection, we have improved the best-known results on the complexity of computing a k-stable for unweighted games, for every fixed k.

4.3.2 Closed formula for the worst-case time of convergence of better-response dynamics ($k \leq 2$)

Polynomial-time solvable problems are conjectured to be strictly contained in PLS [JPY88]. In this section, we are interested in characterizing for which values of k the problem of computing a k-stable partition is in P. As a partial answer to this question, we aim at characterizing for which values of k the corresponding better-response dynamic converges within a polynomial number of steps.

It was proved in various papers [PS08, KL13, EGM12] that better-response dynamics converge in polynomial-time for every fixed $k \leq 3$. The proofs in these papers rely on a potential function argument. We now give an alternative proof of this result for the case $k \leq 2$. It is based on a more combinatorial argument and it allows us to obtain the *exact* worst-case time of convergence.

Theorem 64. *Let G^- be an n-vertex conflict graph. We consider the unweighted game that is played on G^-. Let m and r be the unique non negative integers such that $n = \frac{m(m+1)}{2} + r$, and $0 \leq r \leq m$.*

Then, for every $k \leq 2$, the better-response dynamic applied to this above game converges to a k-stable partition within no more than $2\binom{m+1}{3} + mr \sim \frac{2\sqrt{2}}{3}n\sqrt{n}$ steps.

[3]Each step of the algorithm takes polynomial time, but the number of steps may be superpolynomial.

Moreover this worst-case upper-bound is reached if the conflict graph G^- has no edges.

The remaining of this subsection is devoted to the proof of Theorem 64.

At first glance, it might look counter intuitive that the worst-case convergence time of the dynamic is reached for the edgeless conflict graph. Indeed, when the conflict graph has no edges there is a unique stable partition, with all agents having the same color. However, this can be better understood by noticing that every proper coloring of a conflict graph G^- is also a proper coloring of the edgeless conflict graph $G^\emptyset$ with same vertices. In particular, if we color accordingly G^- and $G^\emptyset$ then a k-deviation for G^- is also a k-deviation for $G^\emptyset$. It directly follows from this observation that the worst-case convergence time for better-response dynamics is always reached with $G^\emptyset$.

The proof of Theorem 64 also makes use of partition vectors. As for Lemma 63, we show that every time the coloring is changed by using a 1-deviation (resp., a 2-deviation), the corresponding partition vector increases with respect to some ordering. However, in order to prove a polynomial upper-bound for the time of convergence, we cannot use anymore the lexicographical ordering, since it is a *total ordering* and the number of partition vectors is superpolynomial [HW79]. Instead, we will use a partial ordering that was introduced by Brylawski in [Bry73], in a somewhat different context.

Integer partitions. We first observe that when the game is played on an n-vertex conflict graph, each partition vector of its colorings defines a unique way to write n as a sum of positive integers. The latter means that partition vectors are in bijective correspondance with the nonincreasing sequences of n nonnegative integers whose terms sum up to n. More precisely, every vector $\overrightarrow{\Lambda}$ is related to the nonincreasing sequence $Q(\overrightarrow{\Lambda})$, with its $n - \sum_{i=1}^{n} \lambda_i$ lowest terms equal to zero, and exactly λ_i terms equal to i for every $1 \leq i \leq n$. These sequences are called integer partitions in the literature [Bry73, HW79].

Dominance ordering. Brylawski has defined an ordering over the integer partitions, sometimes called the dominance ordering [Bry73]. Namely, given two partitions, one is greater than the other if and only if for every $1 \leq i \leq n$, the sum of its i largest terms is greater than or equal to the sum of the i largest terms of the other. The latter ordering is a direct application of the theory of majorization to integer partitions [OM16].

For instance, let us consider two trivial colorings of $G^\emptyset$: one with every agent having a different color, and another with every agent having the same color. In the first case, the partition vector is $\overrightarrow{\Lambda} = (0, \ldots, 0, n)$ so that $\lambda_1 = n$ and $\lambda_i = 0$ for every $i > 1$; in the second case, the partition vector is $\overrightarrow{\Lambda'} = (1, 0, \ldots, 0)$ so that $\lambda'_n = 1$ and $\lambda'_i = 0$ for every $i < n$. The corresponding integer partitions are $Q(\overrightarrow{\Lambda}) = (1, 1, 1, \ldots, 1)$ and $Q(\overrightarrow{\Lambda'}) = (n, 0, 0, \ldots, 0)$. In particular, the i largest terms of $Q(\overrightarrow{\Lambda'})$ always equal n, whereas the i largest terms of $Q(\overrightarrow{\Lambda})$ equal $i \leq n$. Hence, $\overrightarrow{\Lambda'}$ is greater than $\overrightarrow{\Lambda}$ w.r.t. the dominance ordering.

Relationship with 2-deviations. The dominance ordering gives rise to a lattice on the integer partitions. Furthermore, it has been proved in [GK86] that a longest chain in this lattice has length $2\binom{m+1}{3} + mr$, with m and r being the unique non negative integers such that $n = \frac{m(m+1)}{2} + r$, and $0 \leq r \leq m$. Therefore, in order to prove Theorem 64 we have been left to prove a correspondance between the valid sequences of 2-deviations in $G^{\emptyset}$ and the chains of integer partitions in the Dominance lattice. Note that this correspondance holds true only for the edgeless conflict graph $G^{\emptyset}$. Below, we first prove this correspondance in the case of 1-deviations.

Lemma 65. *Assuming $G^- = G^{\emptyset}$ is edgeless, let Q, Q' be two integer partitions of $n = |V|$.*

Then, Q' dominates Q if and only if there exist two colorings c, c' of G^- with respective partition vectors $\overrightarrow{\Lambda}$ and $\overrightarrow{\Lambda'}$ such that: $\mathcal{Q}(\overrightarrow{\Lambda}) = Q$, $\mathcal{Q}(\overrightarrow{\Lambda'}) = Q'$, and there is a valid sequence of 1-deviations from c to c'.

Proof. ($\Rightarrow$) Suppose that Q' dominates Q. We may assume w.l.o.g. that there is no intermediate integer partition Q'' such that Q' dominates Q'' and Q'' dominates Q. Indeed, then we can prove the result in general by induction on the length of a longest chain from Q to Q'. In this situation, we say that Q' covers Q. Brylawski [Bry73] has proposed a combinatorial characterization of the covering relation. Precisely, Q' covers Q if and only if there exist indices j, k satisfying:

- $k = j + 1$ or $q_j = q_k$;
- $q'_j = q_j + 1$, $q'_k = q_k - 1$, and for all i such that $i \notin \{j, k\}$, $q'_i = q_i$.

In particular, since $k = j + 1$ or $q_j = q_k$, we get $q_j \geq q_k$.

Let c be any coloring with partition vector $\overrightarrow{\Lambda}$, so that $\mathcal{Q}(\overrightarrow{\Lambda}) = Q$. We order the color classes by nonincreasing size, naming L_i the i^{th} largest class, in a way so that $|L_i| = q_i$. Then, we pick any $v \in L_k$, that exists since $|L_k| = q_k > 0$. Since by construction there are $|L_j| = q_j \geq q_k$ agents with color j, and there is no edge incident to v and to another agent with color j by the hypothesis, therefore, we can increase the payoff of v by changing her color for j. By doing so, we obtain a new coloring c' with partition vector $\overrightarrow{\Lambda'}$ such that $\mathcal{Q}(\overrightarrow{\Lambda'}) = Q'$.

Conversely, ($\Leftarrow$) let c and c' be two colorings with respective partition vectors $\overrightarrow{\Lambda}$ and $\overrightarrow{\Lambda'}$ such that $\mathcal{Q}(\overrightarrow{\Lambda}) = Q$ and $\mathcal{Q}(\overrightarrow{\Lambda'}) = Q'$. Assume that c' can be obtained from c after a 1-deviation. In particular, let v change her color. We can order the color classes by nonincreasing size, naming L_i the i^{th} largest class, in a way so that:

- v changes her color $c(v) = k$ for $c'(v) = j$, with $j \leq k$;
- every color class L_i, $i < j$, has size $|L_i| > |L_j|$;
- every color class L_i, $i > k$, has size $|L_i| < |L_k|$.

Note that $Q = (|L_1|, |L_2|, \ldots, |L_j|, \ldots, |L_k|, \ldots, |L_n|)$ by construction. In particular, Q' is such that $q'_i = q_i = |L_i|$ if $i \notin \{j, k\}$, and $q'_j = |L_j| + 1$, $q'_k = |L_k| - 1$. As a consequence, we have that Q' dominates Q by the hypothesis. Note that this second part of the proof holds for any conflict graph G^-. $\square$

To complete the proof of Theorem 64, we need to show that 2-deviations cannot make the time of convergence of the dynamic increase. We prove this below with a finer-grained analysis of the partition vectors that are obtained after 2-deviations.

Lemma 66. *Assuming $G^- = G^\emptyset$ is edgeless, let Q, Q' be two integer partitions of $n = |V|$. Suppose that there exist two colorings c, c' of G^- with respective partition vectors $\overrightarrow{\Lambda}$ and $\overrightarrow{\Lambda'}$ such that: $\mathcal{Q}(\overrightarrow{\Lambda}) = Q$, $\mathcal{Q}(\overrightarrow{\Lambda'}) = Q'$, and c' is obtained from c after a 2-deviation. Then, Q' dominates Q.*

Proof. Let $S = \{u, v\}$ be a 2-deviation w.r.t. c so that c' is obtained from c by assigning a same color j to u and v. Furthermore, let $i = c(u)$ and let $i' = c(v)$. In what follows, we denote by $L_i, L_{i'}, L_j$ the color classes of c that correspond, respectively, to the colors i, i' and j.

We note that if $|L_j| \geq |L_i|$ then u can increase her payoff by changing her current color i for j. In this situation, c' can be obtained from c after a sequence of two 1-deviations, with u followed by v changing their respective colors for j sequentially. Therefore, Q' dominates Q by Lemma 65. Similarly, if $|L_j| \geq |L_{i'}|$ then c' can be obtained from c by changing the respective colors of v then u for color j sequentially. Therefore, we also have in this case that Q' dominates Q by Lemma 65. From now on, let us assume that $|L_j| = |L_i| - 1 = |L_{i'}| - 1$. There are two cases to be considered:

- Suppose that $i = i'$. Then the numbers of agents colored by i and j in c' are respectively $|L_i \setminus \{u, v\}| = |L_i| - 2$ and $|L_j \cup \{u, v\}| = |L_j| + 2 = |L_i| + 1$. In particular, another coloring c'' can be obtained from c with a 1-deviation as follows. We pick any agent $u_j \in L_j$ and we make her payoff increase from $|L_j| - 1 = |L_i| - 2$ to $|L_i| = |L_j| + 1$ by changing her current color j for i. By doing so, the coloring c'' so obtained has the same partition vector as c'. Therefore, since c'' is obtained from c after a 1-deviation, Q' dominates Q by Lemma 65.
- Otherwise, $i \neq i'$. Then the numbers of agents colored by i, i' and j in c' are respectively $|L_i \setminus \{u\}| = |L_i| - 1$, $|L_{i'} \setminus \{v\}| = |L_{i'}| - 1 = |L_i| - 1$ and $|L_j \cup \{u, v\}| = |L_j| + 2 = |L_i| + 1$. Again, another coloring c'' with the same partition vector as c' can be obtained from c after a 1-deviation, this time by modifying the color of v from i' to i. Since c'' is obtained from c after a 1-deviation, Q' dominates Q by Lemma 65.

$\square$

By Lemma 66, the maximum number of consecutive 2-deviations in better-response dynamics is upper-bounded by the length of a longest chain in the Dominance lattice. Since Lemma 65 proves that it can be obtained a sequence of 1-deviations with exactly this length, Theorem 64 follows.

Perspectives. In [PS08], Panagopoulou and Spirakis proved that for every conflict graph G^- with independent number $\alpha(G^-)$, the better-response dynamic converges to a Nash equilibrium within $\mathcal{O}(n \cdot \alpha(G^-))$ steps. This improves upon the upper-bound of Theorem 64 for the graphs with independent set $\alpha(G^-) = o(\sqrt{n})$. I conjecture that the worst-case time of convergence of the dynamic is an $\mathcal{O}(n \cdot \sqrt{\alpha(G^-)})$, that would be the best possible.

4.3.3 Lower-bounds for the worst-case time of convergence of better-response dynamics ($k \geq 4$)

Finally, on the negative side we lower-bound the worst-case running-time of better-response dynamics for $k = 4$. It has been conjectured in [EGM12] that in the case of unweighted games, better-response dynamics always converge in polynomial time for every fixed k. Our results for $k = 4$ disprove this conjecture.

Theorem 67. *Let $G^\emptyset$ be an edgeless conflict graph with n vertices. We consider the unweighted game played on $G^\emptyset$.*

Then, for every $k \geq 4$, better-response dynamics applied to this above game converge in $\Omega(n^{\Theta(\log n)})$ steps in the worst-case.

Due to its high level of technicality, the proof of Theorem 67 will be only sketched in what follows. The full proof can be found in [DMC17].

4.3.3.1 Cascade sequences: overview

In order to give a flavor of the method, let us consider some coloring of $G^\emptyset$, with partition vector $\overrightarrow{\Lambda}$ so that $\lambda_p \geq 4$ and $\lambda_{p-3} \geq 1$ for some p. We take a subset S of four agents, each with a distinct color and receiving payoff $p-1$. Such a subset surely exists since $\lambda_p \geq 4$. Then, since $\lambda_{p-3} \geq 1$, there exists some color c that is assigned to exactly $p-3$ agents. Assigning color c to the four agents in S would increase their respective payoff from $p-1$ to p, so, S is a 4-deviation. This case is interesting because after the 4-deviation, the length of a longest chain, in the Dominance lattice, from the current coloring to the *unique* stable partition of $G^\emptyset$ (where all the agents have the same color) has been increased. Hence, we aim at using this type of 4-deviations in order to maximize the number of steps for the better-response dynamic.

With that goal in mind, we now define *cascade sequences.* Indeed, suppose now that for some p, we have as before $\lambda_p \geq 4$ and $\lambda_{p-3} \geq 1$, but also $\lambda_i \geq 1$ for every $i \leq p-4$. As it is described above, we modify the current coloring with a 4-deviation, thereby obtaining as the new partition vector $\overrightarrow{\Lambda'}$ so that:

$$\begin{cases} \lambda'_{p+1} &= \lambda_{p+1} + 1 \\ \lambda'_p &= \lambda_p - 4 \\ \lambda'_{p-1} &= \lambda_{p-1} + 4 \\ \lambda'_{p-3} &= \lambda_{p-3} - 1 \\ \lambda'_i &= \lambda_i \text{ otherwise.} \end{cases}$$

Then, since $\lambda'_{p-1} \geq 4$ and $\lambda'_{p-4} = \lambda_{p-4} \geq 1$, we can modify the new coloring with another 4-deviation, and so on. As an example, the following is a cascade sequence of size four. Each configuration is represented with an integer partition:

$$\mathcal{Q}_0 = (7,7,7,7,4,3,2,1),$$

$$\mathcal{Q}_1 = (8,6,6,6,6,3,2,1),$$

$$\mathcal{Q}_2 = (8,7,5,5,5,5,2,1),$$

$$\mathcal{Q}_3 = (8,7,6,4,4,4,4,1),$$

$$\mathcal{Q}_4 = (8,7,6,5,3,3,3,3).$$

In order to lower-bound the time of convergence in the worst-case, we aim at maximizing the size and the number of cascade sequences during the steps of the dynamic. The latter is achieved through a complex recursive procedure, where we define larger and larger cascades (but in fewer and fewer number) by inserting complex sequences of "adaptive" 1-deviations in-between. In the following Section 4.3.3.2, we will introduce new technical notions that we use in [DMC17] in order to formally define this procedure.

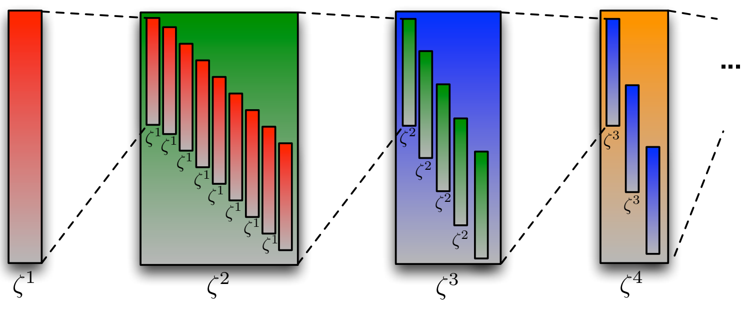


Figure 4.4: A recursive procedure in order to increase the size of cascade sequences (sketch).

4.3.3.2 Representing long sequences of 4-deviations with vectors

Our construction can be best defined by using a vectorial representation of 4-deviations. More precisely, when we change a coloring with partition vector $\overrightarrow{\Lambda}$ for another coloring with partition vector $\overrightarrow{\Lambda'}$, the deviation corresponding to that change can be represented with the difference vector $\overrightarrow{\Lambda'} - \overrightarrow{\Lambda}$. As an example, if after a 1-deviation some agent increases her payoff from $p-1$ to $p+1$ then she leaves a group of size p for some other group of size $p+1$. In particular, her former color class has size $p-1$ after her departure, and her new color class has size $p+2$ after her arrival. Therefore, the corresponding difference vector $\overrightarrow{\Delta} = \overrightarrow{\Lambda'} - \overrightarrow{\Lambda}$ satisfies:

$$\begin{cases} \delta_{p+2} &= 1 \\ \delta_{p+1} &= -1 \\ \delta_p &= -1 \\ \delta_{p-1} &= 1 \\ \delta_i &= 0 \text{ otherwise.} \end{cases}$$

Symmetric property. Our recursive cascades are easier to represent this way, *i.e.*, as a vectorial sequence satisfying some "symmetric properties", that we define next.

Definition 68. The minimum-size sub-vector that contains all non-zero entries of a vector is called the *support* of the vector. We say a vector has the *symmetric property* if, and only if, the coordinates of its support are invariant under the reverse permutation (in which case, it is said "symmetric").

On the one hand, we show in [DMC17] that except for a few pathological cases, every 1-deviation yields an elementary vector that has the symmetric property. But the property does not hold in general for k-deviations whenever $k \geq 3$. This might give a hint of what changes in the nature of the problem when larger deviations are allowed.

On the other hand, the use of this above vectorial representation might lead to define vectorial sequences that do not truly represent sequences of 4-deviations. Thus, we need to define additional constraints in order to prevent that case from happening, which unfortunately level up the technicality of the proof. We give a flavour of it by introducing the notion of **balanced sequences**.

Definition 69. Given any integer $h > 0$, let $\overrightarrow{\varphi}^1, \overrightarrow{\varphi}^2, \ldots, \overrightarrow{\varphi}^t$ be vectors. We call this sequence h-balanced if, for any $1 \leq i \leq t$, the sum of the i first vectors, namely $\sum_{j=1}^{i} \overrightarrow{\varphi}^j$, has all its entries greater than or equal to $-h$.

As an example, since agents in a k-deviation can be in no more than k distinct color classes, the vector gotten after any k-deviation is always k-balanced.

Given a h-balanced sequence $(\overrightarrow{\varphi}^1, \overrightarrow{\varphi}^2, \ldots, \overrightarrow{\varphi}^t)$ of k-deviations, let $\overrightarrow{\Phi} = \sum_{i=1}^{t} \overrightarrow{\varphi}^i$ be the sum of all deviations. In what follows, we will say that $\overrightarrow{\Phi}$ *represents* the sequence. Let $p_{\max}$ be the largest index j that satisfies $\overrightarrow{\Phi}_j \neq 0$. Equivalently, $p_{\max}$ is the largest size of a group modified (hence created) after some deviation in the sequence happens (*i.e.*, $\forall l, \forall p > p_{\max}, \varphi_p^l = 0$). Then, one can observe that a sufficient condition so that the sequence is valid is that it starts from a coloring with at least h color classes of each size j, for $1 \leq j \leq p_{\max}$.

The following claim will be used in our sketch proof for Theorem 67.

Claim 70. *Suppose that $\overrightarrow{\Phi^1}$ and $\overrightarrow{\Phi^2}$ respectively represent a h_1-balanced sequence and a h_2-balanced sequence. Then, $\overrightarrow{\Phi} = \overrightarrow{\Phi^1} + \overrightarrow{\Phi^2}$ represents a $\left(\max\{h_1, h_2 - \min_i \Phi^1_i\}\right)$-balanced sequence, that is the concatenation of the two sequences represented by $\overrightarrow{\Phi^1}$ and $\overrightarrow{\Phi^2}$.*

Proof. Clearly, $\overrightarrow{\Phi}$ represents the sequence obtained by the concatenation of the two sequences that are respectively represented by $\overrightarrow{\Phi^1}$ and $\overrightarrow{\Phi^2}$. In particular, the subsequence represented by $\overrightarrow{\Phi^1}$ is h_1-balanced by the hypothesis. The remaining subsequence is represented by $\overrightarrow{\Phi^2}$, that is h_2-balanced by the hypothesis. Since it follows the first subsequence, and all the entries of $\overrightarrow{\Phi^1}$ are greater than or equal to $\min_i \Phi^1_i$, therefore, this second subsequence is $(h_2 - \min_i \Phi^1_i)$-balanced. ◇

Sketch of the construction. Our proof for Theorem 67 relies on a "shift" operator: given a vector $\overrightarrow{\varphi}$ whose support ranges between indices $p_{\min}, p_{\max}$, the vector ${}^{\mathtt{tr}(i)}\overrightarrow{\varphi}$, $i < p_{\min}$, is a vector of the same size *and the same support* as $\overrightarrow{\varphi}$, but whose support ranges between indices $p_{\max} - i, p_{\min} - i$. For instance, we have ${}^{\mathtt{tr}(1)}(0, 1, -2, 1, 0, 0, 0) = (0, 0, 1, -2, 1, 0, 0)$. In particular, if $\overrightarrow{\varphi}$ represents a k-deviation, then ${}^{\mathtt{tr}(i)}\overrightarrow{\varphi}$ represents the same k-deviation, up to a decrease by i of the size of all color classes involved.

One can extend the operator and its meaning to sequences of k-deviations as well. Formally, let $\overrightarrow{\varphi}^1, \ldots, \overrightarrow{\varphi}^t$ be a sequence of k-deviations, and let $\overrightarrow{\Phi} = \sum_{l=1}^t \overrightarrow{\varphi}^l$ represent this sequence. Then, if no group of size less than $i+1$ is modified nor created by the sequence (*i.e.*, $\forall l, \forall p \leq i, \varphi^l_p = 0$), we obtain by linearity of the operator that ${}^{\mathtt{tr}(i)}\overrightarrow{\Phi} = \sum_{l=1}^t {}^{\mathtt{tr}(i)}\overrightarrow{\varphi}^l$.

Let us prove two important properties of the so-called "shift operator":

Claim 71. *Let $\overrightarrow{\phi}$ be any vector that has a support of size $s = p_{\max} - p_{\min} + 1$, and with the symmetric property. For any positive integers r and d such that $1+(r-1)d \leq p_{\min}$, the vector $\overrightarrow{\phi}' = \sum_{h=0}^{r-1} {}^{\mathtt{tr}(hd)}\overrightarrow{\phi}$ also has the symmetric property.*

Proof. The support of vector $\overrightarrow{\phi}'$ has size $s' = (r-1)d + s$. In the following, we will assume up to padding the vector $\overrightarrow{\phi}$ with additional null entries that it is unbounded *i.e.*, it is indexed by $\mathbb{Z}$. By the hypothesis the vector $\overrightarrow{\phi}$ has the symmetric property and so, $\forall 1 \leq j \leq p_{\max} + p_{\min} - 1, \phi_j = \phi_{p_{\min}+p_{\max}-j}$. Let $0 \leq j \leq s'/2 - 1$. We have that:

$$\phi'_{p_{\max}-j} = \sum_{h=0}^{r-1} \phi_{p_{\max}-j+hd} = \sum_{h=0}^{r-1} \phi_{p_{\max}+p_{\min}-(p_{\max}-j+hd)}$$

$$= \sum_{h=0}^{r-1} \phi_{p_{\min}+j-(r-1-h)d} = \sum_{h=0}^{r-1} \phi_{p_{\min}-(r-1)d+j+hd} = \phi'_{p_{\min}-(r-1)d+j}.$$

Thus, $\overrightarrow{\phi}'$ also has the symmetric property. ◇

Claim 72. *For any positive integers r and d, if $\overrightarrow{\Phi}$ represents a h-balanced sequence then $\overrightarrow{\Phi}' = \sum_{j=0}^{r-1} {}^{tr(jd)}\overrightarrow{\Phi}$ represents a $(h+e_\Phi)$-balanced sequence, with $e_\Phi = -\min_{i_1 \le i_2} \sum_{j=i_1}^{i_2} \Phi_j$.*

Proof. We prove the claim by induction on r. If $r = 0$ then $\overrightarrow{\Phi'} = \overrightarrow{\Phi}$ and so the claim holds vacuously in this base case. Otherwise, let us write $\overrightarrow{\Phi'} = \left(\sum_{j=0}^{r-2} {}^{\texttt{tr}(jd)}\overrightarrow{\Phi}\right) + {}^{\texttt{tr}((r-1)d)}\overrightarrow{\Phi} = \overrightarrow{\Phi''} + {}^{\texttt{tr}((r-1)d)}\overrightarrow{\Phi}$. Note that ${}^{\texttt{tr}((r-1)d)}\overrightarrow{\Phi}$ represents a h-balanced sequence, and by the induction hypothesis $\overrightarrow{\Phi''}$ represents a $(h+e_\Phi)$-balanced sequence. Since all entries of $\overrightarrow{\Phi''}$ are greater than or equal to $-e_\Phi$, therefore, $\overrightarrow{\Phi}$ represents a $(h+e_\Phi)$-balanced sequence by Claim 70. ◇

Finally, in order to prove Theorem 67, we construct vectors $\overrightarrow{\zeta}^i$ that represent sequences of deviations. The construction is recursive. To construct the vector $\overrightarrow{\zeta}^{i+1}$ from $\overrightarrow{\zeta}^i$, we follow a particular construction that we will show valid and that is illustrated in Figure 4.4. The construction is composed of a repetition of the sequence defined by $\overrightarrow{\zeta}^i$ a certain number of times (linear in some parameter $t = \Theta(\log n)$) shifting the "starting point" of each sequence by the same value. The construction then adds 1-deviations in order to get a technical generalization of the symmetric property, called *Good property* (see [DMC17]).

Claim 73. *There exists a sequence of vectors $\overrightarrow{\zeta}^i$ such that the following hold true for every i:*

- *There exist two positive integers denoted by a_i, t_1^i, and there exists a sequence of 1-deviations represented by $\overrightarrow{\xi}^{i+1}$ so that:*

$$\overrightarrow{\zeta}^{i+1} = \sum_{j=0}^{a_i} {}^{tr(jt_1^i)}\overrightarrow{\zeta}^i + \overrightarrow{\xi}^{i+1}.$$

- *If $\overrightarrow{\zeta}^i$ represents a h_i-balanced sequence then $\overrightarrow{\zeta}^{i+1}$ represents a (h_i+1)-balanced sequence.*
- *Furthermore, $s_i \le s_{i+1} < \frac{3}{2}s_i$ where s_i and s_{i+1} denote the respective sizes of the support of $\overrightarrow{\zeta}^i$ and $\overrightarrow{\zeta}^{i+1}$, and $\overrightarrow{\zeta}^{i+1}$ represents a sequence of at least $(\frac{s_i}{2^{i+2}} - 5)$-times more deviations than in the sequence represented by $\overrightarrow{\zeta}^i$.*

Sketch Proof of Claim 73. Our constructions will ensure that every $\overrightarrow{\zeta}^i$ satisfies a so-called *Good Property*, namely:

- $\overrightarrow{\zeta}^i$ has the symmetric property, with its nonzero entries being equal to $1, -1, -1, 1$ and (by symmetry) $1, -1, -1, 1$;
- it has a support $\overrightarrow{supp(\zeta^i)}$ of even size s_i with its two middle entries being equal to 1;
- last, the two least entries of $\overrightarrow{supp(\zeta^i)}$ that are valued -1 are indexed by t_1^i, t_2^i with $1 < t_1^i < t_2^i < 2t_1^i$, and $t_2^i \le 2^{i+1}$.

Before entering in the details of the construction, let us sketch how we use this Good property in what follows. Let h_i be the least integer such that the vector $\overrightarrow{\zeta}^i$ represents a h_i-balanced sequence. Our main objective is to maximize the size of this sequence while minimizing h_i.

- In particular, if $\overrightarrow{\zeta}^i$ satisfies the Good property then its nonzero entries are constrained to $1, -1, -1, 1, 1, -1, -1, 1$, and so, $\overrightarrow{\zeta}^i$ is h_i-balanced implies that $\sum_{j=0}^{a_i} {}^{\texttt{tr}(jt_1^i)}\overrightarrow{\zeta}^i$ is (h_i+2)-balanced by Claim 72. We will ensure in addition that $\overrightarrow{\xi}^{i+1}$ represents a 1-balanced sequence of 1-deviations, so, altogether combined this will show that $\overrightarrow{\zeta}^{i+1} = \sum_{j=0}^{a_i} {}^{\texttt{tr}(jt_1^i)}\overrightarrow{\zeta}^i + \overrightarrow{\xi}^{i+1}$ is (h_i+2)-balanced by Claim 70 (a little more work is needed in order to prove that $\overrightarrow{\zeta}^{i+1}$ is (h_i+1)-balanced).

- Moreover, we note that since $\overrightarrow{\zeta}^{i+1} = \sum_{j=0}^{a_i} {}^{\texttt{tr}(jt_1^i)}\overrightarrow{\zeta}^i + \overrightarrow{\xi}^{i+1}$, it represents a sequence of at least a_i-times more deviations than $\overrightarrow{\zeta}^i$. We will choose a_i (used for the shiftings) to be the largest even integer j such that $jt_1^i + t_2^i < s_i/2+1$. The latter choice implies that $a_i \leq \frac{s_i-4-2t_2^i}{2t_1^i}$. Then, since $1 < t_1^i < t_2^i < 2t_1^i$, and $t_2^i \leq 2^{i+1}$, we obtain that $\frac{s_i-4-2t_2^i}{2t_1^i} > \frac{s_i}{2^{i+2}} - \frac{1}{2^i} - 1$, and so, $a_i \geq \left\lfloor \frac{s_i}{2^{i+2}} - \frac{1}{2^i} - 1 \right\rfloor - 2 \geq \frac{s_i}{2^{i+2}} - 5$, as desired.

As a result, the Good property is a sufficient condition for the two requirements of the claim. Let us now sketch the construction of the vectors $\overrightarrow{\zeta}^i$.

Base case. Let $L = \Theta(\sqrt{n})$ and $t = \Theta(\log n)$. We initiate the sequence with a cascade of 4-deviations. This cascade has size t^2 and it starts with four agents in different color classes of size $L-1$ leaving for a new color class of size $L-4$ (until four agents in different classes of size $L-t^2$ leave for a new color class of size $L-3-t^2$). Then, in order to satisfy some technical requirements we complete the cascade with a small sequence of 1-deviations. Let $\overrightarrow{\Phi}^1$ represent this subsequence. By the calculation, all its entries are equal to zero except for: $\Phi_L^1 = \Phi_{L-5}^1 = \Phi_{L-t^2-1}^1 = \Phi_{L-t^2-6}^1 = 1$, and $\Phi_{L-1}^1 = \Phi_{L-2}^1 = \Phi_{L-t^2-4}^1 = \Phi_{L-t^2-5}^1 = -1$. Note that this intermediate sequence does not satisfy the Good property.

We finally construct $\overrightarrow{\zeta}^1$ by repeating $\overrightarrow{\Phi}^1$ many times, namely from $\sum_{i=0}^{t^2-5} {}^{\texttt{tr}(i)}\overrightarrow{\Phi}^1$, and then ending with "adjusting" sequences of 1-deviations.

To better understand the role played by the latter sequences, let p, q, h be three nonnegative integers such that $p > q + 2h$. Let us consider the sequence where an agent leaves a group of size $q+1$ for a group of size $p-1$, then another agent leaves a group of size $q+2$ for a group of size $p-2$, and so on util a final agent leaves a group of size $q+h$ for a group of size $p-h$. This sequence is represented by a vector $\overrightarrow{\phi}$ such that: $\phi_p = \phi_q = 1$, and $\phi_{p-h} = \phi_{q+h} = -1$. We use this type of sequence so as to position the nonzero entries of $\overrightarrow{\zeta}^1$ as desired in order to satisfy the Good property.

Inductive step. It turns out that all the main ideas for the construction are already present in the base case. Indeed, suppose the vector $\overrightarrow{\zeta}^i$ to be constructed in order to satisfy the Good property. As already stated, we choose a_i to be the largest even integer j such that $jt_1^i + t_2^i < s_i/2+1$. Then, let $\overrightarrow{\Phi}^{i+1} = \sum_{j=0}^{a_i} {}^{\texttt{tr}(jt_1^i)}\overrightarrow{\zeta}^i$, that is a vector with the symmetric property by Claim 71. By construction, this vector has a support of size $s_{i+1} = s_i + a_i t_i^1 < \frac{3}{2}s_i$, that is even because s_i and a_i are even, and that will also be the size of the support of $\overrightarrow{\zeta}^{i+1}$.

In fact, $\overrightarrow{\Phi}^{i+1}$ "almost" satisfies the Good property, but is has more nonzero entries than what is required. So, we set to zero this surplus of nonzero entries using four sequences of 1-deviations, thereby obtaining $\overrightarrow{\zeta}^{i+1}$. □

It can be proved by induction on i that the above-defined sequence $\overrightarrow{\zeta}^i$ is $\mathcal{O}(i)$-balanced and with support of size $o\left(\left(\frac{3}{2}\right)^i\right)$. In particular, this sequence is valid if we start from a coloring with $\mathcal{O}(i)$ color classes of size s for every $1 \leq s \leq o\left(\left(\frac{3}{2}\right)^i\right)$ — in which case, we must ensure $n \geq \mathcal{O}\left(i \cdot \left(\frac{3}{2}\right)^i\right)$. Hence, we can construct the sequence $\overrightarrow{\zeta}^i$ for some polynomial $i = \Omega(n^{1/6}/\log n)$. Altogether combined with the lower-bound on the size of the sequence that is represented by $\overrightarrow{\zeta}^i$, the latter achieves proving Theorem 67. We refer to [DMC17] for the full calculation.

Discussion and open questions. To sum up this section, we have by Theorem 64 that better-response dynamics cannot be used in order to compute 4-stable partitions in polynomial time. As a byproduct of our vectorial approach, we also get an $\Omega(n^2)$ lower-bound on the convergence time of the dynamic for $k = 3$ (see [DMC17]). We conjecture that the worst-case convergence time of the dynamic in this case is indeed $\mathcal{O}(n^2)$, that would improve upon the known $\mathcal{O}(n^3)$ upper-bound.

Finally, it is open whether the problem of computing a 4-stable partition can be solved in polynomial time. In particular, is this problem complete for the complexity class PLS ?

4.4 The parallel complexity of coloring games

In the line of prior Section 4.3, we keep studying the complexity of computing stable partitions for unweighted games. However, the present section is focused on the complexity of computing Nash equilibria (1-stable partitions).

By Theorem 64, for every unweighted game, the better-response dynamic converges to a Nash equilibrium in polynomial time. However, we know by Theorem 67 that the same does not hold for k-stable partitions, with $k \geq 4$. Therefore, it might be desirable to have a better understanding of the complexity of computing Nash equilibria for these games.

4.4.1 Overall approach and main result

I shall investigate on the belonging of the problem – the computation of a Nash equilibrium in coloring games – to some complexity classes that are related to parallel and space complexity. The goal in doing so is to bring more insights on the complexity of the problem.

Complexity classes. In what follows, computations are performed on a parallel random-access machine (PRAM, see [GHR95]) with an unlimited amount of (numbered) processors. We will handle with read/write conflicts between processors with the strategy CREW-PRAM (concurrent read, exclusive write).

Let PTIME contain the decision problems that can be solved in *sequential* polynomial-time, that is with a single processor. Problem A reduces to problem B if given an oracle to solve B, then A can be solved in polylogarithmic-time with a polynomial number of processors. In particular, a problem B is PTIME-hard if every problem in PTIME reduces to B (this is formally defined as quasi-PTIME-hardness in [GHR95]). Such reductions are finer-grained than the more standard logspace reductions.

On the applicative point of view, we recall that coloring games have been proposed in order to design distributed algorithms on graphs, and to model the behaviour of social network users with limited memory and computing power. We note that any distributed algorithm on graphs can be simulated on a parallel machine with one processor per edge and per vertex. Furthermore, there are strong and well-known relationships between space and parallel complexity [Pap03]. Hence, the following result also brings more insights on the feasability of the proposed applications for coloring games in the literature.

The main result in this section can be stated as follows.

Theorem 74. *Computing a Nash equilibrium for coloring games is PTIME-hard.*

This theorem paves the way to a deepening of the complexity of computing Nash equilibria in graph games. I think that similar investigations should be pursued for other games where it can be computed a Nash equilibrium in polynomial time.

The reduction for proving Theorem 74 is from the standard MONOTONE CIRCUIT VALUE problem. However, the gadgets needed are technically challenging, and we will need to leverage nontrivial properties of coloring games in order to prove its correctness. I detail this reduction in what follows.

4.4.2 The reduction

4.4.2.1 The MONOTONE CIRCUIT VALUE problem

In order to prove Theorem 74, we will reduce from a variation of the well-known MONOTONE CIRCUIT VALUE problem, defined as follows.

Problem 1 (Monotone Circuit Value).

Input: *A boolean circuit $\mathcal{C}$ with m gates and n entries, a word $w \in \{0,1\}^n$ such that:*

- *the gates are either AND-gates or OR-gates;*
- *every gate has exactly two entries (in-degree two);*
- *a topological ordering of the gates is given, with the m^{th} gate being the output gate.*

Question: *Does $\mathcal{C}$ output 1 when it takes w as input ?*

This variation of Monotone Circuit Value is proved to be PTIME-complete in [GHR95]. On the technical point of view, it requires a topological ordering of the gates as part of the input. This non standard add up will be shown to be a key element in the reduction to coloring games.

In what follows, let $\langle \mathcal{C}, w \rangle$ be any instance of Monotone Circuit Value. We will reduce it to a coloring game as follows. Let $\mathcal{G} := (g_1, g_2, \ldots, g_m)$ be the gates of the circuit, that are topologically ordered.

4.4.2.2 Construction of the gate-gadgets

For every $1 \leq j \leq m$, the j^{th} gate will be simulated by a subgraph $G_j = (V_j, E_j)$ with $12(n+j) - 9$ vertices. We refer to Figure 4.5 for an illustration.

Let us give some intuition for the following construction of G_j. We aim at simulating the computation of the (binary) output of all the gates in $\mathcal{C}$ when it takes w as input. To do that, we will construct a supergraph G^- of G_j (to be defined later), then we will consider the unweighted game that is played on G^-. The goal of the construction will be to ensure that given a fixed Nash equilibrium for this game, we can guess the output of the j^{th} gate from the subcoloring of G_j. More precisely, the subcoloring will encode a "local certificate" that indicates which values on the two entries of g_j cause the output.

Observe that to certify that an OR-gate outputs 1, it suffices to show that it receives 1 on any of its two entries, whereas for an AND-gate it requires to show that it receives 1 on its two entries. Since by de Morgan's laws [DM47], the negation of an AND-gate can be transformed into an OR-gate and vice-versa, therefore, we need to distinguish between three cases in order to certify the output of the gate. So, the vertices in V_j are partitioned in three subsets of equal size $4(n+j) - 3$, denoted by V_j^1, V_j^2, V_j^3. Furthermore, for every $1 \leq t \leq 3$, every vertex in V_j^t is adjacent to every vertex in $V_j \setminus V_j^t$.

Let us now describe the structure of the three (isomorphic) subgraphs $G_j[V_j^t] = (V_j^t, E_j^t)$ with $1 \leq t \leq 3$. Informally, we will need this internal structure in order to ensure that every of the three subsets V_j^t will behave as a "truthful" certificate to decide on the output of the gate; *i.e.*, only a few vertices of V_j will be used to

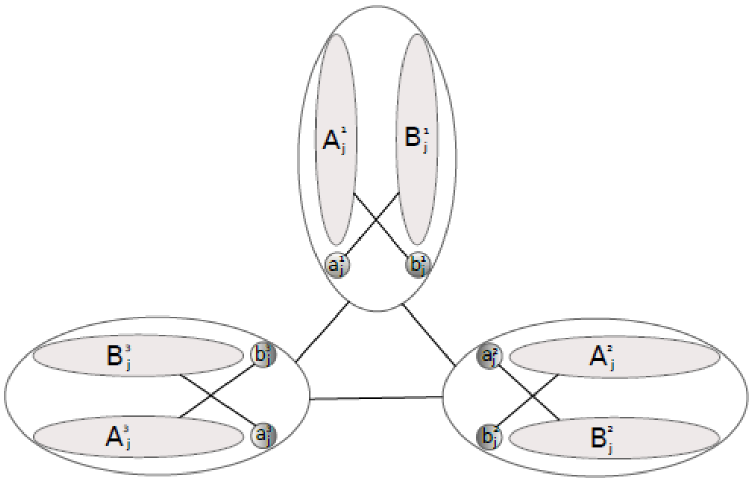


Figure 4.5: Gadget subgraph G_j representing the j^{th} gate. An edge between two subsets of vertices (delimited by an ellipse) denotes the existence of a complete bipartite subgraph.

certify the output of the j^{th} gate, while all others will be divided into artificial aggregates that we name "private groups" whose role is to ensure "truthfulness" of the certificate (this will be made clearer in the following). There are two nonadjacent vertices $a_j^t, b_j^t \in V_j^t$ playing a special role. The other vertices in $V_j^t \setminus \{a_j^t, b_j^t\}$ are partitioned in two subsets A_j^t, B_j^t of respective size $2(n+j)-3$ and $2(n+j)-2$. The sets A_j^t, B_j^t are called the *private groups* of a_j^t, b_j^t. Furthermore, every vertex in A_j^t is adjacent to every vertex in $V_j^t \setminus (A_j^t \cup \{a_j^t\})$, similarly every vertex in B_j^t is adjacent to every vertex in $V_j^t \setminus (B_j^t \cup \{b_j^t\})$.

Computation. Since all edges are defined above independently the one from the other, the graph $G_j[V_j^1] = (V_j^1, E_j^1)$ (encoded by its adjacency lists) can be constructed with $|V_j^1| + |E_j^1| = 4(n+j)^2 - 2(n+j) - 2$ processors simply by assigning the construction of each vertex and each edge to a different processor. Note that each processor can decide on the vertex, resp. the edge, it needs to compute from its number. Overall, it takes $\mathcal{O}(\log(n+j))$-time in order to construct $G_j[V_j^1]$ in parallel. The latter can be easily generalized in order to construct G_j in $\mathcal{O}(\log(n+j))$-time with $|V_j|+|E_j|$ processors. Therefore, the graphs $G_1, G_2, \ldots, G_m$ can be constructed in parallel in $\mathcal{O}(\log(n+m))$-time with $\sum_{j=1}^m(|V_j|+|E_j|)$ processors, that is (huge!) polynomial in $n+m$.

4.4.2.3 Construction of the graph

Let $X = \{x_1, x_1', \ldots, x_i, x_i', \ldots, x_n, x_n'\}$ contain $2n$ nonadjacent vertices, that are two vertices per letter in the binary word w. The (conflict) graph $G^- = (V, E)$ for the reduction has vertex-set $V = X \cup \left(\bigcup_{j=1}^m V_j\right)$. In particular, it has $2n - 9m + 6m(m+2n+1)$ vertices. Furthermore, $G^-[V_j]$ is isomorphic to G_j for every

$1 \leq j \leq m$. In order to complete our reduction, let us now describe how our gadgets are connected the one with the other.

For technical reasons, we will need to make adjacent every vertex in the private group A_j^t (resp. B_j^t), with $1 \leq j \leq m$ and $1 \leq t \leq 3$, to every vertex in $V \setminus V_j$. By doing so, note that every vertex in $V \setminus (A_j^t \cup \{a_j^t\})$ is adjacent to every vertex in A_j^t (resp., every vertex in $V \setminus (B_j^t \cup \{b_j^t\})$ is adjacent to every vertex in B_j^t). Furthermore, each edge is defined independently the one from the other. Hence, similarly as above, $\sum_{j=1}^m \sum_{t=1}^3 (|A_j^t| + |B_j^t|)|V \setminus V_j|$ processors are sufficient in order to construct these edges in $\mathcal{O}(\log(n+m))$-time, that is polynomial in $n+m$.

Finally, we recall that for every j, there are three cases to distinguish in order to decide on the output of the j^{th} gate, with each case being represented with some subset V_j^t. The union of subsets representing a *positive* certificate (output 1) is named Y_j, while the union of those representing a *negative* certificate (output 0) is named N_j. In particular, if the j^{th} gate is an OR-gate, let $Y_j := \{a_j^1, b_j^1, a_j^2, b_j^2\}$ and $N_j := \{a_j^3, b_j^3\}$ (it suffices to receive 1 on one input). Else, the j^{th} gate is an AND-gate, so, let $Y_j := \{a_j^1, b_j^1\}$ and $N_j := \{a_j^2, b_j^2, a_j^3, b_j^3\}$.

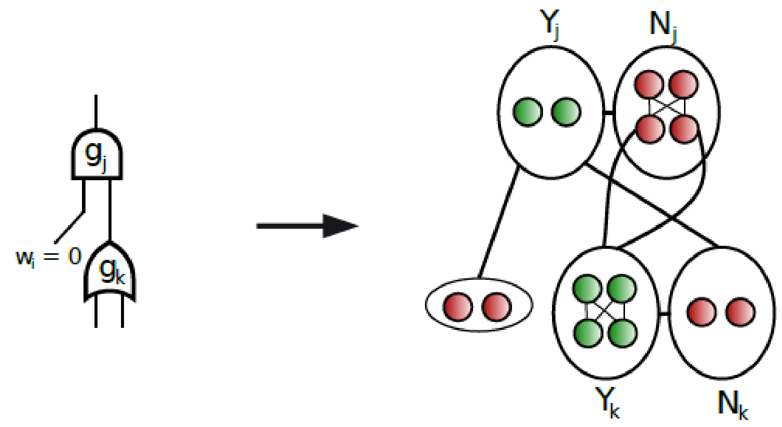


Figure 4.6: Edges in G^- to simulate the two connections of an AND-gate in the circuit.

Suppose the j^{th} gate is an OR-gate (the case where it is an AND-gate follows by symmetry, up to interverting Y_j with N_j, see also Figure 4.6). Let us consider the first entry of the gate. There are two cases.

- Suppose that it is the i^{th} entry of the circuit, for some $1 \leq i \leq n$.
  If $w_i = 0$ then we make both x_i, x_i' adjacent to both a_j^1, b_j^1.
  Else, $w_i = 1$, we make both x_i, x_i' adjacent to both a_j^3, b_j^3.
- Otherwise, the entry is some other gate of the circuit, and so, since gates are topologically ordered, it is the k^{th} gate for some $k < j$. We make every vertex in N_k adjacent to both a_j^1, b_j^1, and we make every vertex in Y_k adjacent to both a_j^3, b_j^3.

The second entry of the gate is similarly considered, up to replacing above the two vertices a_j^1, b_j^1 with a_j^2, b_j^2. We refer to Figure 4.6 for an illustration.

Let us point out that the graph G^-, obtained with our reduction, is *undirected*, whereas the original circuit $\mathcal{C}$ is a DAG (directed acyclic graph). However, since the sizes of private groups are proportional to the positions of the gates in the topological ordering of the circuit, this orientation of the edges can be easily retrieved, from the certificates with smaller privates groups to those with larger ones. Therefore, we do not lose any information.

Computation. Observe that there is only a constant number of edges that are added at this step for each gate. Furthermore, the construction of these new edges only requires to read the two in-neighbours of the gate in the circuit $\mathcal{C}$. As a result, the last step can be done in parallel in $\mathcal{O}(\log(n+m))$-time with m processors.

4.4.3 Proof of the main result

4.4.3.1 Structure of a Nash equilibrium

The (conflict) graph $G^- = (V, E)$ of the reduction defines an unweighted coloring game. Let us fix any Nash equilibrium for this game (that exists by Theorem 64). We will show that it is sufficient to know the color of every vertex in $Y_m \cup N_m$ in order to decide on the output of the circuit $\mathcal{C}$ (recall that the m^{th} gate is the output gate). To prove it, we will need the following technical claims in order to gain more insights on the structure of the equilibrium.

More precisely, we will prove that there are exactly $6m+1$ color classes, that are one color class per private group A_j^t or B_j^t and one additional color for the vertices in X. The intuition is that there are $2(n+m)$ vertices in one special color class (including X) that simulates the computation of the output of $\mathcal{C}$, whereas all other vertices are "trapped" with the vertices in their respective private group. We refer to Figure 4.7 for an illustration.

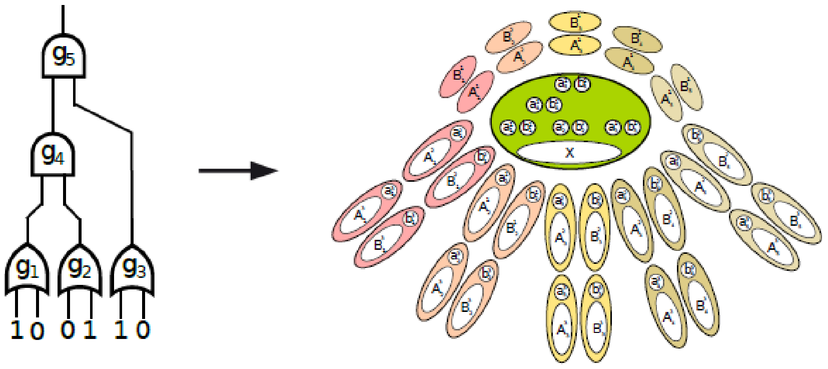


Figure 4.7: A boolean circuit (left) with a Nash equilibrium of the coloring game from our reduction (right). For ease of reading, edges of the graph are not depicted. Each color class is represented with an ellipse. Intuitively, vertices in the central color class simulate the computation of the output. Other color classes contain a private group and they are "inactive".

Full proofs of the claims are delayed to my publication [Duc16]. In what follows, we will denote by $L_c \subseteq V$ the subset of agents colored by c.

Claim 1. *For every j, any color class does not contain more than two vertices in every $Y_j \cup N_j$. Furthermore, if it contains exactly two vertices in $Y_j \cup N_j$ then these are a_j^t, b_j^t for some $1 \leq t \leq 3$.*

Proof. A Nash equilibrium is a proper coloring of G^-. Therefore, since any two vertices in different subsets among V_j^1, V_j^2, V_j^3 are adjacent by construction, they cannot have the same color. Since $Y_j \cup N_j = \{a_j^1, b_j^1, a_j^2, b_j^2, a_j^3, b_j^3\}$ and $a_j^t, b_j^t \in V_j^t$ for every $1 \leq t \leq 3$, the claim follows directly. ◇

Claim 2. *Any two vertices that are in a same private group have the same color. Similarly, x_i and x_i' have the same color for every $1 \leq i \leq n$.*

Proof. Let S be either a private group ($S = A_j^t$ or $S = B_j^t$ for some $1 \leq j \leq m$ and $1 \leq t \leq 3$), or a pair representing the same letter of word w (*i.e.*, $S = \{x_i, x_i'\}$ for some $1 \leq i \leq n$). Let $v \in S$ maximize her payoff and let c be her color. Note that v receives payoff $|L_c| - 1$ with L_c being the color class composed of all the vertices with color c. Furthermore, every $u \in S$ receives payoff lower than or equal to $|L_c| - 1$ by the choice of v. In such case, every $u \in S$ must be colored c, or else, since the adjacency and the nonadjacency relations are the same for u and v (they are twins), furthermore u, v are nonadjacent, the agent u would increase her payoff to $|L_c|$ by choosing c as her new color, thus contradicting the hypothesis that we are in a Nash equilibrium. ◇

The argument we use in Claim 2 is that twin vertices, *i.e.*, nonadjacent agents with the same neighbourhood, must have the same color. In order to prove the following Claim 3, we had to use the same argument under different disguises.

More precisely, consider a union $U \subseteq V$ of color classes. Then, $G^- \setminus U$ defines a coloring subgame, and the constriction of the coloring to the subgraph must be a Nash equilibrium for this subgame. it follows that twin vertices in $G^- \setminus U$ must have the same color, that was the key observation for proving Claim 3.

Claim 3. *Let $1 \leq j \leq m$ and $1 \leq t \leq 3$. Either A_j^t or $A_j^t \cup \{a_j^t\}$ is a color class, and in the same way either B_j^t or $B_j^t \cup \{b_j^t\}$ is a color class. Furthermore, either $B_j^t \cup \{b_j^t\}$ is a color class, or a_j^t and b_j^t have the same color.*

We recall that we aim at simulating the computation of the output of all the gates in $\mathcal{C}$. To do that, we will prove the existence of a special color class containing X and some pair of vertices in $Y_j \cup N_j$ for every j (Claim 5). Intuitively, the two vertices of $Y_j \cup N_j$ are used to certify the output of the j^{th} gate. However, this certificate is "local" in the sense that it assumes the output of the $j-1$ smaller gates to be already certified. Therefore, we need to prove that there can be no "missing gate", *i.e.*, every gate is represented in the special color class. This is where the topological ordering over the gates comes into play. In what follows, we recall that L_c denotes the subset of agents colored by c.

Claim 4. *Let c be a color such that $L_c \not\subseteq X$ and L_c does not intersect any private group (A_j^t or B_j^t for any $1 \leq j \leq m$ and $1 \leq t \leq 3$).*

Then, $X \subseteq L_c$ and there exists an index j_0 such that the following holds true: $|L_c \cap (Y_j \cup N_j)| = 2$ for every $1 \leq j \leq j_0$, and $L_c \cap (Y_j \cup N_j) = \emptyset$ for every $j_0 + 1 \leq j \leq m$.

Proof. By the hypothesis $L_c \not\subseteq X$ and L_c does not intersect any private group, so, there is at least one vertex of $\bigcup_{j=1}^{m}(Y_j \cup N_j)$ with color c. Let j_0 be the largest index j such that there is a vertex in $Y_j \cup N_j$ with color c. Since by Claim 1, there can be no more than two vertices of $Y_j \cup N_j$ that are in L_c for every j, therefore, by maximality of j_0 we get $|L_c| \leq |X| + 2j_0 = 2(n + j_0)$. In particular, observe that if $|L_c| = 2(n+j_0)$ then $X \subseteq L_c$ and for every $1 \leq j \leq j_0$ there are exactly two vertices in $Y_j \cup N_j$ with color c. So, let us prove that $|L_c| = 2(n + j_0)$, that will prove the claim.

By the choice of j_0, there is some $1 \leq t \leq 3$ such that $a_{j_0}^t \in L_c$ or $b_{j_0}^t \in L_c$. In particular, $|L_c| \geq \min\{|A_{j_0}^t|, |B_{j_0}^t|\} + 1 = 2(n + j_0) - 2$ or else, every vertex $v_{j_0}^t \in L_c \cap \{a_{j_0}^t, b_{j_0}^t\}$ would increase her payoff by choosing the color of the vertices in her private group (that is a color class by Claim 3), thus contradicting the hypothesis that we are in a Nash equilibrium.

We prove as an intermediate subclaim that for any $1 \leq j \leq j_0 - 1$ such that $L_c \cap (Y_j \cup N_j) \neq \emptyset$, there is some $1 \leq t' \leq 3$ such that $a_j^{t'}, b_j^{t'} \in L_c$. Indeed, in this situation, there is some t' such that $a_j^{t'} \in L_c$ or $b_j^{t'} \in L_c$. If $b_j^{t'} \in L_c$ then we are done as by Claim 3, $a_j^{t'} \in L_c$. Otherwise, $b_j^{t'} \notin L_c$ and we prove this case cannot happen. First observe that $a_j^{t'} \in L_c$ in this case. Furthermore, since $a_j^{t'}$ and $b_j^{t'}$ do not have the same color we have by Claim 3 that $B_j^{t'} \cup \{b_j^{t'}\}$ is a color class. In this situation, $b_j^{t'}$ receives payoff $2(n + j) - 2 \leq 2(n + j_0 - 1) - 2 < |L_c|$. Since in addition $a_j^{t'}$ and $b_j^{t'}$ are twins in $G \setminus (A_j^{t'} \cup B_j^{t'})$, vertex $b_j^{t'}$ could increase her payoff by choosing color c, thus contradicting that we are in a Nash equilibrium. This proves $a_j^{t'}, b_j^{t'} \in L_c$, and so, the subclaim.

By the subclaim, there is an even number $2k$ of vertices in $\bigcup_{j=1}^{j_0-1}(Y_j \cup N_j)$ with color c, for some $k \leq j_0 - 1$. Similarly, since by Claim 2 the vertices x_i, x_i' have the same color for every $1 \leq i \leq n$, $|X \cap L_c| = 2n'$ for some $n' \leq n$. Now there are two cases to be considered.

- Suppose that $b_{j_0}^t \in L_c$. Then, by Claim 3 $a_{j_0}^t \in L_c$. Furthermore $|L_c| \geq 2(n + j_0) - 1$ or else, vertex $b_{j_0}^t$ would increase her payoff by choosing the color of the vertices in $B_{j_0}^t$ (that is a color class by Claim 3), thus contradicting the hypothesis that we are in a Nash equilibrium. As a result, $|L_c| = 2(n'+k+1) \geq 2(n + j_0) - 1$, that implies $n' + k \geq n + j_0 - 1$, and so, $|L_c| \geq 2(n + j_0)$, as desired.
- Else, $b_{j_0}^t \notin L_c$ and we prove this case cannot happen. First observe that $a_{j_0}^t \in L_c$. Furthermore, $|L_c| = 2(n'+k)+1 \geq 2(n+j_0)-2$, that implies $n'+k \geq n+j_0-1$, and so, $|L_c| \geq 2(n + j_0) - 1$. However, since $a_{j_0}^t$ and $b_{j_0}^t$ do not have the same color, $B_{j_0}^t \cup \{b_{j_0}^t\}$ is a color class by Claim 3. In particular, $b_{j_0}^t$ receives payoff

$2(n+j_0)-2 < |L_c|$. Since $a_{j_0}^t, b_{j_0}^t$ are twins in $G \setminus (A_{j_0}^t \cup B_{j_0}^t)$, vertex $b_{j_0}^t$ could increase her payoff by choosing color c, thus contradicting that we are in a Nash equilibrium.

Altogether, $|L_c| \geq 2(n+j_0)$, that proves the claim. $\diamond$

We point out that by combining Claim 1 with Claim 4, one obtains that for every $1 \leq j \leq m$, there are either zero or two vertices in $Y_j \cup N_j$ in each color class not containing a private group, and in case there are two vertices then these are a_j^t, b_j^t for some $1 \leq t \leq 3$. We elaborate on this property in order to prove the following Claim 5.

Claim 5. *Any two vertices in X have the same color. Furthermore, for every $1 \leq j \leq m$, every vertex in $Y_j \cup N_j$ either has the same color as vertices in X or as vertices in her private group.*

Finally, we will need a "truthfulness" property to prove correctness of our reduction. Namely, the value of the output of any gate in the circuit must be correctly guessed from the agents with the same color as vertices in X. We prove this, as for Claim 1, by elaborating on the property that every Nash equilibrium is a proper coloring of G^-. In this situation, the edges added at the last step of the reduction ensure that the agents of two "uncompatible certificates" cannot be assigned the same color.

Claim 6. *Let $1 \leq j_0 \leq m$ such that for every $1 \leq j \leq j_0$, there is at least one vertex in $Y_j \cup N_j$ with the same color c_0 as all vertices in X. Then for every $1 \leq j \leq j_0$, $L_{c_0} \cap Y_j \neq \emptyset$ if and only if the output of the j^{th} gate is 1.*

4.4.3.2 Proof of Theorem 74

Proof of Theorem 74. Let $\langle \mathcal{C}, w \rangle$ be any instance of Monotone Circuit Value. Let $G^- = (V,E)$ be the conflict graph obtained with our reduction. It can be constructed in polylogarithmic-time with a polynomial number of processors. The graph G^- defines an unweighted coloring game. We fix any Nash equilibrium for this game, that exists by Theorem 64. By Claim 5, any two vertices in X have the same color c_0. We will prove that there is at least one vertex in Y_m with color c_0 if and only if the circuit $\mathcal{C}$ outputs 1 when it takes w as input. Since Monotone Circuit Value is PTIME-complete [GHR95], the latter will prove that computing a Nash equilibrium for coloring games is PTIME-hard.

By Claim 6, we only need to prove that for every $1 \leq j \leq m$, there is at least one vertex in $Y_j \cup N_j$ with color c_0. To prove it by contradiction, let j_0 be the smallest index j such that no vertex in $Y_j \cup N_j$ has color c_0. By Claim 5, every vertex in $Y_{j_0} \cup N_{j_0}$ has the same color as her private group. In particular, the three of $a_{j_0}^1, a_{j_0}^2, a_{j_0}^3$ receive payoff $2(n+j_0)-3$. We will prove that one of these three agents could increase her payoff by choosing c_0 as her new color, thus contradicting that we are in a Nash equilibrium.

Indeed, by the minimality of j_0, it follows by Claim 4 that for any $1 \leq j \leq j_0 - 1$, there are exactly two vertices of $Y_j \cup N_j$ with color c_0, while for every $j_0 \leq j \leq m$ there is no vertex in $Y_j \cup N_j$ with color c_0. As a result, $|L_{c_0}| = 2(n + j_0) - 2$. In particular, any agent among $a^1_{j_0}, a^2_{j_0}, a^3_{j_0}$ could increase her payoff by choosing c_0 as her new color — provided she is nonadjacent to every vertex in L_{c_0}. We will show it is the case for at least one of the three vertices, that will conclude the proof of the theorem. Assume w.l.o.g. that the j_0^{th} gate is an OR-gate (indeed, since by de Morgan's laws, the negation of an AND-gate can be transformed into an OR-gate and vice-versa, both cases are symmetrical). There are two cases.

- Suppose that the output of the j_0^{th} gate is 1. In such case, there must be an entry of the gate such that: it is the i^{th} entry of the circuit, for some $1 \leq i \leq n$, and $w_i = 1$; or it is the k^{th} gate of the circuit for some $k < j_0$ and the output of that gate is 1. In the latter case, we have by Claim 6 that the two vertices of $Y_k \cup N_k$ with color c_0 are in the set Y_k.
  Assume w.l.o.g. that the above-mentioned entry is the first entry of the gate. By construction, the two vertices $a^1_{j_0}, b^1_{j_0}$ are nonadjacent to every vertex in L_{c_0}.
- Else, the output of the j_0^{th} gate is 0. Therefore, for every entry of the gate: either it is the i^{th} entry of the circuit, for some $1 \leq i \leq n$, and $w_i = 0$; or it is the k^{th} gate of the circuit for some $k < j_0$ and the output of that gate is 0. In the latter case, we have by Claim 6 that the two vertices of $Y_k \cup N_k$ with color c_0 are in the set N_k. By construction, the two vertices $a^3_{j_0}, b^3_{j_0}$ are nonadjacent to every vertex in L_{c_0}.

In both cases, it contradicts our assumption that we are in a Nash equilibrium.

□

Conclusion. Theorem 74 proves that computing a Nash equilibrium for coloring games is PTIME-hard. This may be hint that these games are a too powerful computational mechanism design for "lightweight" distributed applications. In this respect, an interesting open problem would be to determine the classes of conflict graphs for which this hardness result holds.

Furthermore, we recall that computing a Nash equilibrium for generalized coloring games is PLS-complete [BZ03]. Hence, this result reinforces the view that for many PLS-hard "weighted" games, the corresponding "unweighted" game is PTIME-hard [Sch91].

4.5 Weighted games: existence of equilibria

Next, we go back to generalized (weighted) coloring games in this section. Every generalized coloring game admits a Nash equilibrium [BZ03]. So, we are more interested in the existence of k-stable partition, for $k \geq 2$. However, as shown with Figure 4.3, not all generalized coloring games admit a 2-stable partition. Since in contrast, unweighted games admit a k-stable partition for every fixed k, it looks natural to investigate on the impact of a *fixed* set of edge-weights $\mathcal{W}$ on the existence of stable partitions.

We are particularly interested in the special case where all edge-weights of the underlying graph G are comprised in $\mathcal{W} = \{-\infty, 0, 1\}$. Roughly, in this modest extension of the unweighted games, we now allow *indifference* relationships between some agents. More formally, the goal of the agents is now to construct a proper coloring of the conflict graph G^- while maximizing their number of neighbours in the friendship graph G^+ with the same color as theirs. Perhaps surprisingly, we shall prove that even in this slight extension, the existence of stable partitions is much more constrained than it is for the unweighted games.

This is joint work with Dorian Mazauric and Augustin Chaintreau.

4.5.1 Positive results

On the one hand, we relate some structural properties of the underlying graph G with the existence of stable partitions. In particular, we relate the existence of stable partitions with the *girth* (size of a smallest cycle) in the friendship graph:

Theorem 75. *Let $G = (V, w)$ have all its edge-weights in $\{-\infty, 0, 1\} \cup -\mathbb{N}$. If the friendship graph G^+ has girth at least $k + 1$ then the generalized coloring game that is played on G admits a k-stable partition.*

Furthermore, the better-response dynamic applied to this above game converges to a k-stable partition within a quadratic number of steps.

Theorem 75 follows from a potential function argument. More precisely, let us define the global utility of a given coloring as the sum of the individual payoff of every agent. See Figure 4.8 for an example. We prove that it is a potential function which increases after any k-deviation.

In order to see the difficulty, we emphasize that even for unweighted games, this above potential function might decrease after a k-deviation (*e.g.*, see the example of 4-deviation that is given in Section 4.3.3 and the related illustration of Figure 4.8). In fact, if j denotes the color assigned to all the agents in the k-deviation then the global utility increases only if all the agents deviating increase their respective payoff in large part due to the agents already colored j. This may not be the case if there are many agents of this k-subset that are pairwise connected by an edge with positive weight. However, if we now assume that the friendship graph G^+ has a large girth then we can upper-bound the number of edges with positive weights among any small subset of agents (because such small subsets must induce a forest in G^+), thereby preventing that case from happening.

In particular, since any friendship graph has girth at least three, we obtain the following corollary:

Corollary 76. *Let $G = (V, w)$ have all its edge-weights in $\{-\infty, 0, 1\} \cup -\mathbb{N}$. Then, the generalized coloring game that is played on G admits a 2-stable partition.*

Furthermore, the better-response dynamic applied to this above game converges to a 2-stable partition within a quadratic number of steps.

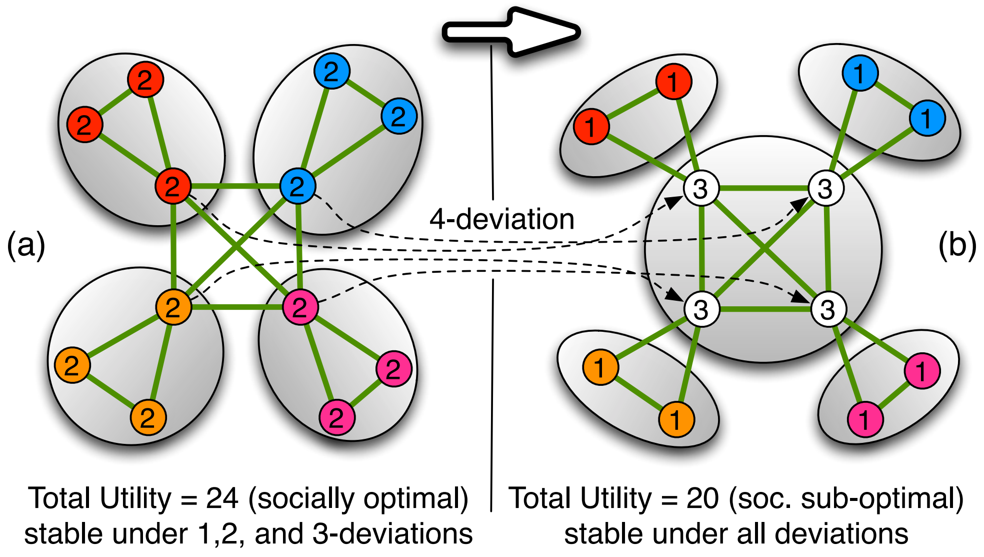

4-deviation
(a)
(b)
Total Utility = 24 (socially optimal)
stable under 1,2, and 3-deviations
Total Utility = 20 (soc. sub-optimal)
stable under all deviations

Figure 4.8: Change of configuration for an unweighted game after a 4-deviation. For ease of readability, only the edges of the friendship graph are represented. Agents are labeled with their payoff.

Perspectives. It is open whether similar results can be obtained for a larger family of sets $\mathcal{W}$. In particular, can it be obtained similar results for some $\mathcal{W}$ with two distinct positive weights ?

4.5.2 The hardness of recognizing games with k-stable partitions

We finally present a more complex construction of weighted games with no k-stable partition for some small value of k. Furthermore, we will explain how the mere existence of a single counter example impacts on the complexity of the recognition of games with k-stable partitions.

On the one hand, as shown with Figure 4.3, there are generalized coloring games that do not admit a 2-stable partition. On the other hand, we proved with Corollary 76 that by constraining the set $\mathcal{W}$ of admissible edge-weights, one obtains a large class of weighted games that admit a 2-stable partition. Surprisingly, this latter result cannot be improved already for $\mathcal{W} = \{-\infty, 0, 1\}$. Precisely, we give in Figure 4.9 an example of a graph G with weights in $\mathcal{W} = \{-\infty, 0, 1\}$ so that the coloring game that is played on G does not admit a 3-stable partition!

The construction in Figure 4.9 borrows from the one of Figure 4.3 (*i.e.*, the nonexistence of 2-stable partitions in generalized coloring games). Roughly, we impose the friendship graph and the conflict graph to be highly symmetric, that ensures that 2-stable partitions for the game are isomorphic. Then, we show that the isomorphism between two distinct 2-stable partitions translates to a 3-deviation from one to the other.

Proposition 77. *There is a graph $G = (V, w)$ whose edge-weights are constrained to $\mathcal{W} = \{-\infty, 0, 1\}$ and such that there does not exist a 3-stable partition for the coloring game defined on G.*

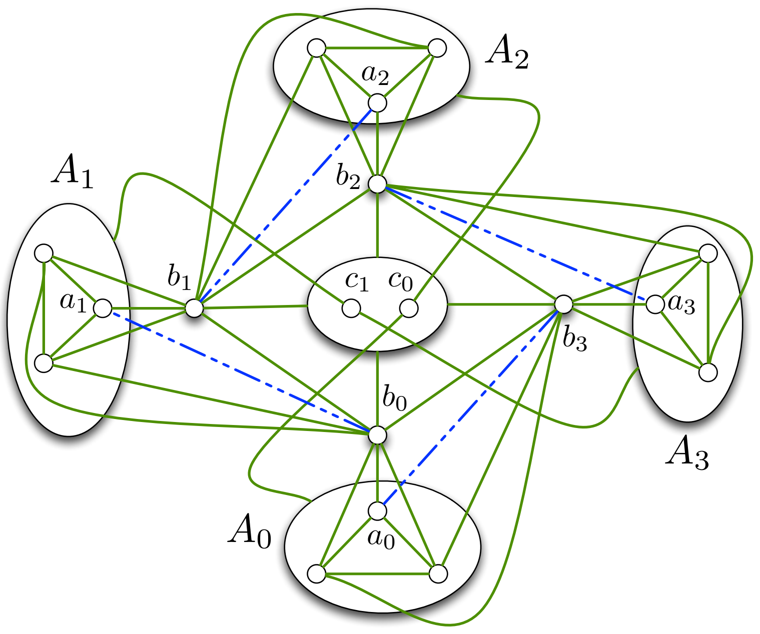


Figure 4.9: A graph $G = (V, w)$ with edge-weights in $\mathcal{W} = \{-\infty, 0, 1\}$. The coloring game played on G does not admit a 3-stable partition. To keep the graph readable, we use conventions. (1) Some sets of nodes are grouped within a circle; an edge from another node to that circle denotes an edge to *all* elements of this set. (2) Edges of the conflict graph are not represented. In particular, all nodes that are not connected by an edge on the figure are connected by an edge with negative weight $-\infty$. (3) Green solid edges represent edges with weight 1, whereas blue dashed edges represent edges with weight 0.

Proof. The set of vertices consists of four sets A_i, $0 \leq i \leq 3$, each of equal size $h \geq 2$ and with a special vertex a_i, plus four vertices b_i, $0 \leq i \leq 3$, and two vertices c_0 and c_1. In what follows, indices are taken modulo 2 for c_j, $j \in \{0, 1\}$, and they are taken modulo 4 everywhere else. Figure 4.9 represents the example with $h = 3$. The friendship graph G^+ here consists of all the edges with weight 1; it contains:

1. all the edges between nodes in A_i ($0 \leq i \leq 3$);
2. edges between b_i and A_i ($0 \leq i \leq 3$);
3. edges between b_i and $A_{i+1} \setminus \{a_{i+1}\}$ ($0 \leq i \leq 3$);
4. edges between b_i and b_{i-1} and b_{i+1} ($0 \leq i \leq 3$);
5. edges between c_0 and all the b_i, and edges between c_1 and all the b_i;
6. edges between c_0 and $A_0 \cup A_2$, and edges between c_1 and $A_1 \cup A_3$.

Moreover, there are four edges with weight 0, namely the edges $\{b_i, a_{i+1}\}$. All the other pairs of agents represent "*enemies*" (they are pairwise connected by an edge with negative weight $-\infty$). That is two nodes in different $A_i, A_{i'}$ are enemies; a user b_i is enemy of b_{i+2} and of the nodes in A_{i+2} and A_{i+3}; c_0 and c_1 are enemies; c_0 is enemy of the nodes in A_1 and A_3, and c_1 is enemy of the nodes in A_0 and A_2. We now assume by contradiction there exists a 3-stable partition for the coloring game defined on $G = (V, w)$.

Full proofs for the following claims are postponed to our paper [DMC17].

Claim 78. *Every agent in A_i picks the same color.*

Our key instrument for proving this claim is a generalization of *false twins* to weighted graphs. We recall that given an *unweighted game* that is played on the conflict graph G^-, for any Nash equilibrium for this game, false twins in G^- must have the same color (see Claim 2).

Now, given an edge-weighted graph $G = (V, w)$, we say that u and u' are *quasi-twins* if $w_{uu'} > 0$ and for all nodes $v \in V \setminus \{u, u'\}$, $w_{uv} = w_{u'v}$ except maybe for one v_0 for which $|w_{uv_0} - w_{u'v_0}| = 1$. We can observe that for unweighted games, quasi-twins are exactly the false twins in the conflict graph. In [DMC17], we prove that for any Nash equilibrium of the coloring game that is played on G, quasi-twins must have the same color. Since in the above construction for Proposition 77, the agents in A_i are pairwise quasi-twins, Claim 78 follows from this result directly.

Claim 79. *b_i picks the same color as the agents in A_i or the agents in A_{i+1}.*

Claim 80. *There is an i such that agents in A_i, b_i and b_{i-1} pick the same color.*

It follows by Claim 80 that there is an i such that the agents in A_i, b_i, b_{i-1}, c_i all pick the same color. Moreover, such a color class is unique in the 3-stable partition due to the conflict graph in G (induced by the conflict edges). In what follows, let L_{i_0} be the color class of a_0 in the 3-stable partition. By symmetry, we will assume $L_{i_0} = \{b_0, b_3, c_0\} \cup A_0$.

Case 1: the agents a_2, b_1, b_2 all have the same color. In particular, by Claims 78 and 79 their color class is $A_2 \cup \{b_1, b_2\}$.

Then, there are two subcases. Suppose that a_1 and c_1 have the same color, in which case their color class is $A_1 \cup \{c_1\}$. In this situation, the agent b_1 would increase her payoff from $1 + (|A_2| - 1) = |A_2| = h$ to $1 + |A_1| = h + 1$ by choosing the same color as a_1 and c_1. So, there is a 1-deviation. Otherwise, a_1 and c_1 do not have the same color, so, their respective color classes are A_1 and either $\{c_1\}$ or $A_3 \cup \{c_1\}$. Then, the agents b_1 and c_1 would increase their respective payoff from $1 + (|A_2| - 1) = |A_2| = h$ and $\leq |A_3| = h$ to $1 + |A_1| = h + 1$ by choosing the same color as a_1. So, there is a 2-deviation.

Case 2: both agents a_2 and b_2 have the same color, but b_1 has a different color. In particular, by Claims 78 and 79 their respective color classes are $A_2 \cup \{b_2\}$ and either $A_1 \cup \{b_1\}$ or $A_1 \cup \{b_1, c_1\}$.

Then, there are two subcases. Suppose that the agents a_3 and c_1 have the same color, in which case their color class is $A_3 \cup \{c_1\}$. Then, both b_2 and b_3 would increase their respective payoff from $|A_2| = h$ and $2 + (|A_0| - 1) = 1 + |A_0| = h + 1$ to $2 + (|A_3| - 1) = |A_3| + 1 = h + 1$ and $2 + |A_3| = h + 2$ by choosing the color of a_3. Otherwise, a_3 and c_1 do not have the same color, in which case the color class of c_1 is either $\{c_1\}$ or $A_1 \cup \{b_1, c_1\}$. But then the three of b_2, b_3, c_1 would increase their respective payoff from $|A_2| = h,\ 2 + (|A_0| - 1) = 1 + |A_0| = h + 1,$ and $\leq 1 + |A_1| = h + 1$ to $2 + (|A_3| - 1) = 1 + |A_3| = h + 1,\ 2 + |A_3| = h + 2,$ and $2 + |A_3| = h + 2$ by choosing the same color as a_3.

Case 3: both agents a_2 and b_1 have the same color, but b_2 has a different color, in which case their respective color classes are $A_2 \cup \{b_1\}$ and either $A_3 \cup \{b_2\}$ or $A_3 \cup \{b_2, c_1\}$ by Claim 79. In that case, b_1 would increase her payoff from $|A_2| - 1 = h - 1$ to $|A_1| = h$ by choosing the color of a_1, so, there is a 1-deviation.

Case 4: the agent a_2 has a different color than b_1 and b_2. In this case, their respective color classes are: A_2, either $A_1 \cup \{b_1\}$ or $A_1 \cup \{b_1, c_1\}$, either $A_3 \cup \{b_2\}$ or $A_3 \cup \{b_2, c_1\}$. In particular, b_2 and a_3 have the same color.

Then, there are two subcases. Suppose that c_1 and a_3 have the same color. In this situation, their color class is $A_3 \cup \{b_2, c_1\}$. So, the agent b_3 would increase her payoff from $2 + (|A_0| - 1) = h + 1$ to $2 + |A_3| = h + 2$ by choosing this color, so, there is a 1-deviation. Otherwise, c_1 and a_3 do not have the same color, in which situation their respective color classes are: either $\{c_1\}$ or $A_1 \cup \{b_1, c_1\}$, and $A_3 \cup \{b_2\}$. But then both b_3 and c_1 would increase their respective payoff from $\leq h + 1$ to $h + 2$ by choosing the color of a_3.

Finally, since in all cases there is a 3-deviation, there does not exist a 3-stable partition for the coloring game defined on G. □

Let us define, for every fixed set $\mathcal{W}$, $k(\mathcal{W})$ to be the largest k such that every coloring game which is played on a graph with edge-weights in $\mathcal{W}$ admits a k-stable partition. As an example, for the special case of unweighted games, we have by [KL13] that $k(\{-\infty, 1\}) = +\infty$. In contrast, we have by the combination of Corollary 76 and Proposition 77 that $k(\{-\infty, 0, 1\}) = 2$. In Table 4.1, we report on the value of $k(\mathcal{W})$ for most sets $\mathcal{W}$.

$\mathcal{W}$	$k(\mathcal{W})$
$\{-\infty, a\}, a > 0$	∞
$\{-\infty, 0, a\}, a > 0$	2
$\{-\infty, a, b\}, b > a > 0$	1
$\{-a, b\}, a > 0, b > 0$	$\leq 2 \cdot \lceil \frac{a+1}{b} \rceil + 1$

Table 4.1: Values of $k(\mathcal{W})$ for different $\mathcal{W}$.

Surprisingly, this above threshold $k(\mathcal{W})$ fully characterizes the complexity of recognizing coloring games with a k-stable partition. More precisely, we have obtained the following dichotomy result for generalized coloring games:

Theorem 81. *Let $\mathcal{W}$ contain $-\infty$ and $k \geq 1$ be fixed. Then, the problem of deciding whether a given coloring game, played on a graph with edge-weights in $\mathcal{W}$, admits a k-stable partition is either:*

- *trivial if $k \leq k(\mathcal{W})$;*
- *or NP-complete if $k > k(\mathcal{W})$.*

In order to get a better intuition for the above Theorem 81, let us consider a minimum-size counter-example $G_0 = (V_0, w_0)$ such that the coloring game played on G_0 does not admit a k-stable partition. Our reduction constructs, from any unweighted graph $G = (V, E)$, an edge-weighted supergraph of G_0 (that is illustrated with Figure 4.10).

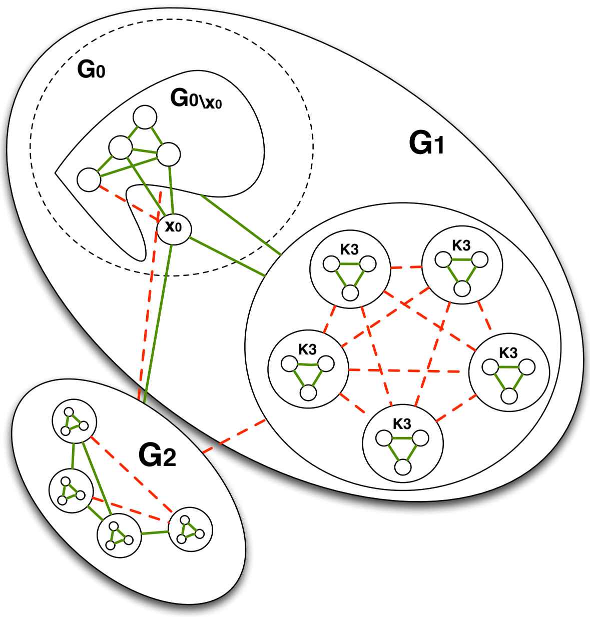


Figure 4.10: Reduction from Maximum independent set. The graph G_0 represents a minimum-size counter-example. Conflict edges with negative weight $-\infty$ are drawn in dashed red whereas all edges drawn in bold green have the same positive weight.

For this graph to have a k-stable partition, one needs a way to force some special agent $x_0 \in V_0$ to pick a different color than the other agents in $V_0 \setminus x_0$. Then, by minimality of the counter-example, the coloring subgame that is played on $G_0 \setminus x_0$ admits a k-stable partition and we are able to extend this subcoloring to a k-stable partition for the game played on the supergraph. Altogether combined, this game played on the supergraph admits a k-stable partition if and only if some agent x_0

can be forced to take a different colour than all other agents in $V_0 \setminus x_0$. Finally, we prove that x_0 indeed takes a different color than the agents of $V_0 \setminus x_0$ if and only if it is part of a large clique in the friendship graph. The latter is shown to correspond to a large independent set in the unweighted graph G that we use for the reduction. As a result, since the MAXIMUM INDEPENDENT SET problem is NP-complete [Dai80], this achieves proving that the problem of recognizing coloring games with a k-stable partition is NP-hard.

4.6 Extensions of coloring games

This section finally covers other games that encompass more aspects of coalition and group formation. We discuss on the extent to which our results for coloring games can be applied to this broader setting. In particular, we intend the following to be a high level description, and so, we made the choice to postpone the proofs of all the results to the research report [DMC12]. These results have not been published elsewhere.

4.6.1 Gossiping

Coloring games with gossip have been introduced by Kleinberg and Ligett in [KL13] for their study of community formation. Such game is still played on an edge-weighted graph $G = (V, E, w)$, with the vertices of G being the agents of the game. However, two agents with distinct colors may now "gossip", in which case both color classes they are part of are merged. Obviously, and as before, this deviation will only take place if it makes increase the utility of the two agents.

Formally, given $G = (V, E, w)$ and $c : V \to \mathbb{N}$, a gossip-deviation w.r.t. c is a 2-subset $\{u, v\}$ such that $c(u) \neq c(v)$ and:

$$\sum_{x | c(x) = c(u)} w_{vx} > 0, \quad \sum_{y | c(y) = c(v)} w_{uy} > 0.$$

The color c represents a k-stable partition for the coloring game with gossip if it is a k-stable partition for the generalized coloring game played on G (without gossip) *and in addition* there is no gossip deviation.

It actually turns out that *unweighted* coloring games with gossip are equivalent to the classical unweighted coloring games. Indeed, consider an unweighted game played on the conflict graph G^-, c a proper coloring of G^-, and suppose that there are two agents u and v gossiping. In particular, u and v cannot be adjacent in G^- to any agent colored by $c(v)$ or $c(u)$ (or else, they would not benefit from merging the two color classes $L_{c(u)}$ and $L_{c(v)}$). Let us assume w.l.o.g. that $|L_{c(u)}| \geq |L_{c(v)}|$. Then, the agent v would also strictly increase her payoff by changing her current color $c(v)$ for $c(u)$. As a result, if there exists a gossip deviation then there is a 1-deviation.

However, in the more general case of weighted games, we prove that there may not exist a 2-stable partition already when there is a unique and fixed positive weight in $\mathcal{W}$. This is in sharp contrast with Corollary 76.

4.6.2 Asymmetry

Another natural variation of coloring games is to make them play on a directed graph. In this situation, colorings of the game and strategies and utility functions of the agents can be defined similarly as before. However, it may now be the case that $w_{uv} \neq w_{vu}$ for some pairs u, v. These games are sometimes called additively separable (asymmetric) Hedonic games [BZ03]. We refer to Figure 4.11 for an illustration.

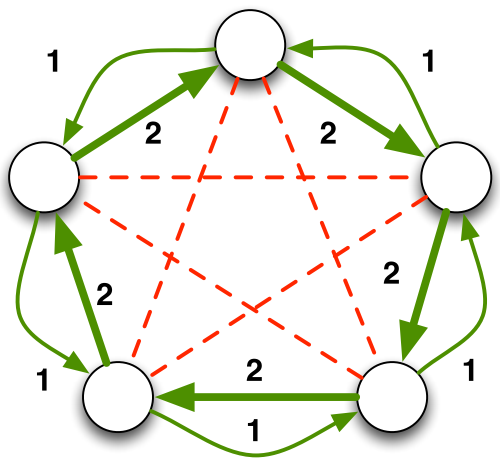


Figure 4.11: A coloring game played on a directed graph. Bidirectional arcs with negative weight $-\infty$ are drawn in dashed red. This game can be shown not to admit a Nash equilibrium.

Even if modest generalization of coloring games, the addition of asymmetrical weights leads to much stronger form of intractability. This can be seen with a simple digraph $D = (\{u, v\}, w)$ such that $w_{uv} > 0$ whereas $w_{vu} < 0$. Clearly, there does not exist any Nash equilibrium for the game played on D.

On the complexity point of view, the problem of deciding whether an asymmetric game admits a Nash equilibrium is NP-hard [SD10]. We prove that this result holds already when there can be no more than two color classes at equilibrium (we prove this by reducing from the well-known PARTITION problem). We recall that in contrast, every generalized coloring games admits a Nash equilibrium, and that such an equilibrium can be computed in quasi-polynomial time with better-response dynamics.

4.6.3 List coloring games

In [DMC12], we introduced a third variation of coloring games, where the strategy of an agent is no more her color, but rather a list of q colors with $q \geq 1$ being a fixed constant. On the social network analysis point of view, our aim in doing so was to allow every user to be part of different communities in order to better represent the community formation process.

In particular, given $G = (V, E, w)$, a configuration of the q-list coloring game played on this graph is a list coloring of G with each vertex having a list of at most q colors, and we name by $\ell(v)$ the list of any agent $v \in V$. Given a fixed q-list coloring of G, the utility function of v now depends on the number of colors that v shares with each peer, that can be written as:

$$\sum_{u \in V} h\left(|\ell(u) \cap \ell(v)|, w_{uv}\right) \tag{4.1}$$

where $h(g, w)$ is a function measuring the utility of sharing g colors with an agent when it is connected to v by an edge with weight w. Note that we assume, without loss of generality, that:

$$h(0, .) = 0,\ h(., 0) = 0 \text{ and } \forall w \in \mathbb{Q},\ h(1, w) = w$$

$$\forall g \in \mathbb{N},\ w \mapsto h(g, w) \text{ is a non-decreasing function,}$$

$$\forall w \in \mathbb{Q},\ g \mapsto w \cdot h(g, w) \text{ is a non-decreasing function.}$$

The last property simply ensures that $h(g, w)$ increases with g when w is positive, and decreases with g when w is negative. In practice, most of our results are proved in the simpler case where $h : (g, w) \mapsto (1 + \varepsilon g)w$, where ε is a small constant.

On the positive side, every q-list coloring game admits a Nash equilibrium. This can be shown by noticing that a q-list coloring game is a potential game, with its potential function being the global utility (sum of the utility functions of every agent). However, for every $q > 1$, we prove that there exist *unweighted* q-list coloring games that do not admit a 3-strong Nash equilibrium (robust to any coalition of at most three agents). The latter result is in sharp contrast with [KL13, EGM12], where the authors prove that every unweighted coloring game admits a k-stable partition for every fixed $k \geq 1$.

Last, we want to emphasize, perhaps counter-intuitively, that a decrease of the parameter q does not preserve the existence of k-strong equilibria. Namely, for every q, there exists $G_q = (V, E, w)$ such that:

- the q-list coloring game played on G_q *does not* admit any 2-strong Nash equilibrium;
- whereas for any other $q' \neq q$, the q'-list coloring game that is played on this same graph G_q does admit a 2-strong Nash equilibrium.

4.6.4 Coloring games on hypergraphs

Finally, we briefly consider the case where we replace the underlying graph $G = (V, E, w)$ by a *hypergraph* $H = (V, E, w)$, with $w : E \mapsto \mathbb{Q} \cup \{-\infty\}$ being a weight function on the hyperedges. On the social network point of view, hyperedges allow one to account for more complex types of relationships between the users.

Formally, given $H = (V, E, w)$ and $c : V \to \mathbb{N}$ a coloring of H, the utility function of any agent $v \in V$ can now be written as the sum of the weights w_e, for all hyperedge e to which v is incident and such that every vertex $u \in e$ satisfies $c(u) = c(v)$. In short, it is:

$$\sum_{e \in E \mid \{v\} \subseteq e \subseteq L_{c(v)}} w_e,$$

with $L_{c(v)} = \{u \in V \mid c(u) = c(v)\}$. This game was studied by Deng and Papadimitriou in [DP94], but with transferable utilities[4].

On the positive side, every coloring game played on a hypergraph is a potential game, with its potential function being the sum of the weights w_e for all *monocolored* hyperedges e (*i.e.*, every two vertices in e must be assigned the same color). If the coloring game is played on a graph then the latter function is equal to half of the global utility. However, this is not true anymore for coloring games on hypergraphs, because hyperedges may now be of arbitrary size.

In particular, we get that every coloring game played on a hypergraph admits a Nash equilibrium, and that one such equilibrium can be computed in quasi-polynomial time with better-response dynamics. We can also extend the positive result of Theorem 75 by taking for cycles the notion of Berge cyclicity (cycles in the incidence graph). Unfortunately, there exist hypergraphs with girth two (w.r.t. Berge cyclicity), so, this extended Theorem 75 has weaker consequences for hypergraphs than it has for graphs. As an example, Corollary 76 does not hold for coloring games on hypergraphs.

4.7 Concluding remarks

Our results in this section shed new lights on the complexity of coloring games. In particular, our results for generalized coloring games in Section 4.5 reinforce the relationship between these games and the MAXIMUM INDEPENDENT SET problem in graphs.

Furthermore, we presented in Section 4.3 an interesting relationship between unweighted games (non generalized coloring games) and the lattice of integer partitions. I believe that an in-depth study of this relationship will help to better understand the structure of stable partitions for unweighted games, and the com-

[4]Informally, there are transferable utilities if arbitrary subsets of agents can share their respective utility functions together, whose total sum is then reparted to these agents w.r.t. some rules.

plexity for computing their equilibria. In particular, the main open question in this field is whether the problem of computing 4-stable partitions is PLS-complete.

My investigations on the parallel and space complexity for computing Nash equilibria, in Section 4.4, have been firstly motivated by this above question. Indeed, I hope that the reduction from the Monotone Circuit Value problem to the computation of Nash equilibria can be transformed into a reduction from FLIP – a circuit computation problem that is the standard PLS-complete problem [JPY88] – to the computation of 4-stable partitions.

On a more general side, an interesting question would be to determine whether conversely, PLS-completeness for a “weighted” game implies PTIME-completeness for some corresponding ’unweighted” game ? Relationships between PLS-completeness and PTIME-completeness have been investigated since the original paper [JPY88] (introducing the complexity class PLS). It was conjectured that PLS-completeness for a search problem implies that checking for the local optimality of a solution is PTIME-complete. However, this conjecture was disproved in [Kre89]. Since for many PLS-complete problems, there exists a local-search algorithm that runs in quasi polynomial time (polynomial in the size, but exponential in the weights), any variation of these games where the weights are bounded is trivially in PTIME. Thus, proving or disproving that these variations are PTIME-hard would make advance our understanding of what makes a search problem PLS-hard.

CHAPTER 5

Learning formulas in a noisy model

Summary

We introduce a new learning model in Section 5.2. This model is motivated by some applications in *Web's transparency*, that is a nascent field where there is a need for uncovering data misuse online. Our objective is to learn an unknown Boolean function that represents the (potentially sensitive) data targeted by a given advertiser.

In Section 5.3, we describe an algorithm for learning the function in the particular case where it depends on a single data input. The cornerstone of this algorithm is a reduction to a SET COVER problem, that is also at the basis of our work in the subsequent sections.

In Section 5.4, we present sufficient conditions – w.r.t. the classification noise in our model – in order to generalize this algorithm for learning every *monotonic* function that only depends on a fixed number of inputs. We also propose an improved algorithm that runs in quasi-linear time, but that can only be applied assuming more restrictive hypotheses on the noise.

Finally, we question in Section 5.5 what can be learnt within our model. On the positive side, we prove that if the function only depends on a fixed number of inputs, positively or negatively, then all these inputs can be computed in quasi-polynomial time with high probability. Under one additional assumption on the classification noise, this algorithm can be extended for learning the function. However, we prove that in general, not all functions can be learnt within our model. Actually, it is impossible to distinguish a conjunction from a disjunction, even if they only depend on two inputs.

My papers on this learning problem [LDL$^+$14, DLCG15, DTC17, CD17] are collected in the appendix.

Contents

5.1 Introduction

This chapter is now devoted to a learning problem on Boolean functions, that we motivate next. Roughly, we aim at making possible for every user online to uncover any misuse of her data. Although *Big Data* promises important societal progress, it exacerbates at the same time the need for algorithmic accountability as more and more decisions affecting millions of users are being automated using personal and private information. Examples of such practices have begun to surface. In a recent incident, Google was found to have used institutional emails from ad-free Google Apps for Education to target ads in users' personal accounts [Gou14, Saf13]. MySpace was found to have violated its privacy policy by leaking personally identifiable information to advertisers [KW10]. Several consumer sites, such as Orbitz and Staples, were found to have adjusted their product pricing based on user location [Mat12, VDSVS12]. And Facebook's 2010 ad targeting was shown to be vulnerable to micro-targeted ads specially crafted to reveal a user's private profile data [Kor11].

The recent area of *Web's transparency* has developed generic methods to reveal which information item or input generates personalization and differentiated treatments [DTD15, LDL$^+$14, LSS$^+$15]. Their output should not be regarded as absolute truth, but rather as evidence for further investigation. In this work, we aim at giving a theoretical framework in order to analyse these methods. We also describe new core algorithms for these methods that are formally analysed in our setting.

Our contributions in this chapter are summarized in Section 5.1.1. Then, an outline of the chapter is provided in Section 5.1.2.

5.1.1 Our results

Simply put, we aim at describing the core algorithms for Web's transparency tools, and to provide the theoretical framework in order to analyse these algorithms. We detail this a bit more below.

5.1.1.1 A theory for ad targeting identification

Let Ad Targeting Detection be defined as the problem of deciding whether some specific input is targeted by a given ad. Similarly, let Ad Targeting Identification be defined as the problem of deciding which inputs are targeted by this ad. First, based on recent experiments [DTD15, LDL+14], we model the problems of Ad Targeting Detection and Ad Targeting Identification as a learning problem, where the hypothesis is a Boolean function that represents the (potentially sensitive) data inputs targeted by a given advertiser[1].

We report on this model and on its motivations in Section 5.2. This is joint work with Augustin Chaintreau.

Furthermore, all the other results that are presented in this chapter are proved in the learning model of Section 5.2.

5.1.1.2 A general approach reducing to Set Cover

In the following two Sections 5.3 and 5.4, we present algorithms for learning a function that only depends on a constant number of inputs and that is *monotonic* (increasing the number of data inputs cannot make decrease the likelihood to receive an ad). These algorithms are based on a reduction to a natural variation of Set Cover, where we seek for a minimum-size family of subsets (*each representing an input that is targeted*) covering a large fraction of a given universal set (*representing all the accounts that receive a given ad*).

This general approach is presented in Section 5.3, along with an algorithm for learning a function when it depends on a single input. Then, this algorithm is generalized in Section 5.4 for learning a monotonic function under the hypothesis that it depends on at most k inputs, for some fixed k. However, this generalized algorithm is proved to be correct only under a technical assumption, namely, if the *classification noise* of the oracle is bounded. The latter assumption implies that it

[1]Note that Ad Targeting Detection can be reduced to a particular case of Ad Targeting Identification where it is asked whether the targeting can be represented by the null-function.

is much likelier for an account within scope to receive an ad than for an account out of scope.

This is joint work with Mathias Lécuyer, Francis Lan, Andrei Papancea, Theofilos Petsios, Riley Spahn, Max Tucker, Augustin Chaintreau and Roxana Geambasu.

5.1.1.3 Necessary and sufficient conditions for learnability

Finally, we give in Section 5.5 a more general algorithmic proof that any function depending on a fixed number of inputs can be learnt — if we make additional assumptions on the oracle. More precisely, we prove that all the relevant inputs on which the function depends can be learnt if an upper-bound on their number is fixed in advance. The latter can be extended to an algorithm for learning any function, but that is proved to be correct only under an additional technical assumption (we call it “strong positive variance” of the oracle). Roughly, we suppose that there can be no population of accounts within scope that are significantly likelier to receive a given ad than all other accounts within scope.

Last, we prove that in general, if no additional assumption is given then only the functions depending on a *single* input can be learnt in our model.

5.1.2 Outline of the chapter

We first introduce a new learning model for Boolean functions in Section 5.2. In Section 5.3, we introduce a generic method in order to design learning algorithms in this model, and to formally analyse these algorithms. We apply this method to the particular case where the function to be learnt only depends on a single input. Then, in Section 5.4 we extend this approach to more general (monotonic) functions, that requires a more in-depth analysis of our probabilistic tools. Finally, in Section 5.5, we delineate the minimal hypotheses to incoporate in the model in order to make *any* function learnable. Note that these hypotheses are not part of the core assumptions for our learning model because they have not been confirmed experimentally. We then conclude this chapter in Section 5.6.

5.2 Learning model

The following presentation of our learning model is kept generic on purpose in order to apply to a broad set of scenarii of online targeting. Let $\mathcal{D} = \{D_1, D_2, \ldots, D_N\}$ be a set of N inputs representing individual information from a given user (typically, keywords extracted from emails in an account, see also [LDL+14]). Our main objective is to identify how these inputs affect a given output of interest (say, an ad or a recommendation). In order to achieve the goal, we here assume that each output is affected through an unknown targeting function f_{output}, that we simply denote by f in the following. The targeting function f is a mapping from the family of all *combinations* (subsets of $\mathcal{D}$) to the Boolean set $\{0; 1\}$. By convention, $f(\mathcal{C}) = 1$ indicates that an account *exactly* containing the inputs in $\mathcal{C}$ is $\underline{\text{targeted}}$, and we denote $f(.) = 0$ if the ad is untargeted. We aim at learning f subject to diverse requirements, each representing one aspect of our experiments for doing so in practice.

A generic framework from learning theory is first presented in Section 5.2.1. Then, we detail how we adapt this framework to our needs in the subsequent Sections 5.2.2, 5.2.3 and 5.2.4. This model is part of our paper [CD17], that is joint work with Augustin Chaintreau.

5.2.1 PAC learning

We refer to [Ang88] for basics of computational learning theory and query complexity. A *hypothesis* $\mathcal{H}$ is a class of Boolean functions. Let $f : \{0,1\}^N \mapsto \{0,1\}$ be an (unknown) function, possibly not in $\mathcal{H}$. In what follows, we are given:

- a function $\mathrm{O}_f : \{0,1\}^N \mapsto \{0,1\}$ (possibly randomized), that is called an *oracle* and whose outputs are assumed to depend on the outputs of f.
  Example: a call to the oracle can represent an observation whether a given account has received the ad;
- a random generator of pairs $\langle x, \mathrm{O}_f(x)\rangle$, that is called a *sampler* and for which every $x \in \{0,1\}^N$ is picked at random w.r.t. some fixed probability distribution Π (denoted by $x \sim \Pi$).
  Example: The sampler can represent our experimental setting. In order to learn the targeting function, we are bound to rely on experiments — to see how it reacts to various inputs. For instance, in [LDL+14] these experiments consist in collecting the ads from Gmail accounts with different subsets of emails.

Let ε, δ be nonnegative[2]. A *PAC-learning* algorithm for f under $\mathcal{H}$ hypothesis (*a.k.a.*, probably approximately correct learning algorithm) is given constant-time access to the sampler, and it must compute, in time polynomial in N and $1/\delta$, the representation of a function $h \in \mathcal{H}$ such that $\mathbb{P}r[h(x) \neq f(x) \mid x \sim \Pi] \leq \varepsilon$. The *query complexity* of the algorithm is its number of calls to the sampler. It is preferrable to keep this complexity small, say, polylogarithmic in N.

In what follows, we will always assume that $\varepsilon = 0$, *i.e.*, we aim at learning f exactly.

There is a vast literature on this problem [Ang88, AR07, FGKP09, MOS04, Val12], with different choices made for: the dependencies between the oracle and the function to be learnt, the distribution for the sampler, the representation of a function, the hypothesis, etc. The main novelty in this work is the set of assumptions on the oracle, and to some extent the choice for the representation of the functions. All the choices made for this work will be presented and discussed in this section.

Outline. In Section 5.2.2, we introduce basic terminology for a specific class of functions called *juntas*, that will be our hypothesis. Our choice for the representation of a function is also discussed in this section. Then, we formally describe our set of

[2]Note that here, δ is no longer related to graph hyperbolicity (defined in Chapter 2).

assumptions on the oracle in Section 5.2.3. In particular, we briefly report on some experiments in Section 5.2.3.1 that have supported the choices made in this work. The axioms on the oracle are given in Section 5.2.3.2. We end this section with our choices made for the sampler in Section 5.2.4.

5.2.2 Juntas

Our choices for the hypothesis $\mathcal{H}$ and the representation of a function are presented in this subsection. Complementary information for the case of monotonic functions is given in Section 5.2.2.1.

The following presentation differs from the standard terminology in the literature of Boolean function learning, but it is shown to be equivalent to it. This change of terminology is motivated by our interpretation of a Boolean word $w \in \{0,1\}^N$ as denoting the content of an online account.

Let $\mathcal{D} = \{D_1, D_2, \ldots, D_N\}$ be a fixed ground set. There is a natural one-to-one mapping between $\{0,1\}^N$ and $2^{\mathcal{D}}$ (power-set of $\mathcal{D}$), defined as $\phi : w \in \{0,1\}^N \mapsto \{D_i \in \mathcal{D} \mid w_i = 1\}$. For simplicity, we will identify f with $f \circ \phi^{-1}$ in what follows. Furthermore, we will call a subset of $\mathcal{D}$ a *combination*. The function f is said to depend on D_i if there exists a combination $\mathcal{C} \subseteq \mathcal{D} \setminus D_i$ such that $f(\mathcal{C}) \neq f(\mathcal{C} \cup \{D_i\})$.

Definition 82 ([BL97]). For every $k \geq 1$, f is a k-junta if it depends on at most k inputs $D_i \in \mathcal{D}$.

In what follows, we will select the class of k-juntas, for some constant k, as our hypothesis. Note that in practice, it is recommended to advertisers to select k in some range between 5 and 20 [Goo].

Representation of a junta. An *implicant* of f is a pair $\langle \mathcal{C}_{in}, \mathcal{C}_{out} \rangle$ of two disjoint combinations of $\mathcal{D}$ with the property that $f(\mathcal{C}) = 1$ for every combination $\mathcal{C}$ such that $\mathcal{C}_{in} \subseteq \mathcal{C}$ and $\mathcal{C} \cap \mathcal{C}_{out} \neq \emptyset$. It is a *prime implicant* of f if for every strict subsets $\mathcal{C}'_{in} \subsetneq \mathcal{C}_{in}$ and $\mathcal{C}'_{out} \subsetneq \mathcal{C}_{out}$, the pair $\langle \mathcal{C}'_{in}, \mathcal{C}'_{out} \rangle$ is not an implicant of f. Every k-junta has $\mathcal{O}(3^k/\sqrt{k})$ prime implicants [CM78].

In what follows, we choose as a representation for any function f the set $\mathcal{S}^{(core)}$ of its prime implicants. Note that we have, for any f:

$$f(\mathcal{C}) = \max_{\langle \mathcal{C}_{in}, \mathcal{C}_{out} \rangle \in \mathcal{S}^{(core)}} \left(\prod_{D_i \in \mathcal{C}_{in}} \mathbb{I}_{\{D_i \in \mathcal{C}\}} \right) \cdot \left(\prod_{D_i \in \mathcal{C}_{out}} (1 - \mathbb{I}_{\{D_i \in \mathcal{C}\}}) \right),$$

with $\mathbb{I}_{\{D_i \in \mathcal{C}\}}$ being an indicator function that takes value 1 only if $D_i \in \mathcal{C}$ (otherwise it is equal to 0). The latter is sometimes called the Blake canonical form of f [Bla38].

5.2.2.1 Case of monotonic functions

A function f is called *monotonic* if for every combination $\mathcal{C} \subseteq \mathcal{D}$ such that $f(\mathcal{C}) = 1$, we have that $f(\mathcal{C}') = 1$ for every superset $\mathcal{C}' \supseteq \mathcal{C}$. Monotonic functions naturally arise in some settings where negative keywords are unavailable, such as (until recently) Facebook [FBE].

In this situation, we simplify the representation of f as follows. A *family* $\mathcal{S}$ of *size* l is any collection of l distinct combinations. The *order* of the family is defined as the largest order of a combination it contains. Interestingly, there is a duality between families and monotonic functions. Indeed on the one hand, one can define for any family $\mathcal{S}$ a function $f : \mathcal{C} \to \max_{\mathcal{C}_j \in \mathcal{S}} \mathbb{I}_{\{\mathcal{C}_j \subseteq \mathcal{C}\}}$ that takes value $f(\mathcal{C}) = 1$ whenever the subset $\mathcal{C}$ contains at least one combination in $\mathcal{S}$. In such case we say that $\mathcal{S}$ *explains* the function. On the other hand, we now show that the converse also holds: given a monotonic function f, there is a *unique* family explaining f that is both of minimum order and minimum size:

Lemma 83. *For each monotonic function f there exists a unique family $\mathcal{S}^{(core)}$ satisfying:*

(i) $\mathcal{S}^{(core)}$ has size l and order r and it explains *f.*

(ii) No family of size $l' < l$ explains f.

(iii) No family of order $r' < r$ explains f.

Proof. We define $\mathcal{S}^{(\text{in})} = \{\mathcal{C} \subseteq \mathcal{D} \mid f(\mathcal{C}) = 1\}$ the set of all combinations for which f takes value 1. Let $\overrightarrow{D}_f$ be the digraph with vertex-set $\mathcal{S}^{(\text{in})}$ and with arc-set $\{(\mathcal{C}, \mathcal{C}') \mid \mathcal{C} \subsetneq \mathcal{C}'\}$. We have that $\overrightarrow{D}_f$ is a DAG (Directed Acyclic Graph) because the subset-containment relation defines a partial order. So, let $\mathcal{S}^{(core)}$ be the non-empty set of combinations with null in-degree in $\overrightarrow{D}_f$. By construction, each combination in $\mathcal{S}^{(\text{in})}$ contains some combination of $\mathcal{S}^{(core)}$ and $\mathcal{S}^{(core)} \subseteq \mathcal{S}^{(\text{in})}$, hence $\mathcal{S}^{(core)}$ explains f. Furthermore, we claim that $\mathcal{S}^{(core)}$ is contained in *any* family $\mathcal{S}'$ explaining f: indeed, since $\mathcal{S}'$ is required to contain a subset of any combination $\mathcal{C} \in \mathcal{S}^{(core)}$, and no combination of $\mathcal{S}^{(\text{in})}$ is strictly contained in $\mathcal{C}$, then it must contain $\mathcal{C}$. This shows that $\mathcal{S}^{(core)}$ satisfies all conditions of Lemma 83. Finally, since another family explaining f needs to include $\mathcal{S}^{(core)}$, then it will necessarily have a higher size l, hence $\mathcal{S}^{(core)}$ is the unique with both minimum size and order. □

For every monotonic function f, the family whose existence is proved in Lemma 83 is called its *core family* and we choose this family as the representation of f.

5.2.3 The oracle

We now introduce specific assumptions on the oracle O_f. We recall that the latter formalizes the observations gathered from different online accounts, *i.e.*, the collection of advertisements received w.r.t. the data inputs contained in the accounts. So, we first report on some experiments in Section 5.2.3.1 in order to motivate our choices for the oracle, presented in Section 5.2.3.2. Finally, an idealized oracle (formerly used in our papers [LDL$^+$14, DLCG15, DTC17]) is discussed in Section 5.2.3.3.

5.2.3.1 Supporting experiments

We briefly report on some experiments whose results and interpretations have motivated our choices for the oracle.

Experiment 1: Correlation of the outcomes with the function to be learnt. In [LDL+14], we posted four Google AdWords campaigns targeted on very specific keywords (Chaldean Poetry, Steampunk, Cosplay, and Falconry). Then, we placed in more than 800 Gmail accounts some emails including these keywords. Overall, the corresponding ads were received by more than 97% of the accounts. The latter shows, as expected, a positive correlation between the outcomes of the experiments and the scope of the campaign.

Experiment 2: Limited coverage. The *coverage* is defined as the true positive rate (*i.e.*, the average probability for an account within the scope of some advertisement campaign to receive this ad). By varying the number N of inputs in our experiments, we have observed that the coverage is a decreasing function in the number of data inputs contained in the accounts. This might come from a larger pool of advertising campaigns for which the accounts are within scope, that makes obtaining an ad slot more competitive. In particular, the probability of receiving an ad cannot be assumed to be a constant that is independent from N.

Experiment 3: Cross-unit effects. The authors in [TDDW15] showed that multiple browser instances running in parallel affect one another. They did so by comparing the diversity of the ads received by browsers running in isolation w.r.t. browsers running in parallel (see [TDDW15] for details). This result suggests that the outcomes of different observations are correlated.

5.2.3.2 Axiomatisation

Let us now introduce our assumptions on the oracle. Formally, O_f is a membership oracle with (asymmetric) classification noise. That is, it outputs the Boolean $f(\mathcal{C})$ for any combination $\mathcal{C}$ with some probability to flip the result. Unlike prior work [Ang88], we do not assume the classification noise to be symmetric, *i.e.*, the oracle may flip the result with some propability *depending on the combination.* Nonetheless, we will assume a few properties for the noise distribution. To our best knowledge, the following assumptions that are made on this probability have not been studied before in the literature.

Histories. Experiment 3 in Section 5.2.3.1 have evidenced that the noise distribution is subject to cross-unit effects. So, in order to handle with these correlations, we find it more suitable to generalize our oracle O_f so that it can take *families of combinations* as inputs. More precisely, let a family be any vector of combinations, denoted by $\mathcal{F} = \langle A_1, A_2, \ldots, A_t \rangle$. The outcome $\mathrm{O}_f(\mathcal{F})$ is simply defined as the binary vector $\mathrm{O}_f(\mathcal{F}) = \langle \mathrm{O}_f(A_1), \mathrm{O}_f(A_2), \dots, \mathrm{O}_f(A_t) \rangle$. Furthermore, let the pair $\mathrm{H}_{\mathcal{F}} = (\mathcal{F}; \mathrm{O}_f(\mathcal{F}))$ be the history of $\mathcal{F}$.

Let $\mathcal{F}_{-i} = \langle A_1, \dots, A_{i-1}, A_{i+1}, \dots, A_t \rangle$. We will assume that each individual outcome $\mathrm{O}_f(A_i)$ is correlated to the partial history $\mathrm{H}_{\mathcal{F}_{-i}}$. However, it may and must be the case that some natural properties hold independently from any history, that we now detail as follows. Let us point out that $\mathcal{S}^{(\mathrm{in})}$ stands for the set of all combinations $\mathcal{C}$ such that $f(\mathcal{C}) = 1$.

Assumption 1 (targeting lift)**.** There exists a universal constant $\varphi \in]0;1[$, called the targeting lift and such that for any $\mathcal{C}_0, \mathcal{C}_1$ with $f(\mathcal{C}_0) = 0, f(\mathcal{C}_1) = 1$:

$$\mathbb{P}r[\mathrm{O}_f(A_i) = 1 \mid A_i = \mathcal{C}_0, \mathrm{H}_{\mathcal{F}_{-i}}] < \varphi \cdot \mathbb{P}r[\mathrm{O}_f(A_i) = 1 \mid A_i = \mathcal{C}_1, \mathrm{H}_{\mathcal{F}_{-i}}].$$

This Assumption 1 is local and it simply ensures that it is more likely to receive an ad for an account within scope than out of scope (conditioned on any fixed history $\mathrm{H}_{\mathcal{F}_{-i}}$). In particular, it implies that the targeting function f is related to the outcome we study.

As we will show in Section 5.4, our most efficient algorithms are proved to be valid only if the targeting lift is bounded.

Assumption 2 (polynomial-growth)**.** There exist positive universal constant α, β, γ with $\alpha \leq 1$ and such that:

$$\mathbb{P}\left[\sum_{i=1}^{t} \mathrm{O}_f(A_i) < \left(\beta \cdot |\mathcal{F} \cap \mathcal{S}^{(\mathrm{in})}|^{\alpha}\right)\right] \leq e^{-\gamma \cdot t}$$

In accordance with Experiment 1 in Section 5.2.3.1, we properly state with Assumption 2 that the amount of accounts receiving an ad must be at least a significant fraction of the account population *within scope* , except on some small event with low probability like, for instance, when the targeting campaign runs out of budget.

Let us point out that if we were assuming that there is some minimum *constant* probability p_{in} for an account within scope to be targeted, Assumption 2 could be shown to be satisfied for $\alpha = 1$ by using standard concentration inequalities. By considering the case $\alpha \leq 1$, we may consider the case where this minimum probability slowly tends to zero when N grows, say, $p_{in} \sim p_o / \log^{\mathcal{O}(1)}(N)$ where p_0 is a constant. The latter case seems to be what happens in practice, as supported by Experiment 2 in Section 5.2.3.1.

Assumption 3 (noninterference)**.** Let the function f only depend on inputs in $V \subseteq \mathcal{D}$. Furthermore, let $A'_i = A_i \cap V$ and let $\mathcal{F}' = \langle A'_1, \dots, A'_t \rangle$.

$$\mathbb{P}r[\mathrm{O}_f(\mathcal{F})] = \mathbb{P}r[\mathrm{O}_f(\mathcal{F}')].$$

Finally, we formalize with Assumption 3 that none of the input that does not affect the function f can impact on the outcome.

5.2.3.3 Discussion: idealized model with independence

For simplicity, we were assuming in [LDL+14] an idealized learning model where the outputs of the oracle were independent random variables and there were two constant p_{in}, p_{out} such that:

$$\mathbb{P}r[\mathrm{O}_f(\mathcal{C})=1 \mid f(\mathcal{C})=1] = p_{in} > p_{out} = \mathbb{P}r[\mathrm{O}_f(\mathcal{C}')=1 \mid f(\mathcal{C}')=0].$$

Limitations. Independence in the model contradicts Experiment 3 in Section 5.2.3.1. Similarly, a constant probability p_{in} to be targeted contradicts Experiment 2 in Section 5.2.3.1. These are the reasons why we are now considering the more general assumptions in Section 5.2.3.2 for the oracle.

Nonetheless, we will see in what follows that our former analysis in the idealized model still holds under more general assumptions. Precisely, the approach presented in this chapter leaves us to analyse a random counting process whose outcome can be lower and upper-bounded by estimating the sum of *independent* random variables (see Lemma 86). In particular, by choosing p_{in}, p_{out} so that:

$$\begin{cases} p_{in} = (1+\mathcal{O}(1)) \cdot \frac{\beta}{\log^{1/\alpha-1}(N)} \\ p_{out} < \varphi \cdot p_{in} \end{cases}$$

all the results obtained with the simpler model in [LDL+14, DLCG15, DTC17] can be generalized to the more general model that is presented in this Section 5.2.

5.2.4 Distribution for the sampler

Last, we present our choices for the distribution and the sampler. The latter formalizes our experimental process, that consists in creating fake Gmail accounts and filling in them with random data.

Exchangeability is defined in [GR86] as the probability that if two accounts were exchanging their data inputs, the probability distribution of the outcome would not be impacted. So, in order to get exchangeability, we take a Bernouilli distribution $\Pi = B(p, N)$, *i.e.*, for every random combination that is sampled, each input $D_i \in \mathcal{D}$ must be present independently at random with probability p.

Interestingly, our process is related with the so-called random intersection model [KSSC99], that can be defined as follows. Let N, M and h be positive integers, and let p be some probability. In order to create a random intersection graph, we first create a bipartite graph B randomly with two sides of respective size N and M, and with each edge being present independently at random with probability p. Then, a new graph is created from B by taking as vertex-set the side of size M and adding an edge between every two vertices that share at least h common neighbours in B, for some constant h. Random intersection graphs have been proposed as a model for complex networks [GL06]. So, it makes sense to mimic this process in order to create random Gmail accounts.

5.3 Single-input targeting

This section addresses the detection and identification of *single-input* targeting, that is when the reception of the output is caused by the presence (or the absence) of a single input. More formally, we propose a PAC-learning algorithm with 1-juntas as hypothesis.

This is joint work with Mathias Lécuyer, Francis Lan, Andrei Papancea, Theofilos Petsios, Riley Spahn, Augustin Chaintreau and Roxana Geambasu.

Outline. Our main result is stated in Section 5.3.1, where we also discuss on its positioning in the nascent field of Web's transparency. Then, the following Sections 5.3.2 and 5.3.3 cover the main tools used in our study. The first tool is algorithmic: we present in Section 5.3.2 a classical technique for learning Boolean functions, of which we use a natural variation as the main brick basis of our algorithm (presented in Section 5.3.2.1). Second, we adapt in Section 5.3.3 standard concentration inequalities to our learning model. The latter will be our main tool in the analysis of the algorithm. Finally, we sketch this algorithm for learning 1-juntas in Section 5.3.4.

Full proofs can be found in our paper [LDL+14]. The version presented in this section also borrows from our paper [CD17] (in preparation).

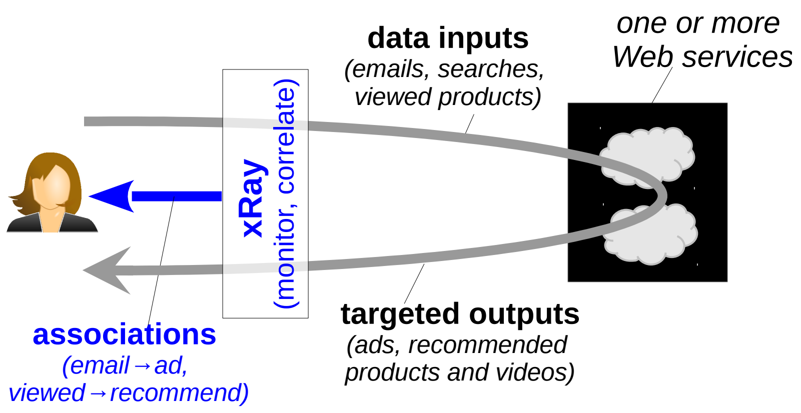

data inputs
(emails, searches, viewed products)
one or more Web services
xRay
(monitor, correlate)
associations
(email→ad, viewed→recommend)
targeted outputs
(ads, recommended products and videos)

Figure 5.1: Xray suggests plausible associations between the emails of a user and the ads she receives, using the core algorithm presented in this section.

5.3.1 Our results

Below, we state our main result in this section.

Theorem 84. *Let $\alpha \leq 1$ be the polynomial-growth (Assumption 2). There is a PAC-learning algorithm such that, for every $\varepsilon > 0$, the targeting function can be learnt with probability $1-\varepsilon$ under 1-juntas hypothesis, in $\mathcal{O}(N \cdot \log^{1/\alpha}(N/\varepsilon))$-time and $\mathcal{O}(\log^{1/\alpha}(N/\varepsilon)))$ queries.*

Theorem 84 is the core algorithm of a prototype called *Xray*, that we introduced in [LDL+14] and on which we now give more emphasis. Roughly, Xray predicts through the help of its core algorithm which data in an arbitrary Web account (such as emails, searches, or viewed products) is being used to target which outputs (such as ads, recommended products, or prices). We refer to Figure 5.1 for an illustration of its functioning. This problem has received some attention in the literature [DTD15, HSMK+13, HSL+14, LDL+14, MGEL12]. However, concurrently with [DTD15], our work on Xray has been the first, to the best of our knowledge, to provide *theoretical* guarantees on the predictions made under plausible assumptions. Furthermore, our core algorithm has (poly)logarithmic query complexity, whereas the authors in [DTD15] (using a different model than in Section 5.2) have proposed an algorithm with *linear* query complexity.

5.3.2 Reduction to Set Cover

The following reduction has been proposed in [AMK03] in order to infer Boolean functions from positive and negative examples. We detail how we can adapt this work to our setting in Section 5.3.2.1

First, suppose that $\mathrm{O}_f = f$ (*i.e.*, there is no classification noise). In this situation, the following lemma holds:

Lemma 85 ([MOS04]). *Let f be a nonconstant k-junta. Suppose that with confidence $1-\varepsilon$, it can be computed an input D_i on which the function f depends in time $n^c \cdot poly(2^k, 1/\varepsilon)$. Then there is an algorithm for exactly learning f which runs in time $n^c \cdot poly(2^k, 1/\varepsilon)$.*

By Lemma 85, if there is no classification noise then learning f can be reduced to compute the inputs on which this function depends. In order to do so, let $\langle \mathcal{C}_1, f(\mathcal{C}_1)\rangle, \langle \mathcal{C}_2, f(\mathcal{C}_2)\rangle, \ldots, \langle \mathcal{C}_m, f(\mathcal{C}_m)\rangle$ be drawn from the sampler. Let us take as our universal set $\mathcal{U} = \{(j_1, j_2) \mid j_1 < j_2 \text{ and } f(\mathcal{C}_{j_1}) \neq f(\mathcal{C}_{j_2})\}$. For every pair $(j_1, j_2) \in \mathcal{U}$, since $f(\mathcal{C}_{j_1}) \neq f(\mathcal{C}_{j_2})$ the two combinations $\mathcal{C}_{j_1}, \mathcal{C}_{j_2}$ must differ in at least one input on which the function f depends. In particular, let us define, for every input $D_i \in \mathcal{D}$, the set $\mathcal{S}_i = \{(j_1, j_2) \mid j_1 < j_2 \text{ and } D_i \in \mathcal{C}_{j_1} \Delta \mathcal{C}_{j_2}\}$, where Δ denotes the symmetric difference between two combinations. Then, it can be proved under some assumptions on the distribution Π of the sampler and the Boolean function f that a minimum set cover for $\mathcal{U}$ with the $\mathcal{S}_i$'s is in one-to-one correspondance with the inputs D_i's on which this function f depends [AMK03].

The obvious drawback of this approach is that computing a minimum set cover is NP-hard [Kar72]. Therefore, greedy heuristics should be used, and the analysis of their output is more delicate [FA05]. However, if the number of relevant variables is assumed to be a constant (that is the case for 1-juntas and more generally, for k-juntas with fixed k), there is no need to rely on such approximations.

5.3.2.1 Set Intersection algorithm

This above machinery cannot be applied to our setting directly because it is strongly dependent on the assumption $\mathrm{O}_f = f$. Indeed, without this assumption, the correspondance between the relevant variables and minimum set covers does not hold. However, based on Assumption 1 (*i.e.*, accounts within scope are much likelier to be targeted than accounts out of scope), it looks intuitive that the relevant variables should still correspond to a set cover for a *large fraction* of the universal set. Hence, in our setting, we propose an alternative reduction to a Set Cover problem with threshold, where we now seek for *x_intersecting subsets* of small size (defined as the subsets intersecting a fraction x of the universal set), for some parameter $x < 1$. The latter problem is formally described with Algorithm 1.

Input: a family $\mathcal{F}$; a threshold parameter $x < 1$; a size parameter s.
Output: the family $\mathcal{S}_x$ of x_intersecting combinations of size at most s.

```
$\mathcal{S}_x \leftarrow \{\}$ ;
foreach $\mathcal{C} \subseteq \mathcal{D}$ s.t. $|\mathcal{C}| \leq s$ do
    if $\mathcal{C}$ intersects $\geq x \cdot |\mathcal{F}|$ accounts in $\mathcal{F}$ then
        $\mathcal{S}_x \leftarrow \mathcal{S}_x \cup \{\mathcal{C}\}$ ;
    end
end
```

Algorithm 1: Set-intersection algorithm.

Discussion: parameter tuning. The reader may observe that Algorithm 1 requires a threshold parameter x as input. For simplicity, we will assume that a good estimate on the *targeting lift* (Assumption 1) is given, and we will show in the following that this information is enough in order to tune x. Nonetheless, we point out that finding this parameter in practice might be cumbersome.

Two methods have been proposed for doing so in [DTC17]. If we are given a ground-truth, *i.e.*, a set of functions f with their representation, then we can use it in order to tune the parameter x by reverse-engineering. However, a ground-truth is not always available. In this situation, we are limited to pick uniformally at random different values for x in a given interval, then to make our algorithms run in parallel. This interval can be chosen so that there can be no false negative (*i.e.*, all the relevant inputs are detected). Then, a final filtering process is used to elect the run whose output has to be taken into account.

5.3.3 Concentration inequalities

We complete Section 5.3.2 by introducing the main tool that will be used to analyse our subsequent algorithms (Lemma 86). Roughly, when using Algorithm 1 as a routine, we aim at approximating some random counting process in order to determine the existence or nonexistence of x_intersecting subsets. Classically, concentration inequalities such as Chernoff bounds [Hoe63] are used in the analysis. However, standard concentration inequalities apply to the sum of *independent* variables, so, they cannot be used in our setting directly. The following is a tedious (but classical) analysis where we show how to adapt Chernoff bounds to our needs.

Lemma 86. *Let $X_1, \dots, X_m$ be random Boolean variables satisfying:*

$$p_{\text{min}} \leq \mathbb{P}r[X_i = 1 \mid X_1, \dots, X_{i-1}] \leq p_{\text{max}}$$

for some constant $p_{\text{min}}, p_{\text{max}}$. Then the following hold for any $0 < \delta < 1$:

$$\mathbb{P}r[\sum_{i=1}^{m} X_i \geq (1+\delta) \cdot p_{\text{max}} \cdot m] \leq e^{-\delta^2 m p_{\text{max}}/3}$$

$$\mathbb{P}r[\sum_{i=1}^{m} X_i \leq (1-\delta) \cdot p_{\text{min}} \cdot m] \leq e^{-\delta^2 m p_{\text{min}}/2}$$

Proof. By symmetry, we will only consider the first inequality. Let $t > 0$. Let us show that:

$$\mathbb{E}[\Pi_{i=1}^{m} e^{t \cdot X_i}] \leq \left(p_{\text{max}}(e^t - 1) + 1\right)^m .$$

The proof is by induction. By the hypothesis,

$$\begin{aligned}
&\mathbb{E}[e^{t \cdot X_m} \mid X_1, \dots, X_{m-1}] \\
&\qquad = e^t \cdot \mathbb{P}r[X_m = 1 \mid X_1, \dots, X_{m-1}] + 1 \cdot \mathbb{P}r[X_m = 0 \mid X_1, \dots, X_{m-1}] \\
&\qquad \leq p_{\text{max}}(e^t - 1) + 1,
\end{aligned}$$

that is the base case. Suppose for the induction hypothesis that:

$$\mathbb{E}[\Pi_{j=i+1}^{m} e^{t \cdot X_j} \mid X_1, \dots, X_i] \leq \left(p_{\text{max}}(e^t - 1) + 1\right)^{m-i} .$$

Then by the law of total probability:

$$\begin{aligned}
&\mathbb{E}[\Pi_{j=i}^{m} e^{t \cdot X_j} \mid X_1, \dots, X_{i-1}] \\
&\qquad = e^t \cdot \mathbb{P}r[X_i = 1 \mid X_1, \dots, X_{i-1}] \cdot \mathbb{E}[\Pi_{j=i+1}^{m} e^{t \cdot X_j} \mid X_1, \dots, X_{i-1}, X_i = 1] \\
&\qquad + 1 \cdot \mathbb{P}r[X_i = 0 \mid X_1, \dots, X_{i-1}] \cdot \mathbb{E}[\Pi_{j=i+1}^{m} e^{t \cdot X_j} \mid X_1, \dots, X_{i-1}, X_i = 0] \\
&\qquad \leq \left(\mathbb{P}r[X_i = 1 \mid X_1, \dots, X_{i-1}] \cdot (e^t - 1) + 1\right) \cdot \left(p_{\text{max}}(e^t - 1) + 1\right)^{m-i} \\
&\qquad \leq \left(p_{\text{max}}(e^t - 1) + 1\right)^{m-i+1},
\end{aligned}$$

which proves the induction hypothesis. The remaining of the proof is now classical computation of Chernoff Bound. By Markoff inequality:

$$\begin{aligned}\mathbb{P}r[\sum_{i=1}^{m} X_i \geq (1+\delta)\cdot p_{\max}\cdot m] &= \mathbb{P}r[e^{t\cdot\sum_{i=1}^{m} X_i} \geq e^{t\cdot(1+\delta)\cdot p_{\max}\cdot m}] \\ &\leq \mathbb{E}[e^{t\cdot\sum_{i=1}^{m} X_i}]/e^{t\cdot(1+\delta)\cdot p_{\max}\cdot m} \\ &= e^{-t\cdot(1+\delta)\cdot p_{\max}\cdot m}\cdot\mathbb{E}[\Pi_{i=1}^{m} e^{t\cdot X_i}] \\ &\leq e^{-t\cdot(1+\delta)\cdot p_{\max}\cdot m}\cdot\left(p_{\max}(e^t-1)+1\right)^m \\ &\leq e^{-t\cdot(1+\delta)\cdot p_{\max}\cdot m}\cdot e^{p_{\max}(e^t-1)\cdot m} \\ &= e^{p_{\max}\cdot m\cdot\left(e^t-1-t\cdot(1+\delta)\right)}\end{aligned}$$

Finally, set $t=\ln(1+\delta)$. One obtains:

$$\mathbb{P}r[\sum_{i=1}^{m} X_i \geq (1+\delta)\cdot p_{\max}\cdot m] \leq \left(\frac{e^{\delta}}{(1+\delta)^{1+\delta}}\right)^{mp_{\max}} \leq e^{-\delta^2 mp_{\max}/3}.$$

□

To summarize Sections 5.3.2 and 5.3.3, we aim at learning the targeting function f by reducing to a natural variation of Set Cover (Section 5.3.2), of which we will analyse the outcome by using concentration inequalities (Section 5.3.3).

5.3.4 Proof overview

Finally, let us sketch the proof of Theorem 84. It is based on the correctness proof of the following Algorithm 2. Note that the ground-set $\mathcal{D}$ and its size N, the targeting lift φ (Assumption 1) and the constants α, β, γ (Assumption 2) are known parameters, so, we don't include them in the input of the algorithms.

Roughly, we use the Set-intersection algorithm (Algorithm 1) in order to detect an input that is significantly present (or missing) among the positive examples (*i.e.*, combinations $\mathcal{C}_i$ such that $\mathrm{O}_f(\mathcal{C}_i)=1$). On the one hand, since irrelevant inputs (on which the targeting function does not depend) cannot affect the outcome, they are present or missing among the positive examples by mere chance. In particular, these inputs can be neither significantly present nor absent among these examples. On the other hand, since it is likelier for the oracle to output 1 for a combination within scope (in $\mathcal{S}^{(\mathrm{in})}$) than for a combination out of scope, there should be slightly more positive examples that are correctly classified than misclassified. Since any input on which f depends positively (resp., negatively) must be present (resp., missing) in all the positive examples that have been correctly classified, this relevant input will be detected by the Set-intersection algorithm with high probability.

Sketch Proof of Theorem 84. Let us set the distribution Π of the sampler to the uniform distribution $B(1/2,N)$. We first make $\Theta(\log^{1/\alpha}(N/\varepsilon))$ queries to the sampler. Note that since f is assumed to depend on only one variable, we have in expectation that $f(\mathcal{C}_i)=1$ for half of the combinations $\mathcal{C}_i$ queried. Hence, by Chernoff

```
**Input**: accuracy $\varepsilon$.
**Output**: the representation $\mathcal{S}^{(core)}$ of $f$ under 1-juntas hypothesis.
/* Parameters tuning */;
Let $x \in ]\frac{1}{2}; \frac{1}{1+\varphi}[$ ;
Let $m \in \Omega\left(\log^{1/\alpha}(N/\varepsilon)\right)$ /*m depends on x*/;
/* Uniform sampling */;
Draw $\langle \mathcal{C}_1, \mathrm{O}_f(\mathcal{C}_1)\rangle, \langle \mathcal{C}_2, \mathrm{O}_f(\mathcal{C}_2)\rangle, \ldots, \langle \mathcal{C}_m, \mathrm{O}_f(\mathcal{C}_m)\rangle$ with $\Pi = B(1/2, N)$ ;
$\mathcal{F} \leftarrow \{\mathcal{C}_i \mid 1 \le i \le m$ and $\mathrm{O}_f(\mathcal{C}_i) = 1\}$ ;
/* Reduction to SET COVER */ ;
$\mathcal{S}_x \leftarrow$ Set-intersection($\mathcal{F}, x, 1$) ;
if $\exists i, \mathcal{S}_x = \{\{D_i\}\}$ then
    //positive targeting;
    $\mathcal{S}^{(core)} \leftarrow \{\langle \{D_i\}, \emptyset\rangle\}$ ;
end
else
    $\overline{\mathcal{F}} \leftarrow \{\mathcal{D} \setminus \mathcal{C}_i \mid 1 \le i \le m$ and $\mathrm{O}_f(\mathcal{C}_i) = 1\}$ ;
    $\mathcal{S}_x \leftarrow$ Set-intersection($\overline{\mathcal{F}}, x, 1$) ;
    if $\exists i, \mathcal{S}_x = \{\{D_i\}\}$ then
        //negative targeting;
        $\mathcal{S}^{(core)} \leftarrow \{\langle \emptyset, \{D_i\}\rangle\}$ ;
    end
    else
        //null function;
        $\mathcal{S}^{(core)} \leftarrow \{\langle \emptyset, \emptyset\rangle\}$ ;
    end
end
```

Algorithm 2: PAC-learning under 1-juntas hypothesis.

Bound, the number of combinations queried that are in $\mathcal{S}^{(\mathrm{in})}$ (within scope) is also an $\Theta(\log^{1/\alpha}(N/\varepsilon))$. By Assumption 2, this is the correct order of magnitude in order to ensure that, with probability $1-\Theta(\varepsilon)$, the oracle O_f will output 1 for at least $\Theta(\log(N/\varepsilon))$ queries.

In particular, let $\mathcal{F}$ be the set of all random combinations $\mathcal{C}_i$ such that $\mathrm{O}_f(\mathcal{C}_i) = 1$. By Assumption 3, the inputs on which the function f does not depend cannot affect the outcome, so, they are contained in half of the combinations of $\mathcal{F}$ in expectation. Furthermore, since these inputs are independently distributed and $|\mathcal{F}| = \Omega(\log(N/\varepsilon))$ is sufficiently large, we can prove by Chernoff bounds that these irrelevant inputs can be neither contained (nor absent) in a large fraction $x > 1/2$ of the combinations in $\mathcal{F}$, with high probability $1-\Theta(\varepsilon)$.

Conversely, it remains to prove that we can detect and identify the unique input on which the function f depends. We claim that for every $A_i \in \mathcal{F}$, $\mathbb{P}r[f(A_i) = 1 \mid \mathrm{O}_f(A_i) = 1, \mathrm{H}_{\mathcal{F}_{-i}}] > 1/(1+\varphi)$, with φ being the targeting lift. Indeed, since f is assumed to be a 1-junta, it is equally likely for a random combination to be in $\mathcal{S}^{(\mathrm{in})}$ than to be out of $\mathcal{S}^{(\mathrm{in})}$. By Assumption 1, combinations out of $\mathcal{S}^{(\mathrm{in})}$ have φ less chances to be in $\mathcal{F}$ than those in $\mathcal{S}^{(\mathrm{in})}$, and so, the claim follows. Then, by using the concentration inequalities of Lemma 86, we obtain that $|\mathcal{F} \cap \mathcal{S}^{(\mathrm{in})}| \geq x|\mathcal{F}|$ with high probability $1-\Theta(\varepsilon)$, provided x is chosen such that $x < 1/(1+\varphi)$. In particular, if f only depends on some input $D_j \in \mathcal{D}$ then there is a large fraction x of the combinations in $\mathcal{F}$ such that either D_j is present (if f depends on the input positively) or absent (if f depends on the input negatively) in these combinations. □

Perspectives. Our work shows that single-input targeting can be *always* detected and identified, under some plausible assumptions. As I mentioned earlier, similar results have been proved under different assumptions, but up to the price of an exponentially larger query complexity [DTD15]. To derive a unifying model where similar results can be proved is, to my mind, an important issue.

5.4 Complex targeting: the case of monotonic functions

This section now addresses complex targeting, *i.e.*, when the targeting function depends on at least two inputs. This is joint work with Mathias Lécuyer, Max Tucker, Augustin Chaintreau and Roxana Geambasu.

It has been argued in [DTD15] that this more challenging case could be reduced to the simpler case of single-input targeting (Section 5.3). In particular, assuming that f strongly depends on some input, this relevant input may still be identified with the algorithms crafted for single-input targeting. However, there is no reason a priori why the targeting function should depend more on some input than on the others. In [DTC17], we describe an experiment where we show that in some cases where two inputs are *simultaneously* targeted (*e.g.*, "programming interview" with "new job"), the corresponding output is misclassified by our prototype Xray [LDL+14] as being untargeted. We detail this a bit more in Figure 5.2. This result has motivated the study of PAC-learning algorithms with k-juntas as hypothesis, for $k > 1$.

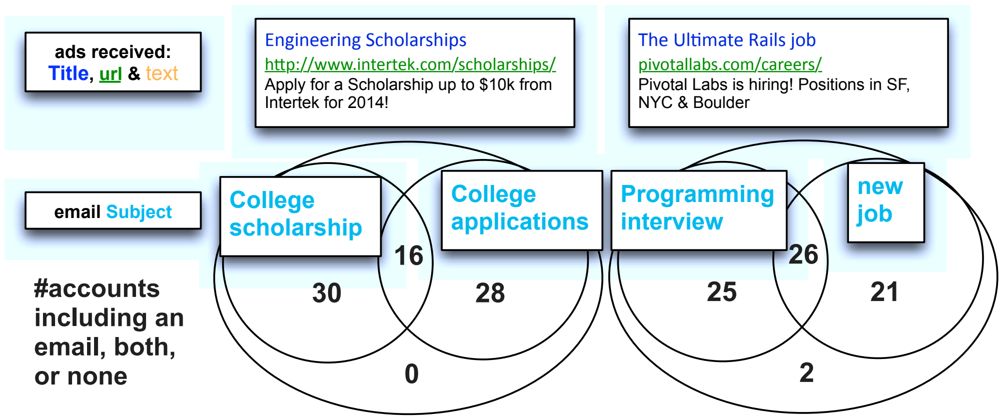


Figure 5.2: A correlation study between random placements of inputs (bottom) and outputs received (top).

More precisely, in this section we only consider *monotonic* k-juntas, that are the functions f such that $\mathcal{C} \subseteq \mathcal{C}'$ implies $f(\mathcal{C}) \leq f(\mathcal{C}')$ (see Section 5.2.2.1). By doing so, we do not pretend to cover *all* the cases of complex targetings that happen in real-life. Our purpose is to generalize our positive results on single-input detection to a broader set of targeting functions, and to investigate on the theoretical limitations of our set cover approach in Section 5.3. Furthermore, we note that in settings such as Facebook (until recently) [FBE], negative keywords are unavailable to the advertisers, and so, every targeting function should be monotonic.

In what follows, our results will be proved under one additional assumption on the oracle. Namely:

Assumption 4 (Nondiscrimination)**.** Let $\mathcal{F}$ be any family. For any $\mathcal{C}_1, \mathcal{C}_1'$ with $f(\mathcal{C}_1) = f(\mathcal{C}_1') = 1$:

$$\mathbb{P}r[\mathrm{O}_f(A_i) = 1 \mid A_i = \mathcal{C}_1, \mathrm{H}_{\mathcal{F}_{-i}}] = \mathbb{P}r[\mathrm{O}_f(A_i) = 1 \mid A_i = \mathcal{C}_1', \mathrm{H}_{\mathcal{F}_{-i}}].$$

Outline. In Section 5.4.1, we present a PAC-learning algorithm with monotonic k-juntas as hypothesis that generalizes our work on single-input targeting. This algorithm is proved to be correct only if some upper-bound on the targeting lift is assumed. Then, we describe more efficient algorithms in Section 5.4.2, but that are proved to be correct under stronger assumptions on the targeting lift. Further discussions on this work are given in the conclusion (Section 5.4.3).

5.4.1 Beyond single-input: the influence of the targeting lift

We first present an extended version of Theorem 84 that can be applied to monotonic k-juntas with additional assumptions. This result has been published in [DLCG15], and it is a joint work with Mathias Lécuyer, Augustin Chaintreau and Roxana Geambasu.

Theorem 87. *Let φ be the targeting lift (Assumption 1) and let $\alpha \leq 1$ be the polynomial-growth (Assumption 2). For every fixed positive integers s and w, there exists a constant $M_{s,w}$ such that the following holds if $\varphi < M_{s,w}$:*

There exists a PAC-learning algorithm such that, for every $\varepsilon > 0$, the targeting function can be learnt with probability $1 - \varepsilon$ under the hypothesis that it has a core with size at most s and order at most w. Furthermore, this algorithm runs in $\mathcal{O}(N^{s+w} \cdot \log^{1/\alpha}(N/\varepsilon))$-time and it has $2^{\mathcal{O}(s+w)} \cdot \log^{1/\alpha}(N/\varepsilon)$ query complexity.

Theorem 87 can be restated under monotonic k-juntas hypothesis by setting $s = w = k$. The main steps of its proof are now sketched. We describe a PAC-learning algorithm under monotonic juntas hypothesis and we prove its correctness.

Sketch of the algorithm. As for Theorem 84, we set the distribution of the sampler to be a binomial distribution $B(p, N)$, and then we make a polylogarithmic number of queries. However, note that here, the probability p will depend on the values for s and w.

The algorithm iterates on all the $\mathcal{O}(N^w)$ subsets $\mathcal{C}$ of size at most w, and it aims at deciding whether $f(\mathcal{C}) = 1$. In order to do so, the following key question is answered: what can be said among the supersets of $\mathcal{C}$ for which the oracle outputs 1 ? By definition, all of those subsets contain all inputs in $\mathcal{C}$ so we are interested in understanding how other inputs affect them. This is where exactly two cases emerge: Firstly, if we assume that $\mathcal{C}$ does contain a combination of the core, it automatically implies that independently of any other inputs, they all receive the ad with the same probability (by Assumption 4 on nondiscrimination). Secondly, if we assume on the other hand the opposite, then among all accounts including $\mathcal{C}$, there will be specific sets of inputs that may complete a combination from the core family and hence be targeted more heavily than others. This latter case resembles the situation of single-input targeting. The former case resembles a situation where f is untargeted (ads appear randomly). We can therefore design a new test as follows, that is sound and complete to determine in which case we are.

Roughly, the algorithms considers all the queried combinations $\mathcal{C}_i$ such that $\mathcal{C} \subseteq \mathcal{C}_i$ and $\mathrm{O}_f(\mathcal{C}_i) = 1$. Then, for all these combinations $\mathcal{C}_i$, the subset $\mathcal{C}_i \setminus \mathcal{C}$ is placed in some family $\Delta^{(ad)}(\mathcal{C})$. The test concludes that $f(\mathcal{C}) = 1$ if and only if $\Delta^{(ad)}(\mathcal{C})$ has no x_intersecting subset of size at most s, for some predefined choice of x. It can be verified in $\mathcal{O}(N^s \cdot \log^{1/\alpha}(N/\varepsilon))$-time by calling upon Algorithm 1. Furthermore, if a combination $\mathcal{C}$ passes the test and it is inclusion wise minimal w.r.t. this property then it is part of the core family of f with high probability.

In what follows (sections 5.4.1.1 and 5.4.1.2), we introduce the two propositions that are the cornerstone of our analysis for this above algorithm. We also explain in Section 5.4.1.3 why there is a need for assuming an upper-bound on the targeting lift in order to prove the correctness of this algorithm.

5.4.1.1 Soundness of the algorithm

First, we need to show that in any family of random subsets, almost asymptotically surely (a.a.s.) there can be no x_intersecting subset of small size (Lemma 88). The following technique is similar to the one used in [NRS04] in order to prove that a.a.s. the minimum size of a dominating set in any n-vertex random graph is $\Theta(\log n)$.

Lemma 88. *Let $1 > x > 0$, $s \in \mathbb{N}$, $p < 1-(1-x)^{\frac{1}{s}}$, and $\mathcal{B}$ a family of combinations that are drawn randomly from a binomial distribution $B(p, N)$. There exists $C > 0$ such that for any $\varepsilon > 0$ and polynomial P, if $m \geq C \cdot (s \ln(n) + \ln P(n) + \ln(1/\varepsilon))$ then with probability $(1 - \varepsilon/P(n))$ no x_intersecting subset of size s exists for this family.*

Proof. Let us consider an arbitrary combination $\mathcal{C} \subseteq \mathcal{D}$ of size s. We introduce Y the variable counting how many random subsets in $\mathcal{B}$ this combination $\mathcal{C}$ intersects, and we note that $\mathcal{C}$ is an x_intersecting subset exactly if $Y \geq xm$. We also observe that Y is a sum of binary independent variables and so, since the probability that $\mathcal{C}$ intersects an arbitrary subset in $\mathcal{B}$ is $1-(1-p)^s$, it has expectation $\mu = (1 - (1 - p)^s)\, m$. Assuming $p < 1 - (1 - x)^{\frac{1}{s}}$ as we do, μ is multiplicatively smaller than xm. Hence we can apply Chernoff Bound to conclude that $\mathbb{P}r[Y \geq xm] \leq \frac{\varepsilon}{P(N)N^s}$ when

$$m \geq C \cdot \ln\left(N^s P(N)/\varepsilon\right) \text{with } C = \frac{3\,(1-(1-p)^s)}{\left(x-(1-(1-p)^s)\right)^2}.$$

Furthermore, since there are $\binom{N}{l} \leq N^s$ choices of $\mathcal{C}$, by the union bound the probability that at least one of them is an x_intersecting subset is at most $\frac{\varepsilon}{P(N)}$. $\square$

By Lemma 88, the test routine of the algorithm will detect all the combinations $\mathcal{C}$ such that $f(\mathcal{C}) = 1$ with high probability. However, the latter result requires a predetermined lower-bound on the threshold parameter x (that depends on the probability p). In particular, the larger the size s of the core family of f, the larger the lower-bound on x.

5.4.1.2 Completeness of the algorithm

Second, we aim at proving that the test routine of the algorithm will reject all the combinations $\mathcal{C}$ such that $f(\mathcal{C}) = 0$ with high probability. This case is quite similar to single-input targeting, as it suffices to show that w.h.p., positive examples in $\Delta^{(ad)}(\mathcal{C})$ (defined above for the test) are likelier to be correctly classified than misclassified. Indeed, if this holds then taking one input in each combination of the core will leave an 1_intersecting subset of size at most s for the subfamily

$\Delta^{(ad)}(\mathcal{C}) \cap \mathcal{S}^{(\mathrm{in})}$ (correctly classified), that will be an x_intersecting subset for the whole family $\Delta^{(ad)}(\mathcal{C})$, for some well-chosen x.

The main difficulty is that it is not equally likely for a random combination to be within scope than out of scope. In particular, the larger the order w (size of a largest combination in the core), the lesser the probability for a random combination to be in $\mathcal{S}^{(\mathrm{in})}$. So, we need to tune the probability p (used for the distribution Π of the sampler) in order to increase in turn the probability for a random account to be within scope. Formally, let us introduce the following function on this probability:

$$\hat{\varphi}^{(k)}_{s,w}(p) = \frac{1 - \frac{s}{k}(1-(1-p)^s)}{\frac{s}{k}(1-(1-p)^s)} \frac{(1-(1-p)^{s/k})^w}{1-(1-(1-p)^{s/k})^w} \tag{5.1}$$

Proposition 89. *Suppose that f has a core family of size at most s and order at most w, and that $\varphi \leq \hat{\varphi}^{(k)}_{s,w}(p)$ for some $k \leq s$. Then, there exist two positive constants x and C (independent of f) such that the following holds for any choice of $\varepsilon > 0$, polynomial P and combination $\mathcal{C}$:*

Let $\mathcal{B}$ be a family of m combinations that are drawn randomly from a binomial distribution $B(p,N)$. If $m \geq p^{-|\mathcal{C}|} \cdot C \cdot (\ln(N) + \ln P(N) + \ln(1/\varepsilon))$, then with probability $(1 - \varepsilon/P(N))$ exactly one of the following claims holds:

(i) $\mathcal{C}$ contains a core combination, i.e. it is in $\mathcal{S}^{(in)}$.

(ii) an x_intersecting subset of size k exists for

$$\Delta(\mathcal{C}) = \{\mathcal{S} \cap \overline{\mathcal{C}} \mid \mathcal{S} \in \mathcal{B}, \mathrm{O}_f(\mathcal{S}) = 1, \mathcal{C} \subseteq \mathcal{S}\}$$

5.4.1.3 Upper-bounds on the targeting lift

Altogether combined, Lemma 88 and Proposition 89 can be proved to be simultaneously correct only if x is chosen in some fixed interval, whose length depends on: the size s of the core, its order w, the targeting lift φ (Assumption 1) and the probability p that is used for the distribution Π of the sampler. Note that the probability p can be tuned in order to maximize the length of this interval, but even then, there will be an upper-limit (depending on φ, s, w) beyond which this interval will be empty. Let us express this limit as an upper-bound $M_{s,w}$ on the targeting lift (only depending on s and w).

Lemma 90. *Let $M_{s,w} = \sup_{p \in]0;1[} \hat{\varphi}^{(s)}_{s,w}(p)$, we have:*

$$\begin{cases} \text{if } s = 1, & M_{1,w} = 1/w, \\ \text{if } w = 1, & M_{s,1} = 1/s, \\ \text{for all } s, w, & \frac{1}{(2^{\max(s,w)}-1)^2} \leq M_{s,w} \leq \frac{1}{(2^{\min(s,w)}-1)^2}, \\ \text{for all } w, s, & M_{s,w} = M_{w,s}, \\ \text{if } s = w = n, & M_{n,n} = 1/(2^n-1)^2. \end{cases}$$

Moreover, if $w > 1$ and $s > 1$ then we have $M_{s,w} = \frac{(p^*)^w}{1-(p^*)^w} \frac{(1-p^*)^s}{1-(1-p^*)^s}$ where p^* is the only solution in $]0;1[$ of:

$$wp^{w+1} - s(1-p)^{s+1} - (w+s)p + w = 0.$$

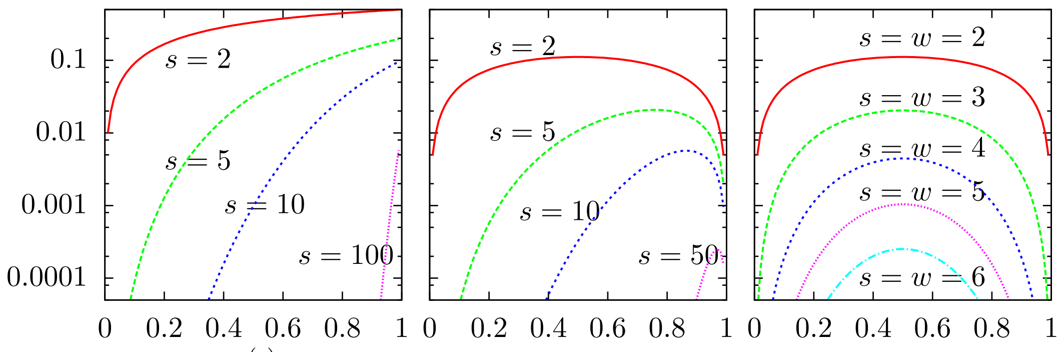


Figure 5.3: Value of $\hat{\varphi}^{(s)}_{s,w}$ as a function of $1-p$ for $w = 1$ (left), $w = 2$ (middle) and $w = s$ (right).

Discussion and perspectives. It is particularly informative to see how this *undetected targeting lift* (upper-bound on the targeting lift) grows with the complexity of the formula used. Figure 5.3 presents the value of the function $\hat{\varphi}^{(s)}_{s,w}$ that defines it (it is drawn up to a change of variable to make it easier to read). As proved in Lemma 90 and shown in the figure, if the targeting solely uses disjunction (resp. conjunction) of inputs, *i.e.*, $w = 1$ (resp., $s = 1$) as shown in Figure 5.3 (left), the undetected targeting lift behaves as $1/s$ and hence it is polynomial. This polynomial expansion remains if s grows while w remains small. Figure 5.3 (middle) presents an example. In contrast, when s and w grow simultaneously, *e.g.*, if they are equal as shown in Figure 5.3 (right) one can show that undetected targeting lift can be decreasing *exponential* fast. While this demonstrates the hardness of *Web's transparency*, we note that such forms of complex targeting combining so many inputs to decide may be relatively rare in practice.

5.4.2 Faster algorithms and tradeoffs

Theorem 87 proves that the set cover approach of Section 5.3 can be generalized for learning the monotonic k-juntas — but under some assumptions on the targeting lift. In this subsection, we present algorithms for this task that achieve a better running-time, but under stronger assumptions on the lift. This is joint work with Max Tucker and Augustin Chaintreau.

Namely, in Section 5.4.2.1 we replace the exact test of Algorithm 1 with a greedy approximation algorithm, thereby decreasing the running time from $\mathcal{O}(N^s \cdot \log^{1/\alpha}(N/\varepsilon))$ to $\mathcal{O}(sN \cdot \log^{1/\alpha}(N/\varepsilon))$. In Section 5.5.1, we introduce a new PAC-learning algorithm that is more intricate than the one presented for Theorem 87 but runs in $\tilde{\mathcal{O}}((sw)! \cdot N)$-time.

5.4.2.1 Faster detection algorithm

Our purpose is to describe a faster test of recognition for the combinations $\mathcal{C}$ such that $f(\mathcal{C}) = 1$.

Theorem 91. *Let φ be the targeting lift (Assumption 1) and let $\alpha \leq 1$ be the polynomial-growth (Assumption 2). For every fixed positive integers s and w, there exists a constant $\hat{M}_{s,w}$ such that the following holds if $\varphi < \hat{M}_{s,w}$:*

Suppose that f has a core family of size at most s and order at most w. Then, for every combination $\mathcal{C}$ and for every $\varepsilon > 0$, it can be decided in $2^{\mathcal{O}(|\mathcal{C}|+s+w)} \cdot N \cdot \log^{1/\alpha}(N/\varepsilon)$-time and with probability $1-\varepsilon$ whether $f(\mathcal{C}) = 1$.

Let us sketch the proof of Theorem 91. We recall that in order to decide whether $f(\mathcal{C}) = 1$ with high probability, it suffices to verify whether some family $\Delta(\mathcal{C})$ has an x_intersecting subset of size at most s, where x is a well-chosen parameter depending on s and w. It can be done in $\tilde{\mathcal{O}}(N^s)$-time by using Algorithm 1. The gist of Theorem 91 is to make this step faster by replacing the (exact) Set-intersection algorithm with a greedy approximation algorithm that we describe next.

Formally, let us set $\mathcal{S} = \Delta(\mathcal{C})$, $\mathcal{C}' = \emptyset$. While $\mathcal{S} \neq \emptyset$ and $|\mathcal{C}'| < s$, we pick any input D_j that maximizes the number of intersected subsets in $\mathcal{S}$. This input D_j is added in $\mathcal{C}'$, then every combination containing D_j is removed from $\mathcal{S}$. This process has already received some attention in the literature of Boolean function learning [FA05], but under a different learning model.

On the one hand, if the resulting combination $\mathcal{C}'$ is an x_intersecting subset then we can conclude, as before for Theorem 87, that $f(\mathcal{C}) = 0$ with high probability. On the other hand, if $\Delta(\mathcal{C})$ does admit an x_intersecting subset of this size then we can prove by using standard arguments on submodular functions that $\mathcal{C}'$ must be an $(1-(1-\frac{1}{s})^{1/s})x$_intersecting subset. It can be proved by Lemma 88 that no such a subset can exist if $f(\mathcal{C}) = 1$ and x is large enough. So overall, we are left to test whether the resulting combination $\mathcal{C}'$ is an x'_intersecting subset with $x' = (1-(1-\frac{1}{s})^{1/s})x$.

As a direct consequence of Theorem 91, we obtain a faster algorithm than the one presented for Theorem 87:

Corollary 92. *Let φ be the targeting lift (Assumption 1) and let $\alpha \leq 1$ be the polynomial-growth (Assumption 2). For every fixed positive integers s and w, there exists a constant $\hat{M}_{s,w}$ such that the following holds if $\varphi < \hat{M}_{s,w}$:*

There exists a PAC-learning algorithm such that, for every $\varepsilon > 0$, the targeting function can be learnt with probability $1-\varepsilon$ under the hypothesis that it has a core with size at most s and order at most w. Furthermore, this algorithm runs in $\mathcal{O}(2^s \cdot N^w \cdot \log^{1/\alpha}(N/\varepsilon))$-time and it has $2^{\mathcal{O}(s+w)} \cdot \log^{1/\alpha}(N/\varepsilon)$ query complexity.

Let us point out that this new algorithm is Fixed-Parameter Tractable in the size s of the core family, but it still depends on its order w exponentially.

5.4.2.2 Faster identification algorithm

We have shown in Section 5.4.2.1 how to improve the detection test in order to recognize the combinations of $\mathcal{S}^{(\text{in})}$. Getting rid of the exhaustive search of all possible subsets of small size (at most the order w of the core) is much more difficult.

We show how to do so by using more properties of the intersecting subsets and a significantly more elaborate algorithm, that has similarities with the one described in [Ang88, Sec. 3.1, Theorem 1].

Theorem 93. *Let φ be the targeting lift (Assumption 1) and let $\alpha \leq 1$ be the polynomial-growth (Assumption 2). For every fixed positive integers s and w, there exists a constant $\overline{M}_{s,w}$ such that the following holds if $\varphi < \overline{M}_{s,w}$:*

There exists a PAC-learning algorithm such that, for every $\varepsilon > 0$, the targeting function can be learnt with probability $1-\varepsilon$ under the hypothesis that it has a core with size at most s and order at most w. Furthermore, this algorithm has $2^{\mathcal{O}(sw \cdot \log(sw))} \cdot \log^{1/\alpha}(N/\varepsilon)$ query complexity, and with probability $1-\varepsilon$ it runs in $2^{\mathcal{O}(sw \cdot \log(sw))} \cdot N \cdot \log^{1/\alpha}(N/\varepsilon)$-time.

```
Input: a family $\mathcal{F}$; and a threshold parameter $x$.
Output: the representation $\mathcal{S}^{(core)}$ of $f$.
$\mathcal{S}^{(core)} \leftarrow \{\}$ ;
$\mathcal{S}_x \leftarrow$ Set-intersection$(\mathcal{F}, x, 1)$; $\mathcal{S} \leftarrow \bigcup_{\{D_i\} \in \mathcal{S}_x} \{D_i\}$;
if $\mathcal{S} \neq \emptyset$ then
    /* Removal of inputs until obtaining a core combination */;
    foreach $D_i \in \mathcal{S}$ do
        $\hat{\mathcal{S}} = \mathcal{S} \setminus D_i$;
        $\hat{\mathcal{F}} = \{A_j \setminus \hat{\mathcal{S}} \mid A_j \in \mathcal{F}, \hat{\mathcal{S}} \subseteq A_j\}$;
        $\hat{\mathcal{S}}_x \leftarrow$ Set-intersection$(\hat{\mathcal{F}}, x, 1)$;
        if $\hat{\mathcal{S}}_x = \emptyset$ then
            /* the subset $\hat{\mathcal{S}}$ is still in $\mathcal{S}^{(in)}$ */;
            $\mathcal{S} \leftarrow \hat{\mathcal{S}}$;
        end
    end
    $\mathcal{S}^{(core)} \leftarrow \mathcal{S}^{(core)} \cup \{\mathcal{S}\}$;
    foreach $D_i \in \mathcal{S}$ do
        /* Recursive call to the algorithm */;
        $\mathcal{S}_i \leftarrow$ GSI$(\mathcal{F} \setminus \{A_j \in \mathcal{F} \mid D_i \in A_j\}, x)$;
        $\mathcal{S}^{(core)} \leftarrow \mathcal{S}^{(core)} \cup \mathcal{S}_i$;
    end
end
```

Algorithm 3: Generalized set-intersection algorithm (GSI).

The proof of Theorem 93 is based on Algorithm 3, that is an intricate variation of the Set-intersection algorithm. Let us first give a better analysis of the detection test that is used in order to recognize the combinations of $\mathcal{S}^{(\text{in})}$ (presented earlier in Section 5.4.1). Given a combination $\mathcal{C}$, this test either asserts that $f(\mathcal{C}) = 1$ or it outputs an x_intersecting subset of size at most s for some family of subsets $\Delta(\mathcal{C})$.

The latter subset can be regarded as a "negative certificate" on which we can extract more information as follows:

Lemma 94. *Suppose that f has a core family of size at most s and order at most w, and let $k \leq s$. Then, provided $\varphi < \overline{M_{s,w}}^{(k)}$ for some constant $\overline{M_{s,w}}^{(k)}$ (only depending on s, k and w), there exist positive constants x (threshold), p (probability for the sampler) and C such that the following holds for any choice of $\varepsilon > 0$, polynomial P and combination $\mathcal{C}$:*

Let $\mathcal{B}$ be a family of m combinations that are drawn randomly from a binomial distribution $B(p, N)$, with $m \geq \alpha^{-|\mathcal{C}|} \cdot C \cdot (\ln(N) + \ln P(N) + \ln(1/\varepsilon))$. The two following claims hold for $S_{x,k} = \{\mathcal{S} \mid \mathcal{S}\ x\_intersecting\ for\ \Delta(\mathcal{C}), |\mathcal{S}| \leq k\}$ with probability $(1 - \varepsilon/P(N))$:

(i) All combinations in $S_{x,k}$ intersect $\bigcup_{\mathcal{S} \in \mathcal{S}^{(core)}} \mathcal{S}$.

(ii) $\mathcal{C} \cup \bigcup_{\mathcal{S} \in S_{x,k}} \mathcal{S}$ is empty or contains a core combination.

From now on, this lemma will be used with $k = 1$.

Let us sketch the main principles behind the algorithm. As before, we set the distribution Π for the sampler to be a binomial distribution $B(p, N)$, for some predetermined value of p. Then, we make a polylogarithmic number of queries to the sampler, and we let $\mathcal{F}$ to be the set of all the combinations $\mathcal{C}_i$ queried such that $\mathrm{O}_f(\mathcal{C}_i) = 1$. If f is not the null-function then under the conditions of Theorem 93, this family $\mathcal{F}$ has x_intersecting subsets of size 1. Furthermore, by calling upon Algorithm 1 (with $s = 1$), all such intersecting subsets of unit size can be computed, in quasi-linear time.

At this step, Lemma 94 comes into play. Indeed, let $\mathcal{S}$ be the union of all x_intersecting subsets of $\mathcal{F}$ of unit size. By Lemma 94(i), every input in $\mathcal{S}$ is in a core combination, hence $|\mathcal{S}| \leq sw$. In addition, we have by Lemma 94(ii) that $\mathcal{S}$ contains a core combination with high probability. The main idea behind Theorem 93 is to extract a core combination $\mathcal{C}$ from $\mathcal{S}$, then to call Algorithm 3 recursively on a constant number of subsets of $\mathcal{F}$ in order to obtain the remaining of the core family. More precisely, there is one recursive call for every input $D_i \in \mathcal{C}$, before which we remove from $\mathcal{F}$ all the combinations that contain D_i in order to obtain different core combinations than $\mathcal{C}$. The main difficulty is to bound the depth of the recursion. This is where we use once more Lemma 94. Indeed, since at each call to Algorithm 3, the superset $\mathcal{S}$ has all its inputs contained in a core combination, and we virtually remove one of them before each recursive call, the depth of the recursion is bounded w.h.p. by $\sum_{\mathcal{C} \in \mathcal{S}^{(core)}} |\mathcal{C}| \leq sw$.

5.4.3 Conclusion and open perspectives

We have generalized the results obtained for single-input targeting to a larger class of targeting functions. A main drawback of this set cover approach, when applied to complex targeting, is that it can be proved to be correct only if the targeting lift is close to zero (the larger the size and the order of the core, the closer the lift to zero). So far, our learning model does not make any assumption on what a "realistic" value for the lift should be. We aim at closing this gap in a near future by using some advertising models in the literature [GEC+13] in order to better evaluate the order of magnitude for this value.

On a more positive side, our approach can be modified in order to give efficient algorithms with quasi-linear time. This is a neat advantage for Web transparency tools such as Xray that, for now, do not cope with complex targeting. To the best of our knowledge, the only prototype which goes beyond the case of single-input targeting is Sunlight [LSS+15], where a different subclass of targeting functions is adressed. Roughly, the core algorithm of this tool is able to detect and to identify a class of "threshold functions" f, where each input is assigned a weight and f outputs 1 only if the sum of the weights of the inputs in presence is greater than some predetermined threshold.

Finally, let us point out that generalizing our approach in this section to *non-monotonic* functions is challenging, at best. Indeed, we recall that our detection test concludes that a combination $\mathcal{C}$ is in $\mathcal{S}^{(\text{in})}$ if and only if there is no $x_$intersecting subset of small size in a given family $\Delta(\mathcal{C})$. This test fails if the targeting function is non-monotonic. As an example, consider a combination $\mathcal{C}$ such that for every prime implicant $\langle \mathcal{C}_{in}, \mathcal{C}_{out} \rangle$ of f, we have $\mathcal{C} \cap \mathcal{C}_{out} \neq \emptyset$. By construction, there can be no superset of $\mathcal{C}$ that is in $\mathcal{S}^{(\text{in})}$. Hence, it may be the case that all these supersets are equally likely to be targeted by mistake, with all the inputs not in $\mathcal{C}$ being present by mere chance. The latter would imply that the family $\Delta(\mathcal{C})$ that is used for the test would not have any $x_$intersecting subset of small size, and so, that $\mathcal{C}$ is mistakenly identified as part of $\mathcal{S}^{(\text{in})}$.

5.5 General case

Finally, this section is about the theoretical limitations of the learning model of Section 5.2. That is, we aim at characterizing what can be learnt in our model. Full proofs can be found in [CD17], which is joint work with Augustin Chaintreau.

Outline. On the positive side, we prove in Section 5.5.1 that all the relevant inputs (on which the targeting depends) can be computed. Furthermore, under one additional assumption on the oracle (generalizing Assumption 4 on nondiscrimination), *any* targeting function can be learnt. However in general (without an additional assumption), it is proved in Section 5.5.3 that monotonic 2-juntas cannot be learnt in our setting. In fact, it is already impossible to distinguish between a conjunction or a disjunction!

Although the proofs in Sections 5.5.1 and 5.5.2 are algorithmic, they do not lead to efficient PAC-learning algorithms.

5.5.1 Identification of the relevant inputs

This subsection presents an algorithm for computing the at most k inputs on which a k-junta depends. Roughly, the relevant inputs will be inferred by virtually "fixing"

$k-1$ inputs from the ground-set $\mathcal{D}$. Such removal will reduce the problem to single-input targeting, and so, the set cover approach of Section 5.3 can be used. This is formalized with the following Algorithm 4.

```
Input: accuracy parameter $\varepsilon$; upper-bound $k$ on the number of relevant
       inputs.
Output: the set of relevant inputs $V$.
$V \leftarrow \{\}$ ;
/* Parameters tuning */;
Let $x \in ]\frac{1}{2}; \frac{1}{1+\varphi}[$ ;
Let $m \in \Omega\left(2^k \cdot \log^{1/\alpha}(N/\varepsilon)\right)$ /*m depends on x*/;
/* Uniform sampling */;
Draw $\langle \mathcal{C}_1, \mathrm{O}_f(\mathcal{C}_1)\rangle, \langle \mathcal{C}_2, \mathrm{O}_f(\mathcal{C}_2)\rangle, \ldots, \langle \mathcal{C}_m, \mathrm{O}_f(\mathcal{C}_m)\rangle$ with $\Pi = B(1/2, N)$ ;
$\mathcal{F} \leftarrow \{\mathcal{C}_i \mid 1 \le i \le m \text{ and } \mathrm{O}_f(\mathcal{C}_i) = 1\}$ ;
/* Exhaustive search for prime implicants */;
foreach $\langle \mathcal{C}_{in}, \mathcal{C}_{out}\rangle$ with $|\mathcal{C}_{in}| + |\mathcal{C}_{out}| \le k-1$ do
    $\hat{\mathcal{F}} \leftarrow \{A_p \in \mathcal{F} \mid \mathcal{C}_{in} \subseteq A_p \text{ and } A_p \cap \mathcal{C}_{out} = \emptyset\}$;
    $\overline{\hat{\mathcal{F}}} \leftarrow \{\mathcal{D} \setminus A_p \mid A_p \in \hat{\mathcal{F}}\}$ ;
    if $|\hat{\mathcal{F}}| \ge \Omega(k \cdot \log(N/\varepsilon))$ then
        $\mathcal{S}_x \leftarrow$ Set-intersection($\hat{\mathcal{F}}, 1, x$) // positive dependency;
        $\overline{\mathcal{S}}_x \leftarrow$ Set-intersection($\overline{\hat{\mathcal{F}}}, 1, x$) // negative dependency;
        $\hat{S} \leftarrow \left(\bigcup_{\{D_i\} \in \mathcal{S}_x \cup \overline{\mathcal{S}}_x} \{D_i\}\right) \setminus \mathcal{C}_{in}$ ;
        $V \leftarrow V \cup \hat{S}$ ;
    end
end
```

Algorithm 4: Inference algorithm for the relevant inputs.

Theorem 95. *Let $\alpha \le 1$ be the polynomial-growth (Assumption 2). There is an algorithm such that, for every $\varepsilon > 0$, the set of relevant variables $V = \{D_i \in \mathcal{D} \mid f$ depends on $D_i\}$ can be learnt with probability $1-\varepsilon$ under k-juntas hypothesis. This algorithm runs in $\mathcal{O}(N^k \cdot \log^{1/\alpha}(N/\varepsilon))$-time and it has $\mathcal{O}(2^k \cdot \log^{1/\alpha}(N/\varepsilon))$ complexity query.*

Sketch Proof of Theorem 95. We give a correctness proof of Algorithm 4. Let $\langle \mathcal{C}_{in}, \mathcal{C}_{out}\rangle$ be fixed, with $|\mathcal{C}_{in}| + |\mathcal{C}_{out}| \le k-1$. Let us define $\hat{\mathcal{B}}$ as the family of all the combinations that have been queried with the sampler, that contain $\mathcal{C}_{in}$ and that do not intersect $\mathcal{C}_{out}$. Furthermore, let $\hat{\mathcal{D}} = \mathcal{D} \setminus (\mathcal{C}_{in} \cup \mathcal{C}_{out})$, let $\hat{f}(\hat{\mathcal{C}}) = f(\hat{\mathcal{C}} \cup \mathcal{C}_{in})$ and $\hat{\mathrm{O}}_f(\hat{\mathcal{C}}) = \mathrm{O}_f(\hat{\mathcal{C}} \cup \mathcal{C}_{in})$ for every combination $\hat{\mathcal{C}} \subseteq \hat{\mathcal{D}}$. In order to reuse the results from

Section 5.3, we will base on the property that $\hat{\mathrm{O}}_f$ "almost" behaves like an oracle for the targeting function $\hat{f}$. That is, it satisfies Assumptions 1 and 2 (trivially), but it only satisfies Assumption 3 partially. More precisely, if f (but not necessarily $\hat{f}$) only depends on some inputs in $\hat{V} \cup \mathcal{C}_{in} \cup \mathcal{C}_{out}$, then Assumption 3 applies for $\hat{V}$. By Lemma 88 (nonexistence of x_intersecting subsets of small size in random families), this weaker version of Assumption 3 implies that the targeting function f depends on every input that is computed by Algorithm 4 with high probability.

In order to complete the proof of the theorem, let D_j be any input on which f depends. Since D_j is relevant, there is a bipartition $\langle \mathcal{C}_{in}, \mathcal{C}_{out} \rangle$ of the relevant inputs from $\mathcal{D} \setminus D_j$ so that $f(\mathcal{C}_{in} \cup \{D_j\}) \neq f(\mathcal{C}_{in})$. So, let us fix any such bipartition $\langle \mathcal{C}_{in}, \mathcal{C}_{out} \rangle$. In such case, $\hat{f}$ is a 1-junta that only depends on D_j, furthermore $\hat{\mathrm{O}}_f$ satisfies Assumption 3 for $\hat{f}$. The average size of $\hat{\mathcal{B}}$ is $m/2^{k-1}$, where m is the number of queries. This case is thus reduced to single-input targeting (Theorem 84). Finally, by taking a union bound over the relevant inputs, every input on which f depends is in V (computed by Algorithm 4) with high probability. □

5.5.2 Filtering technique

In this subsection we now present an algorithm for learning the targeting function f exactly. Suppose that we are given the relevant inputs for the targeting function f. In order to learn $\mathcal{S}^{(\mathrm{in})}$, it suffices to learn all the subsets $\mathcal{C}$ on these (at most k) inputs so that $f(\mathcal{C}) = 1$. Intuitively, this can be achieved by comparing any two combinations $\mathcal{C}_0, \mathcal{C}_1$ and testing whether containing one of these two subsets, say, $\mathcal{C}_1$, increases the chance to be targeted (compared to $\mathcal{C}_0$). On may expect that the latter certifies $f(\mathcal{C}_1) = 1$ and $f(\mathcal{C}_0) = 0$. Algorithm 5 (introduced next) builds upon this intuition.

```
Input: a set of inputs $V$; a family $\mathcal{F}$; a threshold parameter $t$.
Output: the class $\mathcal{T}_k$ of all bipartitions $\langle \mathcal{C}_{in}, \mathcal{C}_{out} \rangle$ of $V$ s.t. $\langle \mathcal{C}_{in}, \mathcal{C}_{out} \rangle \in \mathcal{S}^{(\mathrm{in})}$.
$k \leftarrow |V|$ ;
/* Partition of the family w.r.t. the relevant inputs */;
Partition $\mathcal{F}$ into $\mathcal{F}_1, \mathcal{F}_2, \ldots, \mathcal{F}_{2^k}$ s.t.:
  • $\forall 1 \leq i < 2^k,\ |\mathcal{F}_i| \geq |\mathcal{F}_{i+1}|$ ;
  • $\forall A_p, A_q \in \mathcal{F},\ A_p \cap V = A_q \cap V \iff A_p, A_q \in \mathcal{F}_i$ for some $i$;
/* Ordering of the bipartitions of V by decreasing presence in the family */;
for $i \in \{1, \ldots, 2^k\}$ do
    $V_i \leftarrow A_p \cap V$ with $A_p \in \mathcal{F}_i$ ;
end
/* Identification of the targeting lift */;
$i_{\lim} \leftarrow \min\{1 \leq i \leq 2^k \mid |\mathcal{F}_i| \geq t \cdot |\mathcal{F}_{i+1}|\}$;
$\mathcal{T}_k \leftarrow \{\langle V_i, V \setminus V_i \rangle \mid 1 \leq i \leq i_{\lim}\}$ ;
```

Algorithm 5: Recognition algorithm for the targeting function.

However, it turns out that subtle complications occur which may lead our approch in this section to failure. The reason is that we obtain an ordering over all the bipartitions of the relevant inputs, that somewhat represents the combinations of these inputs by nonincreasing importance, but we have no clue on where the non-targeted combinations should start in this ordering. So, intuitively, the targeting function f can be learnt only if the *targeting lift* can be detected, for the latter delineates the border between combinations within scope and those out of scope.

We next introduce a new parameter on the oracle that will be used in order to prove correctness of our approach under some additional assumptions.

Definition 96. The oracle has *positive variance* ψ if for any family $\mathcal{F} = \langle A_1, \ldots, A_t \rangle$ the following holds for any $\mathcal{C}_1, \mathcal{C}_1' \in \mathcal{S}^{(\mathrm{in})}$:

$$\mathbb{P}r[\mathrm{O}_f(A_i) = 1 \mid A_i = \mathcal{C}_1, \mathrm{H}_{\mathcal{F}_{-i}}] \geq \psi \cdot \mathbb{P}r[\mathrm{O}_f(A_i) = 1 \mid A_i = \mathcal{C}_1', \mathrm{H}_{\mathcal{F}_{-i}})].$$

Assumption 4 (introduced in Section 5.4 corresponds to the extremal case where the oracle has positive variance $\psi = 1$. Roughly, a large positive variance implies that there cannot exist a combination within scope that is significantly more targeted than the other combinations of $\mathcal{S}^{(\mathrm{in})}$. If so then the targeting lift can be detected using a simple leftmost approach (see Algorithm 5).

Theorem 97. *Let φ be the targeting lift (Assumption 1) and let $\alpha \leq 1$ be the polynomial-growth (Assumption 2). The following holds if the oracle has positive variance $\psi > \varphi$:*

There exists a PAC-learning algorithm such that, for every $k \geq 1$ and for every $\varepsilon > 0$, the targeting function can be learnt with probability $1 - \varepsilon$ under the k-juntas hypothesis. Furthermore, this algorithm runs in $\mathcal{O}(N^k \cdot \log^{1/\alpha}(N/\varepsilon))$-time and it has $\mathcal{O}(2^k \cdot \log^{1/\alpha}(N/\varepsilon))$ query complexity.

Let us point out that even when there is no classification noise ($\mathrm{O}_f = f$), the best known PAC-learning algorithm under the k-juntas hypothesis has time complexity $N^{\mathcal{O}(k)}$ [MOS04]. Therefore, improving upon this time complexity will probably require additional assumptions.

5.5.3 Impossibility results

We end up this section with a proof that not all targeting functions can be learnt with respect to our learning model.

Proposition 98. *It is impossible to learn the targeting function f in general. In particular, there is a given monotone 2-junta that cannot be learnt even if the targeting lift is arbitrarily small.*

Proof. In order to prove the result, we will construct an oracle O_f that satisfies Assumptions 1, 2 and 3 for two distinct targeting functions. The latter is enough to prove the proposition since in such case, O_f could be used in our model for any of the two functions, and so, these cannot be distinguished with high probability. More precisely, fix $0 < p_0 < 1/5$. Let us define O_f such that for any combination $\mathcal{C}$:

$$\mathbb{P}r[\mathrm{O}_f(\mathcal{C}) = 1] = p_0 \cdot (1 + 2 \cdot \mathbb{I}_{\{D_1 \in \mathcal{C}\}} + 2 \cdot \mathbb{I}_{\{D_2 \in \mathcal{C}\}}).$$

Note that for any combination $\mathcal{C}$, we have $\mathbb{P}r[\mathrm{O}_f(\mathcal{C}) = 1] \leq 5p_0 < 1$.

Since every combination has positive probability to be targeted and the above oracle considers the combinations independently, by Chernoff bound, O_f satisfies Assumption 2 with $\alpha = 1$ for any targeting function[3]. Furthermore, O_f satisfies Assumption 3 for any targeting function that only depends on the two inputs D_1, D_2. In particular, let $f_1(\mathcal{C}) = \max\{\mathbb{I}_{\{D_1 \in \mathcal{C}\}}, \mathbb{I}_{\{D_2 \in \mathcal{C}\}}\}$ (disjunction) and let $f_2(\mathcal{C}) = \mathbb{I}_{\{D_1 \in \mathcal{C}\}} \cdot \mathbb{I}_{\{D_2 \in \mathcal{C}\}}$ (conjunction). These two functions are monotone. In fact, they are linear combinations since $f_1(\mathcal{C}) = 1 \iff \mathbb{I}_{\{D_1 \in \mathcal{C}\}} + \mathbb{I}_{\{D_2 \in \mathcal{C}\}} \geq 1$, and similarly $f_1(\mathcal{C}) = 1 \iff \mathbb{I}_{\{D_1 \in \mathcal{C}\}} + \mathbb{I}_{\{D_2 \in \mathcal{C}\}} \geq 2$. For both functions, the oracle O_f satisfies Assumption 1 with any targeting lift $\varphi > 1/2$.

Finally, note that in order to extend this negative result to lifts arbitrarily smaller than $1/2$, one may just consider a slightly more complex oracle for the above two functions f_1, f_2, namely:

$$\mathbb{P}r[\mathrm{O}_f(\mathcal{C}) = 1] = q_0^{3 - \mathbb{I}_{\{D_1 \in \mathcal{C}\}} - \mathbb{I}_{\{D_2 \in \mathcal{C}\}}},$$

for some nonzero probability q_0 that can be taken arbitrarily small. □

Let us emphasize that the negative result of Proposition 98 already holds for *monotonic* and *threshold* functions (see Section 5.4.3). In particular, it applies to the theory behind the Web's transparency tools XRay [LDL+14] and Sunlight [LSS+15].

5.6 Conclusion

We have proved in this chapter that the theory behind two recent Web's transparency tools – namely, Xray [LDL+14] and Sunlight [LSS+15] – can be applied to cope with complex targeting, but that it requires stronger assumptions on the oracle. When these assumptions do not hold, we show that not all targeting functions can be learnt.

It is equally likely that not all (learnable) functions can be learnt efficiently. Indeed, even in a simpler learning model where there is no classification noise, learning k-juntas takes $N^{\mathcal{O}(k)}$-time [MOS04, Val12]. Furthermore, given a set of positive and negative examples, learning a function that is compatible with these examples under k-juntas hypothesis is $W[2]$-hard [AKL07]. The same negative result holds under monotonic k-juntas hypothesis [AKL07], which makes the existence of $N^{o(k)}$-time PAC-learning algorithms unlikely. I believe that the existence or

[3]Note that we must also choose the same constants β and γ. Here, the two functions considered are such that the scope of one is contained into the scope of the other. So, we can choose β, γ w.r.t. the function with smallest scope.

nonexistence of quasi-linear time algorithms in our setting is strongly related to the value of the targeting lift — as supported by the results of Section 5.4.

For this reason, I would find it interesting to mix up our learning model with some advertising models of the literature (*e.g.*, [GEC+13]) in order to fix some "plausible" estimate for the lift. This project is part of my on-going work.

Another interesting problem would be to enhance our learning model by including a natural graph structure between the accounts. Namely, as we stated in Section 5.2.4, the online accounts of users can be seen as the vertices of a random intersection graph [KSSC99], where an edge represents two accounts sharing a certain number of inputs. The influence of these edges on the outcome is largely ignored by our model, but it has received some attention in [LMT17]. Combining our model with the approach proposed in [LMT17] is thus an important issue.

Finally, on the practical point of view, one hidden drawback of the algorithms that are proposed in this chapter is that each query to the sampler represents, in real-life, a fake account which needs to be created and maintained [LDL+14]. This task is hard to automate, because online accounts have to respect a policy and they can be quickly closed if they don't. Ideally, we would like to find a different implementation of our algorithms that would require fewer account creations. For instance, could we avoid creating fake accounts by making some existing accounts collaborate (with each of them representing one query to the sampler) ? This simple idea would raise privacy concerns, that would require a computational mechanism design in order to handle with the communications between two accounts.

Overall, new guidelines than our "SET COVER approach" should be investigated, such as for instance the use of different oracles (that would represent accounts on different online platforms) [AM10]. Our work may also benefit from a bio inspired algorithm named Ant-miner [HLC07, PLF02] whose objective is to uncover classification rules from a dataset.

Chapter 6

Conclusion

Contents

As networks more and more impact our lives, the world is turned to be ruled by algorithms. This situation has motivated the need for more efficiency in algorithmic and more transparency in the use of algorithms. In this thesis, we have adressed these two issues by studying metric tree-likeness in graphs – related to the way the information flows in complex networks – and a collection of privacy oriented problems. We provide a finer-grained analysis for the complexity of all the problems studied, so as to question their scalability.

The contributions of my thesis are summarized in Section 6.1, with an emphasis on future work.

6.1 Open perspectives

We summarize our results in Chapters 2–5 and raise interesting questions for future work. In what follows, we borrow from the concluding sections of these different chapters.

First, we have given a survey on graph hyperbolicity in Chapter 2 where known lower and upper bounds are collected and the best known results on the complexity for computing this parameter are covered. In particular, we have introduced a general framework in order to sharply estimate the distortion of hyperbolicity that may be caused by various graph operations and so, conversely, by various graph decompositions. We also have proved new sufficient conditions in order to lower or upper-bound the hyperbolicity in some graph classes that are used for the design of data center interconnection networks. We expect our techniques to apply to even more graph classes, that is left as an interesting open question.

Furthermore, on the complexity point of view, we have proposed a preprocessing method that is based on clique-decomposition. Interestingly, the core arguments that are used for our analysis of the preprocessing can be applied to any other "tree-like" decomposition: where the subgraphs are the bags of a tree decomposition with bounded-diameter adhesion sets. Now, the question is whether they can be applied to more general decompositions, say where the subgraphs are the sets of some family with a "tree-representation" [BXHR12]? If so, then the latter result would subsume all known results on the preservation of hyperbolicity under modular, split and clique decomposition. Another interesting open question is whether the recognition of graphs with "large" hyperbolicity can be done faster than computing this parameter for general graphs. Indeed, we recall that all the hardness results proved for this parameter have been obtained for graphs with small hyperbolicity (bounded by a constant). This is further supported by the experiments presented in [CCL15, BCC15]: where the practical running-time is dominated by the computation of the all-pairs shortest-paths except for some hard instances that have been observed to have a small hyperbolicity.

Chapter 3 is devoted to an in-depth (complexity) study of some tree decompositions in graphs where the bags must satisfy metric constraints. More precisely, we have proved that computing the clique-decomposition is computationally equivalent to TRIANGLE DETECTION under the standard assumption that the latter problem is equivalent to MATRIX MULTIPLICATION. We have also proved that computing the parameters treebreadth, pathbreadth and pathlength (recently introduced in [DK14, DKL14]) is NP-hard and not FPT. However, on a more positive side, the clique-decomposition of planar graphs and bipartite graphs can be computed in linear time, and in the same way it can be decided in polynomial time whether a given bipartite graph or planar graph has treebreadth one.

In particular, let us point out that all our hardness results have been obtained for classes of graphs with a large clique or clique-minor, whereas all our positive results have been proved for classes of graphs with bounded clique-number or clique-minor. Therefore, it would be interesting to find new results (positive or negative) that could better clarify the role of the clique-number and the Hadwiger number (size of a largest clique-minor) in the parameterized complexity of the tree decomposition problems studied in this chapter. In this respect, we might be helped by a central result in Chapter 3: stating that treewidth and treelength can only differ by at most a constant-factor in the classes of graphs with bounded-length isometric cycles and bounded genus.

Furthermore, whereas our tools in Part I have been mainly graph-theoretical, we have used a more diverse toolkit in Part II based on combinatorics, game theory and learning theory. This diversification of our techniques has conduced to open questions of a different nature, that we will expose next.

In particular, we have studied coloring games in Chapter 4, exhibiting new results on the complexity of computing strong Nash equilibria in these games and in some of their variations. More precisely, we have proved that a k-strong Nash equilibrium can be computed with better-response dynamics for every fixed $k \geq 1$, however the dynamics do not converge in polynomial time as soon as $k \geq 4$. So, it may be the case that computing a k-strong Nash equilibrium in coloring games is PLS-complete for some fixed $k \geq 4$. Such a result would be interesting because coloring games are played on an *unweighted* graph whereas the classical PLS-complete problems are "weighted", *i.e.*, they can be solved in quasi-polynomial time with respect to some set of input weights.

Note that as a way to deepen our understanding of coloring games, we have proved that computing a Nash equilibrium in these games is PTIME-hard. It has been proved that computing a Nash equilibrium in generalized coloring games (played on an edge-weighted graph) is PLS-complete. Can we prove that conversely, if a "weighted" game is PLS-hard then any corresponding "unweighted" game (where all the input weights are bounded) is PTIME-hard ? Such a result would make advance our understanding of the complexity of search problems.

Finally, we have studied in Chapter 5 the problem of learning a Boolean function that only depends on a fixed number of variables, under new hypotheses on the classification noise. Our problem is motivated by online advertising in the Internet (we aim at unveiling data misuse), and so, it has a natural graph structure. However, this structure has not been exploited in our algorithms. Hence, an important issue would be to better account for this underlying graph.

As an example, is this graph hyperbolic ? If it were the case, could we take advantage of this fact in order to obtain efficient approximation algorithms for Set Cover, that could be used in our approach for learning the function ?

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Appendix A

Résumé de la thèse

A.1 Contexte

Le *partage d'information* en ligne a gagné en importance au cours de ces dernières décennies. Les chiffres parlent d'eux mêmes: en 2015 il y a eu 205 milliards de courriels échangés quotidiennement [Ema]; sur la même période, près de 500 millions de tweets par jour ont été envoyés [Twi]; on observe plus généralement une hausse du trafic Internet, qui est passé de 100 GB par jour en 1992 à 20 235 GBps en 2015 [Cisa]. De même le volume des données stockées a explosé, avec des prévisions de l'ordre de 40 zettaoctets pour 2020 [IDC].

Alors que nous entrons de plain-pied dans cette "ère du zettaoctet", les techniciens de l'information se retrouvent confrontés à diverses problématiques qui sont régulièrement relayées par les médias. Dans cette thèse, nous nous intéressons à deux de ces problématiques:

- **Le Passage à l'échelle** – défini dans [Ten16] comme l'impératif d'obtenir des algorithmes en temps quasi-linéaire en la taille des réseaux. Dans une perspective plus large, il y a une demande croissante d'algorithmes efficaces pour gérer les réseaux de communication. Ces demandes émanent de nombreux domaines scientifiques tels que ceux des télécommunications, de la bio-informatique, de la vision artificielle et de l'économie. La difficulté principale est qu'avec l'essor des échanges d'information et des collectes de données en ligne la taille des réseaux a augmenté, avec à présent des millions de serveurs dans certains centres de données [DCM], des milliards d'utilisateurs sur les réseaux sociaux [FBN], etc. Devant pareilles tailles mêmes les algorithmes cas d'école ne passent pas tous à l'échelle, ce qui accroît le fossé entre ce qui est calculable et ce qu'on veut calculer. Il y a donc lieu de redéfinir ce que signifie un calcul efficace, ou qui passe à l'échelle, dans ce contexte.

  Nous proposons des avancées dans cette direction en nous basant sur des outils de la théorie des graphes et de la complexité.

- **Le respect de la vie privée** – est défini dans [EDP] comme "*un droit qui interdit aux autorités publiques [et à toute autre organisation ou individu] d'exercer des mesures [de nature à rendre publique la vie privée des gens] à moins que certaines conditions soient vérifiées.*" Plus précisément, des inquiétudes naissent de la collecte effrénée de données par les entreprises en ligne, dont les dérives se font jour fréquemment [Gou14, Mat12, VDSVS12, The14]. De là le besoin de modèles prédictifs afin que chaque individu puisse détecter ces dérives, voire même les identifier.

Nos principaux outils pour cette tâche sont ceux de la théorie de l'apprentissage et la théorie algorithmique des jeux.

Avant d'annoncer nos résultats dans la Section A.2, nous commençons par esquisser notre approche pour cette thèse. Le travail présenté est la somme de plusieurs problèmes combinatoires sur les graphes, dont l'étude est motivée par les deux problématique exposées ci-dessus. Puisque les solutions proposées pour ces problèmes doivent passer à l'échelle sur les grands réseaux, on s'intéresse tout particulièrement à l'étude *fine* de leur complexité.

En particulier, la Partie I est dédiée à l'étude de paramètres dans les graphes dont les relations avec les problématiques ci-dessus ont été montrées dans d'autres travaux [NS11]. L'étude des propriétés des "réseaux complexes", ainsi que de leurs applications, est un sujet bien établi [LLDM09, BAJ00, BKC09, WS98, DGM06]. Dans notre cas, l'accent est mis sur la proximité des métriques de graphes avec les métriques d'arbres [Gro87]. Ce sujet a reçu une attention croissante au cours des dernières décennies. Nous détaillons dans la Partie I comment les avantages et les inconvénients des arbres (avec d'un côté d'importantes applications algorithmiques mais de l'autre côté des vulnérabilités bien connues) peuvent s'étendre aux graphes qui sont (métriquement) proches des arbres.

Cette ligne principale de la thèse sera complétée dans la Partie II par l'analyse de deux processus dynamiques sur les graphes. Ces deux processus modélisent des aspects fondamentaux de la problématique du respect de la vie privée dans les réseaux de communications. En d'autres termes, l'objectif dans cette ligne secondaire de la thèse est de concevoir des outils (qui passent à l'échelle) afin de renforcer le respect de la vie privée dans ces réseaux.

A.2 Contributions

Notre travail est exposé dans deux parties disjointes et indépendantes l'une de l'autre. Leur contenu est présenté dans les Sections A.2.1 et A.2.2 ci-dessous.

Par ailleurs, l'annexe regroupe l'ensemble des articles par lesquels les résultats de cette thèse ont été publiés. En effet, nous avons fait le choix de ne pas inclure toutes les preuves dans le corps des chapitres, en partie pour des raisons de lisibilité car certaines d'entre elles dépassent allègrement la douzaine de pages. Seront seulement données les preuves qui, de notre point de vue, illustrent le mieux les techniques utilisées. Le tout accompagné d'esquisses des preuves les plus longues.

A.2.1 Partie I: Sur les graphes dont la métrique est proche de celle d'un arbre

Nous étudions dans la Partie I des propriétés métriques des graphes et des décompositions de graphes. L'objectif majeur de cette partie est l'étude fine de la complexité de leur calcul. En particulier, ces propriétés peuvent-elles être calculées sur de très grands graphes, avec parfois des millions de noeuds et des milliards d'arêtes ? Nos pistes pour répondre à ces questions nous ont amené à étudier les relations entre les propriétés métriques d'un graphe et ses propriétés structurelles, topologiques, algébriques, etc.

A.2.1.1 Chapitre 2: Une vue d'ensemble sur l'hyperbolicité dans les graphes

Ce chapitre introduit la notion d'hyperbolicité dans les graphes. Ce paramètre donne des bornes sur la meilleure distorsion possible des distances dans un graphe quand il est plongé dans un arbre.

Tout d'abord nous démontrons plusieurs résultats, positifs comme négatifs, sur la complexité du calcul de ce paramètre. Plus précisément, sur le plan positif nous proposons une méthode de pré calcul afin de réduire la taille des graphes en entrée de nos algorithmes. Cette méthode utilise une décomposition des graphes bien connue, selon les cliques-séparatrices [BPS10]. Nous en faisons une analyse poussée. Sur un plan plus négatif, nous prouvons que reconnaître les graphes de petite hyperbolicité (au plus 1/2) est un problème de complexité équivalente à la détection de carrés induits dans un graphe. Ce résultat implique, sous certaines hypothèse de complexité standard, que calculer l'hyperbolicité d'un graphe est impossible en temps sous-cubique. Ces travaux ont été réalisés en collaboration avec Nathann Cohen, David Coudert et Aurélien Lancin [CD14, CCDL17].

Ensuite, nous établissons de nouvelles bornes sur ce paramètre dans des classes de graphes utilisées dans la conception des réseaux d'interconnexion de centre de données. Dans la pratique, nous avons utilisé ce résultat pour estimer fidèlement l'hyperbolicité de graphes de très grande taille sans le moindre calcul. Nous complétons ce résultat par une analyse fine des variations de l'hyperbolicité sous certaines opération bien connues sur les graphes telles que le graphe adjoint, le graphe des cliques, etc. Cette analyse prend une tout autre saveur dans les cas où l'opération peut facilement s'inverser (par exemple, la racine d'un graphe adjoint se calcule en temps linéaire [Whi92]), car elle donne alors de nouvelles méthodes de pré calcul pour le calcul de l'hyperbolicité d'un graphe. Ce travail a été réalisé en commun avec David Coudert [CD16a, CD16b].

A.2.1.2 Chapitre 3: Décompositions arborescentes avec des contraintes sur les distances dans les sacs

De nouveaux résultats sont présentés sur la complexité du calcul de *décompositions arborescentes* avec des contraintes sur les distances dans les sacs (*ç.a.d.* les sous-graphes résultant de la décomposition).

D'abord, on présente une analyse fine de la complexité du calcul de la décomposition d'un graphe selon ses cliques-séparatrices. La complexité de ce problème est prouvée équivalente, sous des hypothèses de complexité standard, à la détection de triangles dans un graphe et au produit de deux matrices carrées. Sur un plan plus positif nous montrons que cette décomposition est calculable en temps quasi-linéaire pour des classes de graphes où la taille d'une plus grande clique est bornée par une constante. Ce travail a été réalisé en commun avec David Coudert [DC17].

Dans un deuxième temps, nous répondons à des questions ouvertes de la littérature sur la complexité du calcul de différents paramètres métriques des graphes, tous reliés à l'hyperbolicité (treebreadth, pathbreadth et pathlength). Nous prouvons que pour tous ces paramètres, leur calcul est un problème NP-difficile. En particulier, nous montrons que reconnaître les graphes de treebreadth au plus une est NP-complet. Cependant, nous prouvons que ce dernier problème devient polynomial si l'on se restreint aux graphes bipartis et aux graphes planaires. Ce travail a été réalisé en collaboration avec Sylvain Legay et Nicolas Nisse [DLN16a].

Enfin, nous étudions les relations entre une autre propriété métrique des graphes: la *treelength*, et une propriété *structurelle* bien connue: la *treewidth* des graphes. Nous bornons la treewidth par deux fonctions affines de la treelength dans les classes de graphes sans long cycle isométrique et de genre borné. Sur le plan algorithmique, on mentionne plusieurs applications de ce résultat. C'est un travail effectué en commun avec David Coudert et Nicolas Nisse [CDN16].

A.2.2 Partie II: Le respect de la vie privée à grande échelle dans les réseaux sociaux

Deux problèmes autour du respect de la vie privée sont introduits et étudiés dans cette partie. Notre objectif est d'obtenir une analyse fine de leur complexité.

A.2.2.1 Chapitre 4: le calcul d'équilibres dans les jeux de coloration

Nous considérons un jeu de coloration sur les graphes. Ce jeu a été proposé dans [KL13] pour modéliser la dynamique des communautés dans les réseaux sociaux. D'autres applications avaient été précédemment suggérées pour ce jeu, dont la sécurisation de groupes de communication [CKPS10].

Nous présentons de nouveaux résultats sur la complexité du calcul d'équilibres dans ce jeu. Pour être plus précis, nous nous concentrons tout d'abord sur le calcul d'équilibres par *meilleure réponse*. Cette méthode de recherche locale permet de calculer, pour tout entier k, un équilibre de Nash robuste contre toutes les coalitions d'agents possibles de taille au plus k. Sur le plan positif, nous établissons le temps de convergence exact de cette méthode dans le pire cas, pour $k \leq 2$. Toutefois, sur le plan négatif, nous prouvons que ce temps de convergence n'est pas polynomialement borné dès que $k \geq 4$. Ce résultat négatif répond aux questions ouvertes de [EGM12, KL13]. Ce travail a été effectué en commun avec Dorian Mazauric et Augustin Chaintreau [DMC13a, DMC17].

Nous complétons ce dernier résultat par une analyse plus fine de la complexité du calcul d'un équilibre de Nash dans le jeu de coloration (robuste contre les déviations de n'importe quel agent). On montre que ce problème est P-difficile, ce qui suggère qu'il est intrinsèquement séquentiel [Duc16].

Enfin, le reste du chapitre est dédié à une généralisation naturelle du jeu de coloration sur les graphes arêtes-pondérés. Nous donnons des conditions suffisantes pour l'existence d'équilibres dans ces jeux qui dépendent de la structure du graphe sous-jacent (notamment, de sa maille). Nous proposons également des constructions surprenantes de jeux pour lesquels de tels équilibres n'existent pas. Pour finir, il est prouvé que reconnaître les jeux de coloration généralisés qui admettent de tels équilibres est un problème NP-complet. Des extensions de tous ces résultats à des classes de jeux plus générales sont aussi discutées. C'est un travail commun avec Dorian Mazauric et Augustin Chaintreau [DMC12, DMC13a, DMC17].

A.2.2.2 Chapitre 5: Apprentissage de formules logiques dans un modèle bruité

Nous consacrons le dernier chapitre à un problème d'apprentissage dont le contexte peut s'énoncer comme suit. Soient un ensemble $\mathcal{D}$ (qui représente des mots-clefs) et un graphe où chaque sommet est étiqueté par un sous-ensemble de $\mathcal{D}$ (*ç.a.d.* une collection de mots-clefs présents dans les courriels d'un utilisateur). On assigne un Booléen à chaque sommet selon un processus (boîte noire) aléatoire, qui lui-même est corrélé à une certaine fonction Booléenne (inconnue) sur les étiquettes. Le problème posé est l'apprentissage de cette fonction. Nous entendons ainsi modéliser le problème de la détection de l'utilisation des données utilisateur dans les campagnes publicitaires en ligne.

D'abord nous proposons un algorithme pour apprendre la fonction dans un cas simple où elle dépend d'au plus une variable. Cet algorithme est à la base de méthodes d'apprentissage plus sophistiquées pour d'autres classes de fonctions — mais sous des hypothèses plus contraignantes. Par ailleurs il est montré que sans ces hypothèses supplémentaires, il est impossible d'apprendre la fonction dès qu'elle dépend d'au moins deux variables. Ce travail a été effectué en collaboration avec Mathias Lécuyer, Francis Lan, Max Tucker, Riley Sphan, Andrei Papancea, Theofilos Petsios, Augustin Chaintreau et Roxana Geambasu [LDL+14, DLCG15, DTC17, CD17].

Papers on graph hyperbolicity

Appendix B

Applying clique-decomposition for computing graph hyperbolicity

Applying clique-decomposition for computing Gromov hyperbolicity

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Abstract

Given a graph, its *hyperbolicity* is a measure of how close its distance distribution is to the one of a tree. This parameter has gained recent attention in the analysis of some graph algorithms and the classication of complex networks. We study on practical improvements for the computation of hyperbolicity in large graphs. Precisely, we investigate on relations between the hyperbolicity of a graph G and the hyperbolicity of its *atoms*, that are the subgraphs output by the clique-decomposition invented by Tarjan [44, 56]. We prove that the maximum hyperbolicity taken over the atoms is at most one unit off from the hyperbolicity of G and the bound is sharp. We also give an algorithm to slightly modify the atoms, which is at no extra cost than computing the clique-decomposition, and so that the maximum hyperbolicity taken over the resulting graphs is *exactly* the hyperbolicity of G. An experimental evaluation of our method for computing the hyperbolicity of a given graph from its atoms is provided for large collaboration networks. Finally, on a more theoretical side we deduce from our results the first *linear-time* algorithm for computing the hyperbolicity of an outerplanar graph.

Keywords: Gromov hyperbolicity; graph algorithms; clique-decomposition; outerplanar graphs.

1 Introduction

In this paper we aim at improving the computation of hyperbolicity in large graphs, whose size ranges from thousands to tens of thousands of nodes. To this end, we will establish new relations between hyperbolicity and some graph decomposition. Roughly, the hyperbolicity of a metric space is an estimate of how close it is to a metric tree (formal definitions are postponed to the technical sections of this paper). This parameter was first introduced by Gromov in the context of automatic groups [35]. Later on, it was extended to more general metric spaces including graphs equipped with their shortest-path metric. Graph hyperbolicity is now part of the parameters in use to classify complex networks [1, 2, 40]. Furthermore, the study of graphs with bounded hyperbolicity has found applications in the design and the analysis of approximation algorithms [19, 24] and geometric routing schemes [11], as well as in network security [38] and bioinformatics [18, 30], to name a few. As a result, hyperbolicity and its relations to other metric graph parameters has received growing attention over the last decades. The reader may refer to [1, 29] for a recent survey.

Computing the hyperbolicity is useful in some of the above applications. For instance, it allows to compute an embedding of the graph into the Hyperbolic plane with quasi-optimal distortion of the distances in linear-time [58]. The latter is a prerequisite to many algorithms on negatively curved spaces [42]. However, the computational cost of hyperbolicity has only recently received a bit more attention. So far, the best-known algorithm to compute the hyperbolicity [31], though it runs in polynomial-time, is impractical for large-scale graphs such as the graph of the Autonomous Systems of the Internet, road maps, etc. This comes from its challenging implementation, relying on fast square matrix multiplications, and its time complexity which is supercubic. On a more positive side, there have been recent attempts that are much more efficient than the state-of-the-art algorithm in practice, with running time dominated by the computation of the all-pairs-shortest-paths [13, 21]. But on the negative side, it is unlikely that graph hyperbolicity can be computed in subquadratic-time, even for sparse graphs [14, 22, 31]. This motivates us to study which structural properties can help to speed-up the computation of hyperbolicity in large graphs.

Our approach. We build on *graphs decompositions* in order to gain more insights on the internal structure of graphs with bounded hyperbolicity. More precisely, we are given a decomposition of a graph in some of its subgraphs and we aim at computing its hyperbolicity from the hyperbolicity of the subgraphs. This way, for computing the hyperbolicity of a graph, we can preprocess it and replace it with the subgraphs of the decomposition, thereby decreasing the size of the inputs. Although such techniques are unlikely to improve the calculation of hyperbolicity in general (for they may be graphs that are "prime" w.r.t. the decomposition), they are expected to work well on some graph classes of interest, including some classes of real-life graphs. A first step toward this direction was made by Soto in his PHD thesis [51]. He proved that the hyperbolicity of a graph is the maximum hyperbolicity taken over the subgraphs from the modular decomposition [33] or the split-decomposition [23]. Examples of complex networks whose underlying graph has a nontrivial modular decomposition are the protein-protein interaction networks [32].

We here address a similar question for the subgraphs from the *clique-decomposition*, also known as *atoms*. The clique-decomposition was introduced by Tarjan in [56] then made unique by Leimer in [44]. Roughly, it consists in disconnecting the graph using clique-separators, and it is easy to implement. Note that there are studies supporting the existence of clique-separators in real-life graphs, such as the underlying graphs of social and biological networks [1, 7, 26, 39], that makes our approach practical for large graphs. Furthermore, clique-decomposition has been proved useful to preprocess the graphs in the computation of many optimization problems [56] – including the computation of treelength [28], related to hyperbolicity. Therefore, at first glance, it should not come as a surprise if clique-decomposition can be applied to preprocess the graphs in the computation of hyperbolicity. This being said, hyperbolicity is less robust than other metric invariants to graph modifications (for instance, it may increase after an edge-contraction [17]), so, a careful analysis is needed to prove whether it is the case.

Main contributions. In fact, our first result is that, somewhat counter-intuitively, the hyperbolicity $\delta(G)$ of a graph G *cannot* be deduced directly from the hyperbolicity of its atoms (Section 3). We will prove nonetheless that it can be approximated with additive constant 1 by taking the maximum hyperbolicity $\delta^*(G)$ over the atoms (Section 4). This result requires an in-depth analysis of clique-decomposition in order to be proved. Additionally, we characterize when it is the case that $\delta(G) > \delta^*(G)$.

Based on this characterization, we will show in Section 5 how each atom can be "modified" (augmented with few simplicial vertices) in order to compute exactly the hyperbolicity, and provide a complexity analysis of the procedure. Experiments in Section 7 show the benefit of our method in terms of size of the graph, when applied to some real collaboration networks.

Finally, we will apply clique-decomposition for improving the best-known complexity to compute hyperbolicity in the class of outerplanar graphs. We will detail in Section 6 the first linear-time algorithm for computing the hyperbolicity of these graphs. We find the latter result all the more interesting that under classical complexity assumptions, the hyperbolicity of sparse graphs cannot be computed in subquadratic-time [14].

Definitions and notations used in this paper will be introduced in Section 2.

2 Definitions and notations

We use the graph terminology of [12, 27]. All graphs considered in this paper are finite, unweighted and simple. Given $G = (V, E)$, let $n = |V|,\ m = |E|$. For every subset of vertices $S \subseteq V$, the open neighborhood of S is the set of all vertices in $V \setminus S$ with at least one neighbor in S. We denote it by $N_G(S)$, or by $N(S)$ when G is clear from the context. The close neighborhood of S is the set $S \cup N(S)$, denoted by $N[S]$.

Given two vertices u and v, a *uv-path* of length $l \geq 0$ is a sequence of vertices $(u = v_0 v_1 \dots v_l = v)$, such that $\{v_i, v_{i+1}\}$ is an edge for every i. In particular, a graph G is *connected* if there exists a uv-path for all pair $u, v \in V$, and in such a case the *distance* $\mathrm{d}_G(u, v)$ is defined as the minimum length of a uv-path in G. Note that it yields a discrete metric space (V, d_G), also known as the shortest-path metric space of G. We will write d instead of d_G whenever G is clear from the context, and we denote by $\mathrm{d}(u, X) = \min_{x \in X} \mathrm{d}(u, x)$ the distance between a vertex u and a set X of vertices.

Our proofs use the notions of subgraphs, *induced* subgraphs, as well as *isometric subgraphs*, the latter denoting a subgraph H of a graph G such that $\mathrm{d}_H(u, v) = \mathrm{d}_G(u, v)$ for any two vertices $u, v \in H$.

2.1 Gromov hyperbolicity

The space (V, d_G) is a tree metric if there exists a distance-preserving mapping from V to the nodes of an edge-weighted tree. In this case, the graph G is called 0-hyperbolic. Several characterizations exist for 0-hyperbolic graphs. Informally, a graph is called δ-hyperbolic if it satisfies one of these characterizations up to a defect at most δ. Different characterizations will lead to different values for δ, but they may differ only by a small constant-factor [6, 25, 35]. We here consider the following 4-point definition for hyperbolicity.

Definition 1 (**4-points Condition, [35]**). *Let G be a connected graph. For every 4-tuple u, x, v, y of vertices of G, we define $\delta(u, v, x, y)$ as half of the difference between the two largest sums among*

$$S_1 = \mathrm{d}(u, v) + \mathrm{d}(x, y),\ S_2 = \mathrm{d}(u, x) + \mathrm{d}(v, y) \text{ and } S_3 = \mathrm{d}(u, y) + \mathrm{d}(v, x).$$

The hyperbolicity of G, denoted by $\delta(G)$, is equal to $\max_{u,x,v,y \in V(G)} \delta(u, v, x, y)$. Moreover, we say that G is δ-hyperbolic, *for every $\delta \geq \delta(G)$.*

It is straightforward, by the above definition, to compute graph hyperbolicity in $\theta(n^4)$-time. In theory, it can be decreased to $\mathcal{O}(n^{3.69})$ by using clever (max, min) matrix product [31]. But in practice, the best-known algorithms still run in $\mathcal{O}(n^4)$-time [13, 21]. Graphs with small hyperbolicity can be recognized faster. In fact, 0-hyperbolic graphs coincide with *block graphs*, that are graphs whose all biconnected components are complete subgraphs [5, 37]. Hence it can be decided in linear $\mathcal{O}(n+m)$-time whether a graph is 0-hyperbolic. The latter characterization of 0-hyperbolic graphs follows from a more general result saying that the hyperbolicity of a graph is the maximum hyperbolicity from its biconnected components (our work will give a new proof of this well-known result). More recently, it was proved that the recognition of $\frac{1}{2}$-hyperbolic graphs is computationally equivalent to decide whether there is a chordless cycle of length 4 in a graph [22]. The latter problem can be solved in deterministic $\mathcal{O}(n^{3.26})$-time [43] and in randomized $\mathcal{O}(n^{2.373})$-time [57] by using fast matrix multiplication.

2.2 Clique-decomposition

Given $G=(V,E)$, we name *separator* a subset of vertices $X \subset V$ such that the removal of X disconnects the graph. We call X a *clique-separator* when the induced subgraph $G[X]$ is a complete graph. A graph is *prime* if it does not contain a clique-separator. Examples of prime graphs are complete graphs and cycles. Finally, the *clique-decomposition* of G is the collection of its maximal sets of vertices that induce prime subgraphs of G (we will call them *atoms*). See Figure 1 for an illustration. The decomposition is unique and it can be computed in $\mathcal{O}(nm)$-time [44, 56]. We refer to [8] for a survey on clique-decomposition.

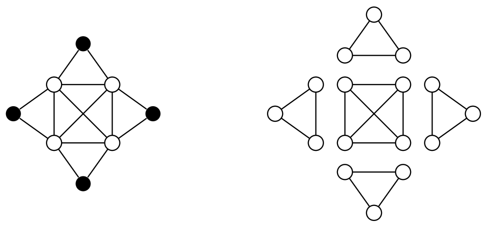


Figure 1: Clique-decomposition of a graph in five atoms. A 4-tuple with hyperbolicity 1 is drawn in bold.

Notations. Let us fix some notations for the proofs. Given $G=(V,E)$, let X be a separator of G. Let A, B denote two sets of vertices such that $A \cap B \subseteq X$ and $A \setminus X$, resp., $B \setminus X$, is nonempty. We will call X a $(A|B)$-separator. Let us denote by $(a|b_1, b_2, b_3)$ a 4-tuple such that $a \in A$ and $b_1, b_2, b_3 \in B$. In the same way, let us denote by $(a_1, a_2|b_1, b_2)$ a 4-tuple such that $a_1, a_2 \in A$ and $b_1, b_2 \in B$. Note that we allow some vertices of the 4-tuple to be in X with this notation.

3 Hyperbolicity and clique-separators

It happens that every atom of the graph is δ-hyperbolic whereas it has hyperbolicity strictly greater than δ. As example, consider the chordal graph of Figure 1. It is 1-hyperbolic, with a 4-tuple of maximum hyperbolicity being drawn in black. However, its five atoms are complete graphs, hence they are 0-hyperbolic.

The purpose of the next two sections is to upper-bound the gap between $\delta(G)$ and $\delta^*(G)$ for every graph G, where $\delta^*(G)$ denotes the maximum hyperbolicity from the atoms of G. To this end, we analyze in this section the relationship between the hyperbolicity of a graph and a given clique-separator, leading to the approximation with additive constant of Theorem 12. It begins with an observation about $(a_1, a_2|b_1, b_2)$ 4-tuples and the diameter $\text{diam}(X) = \max_{u,v\in X} \text{d}_G(u, v)$ of a $(A|B)$-separator X.

3.1 Hyperbolicity of $(a_1, a_2|b_1, b_2)$ 4-tuples

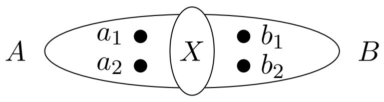


Figure 2: Illustration of a $(A|B)$-separator.

Lemma 2. *Let X be a $(A|B)$-separator of a connected graph G. For every $(a_1, a_2|b_1, b_2)$ 4-tuple, we have $\delta(a_1, a_2, b_1, b_2) \leq \text{diam}(X)$.*

Proof. By Definition 1, we have $\delta(a_1, a_2, b_1, b_2) = (L - M)/2$ where L and M are the two biggest sums among the following:

$$S_1 = \text{d}(a_1, a_2) + \text{d}(b_1, b_2),\ S_2 = \text{d}(a_1, b_1) + \text{d}(a_2, b_2),\ S_3 = \text{d}(a_1, b_2) + \text{d}(a_2, b_1).$$

Let us upper-bound L. By the triangular inequality we have that for every $u, v \in \{a_1, a_2, b_1, b_2\}$, $\text{d}(u, v) \leq \text{d}(u, X) + \text{d}(v, X) + \mathit{diam}(X)$. Thus, for every $i \in \{1, 2, 3\}$ we have (by applying twice the triangular inequality) that $S_i \leq \text{d}(a_1, X) + \text{d}(a_2, X) + \text{d}(b_1, X) + \text{d}(b_2, X) + 2 \cdot \mathit{diam}(X)$. In particular, $L \leq \text{d}(a_1, X) + \text{d}(a_2, X) + \text{d}(b_1, X) + \text{d}(b_2, X) + 2 \cdot \mathit{diam}(X)$.

Furthermore, since X is assumed to be a $(A|B)$-separator, we have that for every $i, j \in \{1, 2\}$, all a_ib_j-paths in G must intersect X, and so, $\text{d}(a_i, b_j) \geq \text{d}(a_i, X) + \text{d}(b_j, X)$. Hence, $\text{d}(a_1, X) + \text{d}(a_2, X) + \text{d}(b_1, X) + \text{d}(b_2, X) \leq \text{d}(a_1, b_1) + \text{d}(a_2, b_2) = S_2$, and in the same way $\text{d}(a_1, X) + \text{d}(a_2, X) + \text{d}(b_1, X) + \text{d}(b_2, X) \leq S_3$. Altogether it implies that $L \leq \min\{S_2, S_3\} + 2 \cdot \mathit{diam}(X)$. By noticing that $\min\{S_2, S_3\} \leq M$, one finally obtains that $L \leq M + 2 \cdot \mathit{diam}(X)$, and so, $\delta(a_1, a_2, b_1, b_2) \leq \mathit{diam}(X)$, as desired. $\square$

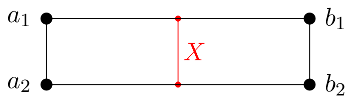


Figure 3: An $(a_1, a_2|b_1, b_2)$ 4-tuple with hyperbolicity 1.

Corollary 3. *Let X be a $(A|B)$-clique-separator of a connected graph G. For every $(a_1, a_2|b_1, b_2)$ 4-tuple, we have $\delta(a_1, a_2, b_1, b_2) \leq 1$.*

The upper-bound of Corollary 3 is sharp, as shown with the grid of Figure 3. By taking larger grids, it can also be shown that the upper-bound of Lemma 2 is sharp.

3.2 Hyperbolicity of $(a|b_1, b_2, b_3)$ 4-tuples

In contrast to $(a_1, a_2|b_1, b_2)$ 4-tuples, the hyperbolicity of a $(a|b_1, b_2, b_3)$ 4-tuple can be arbitrarily large. We will relate $(a|b_1, b_2, b_3)$ 4-tuples with some 4-tuples of $B \cup X$ in order to upper-bound their hyperbolicity. Precisely, note that X being a clique, each vertex $a \in A$ is at distance at least $\mathrm{d}(a, X)$ and at most $\mathrm{d}(a, X) + 1$ from any vertex of X. We now show how this can be used with respect to the hyperbolicity.

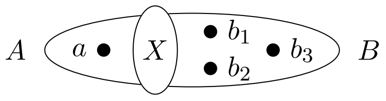


Figure 4: Illustration of a $(a|b_1, b_2, b_3)$-separator.

Lemma 4. *Let X be a $(A|B)$-clique-separator of a connected graph G, and let $a \in A$. We consider the graph G' obtained from G by adding a vertex a^* adjacent to $\{x \in X : \mathrm{d}_G(a, x) = \mathrm{d}_G(a, X)\}$. Then for every $b_1, b_2, b_3 \in B$ we have $\delta(a, b_1, b_2, b_3) = \delta(a^*, b_1, b_2, b_3)$.*

Proof. By construction G is an isometric subgraph of G' and so, $\forall\, u, v \in V(G)$, $\mathrm{d}_{G'}(u, v) = \mathrm{d}_G(u, v) = \mathrm{d}(u, v)$. In particular, the value $\delta(a, b_1, b_2, b_3)$ is not modified by the construction.

Let us relate $\mathrm{d}(a^*, b)$ with $\mathrm{d}(a, b)$ for every $b \in B$. Precisely, let us prove that $\mathrm{d}(a, b) - \mathrm{d}(a^*, b)$ is a constant (*i.e.*, not depending on b), that will prove by Definition 1 that $\delta(a, b_1, b_2, b_3) = \delta(a^*, b_1, b_2, b_3)$ for every $b_1, b_2, b_3 \in B$. In order to prove it, first observe that $\forall\, x \in X$, $\mathrm{d}(a, x) \in \{\mathrm{d}(a, X), \mathrm{d}(a, X) + 1\}$ holds as X is a clique. Since a^* is adjacent to $\{x \in X : \mathrm{d}(a, x) = \mathrm{d}(a, X)\}$, this implies that $\forall\, x \in X$, $\mathrm{d}(a, x) = \mathrm{d}(a^*, x) + (\mathrm{d}(a, X) - 1)$. Furthermore, X is a $(A \cup \{a^*\}|B)$-separator of G'. Hence $\forall\, b \in B$, all a^*b-paths of G', resp. all ab-paths of G', intersect X. As a result, we have that for every $b \in B$, $\mathrm{d}(a, b) = \mathrm{d}(a^*, b) + \mathrm{d}(a, X) - 1$ and replacing a with a^* does not change the hyperbolicity of the 4-tuple a, b_1, b_2, b_3. □

Note that it may be the case that $\delta(G') > \delta(G)$, where G' is the graph defined in Lemma 4. However this is no big deal at this step of the proof, for we are only interested in upper-bounding $\delta(a, b_1, b_2, b_3)$. We will come back to the difference between $\delta(G)$ and $\delta(G')$ later on, in Section 5.

Lemma 5. *Let X be a $(A|B)$-clique-separator of a connected graph G. Given a $(a|b_1, b_2, b_3)$ 4-tuple, let $x \in X$ be such that $\mathrm{d}(a, x) = \mathrm{d}(a, X)$. We have $\delta(a, b_1, b_2, b_3) \leq \delta(x, b_1, b_2, b_3) + 1/2$.*

Proof. Let G' be obtained from G by adding a vertex a^* adjacent to $\{x \in X : \mathrm{d}(a, x) = \mathrm{d}(a, X)\}$. By construction, G is an isometric subgraph of G', and so, the respective values of $\delta(a, b_1, b_2, b_3)$ and $\delta(x, b_1, b_2, b_3)$ are not modified by the addition of a^*. However, $\delta(G') \geq \delta(G)$ with the inequality possibly being strict, but we don't use $\delta(G')$ in the proof.

By Lemma 4 we have $\delta(a^*, b_1, b_2, b_3) = \delta(a, b_1, b_2, b_3)$. Furthermore, we claim that $\forall b \in B, \mathrm{d}(b, x) \leq \mathrm{d}(b, a^*) \leq \mathrm{d}(b, x) + 1$. Indeed, since a^* and x are adjacent in G', by the triangular inequality $\mathrm{d}(b, a^*) \leq \mathrm{d}(b, x) + 1$. Since in addition X is a $(A \cup \{a^*\}|B)$-separator of G', all a^*b-paths of G' must intersect X. As a result, and since $x \in X$ and X is a clique, $\mathrm{d}(b, x) \leq \mathrm{d}(b, a^*)$, that proves the claim.

Let us assume w.l.o.g. that $S_1 \geq S_2 \geq S_3$, where $S_1 = d(a^*, b_1) + d(b_2, b_3)$, $S_2 = d(a^*, b_2) + d(b_1, b_3)$ and $S_3 = d(a^*, b_3) + d(b_1, b_2)$. Since $\forall i \in \{1, 2, 3\}$, by the above claim $\mathrm{d}(b_i, x) \leq \mathrm{d}(b_i, a^*) \leq$

$d(b_i, x)+1$, any sum $S'_i = d(x, b_i) + d(b_j, b_k)$, where $\{j, k\} = \{1, 2, 3\} \setminus \{i\}$, satisfies $S'_i \leq S_i \leq S'_i + 1$. Therefore, we have that for every $i \in \{2, 3\}$:

$$\begin{aligned}\delta(a^*, b_1, b_2, b_3) \leq& (S_1 - S_i)/2 \\ \leq& (S'_1 + 1 - S'_i)/2 \\ \leq& (S'_1 - S'_i)/2 + 1/2.\end{aligned}$$

In particular, if $S'_1 \neq \max\{S'_1, S'_2, S'_3\}$, then we have $\delta(a^*, b_1, b_2, b_3) \leq \frac{1}{2}$ by the choice of $S'_i = \max\{S'_1, S'_2, S'_3\}$. Otherwise, we have $\delta(a^*, b_1, b_2, b_3) \leq \delta(x, b_1, b_2, b_3) + \frac{1}{2}$ by the choice of $S'_i = \max\{S'_2, S'_3\}$. □

3.3 Disconnection by a clique-separator

Summing up the two previous Sections 3.1 and 3.2, we can upper-bound the difference between the respective hyperbolicity of a graph and of its atoms in the particular case when there is a unique clique-separator. The following Theorem 6 was proved independently in [51, 60] for separators of any diameter. We prove it here for self-containment of the paper. Lemmas 2 and 5 will be reused in the following sections.

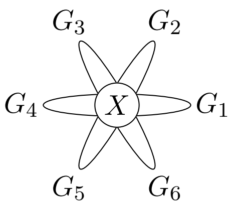


Figure 5: Illustration of a clique-separator X with the connected components of $G \setminus X$.

Theorem 6. *Let X be a clique-separator of a connected graph G, and let $C_1, \ldots, C_l$ be the connected components of $G \setminus X$. We define $G_i = G[C_i \cup X]$. We have :*

$$\max\{\delta(G_1), \ldots \delta(G_l)\} \leq \delta(G) \leq \max\{1/2, \delta(G_1), \ldots \delta(G_l)\} + 1/2.$$

Proof. Since X is a clique, and so, $G[X]$ is an isometric subgraph, every subgraph G_i is isometric as well. Hence, the lower-bound follows from the 4-point definition (Definition 1).

Let us now prove that $\delta(a, b, c, d) \leq \max\{1/2, \delta(G_1), \ldots \delta(G_l)\} + 1/2$ holds for any $a, b, c, d \in V$. We consider a connected component C_i minimizing the number of vertices in the 4-tuple a, b, c, d that are *not* in the block $C_i \cup X$. There are three cases to be considered.

- If $a, b, c, d \in C_i \cup X$ we are done as $\delta(a, b, c, d) \leq \delta(G_i)$.
- If all of a, b, c, d but one vertex are in $C_i \cup X$ let us assume w.l.o.g. that $a \notin C_i \cup X$. Then a, b, c, d is a $(a|b_1, b_2, b_3)$ 4-tuple, for the choices of $B = C_i \cup X$ and $A = V \setminus C_i$. By Lemma 5 it follows that $\delta(a, b, c, d) \leq \delta(G_i) + 1/2$.

- Else, there are no more than two vertices among a, b, c, d that are in $C_i \cup X$. Suppose w.l.o.g. $a, c \notin C_i \cup X$. Let j, k satisfy $a \in C_j$ and $c \in C_k$. By minimality of $|\{a, b, c, d\} \setminus (C_i \cup X)|$ we have $b, d \notin C_j \cup C_k$. Therefore, a, b, c, d is a $(a_1, a_2 | b_1, b_2)$ 4-tuple, for the choices of $A = C_j \cup C_k \cup X$ and $B = V \setminus (C_j \cup C_k)$, and we conclude by Corollary 3 that $\delta(a_1, a_2, b_1, b_2) \leq 1$ in this case. $\square$

The upper-bound of Theorem 6 is sharp. It can be shown using the graph in Figure 6, constructed from a cycle C_7 of length 7 to which we add a triangle.

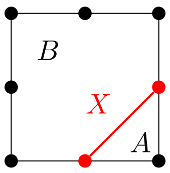


Figure 6: X is a $(A|B)$-clique-separator: we have $\delta(G) = 3/2$, while $\delta(G[B]) = 1$, and $\delta(G[A]) = 0$.

4 Hyperbolicity and clique-decomposition

In Section 3, we gave a sharp upper-bound on the distortion of hyperbolicity when the graph is disconnected by a single clique-separator. The atoms of the graph result from its disconnection by some clique-separators [44]. However, Theorem 6 does not apply to a whole clique-decomposition as the successive approximations would add up. We thus need to find additional properties to approximate the hyperbolicity of a graph from computations on its atoms in order to prove Theorem 12.

Our proofs in this section is based on the property that the atoms of a graph can be organized into a tree (sometimes called an atom tree [9] or a maximal prime subgraph junction tree [48]). Using this tree, any 4-tuple with large hyperbolicity can be related to an atom that is most "central" to it (this will be made more precise in the following). We can then upper-bound the difference between the hyperbolicity of the 4-tuple and the hyperbolicity of this atom. For the latter, a delicate technical argument will be needed in order to obtain the sharp upper-bound on the difference.

4.1 Relating atoms and 4-tuples with large hyperbolicity

We aim at relating every 4-tuple a, b, c, d with a sufficiently large hyperbolicity to some atom by which all the paths between a, b, c, d go through. The difference between $\delta(a, b, c, d)$ and the hyperbolicity of this atom will be studied next. Our result in this section involves basic knowledge about *tree-decomposition* (see [10]). A *tree-decomposition* $(T, \mathcal{X})$ of a graph $G = (V, E)$ is a pair consisting of a tree T and of a family $\mathcal{X} = (X_t)_{t \in V(T)}$ of subsets of V indexed by the nodes of T and satisfying:

- $\bigcup_{t \in V(T)} X_t = V$;
- for any edge $e = \{u, v\} \in E$, there exists $t \in V(T)$ such that $u, v \in X_t$;
- for any $v \in V$, $\{t \in V(T) \mid v \in X_t\}$ induces a subtree of T, denoted by T_v.

The sets X_t are called *the bags* of the decomposition. In the following, we will use the property that there exists a tree-decomposition where the bags are exactly the atoms [9, 48].

Lemma 7. *Let $a, b, c, d \in V$ be a 4-tuple satisfying $\delta(a,b,c,d) \geq \frac{3}{2}$ in a connected graph $G = (V, E)$. There exists an atom A_0 such that $\forall u \in \{a,b,c,d\} \backslash A_0$, there is a clique-separator $X_u \subseteq A_0$ which separates u from $\{a,b,c,d\} \setminus \{u\}$.*

Proof. Let $(T, \mathcal{X})$ be a tree-decomposition of G where the bags are the atoms of G. Such a tree-decomposition was proved to exist in [9, 48]. In order to prove the lemma, we shall seek for an atom A_0 with the property that no more than two vertices among $\{a,b,c,d\} \setminus A_0$ are in the same connected component of $G \setminus A_0$. To find this atom, we will weight the bags of $\mathcal{X}$ and then we will choose the atom A_0 in the weighted centroid of T.

Precisely, for every of a, b, c, d pick an atom containing the vertex. The weight of an atom is the number of times it has been picked. In particular, an atom has weight between 0 and 4, and the sum of weight of the atoms is equal to $\mathcal{W} = 4$. It is well-known that for any node-weighted tree with sum of weights $\mathcal{W}$, there is a node whose removal splits the tree into connected components where the sum of weight of the nodes is at most $\mathcal{W}/2$ [34]. So, let A_0 be an atom of G such that no component of $T \setminus \{A_0\}$ has sum of weight of its bags greater than 2. We claim that $\forall u \in \{a,b,c,d\} \backslash A_0$, there is a clique-separator $X_u \subseteq A_0$ which separates u from $\{a,b,c,d\} \setminus \{u\}$, that will prove the lemma.

Indeed, let $u \in \{a,b,c,d\} \backslash A_0$ be arbitrary. By the properties of a tree-decomposition, T_u (induced by the atoms containing u) is the subtree of a component C_u of $T \setminus \{A_0\}$. Let $V_u \subseteq V$ be the subset of vertices that are contained in an atom in C_u, and let $A_u \in C_u$ be the atom that is adjacent to A_0 in T. Since A_u and A_0 are atoms of G, their intersection, denoted by $X_u = A_u \cap A_0$, is a clique [8]. Furthermore, by the properties of a tree-decomposition, X_u is a $(V_u | V \setminus V_u)$-separator of G. Therefore, we are left to prove that no vertex of $\{a,b,c,d\} \setminus \{u\}$ is in V_u, for the latter will prove that X_u is a clique-separator which separates u from $\{a,b,c,d\} \setminus \{u\}$. Assume for the sake of contradiction the existence of a vertex $v \in \{a,b,c,d\} \setminus \{u\}$ that is contained in V_u. We distinguish between two cases.

- Suppose that $v \notin X_u$. In this situation, T_u, T_v are subtrees of C_u. It implies that the sum of weight of the atoms in C_u is at least 2, and so, by the choice of atom A_0, it is equal to 2. In particular, u, v are the only two vertices of the 4-tuple that are in $V_u \setminus X_u$ (else, the sum of weights of the atoms in C_u should be at least 3). Let $X = X_u,\ A = V_u,\ B = (V \setminus V_u) \cup X_u$. The 4-tuple a, b, c, d is a $(a_1, a_2 | b_1, b_2)$ 4-tuple with $a_1 = u,\ a_2 = v$. Therefore, $\delta(a,b,c,d) \leq 1$ by Corollary 3, that contradicts the hypothesis that $\delta(a,b,c,d) \geq \frac{3}{2}$.
- Else, $v \in X_u$ and we can assume w.l.o.g. that no vertex of $\{a,b,c,d\} \setminus \{u\}$ is in $V_u \setminus X_u$ (else, we go back to the previous case). In this situation, let $X = X_u,\ A = V_u,\ B = (V \setminus V_u) \cup X_u$ as before, the 4-tuple a, b, c, d is a $(a_1, a_2 | b_1, b_2)$ 4-tuple with $a_1 = u,\ a_2 = v$. Therefore, similarly as for the previous case, we have that $\delta(a,b,c,d) \leq 1$ by Corollary 3, that contradicts the hypothesis that $\delta(a,b,c,d) \geq \frac{3}{2}$.

As a result, no vertex of $\{a,b,c,d\} \setminus \{u\}$ is in V_u, and so, X_u is a clique-separator which separates u from $\{a,b,c,d\} \setminus \{u\}$. Since $X_u \subseteq A_0$, the latter proves the claim on A_0, hence the lemma. □

As an illustration, one may notice that the central atom in Figure 7 satisfies the property of Lemma 7 with respect to the 4-tuple v_0, v_1, v_2, v_3. Indeed, none of the four vertices is contained in this atom, but each of them is simplicial and can be separated from the three others by its two neighbors.

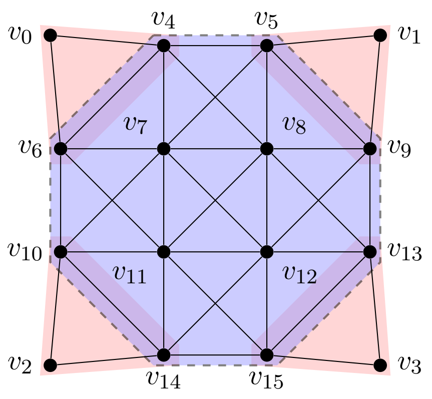


Figure 7: A 2-hyperbolic graph with five atoms: four are 0-hyperbolic, one is 1-hyperbolic. The 4-tuple v_0, v_1, v_2, v_3 has maximum hyperbolicity 2.

Discussion. It is tempting to attempt a generalization of Lemma 7 to some other graph decompositions. In particular, we may wish to consider a decomposition of the graph by separators of diameter at most k, where k is a small constant (the case $k = 1$ corresponds to the clique-decomposition). If we assume in addition that the subgraphs are organized into a tree (*i.e.*, they are the bags of a tree-decomposition), the generalization of Lemma 7 to that case is easy. However, in general there is no such a tree-decomposition, which kills all the arguments in our proof.

We can go one step further and prove the following claim.

Proposition 8. *For every $G = (V, E)$, let $G_1, G_2, \ldots, G_l$ denote the isometric subgraphs of G that do not contain any isometric separator of diameter at most two*[1]*. The difference between $\delta(G)$ and $\max_i \delta(G_i)$ can be arbitrarily large.*

Proof. We shall prove that the result follows from some properties of bridged graphs. Indeed, we recall that a vertex is dominated if its close neighborhood is included in the close neighborhood of another vertex, and a graph is bridged if every of its isometric subgraphs contains a dominated vertex [3]. We claim that for every bridged graph G, all the subgraphs G_i have hyperbolicity at most one. Since the hyperbolicity of bridged graphs can be arbitrarily large [41], the result follows.

In order to prove the claim, let G be a bridged graph and let G_i be an isometric subgraph of G where there is no isometric separator of diameter at most two. If G_i has order at most 1, then we are done as $\delta(G_i) = 0$ in this case. So, let us assume G_i contains at least two vertices. Since G is bridged, G_i contains a dominated vertex v_i. Let $u_i \in V(G_i)$ be a vertex dominating v_i. In this situation, u_i is universal in G_i, or else $N_G[u_i] \setminus v_i$ would be an isometric separator of G_i of diameter at most two. Therefore, G_i has diameter at most two, and so, $\delta(G_i) \leq 1$ [21], that proves the claim, hence the result. □

4.2 Substitution method

From Lemma 7 we can associate a specific atom to a 4-tuple of large hyperbolicity. Four applications of Lemma 5 are then sufficient to prove that the hyperbolicity of this 4-tuple and the hyperbolicity

[1]We name a separator isometric when it induces an isometric subgraph.

of the atom differ by at most 2. The purpose of this section is to prove that this difference is in fact at most 1. To do this, we refine the results of Section 3.2.

We recall that our substitution method in Section 3.2 consists in relating a $(a|b_1, b_2, b_3)$ 4-tuple to a 4-tuple x, b_1, b_2, b_3, with $x \in X$, such that $\delta(a, b_1, b_2, b_3) - \delta(x, b_1, b_2, b_3) \leq 1/2$. The difference between the hyperbolicity of the 4-tuples depends on the choice of x and on some properties of the $(a|b_1, b_2, b_3)$ 4-tuple. So, we will first deepen our analysis of the worst-case when it is equal to $1/2$. We will finally prove that when we apply twice the substitution method to a 4-tuple with a large hyperbolicity, this maximum difference of $1/2$ can occur at most once.

We will need the following lemma, that is a technical generalization of Lemma 5.

Lemma 9. *Let X be a $(A|B)$-clique-separator of a connected graph G. Given a $(a|b_1, b_2, b_3)$ 4-tuple, write:*

$$S_1 = \mathrm{d}(a, b_1) + \mathrm{d}(b_2, b_3),\ \ S_2 = \mathrm{d}(a, b_2) + \mathrm{d}(b_1, b_3),\ \ S_3 = \mathrm{d}(a, b_3) + \mathrm{d}(b_1, b_2).$$

Assume w.l.o.g. that $S_1 \geq S_2 \geq S_3$, and let $x_2 \in X$ be such that $\mathrm{d}(a, b_2) = \mathrm{d}(a, x_2) + \mathrm{d}(x_2, b_2) = \mathrm{d}(a, X) + \mathrm{d}(x_2, b_2)$. If $\delta(a, b_1, b_2, b_3) > \delta(x_2, b_1, b_2, b_3)$, then we have:

- *$S_1 > S_2 = S_3$.*
- *$\mathrm{d}(a, b_1) = \mathrm{d}(a, x_2) + \mathrm{d}(x_2, b_1)$.*

Proof. For ease of calculation, we first reduce to the case when $\mathrm{d}(a, X) = 1$. Let G' be obtained from G by adding a vertex a^* with neighbors $\{x \in X \mid \mathrm{d}(a, x) = \mathrm{d}(a, X)\}$. By construction, G is an isometric subgraph of G', and so, the hyperbolicity of 4-tuples of $V(G)$ is not modified by the construction. Furthermore, by Lemma 4 we have $\delta(a^*, b_1, b_2, b_3) = \delta(a, b_1, b_2, b_3)$. In this situation, we can safely replace a with a^* in the 4-tuple, hence we may assume w.l.o.g. that $\mathrm{d}(a, X) = 1$ for the remaining of the proof.

For every i, let $x_i \in X$ denote a vertex on a shortest ab_i-path such that $\mathrm{d}(a, x_i) = \mathrm{d}(a, X) = 1$. In this situation, $\mathrm{d}(a, b_i) = \mathrm{d}(b_i, x_i) + 1$. Let us introduce the indicator $\varepsilon_i = \mathrm{d}(x_2, b_i) - \mathrm{d}(x_i, b_i)$. We claim that $\varepsilon_i \in \{0, 1\}$, and $\varepsilon_i = 0$ if and only if x_2 is on a shortest ab_i-path. Indeed, since by the triangular inequality, $1 + \mathrm{d}(x_i, b_i) = \mathrm{d}(a, b_i) \leq \mathrm{d}(a, x_2) + \mathrm{d}(x_2, b_i) = 1 + \mathrm{d}(x_2, b_i)$, we have that $\varepsilon_i \geq 0$. Furthermore, since $x_2, x_i \in X$ and X is a clique, we also have by the triangular inequality that $\varepsilon_i \leq \mathrm{d}(x_2, x_i) \leq 1$. Altogether, $\varepsilon_i \in \{0, 1\}$, and we have $\varepsilon_i = 0$ if and only if $\mathrm{d}(a, b_i) = \mathrm{d}(b_i, x_2) + \mathrm{d}(a, x_2)$, that proves the claim. In particular $\varepsilon_2 = 0$.

Let us denote by S'_i the sum $\mathrm{d}(x_2, b_i) + \mathrm{d}(b_j, b_k)$, where $\{j, k\} = \{1, 2, 3\} \setminus \{i\}$. We aim to exhibit a relation between S_i and S'_i, that would yield in turn a relation between the values $\delta(a, b_1, b_2, b_3)$ and $\delta(x_2, b_1, b_2, b_3)$. At first we notice that $\mathrm{d}(a, b_i) = \mathrm{d}(x_i, b_i) + 1 = \mathrm{d}(x_2, b_i) + 1 - \varepsilon_i$. So, we have:

$$\begin{aligned} S_i &= \mathrm{d}(a, b_i) + \mathrm{d}(b_j, b_k) \\ &= \mathrm{d}(x_2, b_i) + \mathrm{d}(b_j, b_k) + 1 - \varepsilon_i \\ &= S'_i + 1 - \varepsilon_i. \end{aligned}$$

Furthermore, by the hypothesis $S_1 \geq S_2 \geq S_3$ and $\delta(a, b_1, b_2, b_3) > 0$. Thus, by Definition 1 we have $S_1 = S_2 + 2\delta(a, b_1, b_2, b_3)$, and so, it holds that $S_1 > \max\{S_2, S_3\}$. The latter implies $S'_1 \geq S_1 - 1 \geq \max\{S_2, S_3\} \geq \max\{S'_2, S'_3\}$. More precisely:

- Suppose $S'_2 \geq S'_3$. In this situation, $\delta(a,b_1,b_2,b_3) = \frac{S_1-S_2}{2} = \frac{(S'_1+1-\varepsilon_1)-(S'_2+1-\varepsilon_2)}{2}$. Since $\varepsilon_2 = 0$, we have $\delta(a,b_1,b_2,b_3) = (S'_1 - S'_2)/2 - \varepsilon_1/2 = \delta(x_2,b_1,b_2,b_3) - \varepsilon_1/2 \leq \delta(x_2,b_1,b_2,b_3)$. However, this case contradicts the hypothesis that $\delta(a,b_1,b_2,b_3) > \delta(x_2,b_1,b_2,b_3)$.

- Else, $S'_3 > S'_2$. Since $S_2 \geq S_3$, we have $\varepsilon_3 = 1$, which implies $S_2 = S_3$. This, in turn, implies that $\delta(x_2,b_1,b_2,b_3) = (S'_1 - S'_3)/2 = (S_1 - 1 + \varepsilon_1 - S_3)/2 = (S_1 - S_2)/2 - (1-\varepsilon_1)/2 = \delta(a,b_1,b_2,b_3) - (1-\varepsilon_1)/2 \leq \delta(a,b_1,b_2,b_3)$.

  In such a case, $\delta(x_2,b_1,b_2,b_3) < \delta(a,b_1,b_2,b_3)$ if and only if we have $\varepsilon_1 = 0$, *i.e.*, x_2 is on a shortest ab_1-path.

□

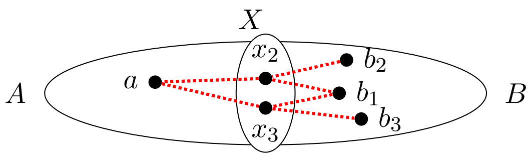


Figure 8: An illustration of the metric property of Lemma 9. The dashed lines represent shortest paths.

The metric property of Lemma 9 is illustrated with Figure 8. We use it to strengthen our results in Section 3.2 as follows.

Lemma 10. *Let a,b,c,d be a 4-tuple of a connected graph G, and X_a, X_d be two cliques of G satisfying:*

- *X_a is a $(a|b,c,d)$-separator;*
- *X_d is a $(d|a,b,c)$-separator;*
- *all vertices of $X_a \backslash X_d$ and a,b,c are in the same connected component of $G \setminus X_d$.*

Then there exist $x_a \in X_a$ and $x_d \in X_d$ such that

$$\delta(a,b,c,d) \leq \delta(x_a,b,c,x_d) + 1/2.$$

Proof. Consider the three sums S_1, S_2, S_3 from Definition 1. For ease of reasoning, let us order the sums by decreasing value, *i.e.*, let T_1, T_2, T_3 be such that $\{T_1,T_2,T_3\} = \{S_1,S_2,S_3\}$ and $T_1 \geq T_2 \geq T_3$. Accordingly, let u_1,u_2,u_3 be such that $\{u_1,u_2,u_3\} = \{b,c,d\}$ and for every $i \in \{1,2,3\}$, $T_i = \mathrm{d}(a,u_i) + \mathrm{d}(u_j,u_k)$ where $\{j,k\} = \{1,2,3\} \setminus \{i\}$. We distinguish between two cases:

- Suppose there is $x_a \in X_a$ satisfying $\delta(a,b,c,d) \leq \delta(x_a,b,c,d)$. By the hypothesis, the clique X_d is a $(d|x_a,b,c)$-separator. Hence by Lemma 5 there exists $x_d \in X_d$ such that $\delta(x_a,b,c,d) \leq \delta(x_a,b,c,x_d) + \frac{1}{2}$. Altogether, $\delta(a,b,c,d) \leq \delta(x_a,b,c,d) \leq \delta(x_a,b,c,x_d) + \frac{1}{2}$, so, the lemma holds true in this case.

- Else, no vertex of X_a satisfies the above property. In particular, let $x_a \in X_a$ be such that $\mathrm{d}(a,x_a) = \mathrm{d}(a,X_a)$, and x_a is on a shortest au_2-path. By the hypothesis, the clique X_a is a $(a|b,c,d)$-separator. Hence, we can deduce the following information on the 4-tuple:

– by Lemma 5 $\delta(a,b,c,d) \leq \delta(x_a,b,c,d) + \frac{1}{2}$, and so, $\delta(a,b,c,d) = \delta(x_a,b,c,d) + \frac{1}{2}$;

– moreover, by Lemma 9 we have that $T_1 > T_2 = T_3$ and x_a is also on a shortest au_1-path.

We shall prove that there exists $x_d \in X_d$ such that $\delta(x_a,b,c,d) \leq \delta(x_a,b,c,x_d)$, that will prove the lemma in this case.

For every i, let $T'_i = \mathrm{d}(x_a,u_i) + \mathrm{d}(u_j,u_k)$ where $\{j,k\} = \{1,2,3\} \setminus \{i\}$. Observe that when x_a is on a shortest au_i-path, we have that $T'_i = T_i - \mathrm{d}(a,x_a) = T_i - \mathrm{d}(a,X_a)$. As a result,

$$T'_1 = T_1 - \mathrm{d}(a,X_a),\ T'_2 = T_2 - \mathrm{d}(a,X_a) \text{ and } T'_3 = T_3 - \mathrm{d}(a,X_a) + 1.$$

Indeed, the two first equalities follow from the fact that x_a is on a shortest au_1-path, resp. on a shortest au_2-path. The third equality follows from the fact that $\delta(x_a,b,c,d) = (T'_1 - \max\{T'_2,T'_3\})/2 = \delta(a,b,c,d) - 1/2$. In particular, we have $T'_1 \geq T'_3 > T'_2$.

Furthermore, by the hypothesis X_d is a $(d|x_a,b,c)$-separator. Let v_1,v_2,v_3 be such that $\{v_1,v_2,v_3\} = \{x_a,b,c\}$ and for every i, $T'_i = \mathrm{d}(v_i,d) + \mathrm{d}(v_j,v_k)$ where $\{j,k\} = \{1,2,3\} \setminus \{i\}$. Finally, let $x_d \in X_d$ be a vertex satisfying $\mathrm{d}(d,x_d) = \mathrm{d}(d,X_d)$ and x_d is on a shortest v_3d-path. We claim that $\delta(x_a,b,c,d) \leq \delta(x_a,b,c,x_d)$, that will prove the lemma in this case. Indeed, suppose for the sake of contradiction that $\delta(x_a,b,c,x_d) < \delta(x_a,b,c,d)$. By Lemma 9, it implies that $T'_1 > T'_3 = T'_2$, which contradicts the fact that $T'_3 > T'_2$.

As a result, in both cases there exist $x_a \in X_a$ and $x_d \in X_d$ such that $\delta(a,b,c,d) \leq \delta(x_a,b,c,x_d) + 1/2$. □

Corollary 11. *Let a,b,c,d be a 4-tuple of a connected graph G satisfying $\delta(a,b,c,d) \geq 3/2$. There exists an atom A of G such that $\delta(a,b,c,d) \leq \delta(G[A]) + 1$.*

Proof. The atom A is obtained by applying Lemma 7. For every vertex $u \in \{a,b,c,d\} \setminus A$, let $X_u \subseteq A$ be a clique-separator disconnecting u from $\{a,b,c,d\} \setminus \{u\}$.

We claim that all vertices of $A \setminus X_u$ and $\{a,b,c,d\} \setminus \{u\}$ are in the same connected component of $G \setminus X_u$. Indeed, since A is an atom, all vertices of $A \setminus X_u$ are in the same connected component C of $G \setminus X_u$. Suppose for the sake of contradiction that there exists $v \in \{a,b,c,d\} \setminus \{u\}$ such that $v \notin C$. Since $v \notin A$, there exists a clique $X_v \subseteq A$ which separates v from $\{a,b,c,d\} \setminus \{v\}$, and so, no vertex of $\{a,b,c,d\} \setminus \{v\}$ is in the same connected component of $G \setminus X_u$ as v. However, in this situation let C_u, C_v be the respective components of u and v in $G \setminus X_u$ and let $X = X_u,\ A = C_u \cup C_v \cup X,\ B = V \setminus (C_u \cup C_v)$. The 4-tuple a,b,c,d is a $(a_1,a_2|b_1,b_2)$ 4-tuple with $a_1 = u,\ a_2 = v$, and so, it implies by Corollary 3 that $\delta(a,b,c,d) \leq 1$, a contradiction. As a result, all vertices of $\{a,b,c,d\} \setminus \{u\}$ are in C, that proves the claim.

In order to prove the corollary, we can then apply our substitution method (at most four times). Precisely, consider the two vertices a,b of the 4-tuple.

- If $a,b \in A$ then we set $a' = a,\ b' = b$. In this situation $\delta(a,b,c,d) \leq \delta(a',b',c,d)$.
- Else, if $a \in A$ and $b \notin A$ then let $x_b \in X_b$ be a vertex satisfying $\mathrm{d}(b,x_b) = \mathrm{d}(b,X_b)$. Let $a' = a,\ b' = x_b$. By Lemma 5, we have $\delta(a,b,c,d) \leq \delta(a',b',c,d) + 1/2$. In the same way, if $a \notin A,\ b \in A$ then we set $a' = x_a,\ b' = b$ where $x_a \in X_a$ is a vertex satisfying $\mathrm{d}(a,x_a) = \mathrm{d}(a,X_a)$.

- Else, $a, b \notin A$. By the claim above, all vertices of $X_a \setminus X_b \subseteq A \setminus X_b$ and a, c, d are in the same connected component of $G \setminus X_b$. Hence, by Lemma 10 there exist $x_a \in X_a$ and $x_b \in X_b$ such that $\delta(a, b, c, d) \leq \delta(x_a, x_b, c, d) + 1/2$. We set $a' = x_a,\ b' = x_b$ in this case.

Overall, in all cases there exist $a', b' \in A$ such that $\delta(a, b, c, d) \leq \delta(a', b', c, d) + 1/2$. We then proceed similarly with c, d in order to find two vertices $c', d' \in A$ such that $\delta(a', b', c, d) \leq \delta(a', b', c', d') + 1/2$. Altogether, $\delta(a, b, c, d) \leq \delta(a', b', c', d') + 1 \leq \delta(G[A]) + 1$. □

4.3 Additive approximation for hyperbolicity

Theorem 12. *Let $A_1, \ldots, A_l$ be the atoms of a connected graph G. Then:*

$$\max_i \delta(G[A_i]) \leq \delta(G) \leq \max_i \delta(G[A_i]) + 1.$$

Proof. As for Theorem 6, the lower-bound of Theorem 12 follows from the fact that the subgraphs $G_i = G[A_i]$ are isometric subgraphs of G. The upper-bound trivially holds when $\delta(G) \leq 1$. We can thus suppose that $\delta(G) \geq 3/2$ and so, that there exist four vertices a, b, c, d such that $\delta(a, b, c, d) = \delta(G) \geq 3/2$. Corollary 11 then yields an atom A such that $\delta(G) \leq \delta(G[A]) + 1$, which proves the second part of our claim. □

Note that the upper-bound is reached by the graph of Figure 7, and by the 1-hyperbolic chordal graph from Figure 1 whose atoms have hyperbolicity 0.

5 Substitution method for an exact computation

As shown with Theorem 12, the hyperbolicity of a graph cannot be deduced from the computation of its clique-decomposition directly. We next introduce a new graph decomposition in order to compute the hyperbolicity of a graph exactly. It bases on clique-decomposition, and it outputs supergraphs of the atoms (we call them *substitute graphs*).

For the remaining of the section, we will consider graphs with hyperbolicity at least 1 (the case of 1/2-hyperbolic graphs will be discussed in the following sections). We will show that under this assumption on the hyperbolicity of the initial graph, it can be computed from the hyperbolicity of the atoms' substitutes.

Outline of the method. We build upon Lemma 4 and other results from the two previous sections. We recall that a *simplicial* vertex is a vertex whose neighborhood induces a complete subgraph. Given a $(A|B)$-clique separator, we add simplicial vertices to the induced subgraphs $G[A]$ and $G[B]$ in order to mimic the maximum $(a|b_1, b_2, b_3)$ 4-tuples that may result from the disconnection (Section 5.1.1). Since the atoms result from the disconnection of the graph by some of its clique-separators, we can repeatedly apply this method and so obtain the atom's substitutes. We finally focus on technical details and additional data structures related to the implementation.

5.1 Substitute graphs

5.1.1 Basic step: single disconnection

Following [8] the clique-decomposition of $G = (V, E)$ can be computed by repeatedly applying the following decomposition step, until none of the subgraphs considered contains a clique-separator.

At first, G is the only subgraph. We find a clique-separator X with some properties[2] in one of the subgraphs G'. The vertex-set of G' is partitioned into two sets A, B so that $A \cap B = X$ and X is a $(A|B)$-separator of G'. Then the subgraph G' is replaced with the two subgraphs $G'[A]$ and $G'[B]$. So, let us first consider the case of a *single* disconnection, of a given graph G' with a $(A|B)$-clique-separator X.

- Let $G_A = G'[A]$. For every $b \in B \setminus X$, we consider the set of vertices $X_b \subseteq X$ which are at distance $\mathrm{d}_{G'}(b, X)$ from b. For every X_b, we add in G_A a (simplicial) vertex s_{X_b} whose neighborhood is X_b. The resulting graph is named G_A^*.
- Let $G_B = G'[B]$. For every $a \in A \setminus X$, we consider the set of vertices $X_a \subseteq X$ which are at distance $\mathrm{d}_{G'}(a, X)$ from a. For every X_a, we add in G_B a (simplicial) vertex s_{X_a} whose neighborhood is X_a. The resulting graph is named G_B^*.

More formally, the *substitute graphs* (or *substitutes* for short) G_A^* and G_B^* of the graphs G_A and G_B with respect to the $(A|B)$-separator X are defined as follows:

Definition 13. *Let X be a $(A|B)$-clique-separator of a connected graph G', where $A \cap B = X$ and $A \cup B = V(G')$. The* substitute graphs *G_A^*, G_B^* are defined as:*

$$V(G_A^*) = A \cup \{s_{X_b} : \exists b \in B \text{ s.t. } X_b = \arg\min_{x \in X} \mathrm{d}(b, x)\} \text{ and } E(G_A^*) = E(A) \cup \{\{s_{X_b}, x\} : x \in X_b\};$$

$$V(G_B^*) = B \cup \{s_{X_a} : \exists a \in A \text{ s.t. } X_a = \arg\min_{x \in X} \mathrm{d}(a, x)\} \text{ and } E(G_B^*) = E(B) \cup \{\{s_{X_a}, x\} : x \in X_a\}.$$

Lemma 14. *Let X be a $(A|B)$-clique-separator of a connected graph G', where $A \cap B = X$ and $A \cup B = V(G')$. Suppose $\delta(G') \geq 1$. We have:*

$$\delta(G') = \max\{1, \delta(G_A^*), \delta(G_B^*)\}.$$

Proof. Let $G_A = G'[A]$, $G_B = G'[B]$. By construction (Definition 13), G_A is an isometric subgraph of G_A^*, resp. G_B is an isometric subgraph of G_B^*.

We claim $\delta(G') \leq \max\{1, \delta(G_A^*), \delta(G_B^*)\}$. In order to prove the claim, let a, b, c, d be a 4-tuple of vertices of G' such that $\delta(a, b, c, d) = \delta(G')$. We distinguish between three cases.

1. **Case** $a, b, c, d \in A$**.** In this situation, $\delta(G') \leq \delta(G_A) \leq \delta(G_A^*)$.

   Similarly, when $a, b, c, d \in B$ we have $\delta(G') \leq \delta(G_B) \leq \delta(G_B^*)$.

2. **Case** $a \in A,\ b, c, d \in B$**.** The 4-tuple is a $(a|b_1, b_2, b_3)$ 4-tuple. In such case, there exists by construction a simplicial vertex a^* of $V(G_B^*) \setminus B$ that is adjacent to $\{x \in X : \mathrm{d}(a, x) = \mathrm{d}(a, X)\}$. Therefore, by Lemma 4 $\delta(G') \leq \delta(a^*, b_1, b_2, b_3) \leq \delta(G_B^*)$.

   In the same way, if $b \in B$ and $a, c, d \in A$ then $\delta(G') \leq \delta(G_A^*)$.

3. Else, it can be assumed w.l.o.g. that the 4-tuple is a $(a_1, a_2|b_1, b_2)$ 4-tuple. By Corollary 3, $\delta(G') \leq 1$ in this case.

[2]The additional properties on the clique-separator ensure the unicity of the decomposition.

Altogether, $\delta(G') \leq \max\{1, \delta(G_A^*), \delta(G_B^*)\}$, as desired.

Conversely, we claim $\delta(G') \geq \max\{1, \delta(G_A^*), \delta(G_B^*)\}$. By the hypothesis, $\delta(G') \geq 1$. Furthermore, let a, b, c, d be a 4-tuple of G_B^* such that $\delta(a,b,c,d) = \delta(G_B^*)$ (the proof for G_A^* is symmetrical to this one). We distinguish between three cases.

1. **Case** $a, b, c, d \in B$**.** In this situation, $\delta(G_B^*) \leq \delta(G_B) \leq \delta(G')$.

2. **Case** $a = a^* \notin B$ **and** $b, c, d \in B$**.** By construction, a^* substitutes to some vertex of A, *i.e.*, there exists $a' \in A$ such that $N(a^*) = \{x \in X : \mathrm{d}(a', x) = \mathrm{d}(a', X)\}$. Furthermore, by Lemma 4 $\delta(a^*, b, c, d) = \delta(a', b, c, d)$. Hence, $\delta(G_B^*) \leq \delta(a', b, c, d) \leq \delta(G')$.

3. Else, there are at least two vertices of the 4-tuple that are not in B. Say w.l.o.g. $a, b \notin B$ and let $A^* = X \cup \{a, b\}$, $B^* = V(G_B^*) \setminus \{a, b\}$. In this situation, the 4-tuple is a $(a_1, a_2 | b_1, b_2)$ 4-tuple with $a_1 = a$, $a_2 = b$. As a result, by Corollary 3 $\delta(G_B^*) \leq 1 \leq \delta(G')$ in this case.

Altogether, $\delta(G_B^*) \leq \delta(G')$. □

We emphasize that some simple rules can be applied to reduce the size of the substitute graphs. In particular, we can remove the pendant vertices which may be added in the construction (we postpone a short analysis of the size of substitutes to Section 5.2.2).

5.1.2 Extension to the atoms

The substitution operation can be naturally extended to the whole clique-decomposition, by mimicking each step of it and applying the basic substitution operation that we describe above at each of these steps. We formalize it by first introducing the following definition of an atom tree.

Definition 15 ([7, 8, 44])**.** *Let G be a connected graph. An* atom tree *of G is a labeled binary rooted tree T, satisfying the following recursive definition:*

- *if G is prime w.r.t. clique-decomposition, then T is reduced to a node labeled with V;*
- *otherwise, the root of T is labeled with a clique-separator X, and there exists two connected components C_1, C_2 of $G \setminus X$ satisfying:*
  - $N_G(C_1) = N_G(C_2) = X$*;*
  - *the left child of the root is labeled with $A_1 = C_1 \cup X$, which does not contain any clique-separator;*
  - *and the right child of the root is an atom tree of $G \setminus C_1$.*

In order to prevent any confusion, the reader has to notice that an atom tree is *not* a tree-decomposition (as defined in Section 4.1). In fact, an atom tree can be seen as the trace of some execution of the algorithm of [44, 56] for computing the clique-decomposition. Indeed, it is proved in [44] that in an atom tree, the leaves are in bijective correspondance with the atoms of the graph. Given a *fixed* atom tree, this yields a natural total ordering of the atoms by increasing depth. We now follow this ordering to construct the substitutes of the atoms from the atom tree. There are as many steps for our substitution method as there are atoms in the graph.

- Starting from $H_1 = G$, we disconnect the first atom A_1 by using the clique-separator X_1 from the atom tree. Applying the substitution operation of Definition 13 to $A = A_1$ and $B = V(G) \setminus (A_1 \setminus X_1)$, we obtain two substitute graphs: $G^*_{A_1}$ which substitutes A_1, and another one denoted by $H_2 = G^*_B$.
- After $i-1$ steps, $i \in \{2, \dots, l-1\}$, we constructed the substitute graphs of atoms $A_1, \dots, A_{i-1}$, plus an additional graph H_i. The graph H_i contains $G[\bigcup_{j \geq i} A_j]$, to which were added simplicial vertices during the previous steps. By using the clique-separator X_i from the atom tree we disconnect the graph H_i and we apply the substitution operation of Definition 13, this time to the set A equal to $C_A \cup X_i$ where C_A is the connected component of $H_i \setminus X_i$ which intersects A_i, and to $B = V(H_i) \setminus (A \setminus X_i)$. We replace H_i with the two substitute graphs, one containing the atom A_i and being its substitute, the other being denoted by $H_{i+1} = G^*_B$.
- We finally stop at the l^{th} step, and we set H_l as the substitute graph of the *last* atom A_l.

Figure 9 illustrates this process. The numbers reported in Tab. 9i illustrate the interest of our pre-processing method for the computation of the hyperbolicity. Indeed, the graph G of Figure 9a has 28 nodes and so, 20 475 4-tuples, while the sum of the numbers of 4-tuples in the graphs G^*_i (Figs. 9c–9h) is 1 800. We thus significantly reduce the size of the search space. Moreover, a simple cutting rule allows us to reduce the number of 4-tuples to consider to 1 575. To do so, we first order the graphs G^*_i by decreasing diameters, then we iteratively compute the hyperbolicity of these graphs in this order, and we stop exploration as soon as the diameter of a graph G^*_j is smaller than twice the largest value of δ computed so far.

5.2 Implementation and complexity analysis

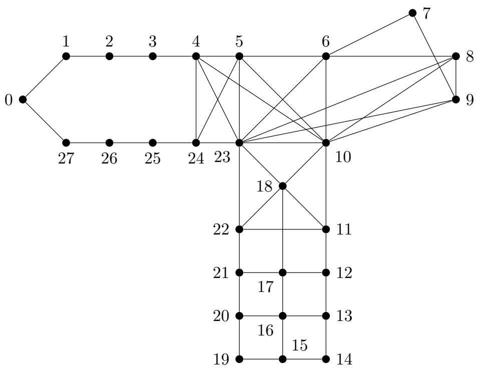
In order to stay competitive with clique-decomposition, the complexity of computing the substitutes needs to be of the same order of magnitude as the one of computing the atoms. A straightforward calculation would require the computation of distances in the graphs $H_1, H_2, \dots, H_l$ (defined in the previous Section 5.1.2), hence the computation of $\mathcal{O}(n)$ all-pairs shortest-paths. Furthermore, the addition of simplicial vertices at each step causes an increase of the size of the graphs, which further complicates the complexity analysis.

The purpose of this section is to show how to compute the atom's substitutes in $\mathcal{O}(nm)$-time (Corollary 20) We achieve the goal by using standard partition refinement techniques and additional properties of clique-decomposition. On the way, we introduce a few rules in order to reduce the size of the substitutes.

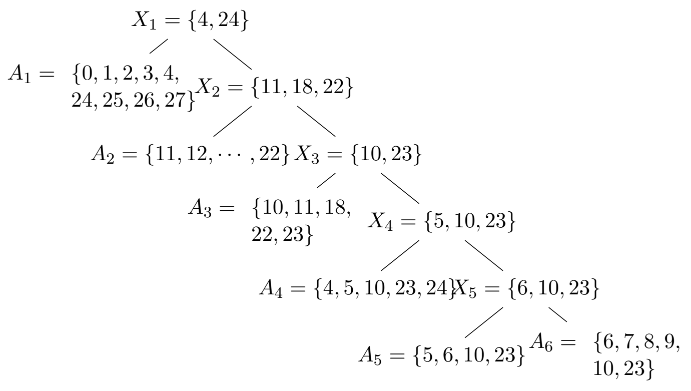
5.2.1 Precomputation step and updates

We first focus on some computational tasks that have to be repeatedly executed at each step of our substitution method. In this section, we provide a high-level description for their implementation.

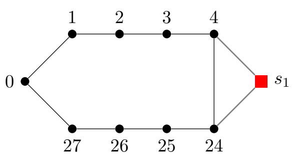
Computation of the distances. Given a $(A|B)$-separator X, we need to compute all distances $\mathrm{d}(v, x)$, $v \in V \setminus X, x \in X$, in order to compute the substitutes. If the distance matrix of the graph is precomputed then each distance can be accessed to in constant-time, hence an $O(n|X|)$-time complexity. However, new vertices are added by our construction. We wish to avoid recomputing



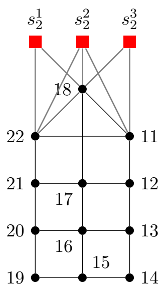
(a) G


$X_1 = \{4, 24\}$
$A_1 = \{0, 1, 2, 3, 4, 24, 25, 26, 27\}$
$X_2 = \{11, 18, 22\}$
$A_2 = \{11, 12, \cdots, 22\}$
$X_3 = \{10, 23\}$
$A_3 = \{10, 11, 18, 22, 23\}$
$X_4 = \{5, 10, 23\}$
$A_4 = \{4, 5, 10, 23, 24\}$
$X_5 = \{6, 10, 23\}$
$A_5 = \{5, 6, 10, 23\}$
$A_6 = \{6, 7, 8, 9, 10, 23\}$

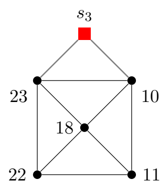
(b) Atom tree of G



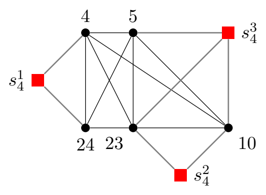
(c) G_1^* built from A_1



(d) G_2^* built from A_2

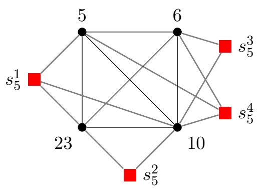


(e) G_3^* built from A_3

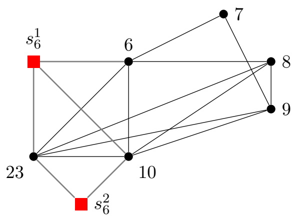


(f) G_4^* built from A_4

	n	m	D	δ	4-tuples
G	28	50	9	2	20 475
G_1^*	10	11	5	2	210
G_2^*	15	25	5	2	1 365
G_3^*	6	10	2	1	15
G_4^*	8	16	3	1/2	70
G_5^*	8	16	2	1/2	70
G_6^*	8	16	3	1	70



(g) G_5^* built from A_5



(h) G_6^* built from A_6

(i) Main characteristics

Figure 9: A connected graph G (Figure 9a), an atom tree of the graph (Figure 9b), the substitute of the atoms of G (Figs. 9c–9h), and the characteristics of these graphs (Tab. 9i).

the distances from scratch at each step of the substitution method (that would result in an $\mathcal{O}(n^2m)$-time complexity). In what follows, we base on Lemma 4 (substitution of a vertex a by a simplicial vertex a^*) in order to reach the goal.

Lemma 16. *Let G be a connected graph. We can embed in quadratic time the distance matrix of G into a data structure, supporting:*

- *$\mathcal{O}(1)$ access to the distance between a non-simplicial vertex and any other;*
- *$\mathcal{O}(|A|)$ updates when G is replaced with the substitute G_B^* (w.r.t. a $(A|B)$-clique-separator X).*

Proof. The gist of such a structure is Lemma 4. Let X be a $(A|B)$-clique separator of G, and s be a simplicial vertex added in the substitute graph of $G[B]$. Let $a \in A \setminus X$ satisfy $N(s) = \{x \in X :$

$d_G(a,x) = d_G(a,X)\}$. Then we have for every $b \in B$, $d(b,s) = d_G(a,b) - d_G(a,X) + 1$.

It thus follows that once the substitution of a with s has been completed, we only need to remember the association of s with a and an offset, so that we can compute the distances in the substitute graphs. The offset can be computed in constant time by picking a neighbor of the simplicial vertex s, as it is the distance $d(a,X)$ between this neighbor and the vertex a which s substitutes. Finally, since there are $l = O(n)$ steps for our substitution method, and that no more than $O(n)$ new simplicial vertices are added at each step, a quadratic-size array is sufficient to store all the pairs $(a, d(a, X_a))$. □

Note that the data structure of Lemma 16 does not support the computation of distances between two vertices added by our construction. We can safely ignore this drawback, as we do not need to compute such distances in our method.

Computation of connected components. Other complexity bottlenecks arise from the computation of connected components in graphs with a superlinear number of edges (up to $\Omega(nm)$ edges). Indeed, at each step i, $1 \leq i < l$, we need to compute the connected component C_A containing the next atom A_i to deal with. Determining the connected components of a graph is linear-time computable. However, as we detailed in Section 5.1.2, here we have to extract the component from a graph $H_i \neq G$, possibly containing more edges than G due to the addition of simplicial vertices at previous steps. Thus it may result in an $\Omega(m)$-time complexity by using the classical algorithm for this problem. Instead, we propose a method to construct the component incrementally, starting from A_i and adding simplicial vertices at every step $1 \leq j \leq i-1$.

Lemma 17. *Let G be a connected graph, T be an atom tree of G, and $A_1, \ldots, A_l$ be its atoms ordered according to their depth in T. We denote by $H_1 = G, H_2, \ldots, H_l$ the sequence of l graphs that are computed by our process, each H_i being decomposed into H_{i+1} and the substitute graph of the i^{th} atom by applying the substitution method of Definition 13. For every (simplicial) vertex $s_i \in H_{i+1} \setminus H_i$, we can compute the index j such that s_i belongs to the substitute graph of the j^{th} atom, in total $O(n|X_i|)$-time.*

Proof. Let $s_i \in H_{i+1} \setminus H_i$ be a simplicial vertex. By construction (Section 5.1.2), we have $N(s_i) \subseteq X_i \subseteq V(G)$. Therefore, if s_i belongs to the substitute graph of the j^{th} atom, $j > i$, then it holds that $N(s_i)$ intersects the connected component containing $A_j \setminus X_j$ —in the graph $H_j \setminus X_j$—. In such case since every vertex in the component either belongs to the atom or is simplicial and not in $V(G)$, then it follows that s_i has a neighbor in $A_j \setminus X_j$. Conversely, if $s_i \in V(H_j)$ and $N(s_i) \cap (A_j \setminus X_j) \neq \emptyset$, then s_i is in the same connected component as $A_j \setminus X_j$ in the graph $H_j \setminus X_j$, hence s_i belongs to the substitute graph of the j^{th} atom. So, at every step of our substitution method, if a simplicial vertex is added by our construction, we consider the minimum index j such that $A_j \setminus X_j$ contains a neighbor of the vertex, and we update the vertex set of the substitute graph of the j^{th} atom by adding this new vertex into it. Since only $O(n)$ vertices are added at step i, and that their neighborhood is contained into X_i, the $O(n|X_i|)$-time complexity follows. □

The two above routines (Lemmas 16 and 17) will be combined in what follows in order to obtain the desired $\mathcal{O}(nm)$-time complexity for our substitution method. Before this, we will show how to reduce the number of simplicial vertices to be added at each step (Section 5.1.1).

5.2.2 Applying simplification rules

The purpose of this section is to reduce the size of the substitutes. Precisely, given $G = (V, E)$ and X a $(A|B)$-clique-separator, we wish to construct a substitute G^*_B from $G[B]$ by adding as few simplicial vertices as possible. A naive implementation would consist in computing the subsets $X_a = \{x \in X : \mathrm{d}_G(a, x) = \mathrm{d}_G(a, X)\}$, for every $a \in A \setminus X$, then adding a simplicial vertex adjacent to X_a. However, by doing so we would add $|A \setminus X|$ new vertices in the substitute, and so, we would lose all the benefit of the separation in terms of size of the graphs. We now define rules in order to avoid this worst-case in some situations. The goal of this section is to give hints on an efficient way to implement these rules.

Partition refinement techniques. We remove pendant and *twin vertices*. Indeed, it may happen that $X_a = \{x_a\}$ for some $a \in A$, and in such a case we needn't add a simplicial vertex for a since the removal of a pendant vertex does not affect the value of hyperbolicity. Furthermore, it may also happen that $X_a = X_{a'}$ for some pair $a, a' \in A$, and in such a case we wish to add only one simplicial vertex in G^*_B.

To do that efficiently, we will use the well-known *partition refinement* techniques (see *e.g.* [36, 49]). Given a partition $\mathcal{P}$ of a set V, and a subset $S \subseteq V$ called the *pivot*, the partition refinement of $\mathcal{P}$ w.r.t. S consists in replacing every group V_i of $\mathcal{P}$ by the non-empty groups among $V_i \cap S$ and $V_i \cap \bar{S}$. This can be achieved in $O(|S|)$-time, up to the precomputation of an appropriate data structure in linear $O(|V|)$-time.

We deduce from this standard technique the following result:

Lemma 18. *Let G be a connected graph given by its distance matrix, and $X \subseteq V(G)$. We define the relation $\equiv_X$ over the set $V(G) \setminus X$ as*

$$u \equiv_X v \overset{def}{\iff} \{x \in X : \mathrm{d}_G(u, x) = \mathrm{d}_G(u, X)\} = \{x \in X : \mathrm{d}_G(v, x) = \mathrm{d}_G(v, X)\}.$$

The equivalence classes of $\equiv_X$ can be computed in $O(n|X|)$-time.

Proof. Since the distance matrix is given, we can compute $X_u = \{x \in X \mid \mathrm{d}_G(u, x) = \mathrm{d}_G(u, X)\}$ for every vertex u, that takes $\mathcal{O}(n|X|)$-time. Then, we start from the partition $\mathcal{P} = \{V \setminus X\}$ which we refine successively for every $x \in X$ with the set $\{u : u \in V \setminus X \text{ s.t. } \mathrm{d}_G(u, x) = \mathrm{d}_G(u, X)\}$. The total cost is $O(\sum_{x \in X} |N_{G_X}(x)|) = O(n|X|)$. □

There are at most $2^{|X|}$ equivalence classes of $\equiv_X$, and we can remove the $|X| + 1$ classes corresponding to the subsets of X of size at most one. Altogether, the substitute G^*_B has at most $|B| + \min\{|A \setminus X|, 2^{|X|} - |X| - 1\}$ vertices when we apply our simplification rules. This bound is sharp, as shown with Figure 10.

Overall, the substitution method will add at most $\sum_{i=1}^{l-1} \min\{n, 2^{|X_i|} - |X_i| - 1\}$ new vertices to the vertex-set of the atoms. In particular, consider the special case when all but at most c clique-separators X_i have size at most k, for some universal constants c and k. In this situation, there are at most $(c + 2^k - k - 1) \cdot n$ new vertices added to the atoms. Hence, the total number of vertices is only increased by a constant-factor. This property will hold for the outerplanar graphs and some real-life graphs that we will study in the next two sections.

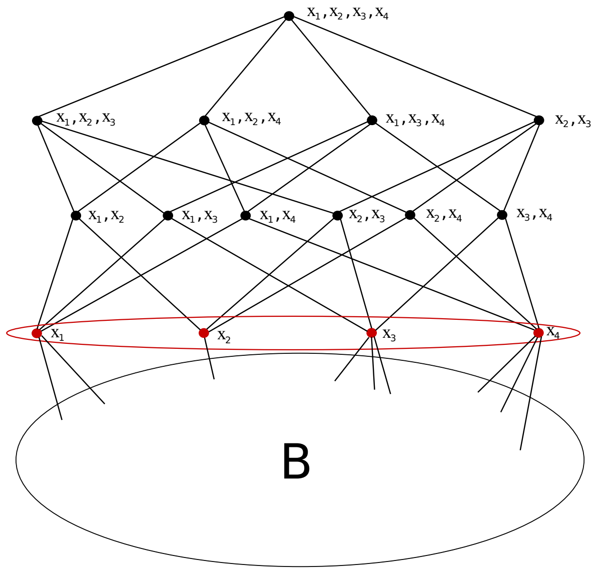


Figure 10: A case when $|A \setminus X| = 2^{|X|} - |X| - 1$ vertices need to be added in G^*_B. The graph $G[A]$ is obtained from the subset lattice of the set $X = \{x_1, x_2, x_3, x_4\}$. Every vertex $a \in A$ is labeled with $\{x \in X \mid \mathrm{d}(a,x) = \mathrm{d}(a,X)\}$.

5.2.3 Complexity analysis

Finally, to determine the time complexity of our substitution method, we will use the following result:

Lemma 19 ([7]). *Let G be a connected graph, and $A_1, \ldots, A_l$ be its atoms. Then $\sum_i |A_i| \leq n + m$.*

Corollary 20. *The substitute of the atoms of a connected graph G can be computed in $O(nm)$-time.*

Proof. The notations are the same as for Section 5.1.2. That is, fix any atom tree T of G and let $A_1, \ldots, A_l$ be the atoms ordered by increasing depth. For every $i < l$, let X_i be the clique-separator of G labeling the father node of leaf A_i in T. By Definition 15, $X_i \subseteq A_i$.

We first precompute the distance matrix of G in $O(nm)$-time, then we embed it in quadratic-time into the data structure of Lemma 16. Also, for every i, we initialize the vertex set of the i^{th} substitute graph with the atom A_i. We then apply each step of our substitution method sequentially.

Precisely, at each step i we are given the vertex set V_i of the graph H_i to be considered. Initially, $V_1 = V(G)$.

- Let us partition the vertices in A and B, where A is the set of all vertices in V_i that are in the i^{th} substitute graph. Since A is known (initialized with A_i then updated at each previous step), it can be done in $\mathcal{O}(|V_i|)$-time.
- Then, we compute the simplicial vertices that result from the substitution operation, and we add them in A and B, respectively. Since we have constant-time access to the distances, we have by Lemma 18 that it can be done in $\mathcal{O}(|V_i||X_i|)$-time.
- For every vertex newly added at this step, we next compute the index of the atom's substitute to which it belongs to. By Lemma 17, it can also be done in $\mathcal{O}(|V_i||X_i|)$-time.

- We set $V_{i+1} = B$ and then we update the distances accordingly. By Lemma 17, it can be done in $\mathcal{O}(|A|)$-time, that is $\mathcal{O}(|V_i|)$.

We can easily show by induction that $|V_i| = \mathcal{O}(n)$. Hence, the i^{th} step can be executed in $\mathcal{O}(n|X_i|)$-time. Overall, our modified clique-decomposition can be computed in $\mathcal{O}(n \sum_i |X_i|)$-time, that is in $\mathcal{O}(n \sum_i |A_i|) = \mathcal{O}(nm)$-time by Lemma 19. □

6 Hyperbolicity of outerplanar graphs

Equipped with the substitution method of Section 5 and our in-depth analysis of clique-decomposition (Sections 3 and 4), we aim at applying these results in order to speed-up the computation of hyperbolicity in some graph classes. In the final two sections, we will review theoretical and practical cases when it is possible to do so. We start with a linear-time algorithm for computing the hyperbolicity of a given outerplanar graph (Theorem 28).

The outerplanar graphs can be characterized in several ways (see [53]). We will use the following ones.

A *planar graph* is a graph drawable in the Euclidean plane so that edges may only intersect at their endpoints. It is *outerplanar* if it stays planar whenever one adds a universal vertex to it. Equivalently, a graph is outerplanar if it is drawable in the Euclidean plane so that edges may only intersect at their endpoints, and all the vertices lie on a common face which is called the *outerface*. Such a drawing is furthermore called an outerplanar embedding, and it can be computed in linear-time [54]. Note that it easily follows from this definition that all cycles are outerplanar graphs.

The class of outerplanar graphs is minor-closed, and a graph is outerplanar if and only if it is K_4-minor-free and $K_{2,3}$-minor-free [53].

We will exploit nontrivial properties of the clique-decomposition of outerplanar graphs to prove Theorem 28. In particular, clique-separators of an outerplanar graph have size at most two, *i.e.*, they are either cut-vertices or edge-separators. More precisely, the atoms of an outerplanar graph are cycles. We will base on the property that the hyperbolicity of a given cycle can be computed in linear time, by using the following formula:

Lemma 21 ([59, 20])**.** *Cycles of order $4p + \varepsilon \geq 3$, with $p \geq 0$ and $\varepsilon \in \{0, 1, 2, 3\}$, are $(p - 1/2)$-hyperbolic when $\varepsilon = 1$, and p-hyperbolic otherwise.*

The main purpose of this section is to obtain a similar characterization for the substitute of cycles (Lemma 26). So, we will analyze the properties of this class of graphs in Section 6.2. We will also need to compute the substitutes of atoms of a given outerplanar graph in linear time. For this purpose, we will rely on the notion of *weak dual* [4].

Definition 22. *Let G be a biconnected outerplanar graph. The weak dual of G is a tree T_G equal to the intersection graph of the atoms of G. Two adjacent nodes of T_G correspond to atoms which share a single edge.*

Note that a weak dual is nothing else than a tree-decomposition whose bags are the atoms of an outerplanar graph. If G is biconnected, then starting from an outerplanar embedding of the graph, we construct it by removing from the dual of the graph the universal vertex corresponding to the outerface (see Figure 13 for an example).

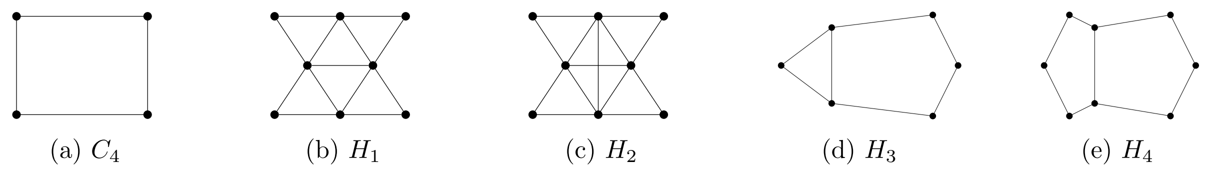

(a) C_4 (b) H_1 (c) H_2 (d) H_3 (e) H_4

Figure 11: Characterization of 5-chordal $\frac{1}{2}$-hyperbolic graphs, in terms of forbidden isometric subgraphs.

We will show that the atoms' substitutes can be computed by dynamic programming on the weak dual (Lemma 27). This combined with Lemma 26 and a characterization of 1/2-hyperbolic outerplanar graphs (Proposition 23) will achieve proving Theorem 28.

6.1 Outerplanar graphs with small hyperbolicity

As observed in Section 5, our substitution method for an exact computation of hyperbolicity requires the hyperbolicity of the graph to be at least 1. To overcome this drawback, we first characterize in this section outerplanar graphs that are $\frac{1}{2}$-hyperbolic. Note that we only consider biconnected graphs, as the hyperbolicity of a graph is the maximum hyperbolicity taken over all its biconnected components, and the biconnected components of a graph are computable in linear-time [55].

Proposition 23. *A biconnected outerplanar graph is $\frac{1}{2}$-hyperbolic if, and only if, either it is isomorphic to C_5, or it is chordal and it does not contain the graph of Figure 11b as a subgraph. Furthermore, these conditions can be checked in linear-time.*

Proof. Let G be a $\frac{1}{2}$-hyperbolic outerplanar biconnected graph. By Lemma 21, the graph C_5 is $\frac{1}{2}$-hyperbolic, and we now assume that G is not isomorphic to C_5. The induced cycles of G are exactly its atoms. As a result, we have by Lemma 21 that G only has induced cycles of length 3 or 5 (else, $\delta(G) \geq 1$). Moreover, Wu and Zhang prove in [59] that a 5-chordal graph is $\frac{1}{2}$-hyperbolic if, and only if, it does not contain any graph of Figure 11 as an isometric subgraph[3].

Since we consider graphs with induced cycles of length 3 or 5, G is C_4-free and so, it does not contain the graph of Figure 11a as an isometric subgraph. Moreover, we claim that G is C_5-free, as otherwise it would contain the graph of Figure 11d, or the graph of Figure 11e, as an isometric subgraph. Thus G has to be chordal. In addition, we claim that G cannot contain the graph of Figure 11c, since it is not outerplanar and being outerplanar is a hereditary property. Consequently, G is $\frac{1}{2}$-hyperbolic if, and only if, it is chordal and it does not contain the graph of Figure 11b as an isometric subgraph.

Let H_1 be the graph of Figure 11b. To complete the proof of the proposition, we are left to prove that every subgraph of G that is isomorphic to H_1 is isometric. Indeed, the latter will prove that G is $\frac{1}{2}$-hyperbolic if, and only if, it is chordal and it does not contain H_1 as a subgraph.

We observe that H_1 is an edge-maximal outerplanar graph, hence every subgraph isomorphic to H_1 must be induced. Suppose for the sake of contradiction that there is an induced subgraph of G that is isomorphic to H_1 but not isometric. In this situation, there is a vertex $x \in V(G \setminus H_1)$ connecting two vertices at distance 3 in H_1. As shown in Figure 12, it implies the existence of a

[3]The characterization of [59] is composed of six forbidden isometric subgraphs, but the sixth one is actually 6-chordal.

$K_{2,3}$-minor in G, thereby contradicting that it is outerplanar. Therefore, the claim is proved, and so, G is $\frac{1}{2}$-hyperbolic if, and only if, it is chordal and it does not contain H_1 as a subgraph.

Being chordal can be checked in linear-time [50]. Furthermore, when G is chordal, all its induced cycles have length three, hence it contains H_1 as a subgraph if and only if there are two adjacent vertices of degree 3 in its weak dual (see Figure 13 for an illustration). Overall, since the weak dual can be computed in linear time, deciding whether a chordal outerplanar graph G is 1/2-hyperbolic can be done in linear time. □

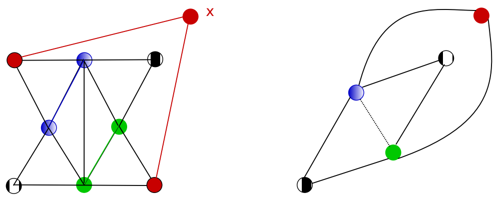


Figure 12: Existence of a $K_{2,3}$-minor in G.

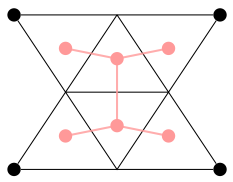


Figure 13: The forbidden subgraph of Figure 11b, and its characterization in the weak dual.

6.2 Substitute graphs of cycles

As we constrain ourselves to outerplanar graphs, recall that the atoms are exactly the induced cycles of the graph. Clearly, a clique-separator contained in a cycle is either a cut-vertex or an edge-separator. Since we never add pendant vertices with our substitution method (cf. Section 5.2.2), we never add a simplicial vertex in the first case, and in the second case we might only add a single vertex which has to be adjacent to both ends of the edge-separator. Substitute graphs of cycles thus fall into the following subclass of outerplanar graphs:

Definition 24. *A biconnected outerplanar graph is called a sunshine graph if it can be obtained from a cycle C by adding, for every edge of C, at most one simplicial vertex that is adjacent to that edge.*

Trivially, all cycles are sunshine graphs. Two other examples of sunshine graphs are given in Figure 14.

We can derive some useful properties of sunshine graphs from their definition. First is that vertices in the cycle C form a dominating set of the graph. Furthermore, the choice of C is unique, except for the particular case of the diamond graph (obtained from two triangles sharing an edge).

Finally, since every sunshine graph G is obtained by adding simplicial vertices to a cycle, it has at most one induced cycle of length at least four, and if it exists this cycle must be C. Thus, we have by Theorem 12 that $\delta(C) \leq \delta(G) \leq \delta(C)+1$. This difference can be decreased by $\frac{1}{2}$ as follows.

Lemma 25. *Let G be a sunshine graph, and C be a dominating cycle of G. Then we have:*

$$\delta(C) \leq \delta(G) \leq \delta(C) + \frac{1}{2}.$$

Proof. By Theorem 12, we have $\delta(C) \leq \delta(G) \leq \delta(C) + 1$. So, our aim is to prove that no 4-tuple of G has a hyperbolicity greater than $\delta(C) + \frac{1}{2}$. By contradiction, let a, b, c, d be such that $\delta(a, b, c, d) = \delta(C) + 1$.

We arbitrarily orient the cycle C. For every $u \in \{a, b, c, d\} \setminus C$, we denote by $e_u = \{h_u, t_u\}$ the edge of C induced by its neighbors, where h_u denotes the head of the edge w.r.t. the orientation. Observe that for every $u, v \in \{a, b, c, d\} \setminus C$, we have $\mathrm{d}(u, v) = 2 + \min\{\mathrm{d}(h_u, t_v), \mathrm{d}(h_v, t_u)\} = 1 + \mathrm{d}(h_u, h_v) = 1 + \mathrm{d}(t_u, t_v)$.

We then claim that there is exactly one vertex among a, b, c, d which belongs to the cycle C. We prove the claim with a case-by-case analysis.

- Since we assume $\delta(a, b, c, d) > \delta(C)$, not all of a, b, c, d belong to the cycle;
- Furthermore, suppose for the sake of contradiction that $a \notin C$ but $b, c, d \in C$. Let $X = N(a)$, $A = N[a]$, and $B = V(G) \setminus a$. The 4-tuple is a $(a|b_1, b_2, b_3)$ 4-tuple, and so, by Lemma 5, there exists $x \in N(a)$ such that $\delta(a, b, c, d) \leq \delta(x, b, c, d) + 1/2$. In this situation, $x, b, c, d \in C$, hence $\delta(a, b, c, d) \leq \delta(C) + 1/2$, thereby contradicting our assumption that $\delta(a, b, c, d) = \delta(C) + 1$.
- In the same way, suppose for the sake of contradiction that $a, d \notin C$ but $b, c \in C$. Let $X_a = N(a)$ and $X_d = N(d)$. These two clique-separators satisfy the conditions of Lemma 10, so, there exist $x_a \in X_a,\ x_d \in X_d$ such that $\delta(a, b, c, d) \leq \delta(x_a, b, c, x_d) + 1/2$. In this situation, $x_a, b, c, x_d \in C$, hence $\delta(a, b, c, d) \leq \delta(C) + 1/2$, thereby contradicting our assumption that $\delta(a, b, c, d) = \delta(C) + 1$.
- So, there are at least three vertices of a, b, c, d that are not in C. Finally, suppose for the sake of contradiction that $a, b, c, d \notin C$. In this situation, for every $u, v \in \{a, b, c, d\}$, we have $\mathrm{d}(u, v) = 1 + \mathrm{d}(h_u, h_v)$. Therefore by the 4-point condition we have $\delta(a, b, c, d) = \delta(h_a, h_b, h_c, h_d) \leq \delta(C)$. The latter contradicts our assumption that $\delta(a, b, c, d) = \delta(C) + 1$.

As a result, there is exactly one vertex of the 4-tuple that is in C, which proves the claim. Assume w.l.o.g. that $a \in C$. In such a case, for every $u \in \{b, c, d\}$ we have $\mathrm{d}(a, h_u) \leq \mathrm{d}(a, u) \leq \mathrm{d}(a, h_u) + 1$.

Let S_1, S_2, S_3 satisfy $\{S_1, S_2, S_3\} = \{\mathrm{d}(a, b) + \mathrm{d}(c, d), \mathrm{d}(a, c) + \mathrm{d}(b, d), \mathrm{d}(a, d) + \mathrm{d}(b, c)\}$ and $S_1 \geq S_2 \geq S_3$. Accordingly, let u_1, u_2, u_3 satisfy $\{u_1, u_2, u_3\} = \{b, c, d\}$ and for every i, $S_i = \mathrm{d}(a, u_i) + \mathrm{d}(u_j, u_k)$ where $\{j, k\} = \{1, 2, 3\} \setminus i$. Finally, let $S'_i = \mathrm{d}(a, h_{u_i}) + \mathrm{d}(h_{u_j}, h_{u_k})$.

We have $\mathrm{d}(a, h_{u_i}) \leq \mathrm{d}(a, u_i) \leq \mathrm{d}(a, h_{u_i}) + 1$ and $\mathrm{d}(u_j, u_k) = \mathrm{d}(h_{u_j}, h_{u_k}) + 1$. Consequently, we have $S'_i + 1 \leq S_i \leq S'_i + 2$ for every i. By the 4-point condition, it implies $\delta(a, h_b, h_c, h_d) \leq \delta(a, b, c, d) + 1/2$. Since in addition $a, h_b, h_c, h_d \in C$, we have $\delta(a, b, c, d) \leq \delta(C) + 1/2$, thereby contradicting our assumption that $\delta(a, b, c, d) = \delta(C) + 1$. Altogether, this proves $\delta(G) \leq \delta(C) + 1/2$. □

We now present a characterization for the hyperbolicity of sunshine graphs, from which it can be easily derived a linear-time algorithm in order to compute it.

Lemma 26. *Let G be a sunshine graph, and C be a dominating cycle for G of length $4p + \varepsilon \geq 3$, with $p \geq 0$ and $\varepsilon \in \{0, 1, 2, 3\}$. Assuming $G \setminus C$ is nonempty we have:*

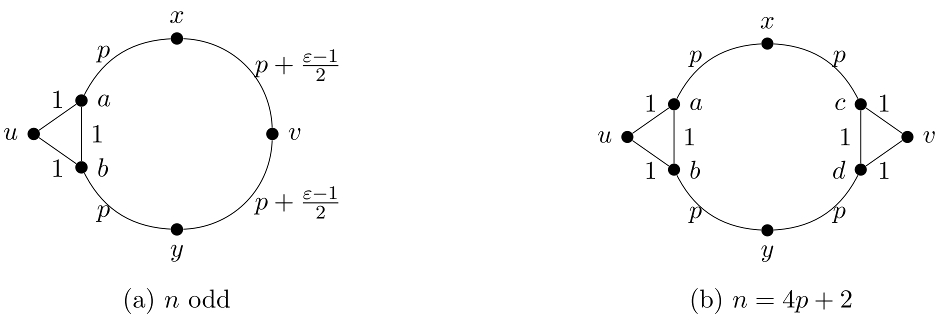


Figure 14: Substitute graphs of the atoms of an outerplanar graph.

- *if ε is odd, then $\delta(G) = \delta(C) + \frac{1}{2}$;*
- *if $\varepsilon = 2$, then $\delta(G) = \delta(C) + \frac{1}{2}$ if, and only if, there is a diametral pair made of two simplicial vertices not in C (otherwise, $\delta(G) = \delta(C)$);*
- *finally, if $\varepsilon = 0$, then $\delta(G) = \delta(C)$.*

Proof. Recall that by the previous Lemma 26, we have $\delta(G) \leq \delta(C) + \frac{1}{2}$. Thus we only focus on finding 4-tuples u, v, x, y of hyperbolicity (at least) this value, and we choose one, if any, maximizing $|C \cap \{u, x, v, y\}|$. In what follows, write $S_1 = \mathrm{d}(u, v) + \mathrm{d}(x, y)$, $S_2 = \mathrm{d}(u, x) + \mathrm{d}(v, y)$ and $S_3 = \mathrm{d}(u, y) + \mathrm{d}(v, x)$. We will assume in addition that $S_1 \geq S_2 \geq S_3$.

Case ε odd Equivalently, we have $\varepsilon \in \{1, 3\}$. In such a case, we have $\delta(C) = p + \frac{\min\{0,\varepsilon-2\}}{2}$ by Lemma 21. Figure 14a exhibits a 4-tuple u, v, x, y satisfying:

$$S_1 = (2p + \frac{\varepsilon+1}{2}) + (2p + \min\{1, \varepsilon-1\}) = 4p + \frac{\varepsilon+1}{2} + \min\{1, \varepsilon-1\};$$
$$S_2 = (p+1) + (p + \frac{\varepsilon-1}{2}) = 2p + \frac{\varepsilon+1}{2};$$
$$S_3 = S_2.$$

Hence, this 4-tuple has hyperbolicity $p + \frac{\min\{1,\varepsilon-1\}}{2} = \delta(C) + \frac{1}{2}$.

Case $\varepsilon = 2$ In such a case, we have $\delta(C) = p$ by Lemma 21. We assume w.l.o.g. that $u \notin C$, and we claim that it implies $v \notin C$. Indeed, by the metric property of Lemma 9, and noticing that $S_1 \geq S_2 \geq S_3$, the vertex v has to be at equal distance l of both neighbors of u, as otherwise u could be replaced with one of its two neighbors, contradicting the maximality of $|C \cap \{u, x, v, y\}|$. Hence $v \in C$ is impossible, as it would yield the length of C is $2l + 1 = 4p + 2$. It thus follows that $v \notin C$, and the length of C is in fact $2(l-1) + 2 = 2l$, yielding $l = 2p + 1$.

Conversely, assume that there exist two simplicial vertices u, v that are diametrically opposed in G. We choose the 4-tuple u, x, v, y as in Figure 14b, and it satisfies:

$$S_1 = (2p+2) + (2p+1) = 4p+3;$$
$$S_2 = 2(p+1) = 2p+2;$$
$$S_3 = S_2.$$

So, we have $\delta(u, v, x, y) = p + \frac{1}{2} = \delta(C) + \frac{1}{2}$.

Case $\varepsilon = 0$ Another application of Lemma 21 yields $\delta(C) = p$. Assuming $u \notin C$, we deduce as for the previous case that $v \notin C$, and v is at equal distance $l = 2p$ from both neighbors of u. Thus, C is partitioned by the neighborhoods of u and v in two paths of length $l - 1 = 2p - 1$, that is in the same way as in Figure 14b. Furthermore, since the diameter of C is $2p$, those paths are geodesics of the cycle.

We recall that on the way to prove Lemma 25, we showed that $u, v, x, y \notin C$ implies $\delta(u, v, x, y) \leq \delta(C)$. Since we assume $\delta(u, v, x, y) > \delta(C)$, it implies the existence of one vertex $z \in \{x, y\}$ among the 4-tuple that must be in C. Furthermore, in this situation we obtain by considering the geodesic containing z that $\mathrm{d}(u, z) + \mathrm{d}(v, z) = 2 + (l - 1) = 2p + 1$. In particular, we have $\min\{\mathrm{d}(u, z), \mathrm{d}(v, z)\} \leq p$. The latter contradicts the assumption that $\delta(u, v, x, y) > \delta(C)$, since we have by [51] that $\delta(u, v, x, y) \leq \min\{\mathrm{d}(u, z), \mathrm{d}(v, z)\}$. Altogether, we always have $\delta(G) = \delta(C)$ if $\varepsilon = 0$. □

6.3 Applying the substitution method in linear-time

Given an outerplanar graph G, we recall that we aim at computing $\delta(G)$ from the substitute of its atoms. From Lemma 26, the hyperbolicity of the substitutes can be computed in linear time. So, we are left to prove that the atom's substitutes can also be computed in linear time.

Lemma 27. *Let G be an outerplanar biconnected graph. The substitute graphs of the atoms of G can be computed in linear-time.*

Proof. We construct the weak dual T_G of G from an outerplanar embedding, that is linear-time computable. Let $C_1, \ldots, C_l$ be the atoms of G. We root T_G on an atom C_1, which is an induced cycle. Then, we claim that the following algorithm for computing the atom's substitutes is correct.

- For every i, we initialize C_i^* with C_i.
- We start a depth-first search from the root, and so obtain a postordering of the nodes of T_G. Then, we visit the atoms following this ordering, and we proceed as follows. For every C_i, we name $e_{ij} = C_i \cap C_j$ an edge shared with a child in the rooted tree. If there is a vertex of C_j^* that is at equal distance to both ends of e_{ij} then we add in C_i^* a new simplicial vertex that is adjacent to e_{ij}. That is, we add such new vertex if either C_j is odd, or there is a simplicial vertex of $C_j^* \setminus C_j$ that is adjacent to the edge opposed to e_{ij}.
- Finally, we start a breadth-first search from the root and for every visited atom $C_i \neq C_1$, we consider its parent atom, denoted by C_k, naming $e_{i,k}$ the edge-separator that it shares with it. As before, we add in C_i^* a simplicial vertex whose neighborhood is $e_{i,k}$ if, and only if, either the length of C_k is odd, or there is a simplicial vertex in $C_k^* \setminus C_k$ whose neighborhood is the edge diametrically opposed to $e_{i,k}$ in the atom C_k.

This algorithm runs in linear time. Furthermore, we note that an atom tree can be obtained from $(T_G; C_1)$ (as defined in Definition 15) by disconnecting at every step an atom that is a leaf of T_G until the clique-decomposition is obtained. Following this atom tree, the atom's substitutes so obtained are isomorphic to the output $C_1^*, C_2^*, \ldots, C_l^*$ of the above algorithm. In particular, for every atom, we use the depth-first search to compute the simplicial vertices resulting from the disconnection of its sons, whereas the breadth-first search is used to compute the single vertex resulting from its own disconnection, if any. Hence, the above algorithm for computing the atom's substitutes is correct, and so, the resulting $C_1^*, \ldots, C_l^*$ are the substitute graphs of the atoms of G. $\square$

Figure 15 shows the substitute graphs resulting from the application of the substitution method to a biconnected outerplanar graph.

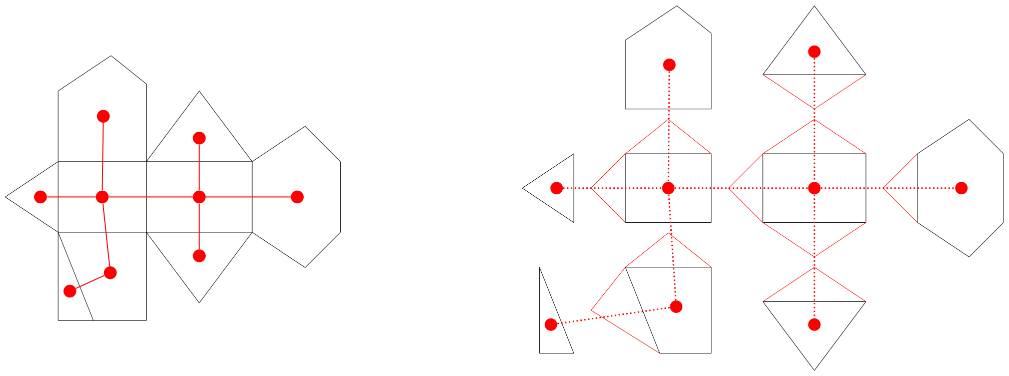


Figure 15: An application of the substitution method to an outerplanar graph.

We finally conclude with the following theorem.

Theorem 28. *The hyperbolicity of a given connected outerplanar graph G is computable in linear time.*

Proof. We can safely assume G to be biconnected by [55]. By [5, 37], G is 0-hyperbolic if, and only if, G is a clique. If it is not, then by Proposition 23, we can check whether it is $\frac{1}{2}$-hyperbolic in linear time.

From now on, assume $\delta(G) \geq 1$. By Lemma 27, we can compute the substitute graphs of the atoms of G in linear time. We can thus conclude by Lemma 14 (*i.e.* the correctness of our substitution method), as these substitute graphs are sunshine graphs and their hyperbolicity is linear-time computable by Lemma 26. $\square$

7 Experimental evaluation

Before concluding the paper, we shall apply the substitution method of Section 5 to some real-life graphs with a large number of vertices. We report in this section on experiments performed with our substitution methodology on the graphs of five collaboration networks. This way, we aim to evaluate the computation time of the substitutes on some empirical graphs, and to better understand the factors impacting their size (compared with the upper-bound of Section 5.2.2).

The section is subdivided as follows. In Section 7.1, we present the graphs from the dataset and we motivate our choice to test the method on these graphs. We report on the reduction on the size of the subgraphs (biconnected components, atoms and substitutes) in Section 7.2. In spite of strong similarities between the graphs from the dataset, the results obtained vary from one graph to the other. So, we conduct a deeper analysis of their clique-decomposition in Section 7.3, reporting on the structure of their atom tree and on the size of the clique-separators, in order to justify the variations in the results. We complete our experiments with a numerical analysis of the time needed for computing the hyperbolicity of these graphs, with and without the clique-decomposition and the substitute decomposition of Section 5. On the way, we report on the hyperbolicity of all graphs in the dataset (Section 7.4).

7.1 Datasets

We apply the algorithm presented in Section 5 to the collaboration networks of five different scientific communities [45], namely:

- `ca-AstroPh`, for the astrophysics community;
- `ca-CondMat`, for the condensed matter physics community;
- `ca-GrQc`, for the general relativity and quantum cosmology community;
- `ca-HepPh`, for the high energy physics-phenomenology community;
- and `ca-HepTh`, for the high energy physics-theory community.

In the `ca-*` graphs, nodes represent scientists and edges represent collaborations (i.e., co-authoring a paper). These graphs are interesting to analyze the behavior of our algorithm, and the size of their substitute graphs, because they have many cliques of various sizes. Indeed, a paper co-authored by k scientists induces a clique of size k in the graph. Furthermore, the number of co-authors per papers varies from one community to another. As noted in Section 5.2.2, there are $\mathcal{O}(2^k)$ vertices newly added in the substitutes for any clique-separator of size k. Therefore, we expect to observe different results in terms of the size of the substitutes, despite the graphs from the dataset share many properties (see [45]).

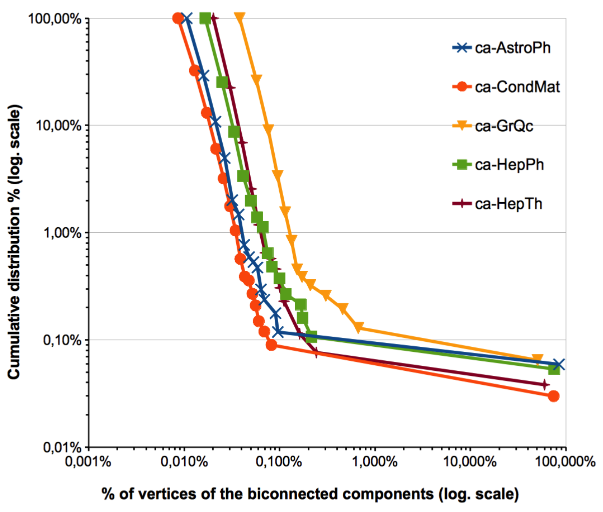
7.2 Empirical results

We modified the clique-decomposition algorithm of [8] to implement the substitution method that we presented in Section 5. We used it here to compute, for every graph, the substitute of each atom of the decomposition.

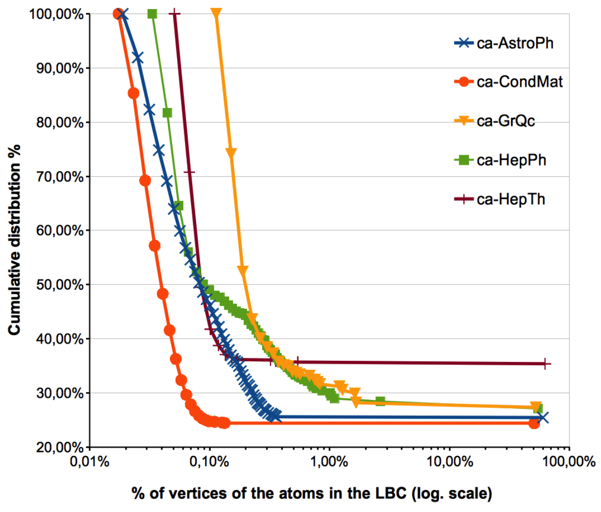
Below, we report on the size of the substitutes. We compare it with the size of the atoms and the biconnected components (see Figure 16 and Table 1). This preliminary analysis also explains why we can ignore almost all substitutes in the computation of hyperbolicity (precisely, all but one substitute), that will further reduce the time of computation.

Decomposition into biconnected components We observed that all of the five graphs are composed of one largest biconnected component, that we call LBC, that includes from 50% to 84.85% of all the vertices. This can be observed from the cumulative distribution of the size of the biconnected components in Figure 16a. The cumulative number of components is given as a percentage of the total number of biconnected components, and the size of the components as a percentage of the total number of vertices in the graph. We noticed that all the biconnected components but the LBC are small: only covering at most 1% of the vertices.

Clearly, the smallest biconnected components can be safely ignored for the computation of hyperbolicity, provided that their diameter is smaller than two times the hyperbolicity of the LBC, which is always the case for these graphs (see [20]). Thus, we now focus on the clique-decomposition of the LBC, and on its resulting substitute graphs.



(a) Biconnected components



(b) Atoms in the LBC

Figure 16: Cumulative distributions of the size of the biconnected components (Figure 16a) and of the atoms in the LBC of each graph (Figure 16b).

Clique-decomposition We plotted in Figure 16b the cumulative distribution of the size of the atoms of the LBC. The cumulative number of atoms is given as a percentage of the total number of atoms and the size of the atoms as a percentage of the total number of vertices in the LBC. Again, for all of the graphs, we observed one largest atom, that we call the LA, that includes from 50% to 60% of all the vertices, and all the other atoms only represent a small fraction of the overall vertices. In the worst case (`ca-HepPh`), all the atoms but the LA solely cover 2.65% of the vertices of the graph.

Moreover, like for the smallest biconnected components and as reported in [20], the substitute graphs of the smallest atoms can be safely ignored for the computation of hyperbolicity. As a result, the only component of the graphs to deal with for computing their hyperbolicity is the substitute graph of the LA. We will denote it by LS in what follows.

Size of the substitute graphs As explained in Section 5, the size of the LS depends on both the initial size of the LA and the number of added simplicial vertices. We have reported in Table 1 the original size n of each graph, the size n_B of its LBC, the size n_{LA} of the LA, and the size n_{LS} of the largest substitute. We have then computed the percentage R_{LA} of vertices that have been removed from the LBC to obtain the LA, that is $R_{LA} = \frac{n_B - n_A}{n_B}$. We observe a significant reduction rate R_{LA}, varying from 37.40% to 49.22%. We have also computed the reduction rate R_{LS} of the LS with respect to the LBC, that is $R_{LS} = \frac{n_B - n_{LS}}{n_B}$. We observe that this reduction rate falls between 11.22% and 20.84%. It indicates that in spite of the simplification rules presented in Section 5.2.2, the substitution method adds many simplicial vertices to the LA when constructing the LS.

We reported in Table 1 as *Cost* the percentage of vertices in the LBC representing the addition of new simplicial vertices.

We first analyze the `ca-CondMat` graph. This graph has the largest reduction rates R_{LS} and

Instance name	n	n_B	n_{LA}	n_{LS}	R_{LA}	R_{LS}	Cost	Time (in sec.)
`ca-CondMat`	23 133	17 234	8 751	13 643	49.22%	20.84%	28.39%	672
`ca-GrQc`	5 242	2 651	1 386	2 107	47.72%	20.52%	27.20%	5
`ca-HepPh`	12 008	9 025	4 925	7 170	45.43%	20.55%	24.88%	167
`ca-AstroPh`	18 772	15 929	9 561	13 407	39.98%	15.83%	24.14%	679
`ca-HepTh`	9 877	5 898	3 692	5 236	37.40%	11.22%	26.18%	53

Table 1: Characteristics of the collaboration networks. The size of the graph is given as n, the size of the LBC as n_b, the size of the LA as n_{LA} and the size of the LS as n_{LS}. The percentage of vertices removed from the LBC to obtain the LA is given as R_{LA}, the reduction rate is $R_{LS} = \frac{n_B - n_{LS}}{n_B}$, and the percentage of vertices in the LBC, representing the addition of simplicial vertices, is given as *Cost*. Finally, the computation time of the substitution method, denoted by *Time*, is given in seconds.

R_{LA} from the dataset. However, despite a R_{LA} of 49.22%, it has almost the same reduction rate R_{LS} as `ca-HepPh` and `ca-GrQc` — ranging from 20.55% to 20.84%. This is the consequence of more simplicial vertices added with our substitution methodology. The new simplicial vertices represent 28.39% of the size of its LBC, whereas for the `ca-HepPh` graph it goes up to only 24.88%.

A similar behavior is observed between `ca-AstoPh` and `ca-CondMat`: even though their R_{LA} differ on 9.25%, the difference of their reduction rate R_{LS} finally falls to 5%. This results from the addition of 4.24% less simplicial vertices in `ca-AstoPh` than in `ca-CondMat`. As an extremal case, the R_{LA} and R_{LS} of the `ca-HepPh` graph are respectively bigger and smaller than the R_{LA} and R_{LS} of `ca-GrQc`.

We thus conclude that the impact of n_{LA} and of the number of new simplicial vertices on the final size n_{LS} differs greatly depending on the graph.

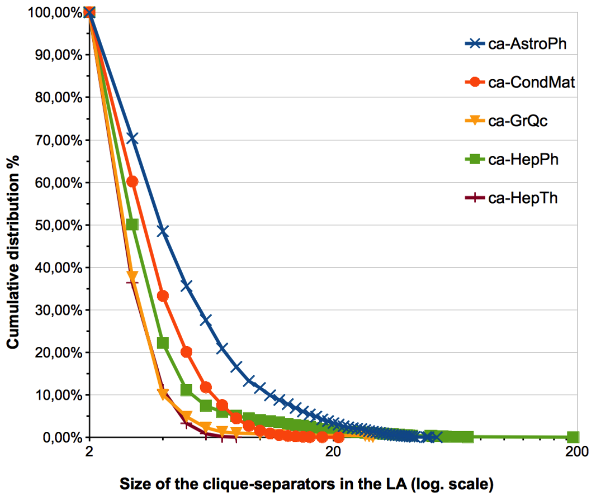
7.3 Decomposition analysis

Having noticed the heterogeneous results of our empirical section, we are now analyzing in more details the properties causing the asymmetry between the various `ca-*` graphs. To do so, we report on the structure of the intersection graph of the atoms (sometimes call the atom graph) and on the size of the clique-separators.

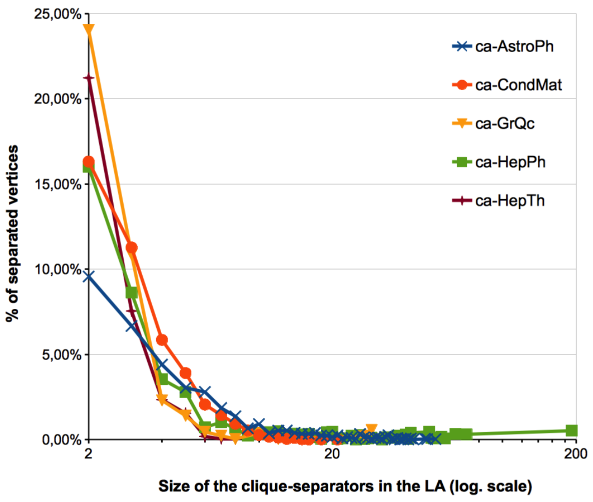
We support through our experiments that most clique-separators are small (with no more than two or three nodes), and they are responsible for the largest part of new simplicial vertices. One plausible explanation for small-size separators are the student interns, publishing one paper with their supervisors before changing their lab or leaving the community.

Clique-decomposition We first analyzed the neighborhood of the LA in the *atom graph*, as it is defined in [7]. That is, we consider the set of atoms $\mathcal{A}_{LA} = \{A_1, \ldots, A_l\}$ that intersect the LA, naming $\mathcal{X}_{LA} = \{X_1 = A_1 \cap LA, \ldots, X_l = A_l \cap LA\}$ the clique-separators at their intersection. We emphasize that there might be other atoms in the graph than the LA and those in $\mathcal{A}_{LA}$. But such atoms, if any, do not overlap the LA.

We plotted in Figure 17a the cumulative distribution of the size of the clique-separators in the



(a) Clique-separators in the LA



(b) Separated vertices from the LA

Figure 17: Cumulative distribution of the size of the clique-separators in the LA (Figure 17a) and percentage of separated vertices as a function of the size of the clique-separators in the LA (Figure 17b).

LA as a percentage of the total number of clique-separators. By doing so, we observed smaller clique-separators for the `ca-HepTh` and `ca-CondMat` graphs, with a maximum size of 8 and 21, respectively, than for the three other graphs `ca-GrQc`, `ca-AstroPh` and `ca-HepPh`, having clique-separators of maximum size 42, 53 and 192, respectively. Also, we reported in Table 2 that the ratio $R_{|\mathcal{X}_{LA}|} = |\mathcal{X}_{LA}|/n_{LA}$ varies from 0.39 for `ca-AstroPh` to 0.54 for `ca-CondMat`. To sum up, there are more clique-separators in `ca-CondMat` than in `ca-AstropPh`, but there are larger clique-separators in `ca-AstropPh` than in `ca-CondMat`.

Recall that our substitution methodology never adds more simplicial vertices than the number of nodes disconnected by the clique-separator. So, to complete our measurements, we related the size of clique-separators with the proportion of vertices that are disconnected by them from the LA. We reported in Table 2 as $\alpha_1 = n_B - n_{LA}$ the total number of vertices separated from the LA in the LBC, and as $\alpha_2 = |\bigcup_{i=1}^{l} A_i \setminus X_i|$ the number of vertices of $LBC \setminus LA$ present in an atom of $\mathcal{A}_{LA}$. Finally, we computed the fraction $\Delta_1 = \frac{\alpha_1 - \alpha_2}{n_B}$, quantifying the percentage of vertices that are neither contained into the LA, nor in any of the atoms in $\mathcal{A}_{LA}$. We reported as $\Delta_2 = R_{LA} - \Delta_1$ the fraction of vertices in some atom of $\mathcal{A}_{LA}$, hence those that are *directly* separated from the LA.

Our results put in evidence that most of the vertices are either contained in the LA, or in some other atom intersecting the LA. Other vertices comprise around 2.88% and 7.03% of the overall vertices. Moreover, as shown with Figure 17b, where we plotted the percentage of separated vertices as a function of the size of clique-separators, smaller clique-separators of size ≤ 5 are responsible for a significant part (w.r.t. Δ_2) of the vertices disconnected from the LA in `ca-CondMat` (37.34% of vertices over 49.22%), whereas in `ca-AstroPh` they solely disconnect 23.67% over 39.98% of vertices. This difference is not balanced with clique-separators of larger size, even though these ones disconnect 13.43% of vertices in `ca-AstroPh`, while only 5.67% in `ca-CondMat`. Comparing `ca-CondMat` with `ca-HepPh` does not change the picture. In contrast, for the graphs `ca-GrQc` and ca-HepTh, we notice that 6.71% and 4.91% more vertices, respectively, than in CondMat, are disconnected by edge-separators. But the rest of the clique-separators only disconnect 16.67% and 11.70% of the vertices from the LA, respectively, whereas 26.70% of them are separated from the LA in ca-CondMat. Therefore, most of the difference for the final size of the substitute graph LS comes from the number of vertices that are disconnected by clique-separators of *small* size.

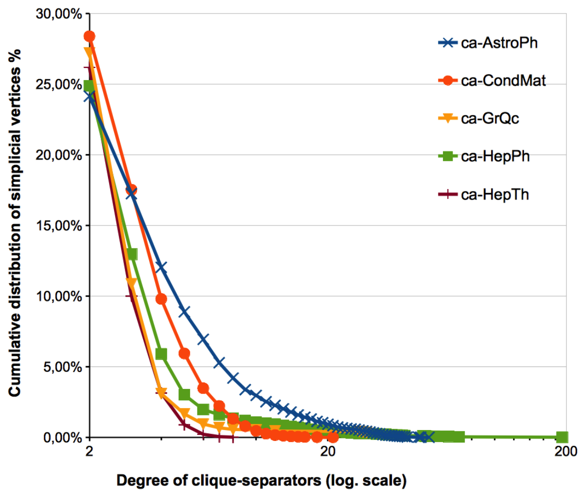
Instance name	α_1	α_2	$\lvert\mathcal{X}_{LA}\rvert$	$R_{\mathcal{X}_{LA}}$	Δ_1%	Δ_2%
ca-CondMat	8 483	7 413	4 702	0.54	6.21%	43.01%
ca-GrQc	1 265	1 079	698	0.5	7.03%	40.69%
ca-HepPh	4 100	3 727	2 166	0.44	4.13%	41.3%
ca-AstroPh	6 368	5 910	3 715	0.39	2.88%	37.1%
ca-HepTh	2 206	1 942	1 506	0.41	4.47%	32.93%

Table 2: Distribution of clique-minimal separators, and of the vertices disconnected from the LA. The total number of vertices separated from the LA in the LBC is given as $\alpha_1 = n_B - n_{LA}$, and the number of disconnected vertices being present in the subset of neighboring atoms $\mathcal{A}_{LA}$ as $\alpha_2 = |V(\mathcal{A}_{LA} \setminus \mathcal{X}_{LA})|$.
Also, the number of clique-minimal separators in the LA is given as $|\mathcal{X}_{LA}|$.
We quantify the percentage of vertices that are neither contained into the LA nor in any of the atoms in $\mathcal{A}_{LA}$ as $\Delta_1 = \frac{\alpha_1 - \alpha_2}{n_B}$; the fraction of vertices in some atom of $\mathcal{A}_{LA}$ that are *directly* separated from the LA is equal to $\Delta_2 = R_{LA} - \Delta_1$.

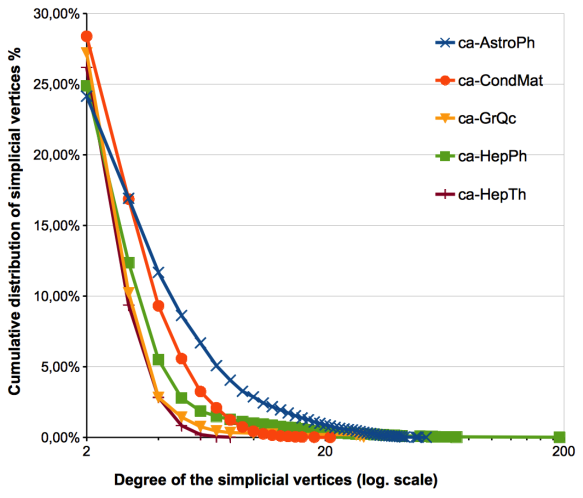
Substitute construction Recall that we assume that the largest number of simplicial vertices are connected to the smallest clique-separators. In order to validate the assumption, we plotted in Figure 18a the cumulative number of simplicial vertices connected to the LA, normalized by the size of the LBC, as a function of the size of the clique-separators. In particular, note that for each graph, such a summation is equal to the value given as Cost in Table 1. By looking only at clique-separators of size two and three, the proportions of simplicial vertices for the graphs ca-CondMat, ca-GrQc, ca-HepPh, ca-AstroPh and ca-HepTh respectively, represent 65.49%, 88.63%, 76.26%, 50.16% and 88.02% respectively, of the total number of simplicial vertices connected to the LA. Thus it highlights the importance of clique-separators of small size, to which a large proportion of simplicial vertices are connected to.

Let us also remark by comparing Figure 18a to Figure 18b that almost all simplicial vertices have *same degree*. In the worst case (ca-GrQc), there are no more than 0.75% of the simplicial vertices whose degree differs from the others. Most of these simplicial vertices have degree two. Hence, the final proportion of simplicial vertices, given in Table 1 as Cost, mostly depends on the size distribution of the clique-separators in the graphs. Also, since there is a worst-case variation of only 4.25% in the proportion of simplicial vertices in our graphs – that is reached with ca-CondMat and ca-AstroPh –, that allows us to make relative comparisons between the graphs from the dataset. Especially we are interested in comparing the proportion of simplicial vertices of small degree (less than four). Such a proportion represents, for ca-CondMat, ca-GrQc, ca-HepPh, ca-AstroPh and ca-HepTh respectively, a percentage of 18.59%, 24.1%, 18.97%, 12.11% and 23.04% respectively, of the simplicial vertices in total. To sum up:

- when comparing ca-AstroPh to ca-CondMat: even if the former has 2.23% more simplicial vertices with degree at least three, this is compensated by its 6.48% less simplicial vertices of



(a) Simplicial vertices connected to the LA as a function of the size of the clique-separators



(b) Degree distribution of the simplicial vertices connected to the LA

Figure 18: Cumulative number of simplicial vertices connected to the LA normalized by the size of the LBC as a function of the size of the clique-separators to which they are connected (Figure 18a), cumulative degree distribution of the simplicial vertices connected to the LA normalized by the size of the LBC (Figure 18b)

degree at most four, which results in overall to 4.25% less simplicial vertices in `ca-AstroPh` than in `ca-CondMat`. The same happens when comparing `ca-AstroPh` to the remaining graphs. Indeed, the lower number of simplicial vertices with degree at most four *always* compensates its larger number of simplicial vertices of higher degree.

- when comparing `ca-CondMat` to `ca-GrQc` and `ca-HepTh`: the two latter graphs respectively have 5.51% and 4.45% more simplicial vertices with degree at most four. However, they respectively have 6.7% and 6.66% less simplicial vertices with degree at least three. As a result, there are 1.19% less simplicial vertices in `ca-GrQc`, and 2.21% less simplicial vertices in `ca-HepTh`, respectively, than in `ca-CondMat`.

- finally, when comparing `ca-CondMat` to `ca-HepPh`: we observe quite similar numbers of simplicial vertices of degree smaller than four. They respectively represent 18.59% and 18.97% of the simplicial vertices in total. Again, the main difference comes from the proportion of simplicial vertices with degree higher than three, with 5.91% more simplicial vertices in `ca-CondMat` than in `ca-HepPh`, resulting in 3.51% less vertices in `ca-HepPh`.

7.4 Computation times

In order to complete the empirical section, we present in Table 3 the computation times of the hyperbolicity on the LS and on the LBC of the `ca-*` graphs. Of course, we expect the computation time to decrease proportionally to the size of the graphs. However, we use the algorithm that we proposed in [21] for computing the hyperbolicity, and so, the computation time may be impacted by other factors.

On the way, we also give in Table 3 the values of the hyperbolicity we obtained and the computation time of the LS using the algorithm given in Section 5. Interestingly, for all graphs from the dataset, the hyperbolicity of the graph always equals the hyperbolicity of its largest atom.

Instance name	n	n_B	n_{LA}	n_{LS}	δ	T_{LS}	$T_{\delta_{LS}}$	$T_{\delta_{LBC}}$	$R1$	$R2$
`ca-GrQc`	5 242	2 651	1 386	2 107	3.5	6s.	1s.	8.8s.	8.8	1.26
`ca-HepTh`	9 877	5 898	3 692	5 236	4	52s.	0.3s.	2.4s.	8	0.046
`ca-HepPh`	12 008	9 025	4 925	7 170	3	162s.	50s.	677s.	13.5	3.19
`ca-AstroPh`	18 772	15 929	9 561	13 407	3	762s.	22s.	202s.	9.2	0.26
`ca-CondMat`	23 133	17 234	8 751	13 643	3.5	1180s.	101s.	2498s.	24.7	1.95

Table 3: Hyperbolicity and computation times on the `ca-*` graphs. The size of the graph is given as n, the size of the LBC as n_b, the size of the LA as n_{LA} and the size of the LS as n_{LS}. The value of the hyperbolicity computed on the LS is given as δ. The computation time in second of the largest substitute is given as T_{LS}. The computation times in second of the hyperbolicity, on the LS and on the LBC respectively, is given as $T_{\delta_{LS}}$ and $T_{\delta_{LBC}}$ respectively. Finally, the ratio $T_{\delta_{LS}}/T_{\delta_{LBC}}$ is given as $R1$ and $(T_{LS} + T_{\delta_{LS}})/T_{\delta_{LBC}}$ is given as $R2$.

We observe that the hyperbolicity can be computed from 8 to 24 times faster on the LS than on the LBC. However, computing the hyperbolicity on the LS also comes at the cost of the time to construct this graph. By combining the two, one improves the time of computation by a smaller factor between 1.26 and 3.19 (for the graphs `ca-GrQC`, `ca-HepPh` and `ca-CondMat`). In some cases (`ca-AstroPh` and `ca-HepTh`), our method even increases the time of computation. However, these cases happen only for small graphs where the hyperbolicity can be computed in a few seconds. For larger graphs, up to 50 000 nodes, we have been able to reduce the times by two, saving from hours to days of computation.

8 Conclusion

We proved a tight relationship between the hyperbolicity of a given graph and the maximum hyperbolicity from its atoms. This gives a new proof that chordal graphs (and other related graph classes such as 2-chordal graphs [46, 47], nearly chordal graphs [15] or quasi-triangulated graph [52]) have a bounded hyperbolicity [16]. Our results also cover some class with unbounded hyperbolicity, namely the outerplanar graphs, for which we give a complete characterization of their hyperbolicity. This extends to a linear-time algorithm for computing the hyperbolicity of these graphs. To the best of our knowledge, this is the first linear-time algorithm for computing the hyperbolicity in these graphs. We let open whether the same can be done for other classes of graphs. Especially, can it be taken advantage of the linear-time algorithm for outerplanar graphs in order to compute the hyperbolicity of planar graphs more efficiently ?

Furthermore, we deduced from our proofs a general substitution method, allowing us to modify the atoms at no extra-cost than the clique-decomposition. For graphs with hyperbolicity at least one, the maximum hyperbolicity from the resulting graphs is exactly the hyperbolicity of the graphs. However, the graphs to be considered may have a larger size than the atoms. Experiments suggest that the final size of the substitute graphs is mostly related with the number of clique-separators of small size, and the disconnections resulting from them. Part of our future work will consist in finding other graph decompositions which are applicable to the computation of the hyperbolicity.

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Appendix C

On the recognition of C_4-free and $1/2$-hyperbolic graphs

RECOGNITION OF C_4-FREE AND 1/2-HYPERBOLIC GRAPHS[*]

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Abstract. The shortest-path metric d of a connected graph G is 1/2-*hyperbolic* if, and only if, it satisfies $\mathrm{d}(u,v)+\mathrm{d}(x,y) \leq \max\{\mathrm{d}(u,x)+\mathrm{d}(v,y), \mathrm{d}(u,y)+\mathrm{d}(v,x)\}+1$, for every 4-tuple u,x,v,y of G. We show that the problem of deciding whether an unweighted graph is 1/2-hyperbolic is *subcubic equivalent* to the problem of determining whether there is a chordless cycle of length 4 in a graph. An improved algorithm is also given for both problems, taking advantage of fast rectangular matrix multiplication. In the worst case it runs in $O(n^{3.26})$-time.

Key words. Hyperbolicity, discrete metric space, graph algorithms, C4-free graphs, rectangular matrix multiplication

AMS subject classifications. 05C85, 65F30, 68Q17, 68Q25, 68R10

1. Introduction.

The primary aim of our work is to study hyperbolicity of simple unweighted graphs. This is a metric parameter, that was first introduced by Gromov in the context of automatic groups (see [23]), then extended to more general metric spaces [5]. Roughly, the hyperbolicity of a connected graph is a measure of how far is the shortest-path metric of the graph from a *tree metric*. One can deduce from this parameter tight bounds for the (worst) additive distortion of the distances in the graph when its vertices are embedded into a weighted tree [10]. Practical applications of hyperbolicity were proposed in the domains of routing [6], network security [27], bioinformatics [18], and in the spread of information in social networks [4].

So far, the best known algorithm for determining the hyperbolicity of a graph has an $O(n^{3.69})$-time complexity [21]. This is however prohibitive for graphs with tens of thousands of nodes such as the graph of the Autonomous Systems of the Internet, road maps, etc. An algorithm with good practical performances has been proposed in [11]. It improves the worst-case running time on certain graph classes, but it cannot be used on graphs with hyperbolicity less than one.

Related work. Our work focuses on a decision version of the problem, namely the recognition of graphs with hyperbolicity (at most) 1/2. Graphs with small hyperbolicity value have already received some attention, as a first characterization of 1/2-hyperbolic graphs was proposed in [1]. However, to the best of our knowledge, there was no known algorithmic application to it prior to this work. We are more interested in a reduction such as the recent one in [21], where the authors proved an equivalence between the problems of finding a 2-approximation for the hyperbolicity and the $(\max, \min)$-matrix multiplication. A recent work [19] further exploits the relation between both problems, yielding constant-factor approximations for the hyperbolicity in subcubic-time. We point out that a similar line of research was followed in [34, 39], where they determined the subcubic equivalence between various combinatorial problems.

Our contribution. We relate the recognition of graphs with hyperbolicity (at most) 1/2 to the search of (induced) cycles of length 4, *e.g.* C_4, in a graph. It

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actually follows from our work that either both problems are solvable in subcubic-time, or none of them is. We first present a linear-time reduction from the C_4-free graph recognition problem to the recognition of 1/2-hyperbolic graphs (§3.1). Then we prove a new characterization of 1/2-hyperbolic graphs, which is based on graph powers [30], and from which it follows that, conversely, deciding whether a graph is 1/2-hyperbolic can be reduced in subcubic-time to the C_4-free graph recognition problem (§3.2). In §4, we finally reduce both problems to the problem of the rectangular matrix product that was defined in [31]. This allows us to solve both of them in $O(n^{3.26})$-time, which beats the previous records established in [21, 37].

We give the notations used in this paper in §2, along with definitions for graph hyperbolicity and C_4-free graphs.

2. Definitions and Notations. A graph G is a pair (V, E), whose n *vertices* are the elements of the set V, and whose m *edges* are the elements of E; every edge is a set of two distinct vertices of G. The *neighborhood* $N(u)$ of a vertex $u \in V$, is the (possibly empty) set of vertices $v \in V$ such that $\{u, v\}$ is an edge. Alternatively, we say that the elements of $N(u)$ are *adjacent* to u. A *clique* is a set of pairwise adjacent vertices. Note that the adjacency relation is clearly symmetric; we also define the (symmetric) adjacency matrix $A = (\mathbb{I}_{\{u \in N(v)\}})_{u,v \in V}$, where $\mathbb{I}$ denotes the Kronecker delta[1].

Finally, an *induced subgraph* of G is a graph $G[X] = (X, F)$ such that $X \subseteq V$ and $F = \{\{u, v\} \in E : u, v \in X\}$. In particular if X is a clique, then it is called a *complete* subgraph. The induced subgraph is a *path of length* $l \geq 0$ if $|X| = l + 1$ and the vertices of X can be linearly ordered into a sequence $(v_0, v_1, \dots, v_l)$ such that for every $0 \leq i, j \leq l$, the vertex v_i is adjacent to v_j if, and only if, $|j - i| = 1$. In such a case, the vertices v_0 and v_l are called the *endpoints* of the path, and the path is a v_0v_l-path. The graph G is *connected* if, for every pair $u, v \in V$, there exists a uv-path. Also, a cycle is a graph such that the deletion of any edge $\{v_0, v_l\} \in F$ yields a v_0v_l-path, and a tree is a connected graph which does not contain any cycle as a subgraph.

Further standard graph terminology can be found in [7, 14].

2.1. 1/2-hyperbolic graphs. Given a connected graph $G = (V, E)$, we define the distance $\mathrm{d}_G(u, v)$ between two vertices $u, v \in V$ as the minimum length of a uv-path in the graph. This yields a (discrete) metric space (V, d_G). For a survey of metric graph theory, the reader may refer to [2]. We define in the space (V, d_G) an interval $[u, v]$ between any two vertices $u, v \in V$, as the set of vertices "in between" u and v, *e.g.* $[u, v] = \{x \in V : \mathrm{d}_G(u, v) = \mathrm{d}_G(u, x) + \mathrm{d}_G(x, v)\}$.

In the sequel, we will call a uv-path of minimum length a *uv-shortest path*, and we will denote the distance function by d instead of d_G whenever G is clear from the context. The graph hyperbolicity of G can now be defined as follows:

DEFINITION 2.1 (**4-points Condition, [23]**). *Let G be a connected graph. For every 4-tuple u, x, v, y of G, we define $\delta(u, v, x, y)$ as half of the difference between the two largest sums amongst*

$S_1 = \mathrm{d}(u, v) + \mathrm{d}(x, y)$,

$S_2 = \mathrm{d}(u, x) + \mathrm{d}(v, y)$, *and*

$S_3 = \mathrm{d}(u, y) + \mathrm{d}(v, x)$.

The graph hyperbolicity, denoted by $\delta(G)$, is equal to $\max_{u,x,v,y} \delta(u, v, x, y)$.

[1]We use the symbol $\mathbb{I}$ instead of the classical symbol δ for the Kronecker delta in order to prevent confusion with hyperbolicity.

Moreover, we say that G is δ-hyperbolic*, for every $\delta \geq \delta(G)$.*

Unlike many well-known graph properties, it is very important to note that the hyperbolicity of an *induced subgraph* of G does not yield any information in general about the hyperbolicity of G. For example, the wheel W_n is 1-hyperbolic, whereas it contains as an induced subgraph the cycle C_n whose hyperbolicity grows linearly with n [11]. A way to deal with this difficulty is to constrain ourselves to distance-preserving, or *isometric* subgraphs. Formally, an induced subgraph H of G is isometric if, and only if, it is connected and for every pair of vertices $u, v \in H$, we have that $\mathrm{d}_H(u,v) = \mathrm{d}_G(u,v)$. We also say that a subgraph which is not isometric is a *bridged* subgraph.

Lower and upper bounds on the hyperbolicity can be deduced from classical parameters such as the girth [33], the circumference [8], the domination number [35], and the chordality [29, 40]. In particular, we have that $\delta(G) \leq \lfloor diam(G)/2 \rfloor$, where $diam(G) = \max_{u,v \in V} \mathrm{d}_G(u,v)$ is the *diameter* of the graph [11, 40].

We inform the reader that Definition 2.1 is not a universal definition for the hyperbolicity of a graph. Some authors actually proposed and studied other definitions (see, for instance [13, 23]). Though the value of $\delta(G)$ may vary depending on the choice of the definition, any δ-hyperbolic graph with respect to (w.r.t.) any of the definitions is $f(\delta)$-hyperbolic w.r.t. any other definition of the hyperbolicity. The function f is linear in δ in most cases. Moreover, the class of trees is always contained into the class of 0-hyperbolic graphs, which makes the graph hyperbolicity a tree-likeness parameter.

We here restrict our study to Definition 2.1, as it has algorithmic applications. Indeed, it is straightforward by using Definition 2.1 to compute the graph hyperbolicity $\delta(G)$ in $\Theta(n^4)$-time (see [11] and [21] for practical and theoretical improvements of the complexity). Also, note that $\delta(G)$ is always a half-integer (w.r.t. Definition 2.1). Our work focuses on graphs with small hyperbolicity, that is hyperbolicity at most 1/2. Those graphs thus satisfy either $\delta(G) = 0$ or $\delta(G) = 1/2$. We address the problem of recognizing those graphs, that we formulate as follows.

PROBLEM 2.2. *Given a connected graph G, is G a 1/2-hyperbolic graph ?*

In [1], Bandelt and Chepoi characterized the 1/2-hyperbolic graphs as the connected graphs that simultaneously satisfy the three following conditions:

CONDITION 2.3. *Every cycle of length at least* 6 *in G is bridged.*

CONDITION 2.4. *For every pair $u, v \in G$, $N(u) \cap [u,v]$ is a clique.*

CONDITION 2.5. *No graph in Figure 1 is an isometric subgraph of G.*

A simpler characterization was previously given for 0-hyperbolic graphs [3, 24]. In fact, 0-hyperbolic graphs are *block-graphs*, that are graphs in which every biconnected component (block) is a clique (possibly reduced to a single vertex). This class includes cliques and trees, and a block-graph can be recognized in $O(n+m)$-time.

2.2. C_4-free graphs. The C_4-free graph recognition problem asks whether a given graph G contains an induced cycle of length 4. In the sequel, such a cycle, if any, is called a C_4, or a *quadrangle*. A graph G which does not contain any C_4 as an induced subgraph is a *C_4-free* graph. Let us define our decision problem in the following way.

PROBLEM 2.6. *Given a graph G, does G contain a C_4 as an induced subgraph ?*

We now remind a well-known, local characterization of those graphs:

FACT 2.7. *A graph $G = (V,E)$ is C_4-free if, and only if, for every pair of non-adjacent vertices u, v, the set $N(u) \cap N(v)$ is a (possibly empty) clique.*

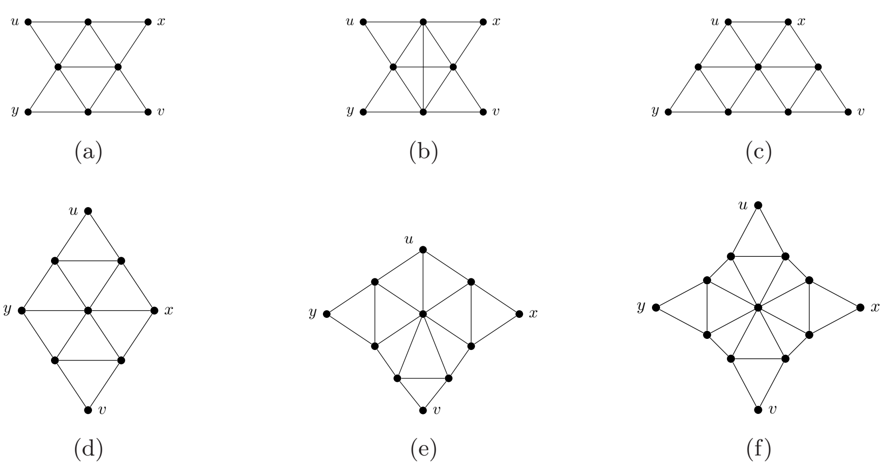


Figure 1: The six forbidden isometric subgraphs.

To see the relation between Problem 2.6 and Problem 2.2, one can observe that the condition of Fact 2.7 is equivalent to Condition 2.4 when considering vertices u, v at distance 2. As a consequence, every 1/2-hyperbolic graph is also C_4-free. In fact, a more direct way to see this is to note that every induced subgraph which is a quadrangle is *isometric* (this comes from the fact that a C_4 is connected and it has diameter 2). Since one can easily check that $\delta(C_4) = 1$, then it indeed follows that a 1/2-hyperbolic graph cannot contain a quadrangle as an induced subgraph.

So far, the best-known algorithm we are aware of to detect an induced C_4 in a graph has $O(n^{\omega(1)+1}) = O(n^{3.3727})$-time complexity [37], with $O(n^{\omega(1)})$ being the complexity of multiplying two $n \times n$ matrices (see §4.1 for details). We will improve this result in §4.

3. The subcubic equivalence. It is straightforward by the definitions that both the 1/2-hyperbolic graph recognition problem (Problem 2.2), and the C_4-free graph recognition problem (Problem 2.6), are polynomial-time solvable [21, 37]. On the other hand, the best-known upper-bound on their time complexity is strictly more than cubic. Thus it motivates the search for *subcubic reductions* between these problems, as they are defined in [39]. Formally, a subcubic reduction from a problem A to a problem B is a subcubic-time Turing reduction, which verifies the following additional properties on the oracle access to problem B. For every positive real μ, there has to exist a positive real ε such that:

(i) the reduction runs in $\tilde{O}(n^{3-\varepsilon})$-time[2], where n denotes the size of the input;

(ii) and given an instance of size n of problem A, $\sum_i \tilde{O}(n_i^{3-\mu}) = \tilde{O}(n^{3-\varepsilon})$, where n_i denotes the size of the i^{th} oracle call to problem B in the reduction.

In particular, a linear-time reduction is a subcubic reduction. More generally, any subcubic-time reduction which satisfies $\sum_i n_i = \tilde{O}(n)$ is also a subcubic reduction. We will only consider subcubic reductions of this kind in the sequel.

[2]The notation $\tilde{O}(f(n))$ is for a complexity $f(n) \cdot \log^{O(1)} n$.

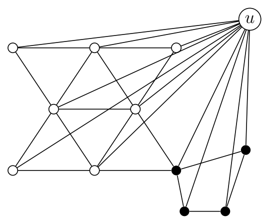


Figure 2: An illustration of the linear-time reduction of Proposition 3.1.

Subcubic reductions are of specific interest in the study of subcubic-time algorithms, because if there exists a subcubic reduction from problem A to problem B, and there is a subcubic-time algorithm which solves problem B, then there also exists a subcubic-time algorithm which solves problem A. In particular, if problems A and B are *subcubic equivalent*, then either both of them are solvable in subcubic-time, or none of them is. In this section, we will show that Problem 2.2 and Problem 2.6 are subcubic equivalent. We first present a linear-time reduction from Problem 2.6 to Problem 2.2 in §3.1 (Proposition 3.1). Then we present a subcubic reduction from Problem 2.2 to Problem 2.6 in §3.2 (Theorem 3.13).

3.1. Reducing the detection of a C_4 to the recognition of a 1/2-hyperbolic graph. PROPOSITION 3.1. *There is a linear-time reduction from the C_4-free graph recognition problem to the problem of deciding whether a graph is 1/2-hyperbolic.*

Proof. Let $G = (V, E)$ be an instance of the C_4-free graph recognition problem. Let $u \notin V$, and let $G' = (V \cup \{u\}, E \cup \{\{u, v\} : v \in V\})$. By construction, G' is connected, and it has diameter at most 2. Thus, we have that $\delta(G') \leq 1$ (*e.g.* see [11]), and all of its isometric subgraphs also have diameter at most 2. Moreover we remind that a cycle of length l has diameter $\lfloor l/2 \rfloor$. In particular, every cycle of length at least 6 is a graph of diameter at least 3 and as such, it cannot be an isometric cycle of G'. Consequently, G' always satisfies Condition 2.3. We can prove that it always satisfies Condition 2.5 in the same way. Finally, since Condition 2.4 is satisfied for every pair $u, v \in V$ of *adjacent* vertices, then G' satisfies Condition 2.4 if, and only if, for every pair $u, v \in V$ of *non-adjacent* vertices, we have that $N_{G'}(u) \cap [u, v]$ is a clique; since $d_{G'}(u, v) = 2$ in such a case, then it is equivalent to have that $N_{G'}(u) \cap N_{G'}(v)$ is a clique, *e.g.* the graph G' is C_4-free by Fact 2.7. Furthermore, we have by construction that any induced C_4 in G' is an induced quadrangle in G, and vice-versa. Consequently, G is C_4-free if, and only if, the graph G' is 1/2-hyperbolic. □

We want to highlight that our reduction from Problem 2.6 to Problem 2.2 here is linear-time, whereas the converse reduction from Problem 2.2 to Problem 2.6, presented in §3.2, is super-linear. It might be of interest to determine whether a linear-time reduction from Problem 2.2 to Problem 2.6 exists.

3.2. Finding quadrangles to recognize non-1/2-hyperbolic graphs. Our aim is now to prove that there exists a subcubic reduction from Problem 2.2 to Problem 2.6 (Theorem 3.13). Ideally, we would ask for a subcubic-time routine for checking whether Conditions 2.3, 2.4 and 2.5 are satisfied. Our reduction is however more complex, as we actually introduce and verify different conditions in subsequent sections. Thus we have to prove that these conditions imply Conditions 2.3, 2.4 and 2.5, and also that they are satisfied by 1/2-hyperbolic graphs.

3.2.1. Quickly excluding long isometric cycles. Let us first deal for our reduction with a tool that we will use later to verify whether Condition 2.3 is satisfied. We recall that Condition 2.3 requires that every cycle of length at least 6 in G is a bridged subgraph. A first naive approach to deal with this condition is to compute the length of a longest isometric cycle of G. This can be done in polynomial-time, but the best-known algorithm runs in $O(n^{2\omega(1)} \log n) = O(n^{4.752} \log n)$-time, which is super-cubic [32]. Instead, we propose in this section a way to weaken Condition 2.3, by only having to consider isometric cycles of *polylogarithmically-bounded* length.

Given a connected graph G, we recall that a c-factor approximation of the hyperbolicity of G is a half-integer $\delta_c(G)$ such that $\delta(G) \leq \delta_c(G) \leq c.\delta(G)$. In this section, we will assume we have a subcubic-time algorithm computing a c-factor approximation of the hyperbolicity, for some fixed choice of $c = \log^{O(1)} n$. Below, we remind possible ways to achieve such a result:

LEMMA 3.2 ([9, 19, 21]). *Let $G = (V, E)$ be a connected graph.*

(i) *There exists an algorithm computing a 2-factor approximation of the hyperbolicity in $O(n^{3-\omega(1)/2}) = O(n^{2.69})$-time [21].*

(ii) *For every $\varepsilon > 0$, there exists an algorithm computing a $(2+\varepsilon)$-factor approximation of the hyperbolicity in $\tilde{O}(\varepsilon^{-1}n^{\omega(1)}) = \tilde{O}(\varepsilon^{-1}n^{2.3727})$-time [19].*

(iii) *There exists an algorithm computing a 1569-factor approximation of the hyperbolicity in $O(\min\{nm, n^{\omega(1)} \log n\} + n^2) = \tilde{O}(n^{2.3727})$-time*[3] *[9].*

Combining results from [10, 15, 21], there also exists a $\theta(\log n)$-factor approximation algorithm of the hyperbolicity in $\tilde{O}(n^2)$-time[4]. In addition, one can deduce from the results from [16, 17, 22] an algorithm which computes a $\theta(\log^2 n)$-factor approximation of the hyperbolicity in $O(m \log n)$-time.

It is well-known that the hyperbolicity of the cycle C_n grows linearly with n. Formally:

LEMMA 3.3 ([11, 40]). *Cycles of order $4p + \varepsilon \geq 3$, with $p \geq 0$ and $\varepsilon \in \{0, 1, 2, 3\}$, are $(p - 1/2)$-hyperbolic when $\varepsilon = 1$, and p-hyperbolic otherwise.*

As a result, it follows from Lemma 3.3 that a (polylogarithmic) upper-bound on the hyperbolicity of G yields a (polylogarithmic) upper-bound on the length of a longest isometric cycle of G; more accurately:

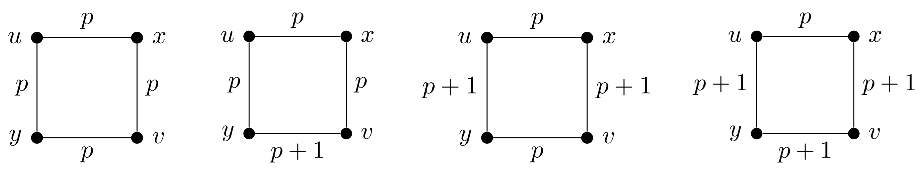
COROLLARY 3.4. *Let $G = (V, E)$ be a connected graph. Then all the isometric cycles of G have length upper-bounded by $4\delta(G) + 3$.*

Proof. First assume $\delta(G)$ is an integer. By Lemma 3.3, the longest $\delta(G)$-hyperbolic cycle has length at most $4\delta(G) + 3$. Otherwise, $\delta(G)$ is a half-integer by Definition 2.1 and so, again by Lemma 3.3, the longest $\delta(G)$-hyperbolic cycle has length at most $4(\delta(G) + 1/2) + 1 = 4\delta(G) + 3$. □

Since we are interested in 1/2-hyperbolic graphs, then Corollary 3.4 implies that every isometric cycle must have length upper-bounded by 5 *i.e.*, Condition 2.3. We introduce in the next section a second tool so that we can detect isometric cycles of polylogarithmically-bounded length.

[3]The term $\min\{nm, n^{\omega(1)} \log n\}$ in the complexity comes from the computation of the all-pairs shortest-paths in the graph (see [36] for an algorithm in $\tilde{O}(n^{\omega(1)})$-time for the problem).

[4]The authors in [21] actually claim a $O(n^2)$-time complexity for their algorithm, but it takes as inputs discrete metric spaces and so, it does not apply to graphs directly. To apply their results on graphs, we can use a $\theta(\log n)$-additive approximation of the all-pairs shortest-paths, which can be computed in $\tilde{O}(n^2)$-time (see [15]).



(a) $l = 4p$ (b) $l = 4p + 1$ (c) $l = 4p + 2$ (d) $l = 4p + 3$

Figure 3: Shrinking long isometric cycles into quadrangles.

3.2.2. Using graph powers. Let us now present the main tool for our reduction, namely graph powers.

Definition 3.5. *Given a connected graph $G = (V, E)$, let i be a positive integer. The i^{th}-*power *of G, denoted by $G^i = (V, E_i)$, is a graph whose set of vertices is the same as for G; two vertices $u, v \in V$ are adjacent in G^i if, and only if, there exists a uv-path of length at most i in G. Formally, $E_i = \{\{u, v\} : 0 < \mathrm{d}_G(u, v) \leq i\}$.*

In particular, the graph power G^1 is G, and the graph power $G^{diam(G)}$ is the complete graph K_n, where $diam(G) = \max_{u,v \in V} \mathrm{d}(u, v)$ is the diameter of G. It is folklore that the graph power G^i can be computed in $O(n^{\omega(1)} \log i)$-time, using fast square matrix multiplication [36].

Recall that we said in §2.2 that every 1/2-hyperbolic graph G is C_4-free. Roughly, most of our reduction will consist in checking whether a *polylogarithmic* number of graph powers of G are C_4-free as well. This is a necessary condition so that G is 1/2-hyperbolic, as stated below.

Lemma 3.6. *If G is a 1/2-hyperbolic graph, then for every positive integer i, the graph G^i is C_4-free.*

Proof. By contradiction, let u, v, x, y be the vertices of an induced quadrangle in G^i, for some positive integer $i \geq 1$. Without loss of generality, assume that $x, y \in N_{G^i}(u) \cap N_{G^i}(v)$. It follows by Definition 3.5 that:

$$\max\{\mathrm{d}_G(u, x), \mathrm{d}_G(u, y), \mathrm{d}_G(v, x), \mathrm{d}_G(v, y)\} \leq i;$$
$$\text{and} \qquad \min\{\mathrm{d}_G(u, v), \mathrm{d}_G(x, y)\} \geq i + 1.$$

As a consequence, we have by Definition 2.1 that:

$$\begin{aligned}\delta(u, v, x, y) &= \frac{1}{2}[(\mathrm{d}_G(u, v) + \mathrm{d}_G(x, y)) \\ &\qquad - \max\{\mathrm{d}_G(u, x) + \mathrm{d}_G(v, y), \mathrm{d}_G(u, y) + \mathrm{d}_G(v, x)\}] \\ &\geq \frac{1}{2}[2(i + 1) - 2i] \\ &\geq 1\end{aligned}$$

which contradicts the fact that G is 1/2-hyperbolic. □

Intuitively, the existence of isometric cycles of length l in G yields the existence of induced quadrangles in some graph power $G^{\theta(l)}$; this shrinking effect is illustrated with Figure 3. As a result, it may be more efficient to search for induced cycles of length 4 in the graph powers rather than computing the length of a longest isometric cycle of G directly.

We emphasize that the converse does not hold: not all the induced quadrangles in G^i yield an isometric cycle in the original graph G. For instance, the square graph H_1^2 of the graph H_1 in Figure 1a contains a quadrangle as an induced subgraph (the vertices of which are u, x, v, y), yet H_1 does not contain an isometric cycle of length more than 3. However, we remind that every graph power has to be C_4-free by Lemma 3.6 and so, *any* induced quadrangle that we detect in some graph power is a certificate to prove that the graph is not 1/2-hyperbolic.

We formalize it as follows.

LEMMA 3.7. *Let $G = (V, E)$ be a connected graph, and let C_l be an isometric cycle of length $l = 4p + \varepsilon$, $p \geq 1$, $\varepsilon \in \{0, 1, 2, 3\}$ and $l \neq 5$. There is an integer $i \in [p, 2p]$ such that the graph power G^i contains a C_4 as an induced subgraph.*

Proof. Let us fix an arbitrary orientation for C_l, and choose a 4-tuple u, x, v, y (in clockwise order) such that:

(i) if $\varepsilon = 0$: $\mathrm{d}_G(u, x) = \mathrm{d}_G(u, y) = \mathrm{d}_G(v, x) = \mathrm{d}_G(u, y) = p$;
(ii) if $\varepsilon = 1$: $\mathrm{d}_G(u, x) = \mathrm{d}_G(u, y) = \mathrm{d}_G(v, x) = p$, and $\mathrm{d}_G(v, y) = p + 1$;
(iii) if $\varepsilon = 2$: $\mathrm{d}_G(u, x) = \mathrm{d}_G(v, y) = p$, and $\mathrm{d}_G(u, y) = \mathrm{d}_G(v, x) = p + 1$;
(iv) if $\varepsilon = 3$: $\mathrm{d}_G(u, x) = \mathrm{d}_G(u, y) = \mathrm{d}_G(v, x) = p + 1$, and $\mathrm{d}_G(v, y) = p$.

An example of such a choice is given in Figure 3. Note that all the above distances are upper-bounded by $p + \lceil \varepsilon/4 \rceil$. Furthermore, recall that C_l is an isometric cycle by the hypothesis. So, we have:

$$\mathrm{d}_G(u, v) = \mathrm{d}_G(x, y) = \begin{cases} 2p & \text{when } \varepsilon \in \{0, 1\} \\ 2p + 1 & \text{when } \varepsilon \in \{2, 3\} \end{cases}$$

Equivalently, we have $\mathrm{d}_G(u, v) = \mathrm{d}_G(x, y) = 2p + \lfloor \varepsilon/2 \rfloor$. As a consequence, by Definition 3.5, we have that $G^i[\{u, x, v, y\}]$ is an induced C_4, for every $p + \lceil \varepsilon/4 \rceil \leq i \leq 2p + \lfloor \varepsilon/2 \rfloor - 1$. To prove that such a value of i always exists, it now remains to prove that:

$$p + \left\lceil \frac{\varepsilon}{4} \right\rceil \leq 2p + \left\lfloor \frac{\varepsilon}{2} \right\rfloor - 1,$$

that is:

$$\left(2p + \left\lfloor \frac{\varepsilon}{2} \right\rfloor - 1\right) - \left(p + \left\lceil \frac{\varepsilon}{4} \right\rceil\right) = p + \left(\left\lfloor \frac{\varepsilon}{2} \right\rfloor - \left\lceil \frac{\varepsilon}{4} \right\rceil\right) - 1 \geq 0.$$

A straightforward calculation shows that:

$$\left\lfloor \frac{\varepsilon}{2} \right\rfloor - \left\lceil \frac{\varepsilon}{4} \right\rceil = \begin{cases} -1 & \text{if } \varepsilon = 1 \\ 0 & \text{otherwise} \end{cases}$$

As a consequence, if $\varepsilon \neq 1$ then we are done. Otherwise, since $l = 4p + 1 > 5$ by the hypothesis, then $p \geq 2$ and so:

$$p + \left(\left\lfloor \frac{\varepsilon}{2} \right\rfloor - \left\lceil \frac{\varepsilon}{4} \right\rceil\right) - 1 \geq 2 - 1 - 1 \geq 0. \qquad \square$$

Note that the only two possible lengths for an isometric cycle of the graph that Lemma 3.7 does not take into account are 3 and 5. This is not a coincidence, as C_3 and C_5 are the only cycles that are 1/2-hyperbolic by Lemma 3.3.

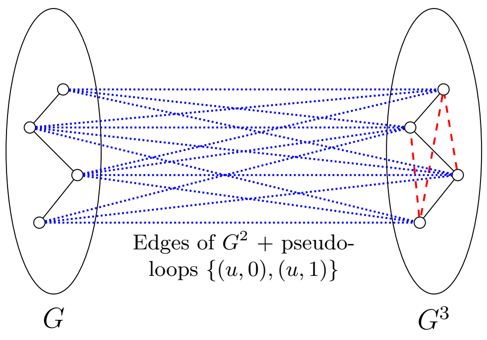


Figure 4: The construction of the graph $G^{[2]}$.

3.2.3. Transforming some obstructions into quadrangles. One of the most fundamental step for our reduction was to prove with Lemma 3.6 that every graph power G^i, $i \geq 1$, has to be C_4-free so that a connected graph G is 1/2-hyperbolic. An interesting question on its own is whether it is also a sufficient condition.

We give a negative answer to this conjecture, using the graph H in Figure 5. The graph H is the union of a C_5 and a C_3 that both share a single edge; using the 4-tuple in bold in Figure 5, one can verify that $\delta(H) \geq 1$. Clearly, H does not contain a quadrangle as an induced subgraph. Moreover, $diam(H) = 3$ and so, for every $i \geq 3$, the graph power H^i is a complete graph. Finally, as there is only one couple x, y of H such that $\mathrm{d}_H(x,y) = 3$, it follows that the square graph H^2 of H only lacks a single edge to be complete; as a result, H^2 is C_4-free as well.

The primary aim of this section is now to show that in order to complete our reduction, we solely need to decide whether only *one* additional graph is C_4-free:

Definition 3.8. *Let $G = (V,E)$ be a connected graph. The graph $G^{[2]} = (V^{[2]}, E^{[2]})$ is defined as follows:*

(i) $V^{[2]} \simeq V \times \{0,1\}$*;*
(ii) $G^{[2]}[V \times \{0\}] \simeq G$*;*
(iii) $G^{[2]}[V \times \{1\}] \simeq G^3$*;*
(iv) *$\forall u, v \in V$, the vertices $(u,0)$ and $(v,1)$ are adjacent in $G^{[2]}$ if, and only if,* $\mathrm{d}_G(u,v) \leq 2$.

In particular, $\forall u \in V$, there is an edge $\{(u,0),(u,1)\} \in E^{[2]}$.

An illustration of the construction of $G^{[2]}$ is presented in Figure 4. It might help to observe that for every edge of G^2 *i.e.*, for every two distinct vertices u, v such that $\mathrm{d}_G(u,v) \leq 2$, there are exactly two corresponding edges in $G^{[2]}$, denoted by $\{(u,0),(v,1)\}$ and $\{(u,1),(v,0)\}$, that connect the sets $V \times \{0\}$ and $V \times \{1\}$. Every other connecting edge of $G^{[2]}$ is a pseudo-loop $\{(u,0),(u,1)\}$, for some vertex $u \in V$.

We interpret the role of $G^{[2]}$ as the role of an "intermediate power" between the square graph G^2 and the cube graph G^3. First, let us prove that it is necessary for $G^{[2]}$ to be C_4-free so that G is 1/2-hyperbolic.

Lemma 3.9. *If G is a 1/2-hyperbolic graph, then the graph $G^{[2]}$ is C_4-free.*

Proof. By contradiction, let a, b, c, d be the vertices of an induced quadrangle in $G^{[2]}$. Without loss of generality, we assume that $\mathrm{d}_{G^{[2]}}(a,b) = \mathrm{d}_{G^{[2]}}(c,d) = 2$. Several cases have to be considered, that we illustrate with Figure 6.

If $a, b, c, d \in V \times \{0\}$, then there is an induced C_4 in G by Definition 3.8. Similarly,

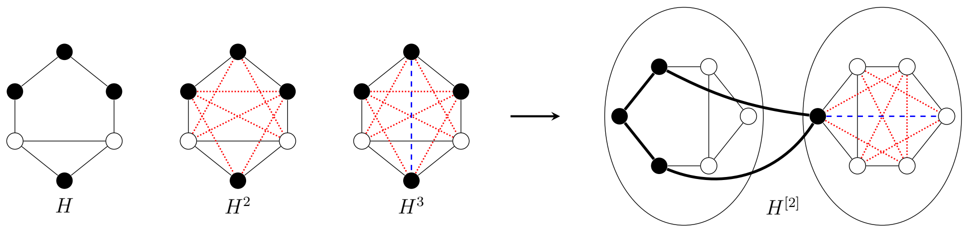


Figure 5: A 1-hyperbolic graph whose powers are C_4-free. A quadrangle in $H^{[2]}$ is drawn in bold.

if $a, b, c, d \in V \times \{1\}$, then there is an induced C_4 in G^3 by Definition 3.8. In both cases, this implies that G is *not* 1/2-hyperbolic, by Lemma 3.6.

For all the remaining cases, we claim that there is no vertex $u \in V$ such that $\{(u,0),(u,1)\} \subseteq \{a,b,c,d\}$. It easily follows from the fact that $N_{G^{[2]}}((u,0)) \cup \{(u,0)\} \subseteq N_{G^{[2]}}((u,1)) \cup \{(u,1)\}$. Thus we can write $(a,b,c,d) = ((u,k),(v,k'),(x,j),(y,j'))$, with $\{k,k',j,j'\} = \{0,1\}$ and vertices u, v, x, y are pairwise distinct.

Case 1: $k = 0$, $k' = j = j' = 1$. Here it comes that:

$$\max\{d_G(u,x) + d_G(v,y), d_G(u,y) + d_G(v,x)\} \leq 2 + 3 = 5,$$
$$\text{whereas} \qquad d_G(u,v) + d_G(x,y) \geq 3 + 4 = 7.$$

In other words, $\delta(G) \geq \delta(u,v,x,y) \geq 1$.

Case 2: $k = 1$, $k' = j = j' = 0$. In such a case:

$$\max\{d_G(u,x) + d_G(v,y), d_G(u,y) + d_G(v,x)\} \leq 2 + 1 = 3,$$
$$\text{whereas} \qquad d_G(u,v) + d_G(x,y) \geq 3 + 2 = 5.$$

So, $\delta(G) \geq \delta(u,v,x,y) \geq 1$.

Case 3: $k = k' = 0$, $j = j' = 1$. It follows that:

$$\max\{d_G(u,x) + d_G(v,y), d_G(u,y) + d_G(v,x)\} \leq 2 + 2 = 4,$$
$$\text{whereas} \qquad d_G(u,v) + d_G(x,y) \geq 2 + 4 = 6.$$

In other words, $\delta(G) \geq \delta(u,v,x,y) \geq 1$.

Case 4: $k = j = 0$, $k' = j' = 1$. Then we have:

$$\max\{d_G(u,x) + d_G(v,y), d_G(u,y) + d_G(v,x)\} \leq \max\{1+3, 2+2\} = 4,$$
$$\text{whereas} \qquad d_G(u,v) + d_G(x,y) \geq 3 + 3 = 6.$$

So, we again conclude that $\delta(G) \geq \delta(u,v,x,y) \geq 1$. □

Recall that in order to decide whether a graph is 1/2-hyperbolic, our aim is to check whether all of the three Conditions 2.3, 2.4 and 2.5 of [1] are satisfied, using stronger necessary conditions. So far, we only dealt with Condition 2.3, developing tools in §3.2.1 and 3.2.2 in order to determine if every cycle of length at least 6 in the graph is bridged. The following two lemmas will show a way to combine the graph $G^{[2]}$ of Definition 3.8 with the graph powers of Definition 3.5, in order to ensure that both Conditions 2.4 and 2.5 are satisfied as well.

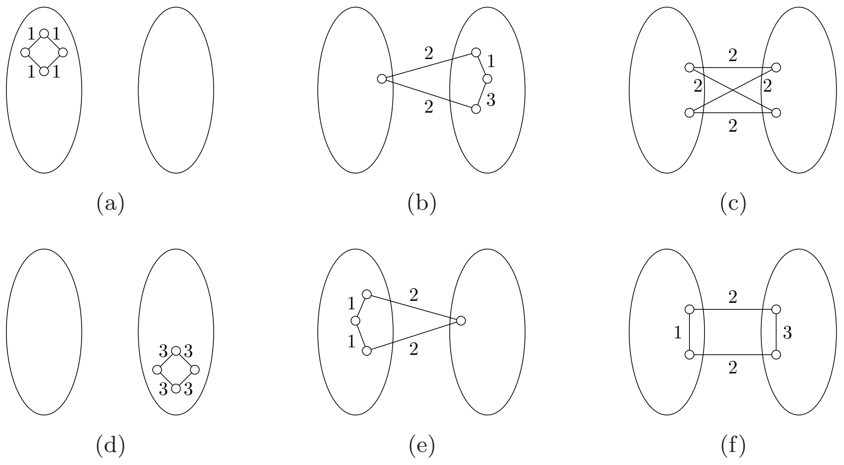


Figure 6: Possible quadrangles in $G^{[2]}$. Edge weights represent distances in G.

Let us start with Condition 2.4:

LEMMA 3.10. *Let $G = (V, E)$ be a δ-hyperbolic graph, for some $\delta \geq 1/2$. Suppose G does not satisfy Condition 2.4. Then $G^{[2]}$ is not C_4-free, or there exists some positive integer $i \leq 2\delta$ such that G^i is not C_4-free.*

Proof. Let $u, v \in V$ be such that $N(u) \cap [u, v]$ is not a clique, and $\mathrm{d}(u, v)$ is minimum w.r.t. this property. Let $x_1, y_1 \in N(u) \cap [u, v]$ such that x_1 and y_1 are not adjacent in G.

- Note that if $\mathrm{d}(u, v) = 2$, then we are done as u, v, x_1, y_1 are the vertices of an induced C_4 in G.
- Similarly, if $\mathrm{d}(u, v) = 3$, then we have:
  (i) $\mathrm{d}(u, x_1) = \mathrm{d}(u, y_1) = 1$;
  (ii) $\mathrm{d}(x_1, y_1) = \mathrm{d}(v, x_1) = \mathrm{d}(v, y_1) = 2$;
  as a consequence, $(u, 0), (x_1, 0), (y_1, 0), (v, 1)$ are the vertices of an induced quadrangle in the graph $G^{[2]}$.

In the sequel, we will assume $\mathrm{d}(u, v) \geq 4$. Let us define the two uv-shortest paths:

$$P_1 = u, x_1, x_2, x_3, \ldots, x_{\mathrm{d}(u,v)-1}, v$$
$$\text{and } P_2 = u, y_1, y_2, y_3, \ldots, y_{\mathrm{d}(u,v)-1}, v$$

Note that for every $i \leq j$ we have $\mathrm{d}(x_i, y_j) \geq \mathrm{d}(y_i, y_j) = j - i$, and in the same way $\mathrm{d}(x_j, y_i) \geq \mathrm{d}(x_j, x_i) = j - i$. We now claim that for every $i \leq j$, the inequalities above are strict, or equivalently $\mathrm{d}(x_i, y_j) > j - i$ and $\mathrm{d}(x_j, y_i) > j - i$. By contradiction, suppose that there is some $i \leq j$ satisfying $\mathrm{d}(x_i, y_j) = j - i$. Then in such a case we have $x_1, y_1 \in N(u) \cap [u, y_j]$, contradicting the minimality of $\mathrm{d}(u, v)$. The case when $d(x_j, y_i) = j - i$ is dealt with similarly. To sum up, by the minimality of $\mathrm{d}(u, v)$ we have that for any $i \leq j$:

$$\mathrm{d}(x_i, y_j) > \mathrm{d}(y_i, y_j) = j - i \text{ and } \mathrm{d}(x_j, y_i) > \mathrm{d}(x_j, x_i) = j - i.$$

In particular, for all i, j this yields that x_i and y_j are pairwise distinct.

Also, note that for all i, $\delta(u, v, x_i, y_i) = \mathrm{d}(x_i, y_i)/2$ and so, we have that for every i:

$$\mathrm{d}(x_i, y_i) \leq 2\delta.$$

Let $l \geq 3$ be the least index greater than 2 such that $\mathrm{d}(x_l, y_l) \leq l - 1$. One has to observe that since for all $i, \mathrm{d}(x_i, y_i) \leq 2\delta$, it holds that $l \leq \min\{2\delta + 1, \mathrm{d}(u, v) - 1\}$. In such a case:

(i) $\mathrm{d}(x_1, x_l) = \mathrm{d}(y_1, y_l) = l - 1$;
(ii) $\mathrm{d}(x_1, y_1)$, $\mathrm{d}(x_l, y_l) \leq l - 1$;
(iii) $\mathrm{d}(x_1, y_l)$, $\mathrm{d}(x_l, y_1) > l - 1$.

Consequently, x_1, y_1, x_l, y_l are the vertices of an induced quadrangle in G^{l-1}. □

Let us finally prove with Lemma 3.11 that we can verify whether Condition 2.5 is satisfied in the same way as we verified Condition 2.4 in Lemma 3.10.

Lemma 3.11. *Let $G = (V, E)$ be a connected graph that does not satisfy Condition 2.5. Then there is an induced C_4 in the graph $G^{[2]}$, or there is an induced C_4 in the square graph G^2.*

Proof. We proceed by contradiction. Let us assume that one of the graphs of Figure 1 is an isometric subgraph of G. For each of the forbidden graphs of Condition 2.5, we will only consider the 4-tuple of vertices that are drawn in bold in Figure 1, denoted by u, y, v, x.

Cases 1a and 1b One can easily check that in both cases, the four vertices in bold are the vertices of an induced quadrangle in the square graph G^2.

Case 1c Observe that $\mathrm{d}(u, x) = 1$, $\mathrm{d}(u, y) = \mathrm{d}(v, x) = 2$, $\mathrm{d}(u, v) = \mathrm{d}(x, y) = \mathrm{d}(v, y) = 3$. So, $(u, 0), (y, 1), (v, 1), (x, 0)$ are the vertices of an induced quadrangle in $G^{[2]}$. A contradiction.

Case 1d We have that all distances but $\mathrm{d}(u, v)$ equal 2, and that $\mathrm{d}(u, v) = 4$. Therefore, $(u, 1), (y, 0), (v, 1), (x, 0)$ are the vertices of an induced C_4 in $G^{[2]}$. Again, this is not possible.

Case 1e Observe that $\mathrm{d}(u, x) = \mathrm{d}(u, y) = 2$, $\mathrm{d}(x, y) = 4$, and all the remaining distances are equal to 3. As a consequence, $(u, 0), (y, 1), (v, 1), (x, 1)$ are the vertices of an induced quadrangle in $G^{[2]}$, which contradicts the fact that $G^{[2]}$ is C_4-free.

Case 1f The vertices $(u, 1), (y, 1), (v, 1), (x, 1)$ induce a C_4 in G^3, hence in $G^{[2]}$, that is once more a contradiction. □

To sum up, we obtain as a byproduct of our reduction, and especially of Lemmas 3.6, 3.7, 3.9, 3.10 and 3.11, the following new characterization of 1/2-hyperbolic graphs:

Characterization 3.12. *A connected graph G is 1/2-hyperbolic if, and only if, every graph power G^i, $i \geq 1$, is C_4-free, and the graph $G^{[2]}$ is C_4-free.*

The condition is necessary by Lemmas 3.6 and 3.9, and it is sufficient by Lemmas 3.7, 3.10 and 3.11.

3.2.4. The reduction. Theorem 3.13. *There is a subcubic reduction from the 1/2-hyperbolic graph recognition problem to the problem of detecting an induced quadrangle in a graph.*

Proof. Let $G = (V, E)$ be a connected graph. Since there exists a linear-time algorithm to recognize 0-hyperbolic graphs[5], we will assume for the proof $\delta(G) >$

[5]Recall that a graph is 0-hyperbolic if, and only if, it is a *block-graph i.e.*, a graph whose biconnected components are complete subgraphs [3, 24].

0, or equivalently $\delta(G) \geq 1/2$. Let us fix any $c = \log^{O(1)} n, c \geq 1$, such that we can compute a c-factor approximation of the hyperbolicity in subcubic-time. Three possible choices for c are given in Lemma 3.2, and two others ones are discussed in §3.2.1.[6]. In the sequel, let $\delta_c(G)$ be a c-factor approximation of the hyperbolicity. Recall that we have $\delta(G) \leq \delta_c(G) \leq c.\delta(G)$ by the hypothesis. So, if $\delta_c(G) > c/2$, then we are done as the graph G is not 1/2-hyperbolic. Let us now assume that $\delta(G) \leq \delta_c(G) \leq c/2$. By Corollary 3.4, every isometric cycle of G has length upper-bounded by $4\delta_c(G) + 3 \leq 2c + 3$, which is polylogarithmically upper-bounded.

We then compute all the graph powers G^i, for $1 \leq i \leq 2\delta_c(G) + 1$. This can be done in subcubic-time, by first computing the distance-matrix of G in $O(n^{\omega(1)} \log n)$-time (see [36]). Moreover every G^i has to be C_4-free by Lemma 3.6. If so, then by Lemma 3.7, there is no isometric cycle C_l of length $6 \leq l \leq 4\delta_c(G)+3$. Consequently, the graph G satisfies Condition 2.3. Finally, let us build $G^{[2]}$, which can also be done in subcubic-time using the distance-matrix of G. By Lemma 3.9, the graph $G^{[2]}$ has to be C_4-free so that G is 1/2-hyperbolic. If it is indeed the case, then we have:

(i) $G^{[2]}$ and all of G^i, $1 \leq i \leq 2\delta_c(G)$ are C_4-free, hence G satisfies Condition 2.4 by Lemma 3.10;

(ii) $G^{[2]}$ and the square graph G^2 are both C_4-free and so, G satisfies Condition 2.5 by Lemma 3.11.

Thus we can conclude by [1] that G is a 1/2-hyperbolic graph. $\square$

Corollary 3.14. *There is a subcubic equivalence between the* 1/2*-hyperbolic graph recognition problem and the* C_4*-free graph recognition problem.*

4. Finding a quadrangle.

We will conclude this paper with an improved algorithm for the C_4-free graph recognition problem, that hence improves the best-known upper-bound on the time complexity of both Problem 2.2 and Problem 2.6 by the subcubic equivalence of Corollary 3.14. While the algorithm proposed in [37] relies on transitive orientation, our algorithm merely reduces the whole Problem 2.6 to a fast rectangular matrix multiplication.

A quick reminding of the problem of matrix multiplication is given in §4.1, before we present our algorithm to detect an induced quadrangle in §4.2.

4.1. Fast rectangular matrix multiplication.

The study of fast matrix multiplication mainly focuses on the $O(n^{\omega(1)})$ time complexity of multiplying two $n \times n$ matrices, also known as the square matrix product. Currently, $\omega(1)$ is known to be less than 2.3727 [38]. The *rectangular* matrix multiplication problem has received less attention, maybe because the product of an $n \times m$ matrix with an $m \times p$ matrix is known to be reducible to square matrix multiplications, yielding an $O(q^{\omega(1)-2}. \max\{mn, mp, np\})$-time complexity, for $q = \min\{m, n, p\}$ [25].

On the other hand, there is evidence that faster methods for the rectangular matrix multiplication which do not rely on the square matrix product may exist. This is known to be the case even for truly practical improvements of the matrix multiplication such as the Strassen algorithm and its variations [26, 28]. As stated below, the conjecture is (numerically) true w.r.t. the best known algorithms for square and rectangular matrix multiplications.

Lemma 4.1 ([12, 25, 31, 38]). *Let* $r \geq 1$ *be a rational number. There exists a non-decreasing function* $\omega : [1; +\infty[\to [2.3727; +\infty[$ *such that multiplying an* $n \times n^r$

[6]A careful reader will remark that the choice of c determines the maximum number of calls in the reduction to the algorithm for detecting an induced quadrangle. There is a trade-off between this number and the running-time of the c-factor approximation algorithm.

matrix with an $n^r \times n$ matrix can be done in $O(n^{\omega(r)})$-time.

Furthermore, $\omega(2) \leq 3.26$, and for every $r \geq 1$ we have $\omega(r) \leq r + \omega(1) - 1$.

Note that reducing the rectangular matrix product to square matrix multiplications would have only yielded $\omega(2) \leq 3.3727$.

A more efficient method is known for sparse matrices (*e.g.* see [41]).

4.2. An algorithm to count quadrangles in a graph. In this section, we essentially apply the local characterization of Fact 2.7. There are two main steps of computation in our algorithm, that are described below.

Fact 4.2 ([36]). *Given a graph $G = (V, E)$, let $A = (A_{u,v})_{u,v \in V}$ be the adjacency matrix of G.*

For every pair $u, v \in V$, we have $A^2_{u,v} = |N(u) \cap N(v)|$.

Hence, $\mathrm{d}(u,v) = 2$ *if, and only if, $u \neq v$, $A_{u,v} = 0$ and $A^2_{u,v} \neq 0$.*

Proof. By the definition of matrix multiplication, we have for every pair $u, v \in V$ that:

$$\begin{aligned} A^2_{u,v} &= \sum_{x \in V} A_{u,x} A_{x,v} = \sum_{x \in V} \mathbb{I}_{\{\{x,u\} \in E\}} \mathbb{I}_{\{\{x,v\} \in E\}} \\ &= \sum_{x \in V} \mathbb{I}_{\{x \in N(u)\}} \mathbb{I}_{\{x \in N(v)\}} = \sum_{x \in V} \mathbb{I}_{\{x \in N(u) \cap N(v)\}} \\ &= |N(u) \cap N(v)|. \end{aligned}$$

Moreover, $\mathrm{d}(u,v) = 2$ if, and only if, $u \neq v$, u and v are not adjacent in G (*e.g.* $A_{u,v} = 0$), and $N(u) \cap N(v) \neq \emptyset$. Clearly, we have that $N(u) \cap N(v) \neq \emptyset$ if, and only if, $A^2_{u,v} \neq 0$. □

Lemma 4.3. *Given a graph $G = (V, E)$, let $T = (T_{u,e})_{u \in V, e \in E}$ be such that $T_{u,e} = \mathbb{I}_{\{e \subseteq N(u)\}}$ for every $u \in V, e \in E$.*

For every pair $u, v \in V$, we have $TT^\top_{u,v} = |\{e \in E : e \subseteq N(u) \cap N(v)\}|$.

Proof. Similarly to the proof of Fact 4.2, we have by the definition of matrix multiplication that for every pair $u, v \in V$:

$$\begin{aligned} TT^\top_{u,v} &= \sum_{e \in E} T_{u,e} T^\top_{e,v} = \sum_{e \in E} T_{u,e} T_{v,e} = \sum_{e \in E} \mathbb{I}_{\{e \subseteq N(u)\}} \mathbb{I}_{\{e \subseteq N(v)\}} \\ &= \sum_{e \in E} \mathbb{I}_{\{e \subseteq N(u) \cap N(v)\}} = |\{e \in E : e \subseteq N(u) \cap N(v)\}|. \end{aligned} \quad \square$$

Combining Fact 4.2 and Lemma 4.3, we can now rely on Fact 2.7 in order to detect, to count and to output induced quadrangles in the graph as follows.

Proposition 4.4. *Counting the number of induced quadrangles in a a graph G, and returning an induced C_4 of G if any, can be done in $O(n^{\omega(\log_n m)}) = O(n^{3.26})$-time.*

Proof. First, it is straightforward that we can compute the adjacency matrix A of G in quadratic-time. Using A, we can compute the matrix $T = (\mathbb{I}_{\{e \subseteq N(u)\}})_{u \in V, e \in E}$, hence the transpose matrix $T^\top$ as well, as they are defined in Lemma 4.3, in $O(nm)$-time.

Let us now compute A^2 and $TT^\top$. This can be done, respectively, in $O(n^{\omega(1)}) = O(n^{2.3727})$-time and in $O(n^{\omega(\log_n m)}) = O(n^{\omega(2)}) = O(n^{3.26})$-time by Lemma 4.1.

By Fact 2.7, G is C_4-free if, and only if, for every pair $u, v \in V$ of non-adjacent vertices, we have that $N(u) \cap N(v)$ is a clique, *e.g.* that:

$$|\{e \in E : e \subseteq N(u) \cap N(v)\}| = \frac{|N(u) \cap N(v)|(|N(u) \cap N(v)| - 1)}{2}.$$

This is equivalent to have that $TT^{\top}_{u,v} = A^2_{u,v}(A^2_{u,v} - 1)/2$ by Fact 4.2 and Lemma 4.3. Hence, it can be checked with an enumeration of all the possible pairs $u, v \in V$, in quadratic-time.

We actually note that if there is some pair $u, v \in V$ of non-adjacent vertices such that $TT^{\top}_{u,v} < A^2_{u,v}(A^2_{u,v} - 1)/2$, then there are exactly $A^2_{u,v}(A^2_{u,v} - 1)/2 - TT^{\top}_{u,v}$ induced quadrangles of G which contain this pair of vertices (that is one quadrangle for each of the missing edges in $G[N(u) \cap N(v)]$). Consequently, there are exactly $1/4 \sum_{u,v \in V}(1 - A_{u,v})(A^2_{u,v}(A^2_{u,v} - 1)/2 - TT^{\top}_{u,v})$ induced quadrangles in the graph, which can also be computed in quadratic-time, by an enumeration of all the possible pairs $u, v \in V$.

To conclude, observe that if $TT^{\top}_{u,v} \neq A^2_{u,v}(A^2_{u,v} - 1)/2$ for some pair $u, v \in V$ of non-adjacent vertices, then it is straightforward to compute an induced quadrangle of G containing u, v in quadratic-time. $\square$

We remind the reader that there is only evidence that a fast rectangular matrix product can be computed faster than up to the reduction to fast square matrix multiplications. However, we want to highlight that, from a *theoretical* point of view, our algorithm for detecting an induced quadrangle is never slower than the algorithm of [37]. The dominant term for the complexity of our algorithm is indeed the fast rectangular matrix multiplication $TT^{\top}$ (*e.g.* Lemma 4.3), which can be computed in $O(mn^{\omega(1)-1})$- time in the worst-case, using the reduction to fast square matrix products that we described earlier in §4.1. In comparison, the time complexity of the algorithm of [37] is $O(n^{\omega(1)+1})$.

Also, we emphasize that for graphs with few C_3's, a speed-up for the computation of $TT^{\top}$ can be achieved using the results from [41] for sparse matrix multiplication. Indeed, the number of non-zero elements in the matrix T is exactly $3.t(G)$, where $t(G)$ denotes the number of C_3 in the graph.

5. Conclusion.

In this work, we proved an interesting equivalence between the complexity of the purely *metric* problem of recognizing 1/2-hyperbolic graphs, and the purely *structural* problem of detecting an induced quadrangle in a graph. This shows a surprising gap in the complexity for recognizing graphs with small hyperbolicity, as in comparison there is a linear-time algorithm to decide whether a graph is 0-hyperbolic.

Our reduction being subcubic, it remains open whether 1/2-hyperbolic graphs can be recognized in linear-time, for some classes of graphs for which detecting an induced quadrangle is easy, like for instance planar graphs [20]. Also, it would be nice to extend our results to find a better upper-bound on the complexity of the problem of deciding if a graph is 1-hyperbolic. Note that this latter problem might be easier than the recognition of 1/2-hyperbolic graphs, as the true difficulty may only lie in the distinction between graphs with hyperbolicity *exactly* 1 and exactly 1/2. Any recognition algorithm in $O(f(n))$-time for 1-hyperbolic graphs would furthermore yield a 4-factor approximation algorithm for the hyperbolicity that runs in $\tilde{O}(f(n) + n^{\omega(1)})$-time.

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Appendix D

On the hyperbolicity of bipartite and intersection graphs

On the hyperbolicity of bipartite graphs and intersection graphs

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Abstract

Hyperbolicity is a measure of the tree-likeness of a graph from a metric perspective. Recently, it has been used to classify complex networks depending on their underlying geometry. Motivated by a better understanding of the structure of graphs with bounded hyperbolicity, we here investigate on the hyperbolicity of bipartite graphs. More precisely, given a bipartite graph $B = (V_0 \cup V_1, E)$ we prove it is enough to consider any one side V_i of the bipartition of B to obtain a close approximate of its hyperbolicity $\delta(B)$ — up to an additive constant 2. We obtain from this result the sharp bounds $\delta(G) - 1 \leq \delta(L(G)) \leq \delta(G) + 1$ and $\delta(G) - 1 \leq \delta(K(G)) \leq \delta(G) + 1$ for every graph G, with $L(G)$ and $K(G)$ being respectively the line graph and the clique graph of G. Finally, promising extensions of our techniques to a broader class of intersection graphs are discussed and illustrated with the case of the biclique graph $BK(G)$, for which we prove $(\delta(G) - 3)/2 \leq \delta(BK(G)) \leq (\delta(G) + 3)/2$.

Keywords: Gromov hyperbolicity; bipartite graph; intersection graph; graph power; line graph; clique graph; biclique graph.

1. Introduction

The purpose of this paper is to bound the hyperbolicity of some classes of graphs that are defined in terms of graph operators. Roughly, hyperbolicity is a tree-likeness parameter that measures how close the shortest-path

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metric of a graph is to a tree metric (the smaller the hyperbolicity the closer the graph is to a metric tree). It has thus been proposed to take hyperbolicity into account to better classify complex networks [22]. For instance, it has been experimentally shown in [22] that social networks and protein interaction networks have bounded hyperbolicity while it is not the case for road networks. Another interest for hyperbolicity is that it helps analyzing some graph heuristics on large-scale networks. A good example to this is the *2-sweep* heuristic for computing the diameter, that provides very good results in practice [23]; such good results can be explained assuming a bounded hyperbolicity [11].

Relating the structural properties of graphs with hyperbolicity can be useful in this context, and it has become a growing line of research (*e.g.*, see [12, 15, 24, 31]). Indeed, we argue that one can obtain from such relations a comprehensive overview of the reasons why some complex networks are hyperbolic and some others are not. Following this line, we proved in [15] that most data center interconnection networks are *not* hyperbolic because they are symmetric graphs. As an attempt to go further in this direction, we here investigate on the hyperbolicity of bipartite graphs. In fact, we were motivated at first to bound the hyperbolicity of *line graphs* [30], that are intersection graphs of edges in a graph and have already received some attention in the literature of graph hyperbolicity [8, 9]. In this paper, we fully characterize what can be the defect between the hyperbolicity of a given graph and the hyperbolicity of its line graph, using an original connection with bipartite graphs. To better depict our novel approach, let us first recall that intersection graphs over a ground set S have for vertices a family of subsets of S with an edge between every two intersecting subsets. Therefore, they can be naturally represented as a bipartite graph — with vertices of the graph on one side, the ground set S on the other side, and an edge between every element of S and the subsets that contain it. Our main contribution is to show how we can use this representation so as to bound the hyperbolicity of intersection graphs—. This simple framework does not only apply to line graphs. We can use it to bound the hyperbolicity of *clique graphs* [20] and (with slightly more work) *biclique graphs* [19]. Overall, our main results can be expressed as follows.

- Given a bipartite graph $B = (V_0 \cup V_1, E)$, for every $i \in \{0, 1\}$ let G_i be the graph with vertex-set the side V_i and with an edge between every two vertices that share a common neighbor in B. We prove that $2\delta(G_i) \leq \delta(B) \leq 2\delta(G_i) + 2$ and the bounds are sharp (Theorem 4).

- We deduce from the above inequalities that $\delta(G) - 1 \leq \delta(L(G)) \leq$

$\delta(G)+1$ for every graph G, with $L(G)$ being the line graph of G (Theorem 6). Furthermore we show that all possible cases (between $\delta(G)-1$ and $\delta(G)+1$) can happen. This complements the bounds in [8, 9] that are proved to be sharp only for cycles (but with an alternative definition of hyperbolicity).

- By applying the same technique as for line graphs, we are the first to bound the hyperbolicity of clique graphs, *a.k.a.*, the intersection graphs of maximal cliques. More precisely, we prove that $\delta(G)-1 \leq \delta(K(G)) \leq \delta(G)+1$ for every graph G, with $K(G)$ being the clique graph of G, and all possible cases between $\delta(G)-1$ and $\delta(G)+1$ can happen (Theorem 8).

- We introduce graph powers [3] in our framework to obtain bounds on the hyperbolicity of other graphs. As example we prove that $(\delta(G)-3)/2 \leq \delta(BK(G)) \leq (\delta(G)+3)/2$ for every graph G, with $BK(G)$ being the biclique graph of G (Theorem 13). Bicliques are maximal induced complete bipartite subgraphs and they have gained recent attention in graph theory and graph algorithms. We refer to [19] and the papers cited therein for details.

- Finally, we bound the hyperbolicity of some other extensions of line graphs using our framework (Section 4.4), namely the *incidence graph*, the *total graph* [5], the *middle graph* [27], and the *k-edge graph* [26] of G.

Definitions and useful notations are given in Section 2.

2. Definitions and notations

We will follow the graph terminology in [6, 17]. Graphs in this study are connected, unweighted and finite (although part of the results extend to infinite weighted graphs). Given a graph $G=(V,E)$, the distance between every two vertices u,v in V equals the minimum number of edges on an uv-path. We will denote the distance between u and v by $\mathrm{d}_G(u,v)$, or simply $\mathrm{d}(u,v)$ when G is clear from the context. Informally, we are interested in this paper in embedding the vertices of G into a tree T (possibly, edge-weighted) while minimizing the additive distortion of the distances in G. Hyperbolicity is both a lower-bound and an $\mathcal{O}(\log|V|)$-approximation for the minimum possible distortion [18]. Finer-grained relations between hyperbolicity and the minimum possible distortion for graphs are discussed in [16].

Definition 1 (**4-points Condition,** [18]). *Let $G = (V, E)$ be a connected graph.*

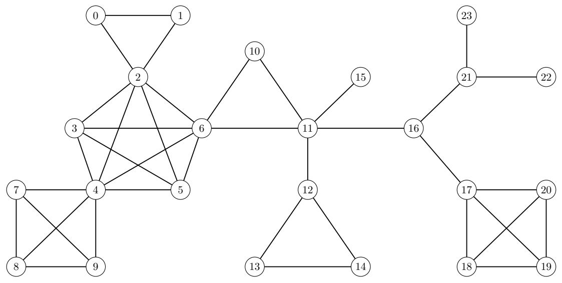
For every 4-tuple u, v, x, y of V, we define $\delta(u, v, x, y)$ as half of the difference between the two largest sums amongst:

$$S_1 = \mathrm{d}(u, v) + \mathrm{d}(x, y),\ S_2 = \mathrm{d}(u, x) + \mathrm{d}(v, y),\ \textit{and}\ S_3 = \mathrm{d}(u, y) + \mathrm{d}(v, x).$$

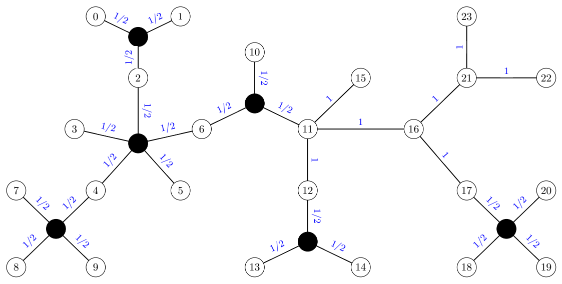
The graph hyperbolicity, denoted by $\delta(G)$, is equal to $\max_{u,v,x,y \in V} \delta(u, v, x, y)$.

*Moreover, we say that G is δ-*hyperbolic *for every $\delta \geq \delta(G)$.*

It is well-known that 0-hyperbolic graphs are exactly those that can be embedded into a tree without any distortion, including trees and complete graphs. In fact, 0-hyperbolic graphs coincide with the *block graphs*, that are graphs whose all biconnected components are cliques (see Figure 1 for an illustration) [4, 21]. The class of 1/2-hyperbolic graphs has also been characterized in [2, 14].



(a) A block graph G.



(b) An embedding of G into an edge-weighted tree with null distortion.

Figure 1: Block graphs are exactly the 0-hyperbolic graphs.

Furthermore, it turns out that not all 4-tuples in the graph need to be considered for the computation of hyperbolicity. This crucial point is the cornerstone of the most efficient algorithms so far to compute this parameter [7, 13]. Here we will use this observation to gain more insights on 4-tuples with maximum hyperbolicity in our proofs. This will require us to introduce the central notion of far-apart pairs.

Definition 2 (**Far-apart pair** [25, 28])**.** *Given $G = (V, E)$, the pair (u, v) is far-apart if for every $w \in V \setminus \{u, v\}$, we have $\mathrm{d}(w, u) + \mathrm{d}(u, v) > \mathrm{d}(w, v)$ and $\mathrm{d}(w, v) + \mathrm{d}(u, v) > \mathrm{d}(w, u)$.*

Said differently, far-apart pairs are the ends of maximal shortest-paths in the graph. Their key property is that there always exists a 4-tuple with maximum hyperbolicity which contains two far-apart pairs.

Lemma 3 ([25, 28])**.** *Given $G = (V, E)$, there exist two far-apart pairs (u, v) and (x, y) satisfying:*

i) $\mathrm{d}_G(u, v) + \mathrm{d}_G(x, y) \geq \max\{\mathrm{d}_G(u, x) + \mathrm{d}_G(v, y), \mathrm{d}_G(u, y) + \mathrm{d}_G(v, x)\}$;
ii) $\delta(u, v, x, y) = \delta(G)$.

3. New bounds on the hyperbolicity of bipartite graphs

Let us start proving our main tool for the remaining of the paper, that is Theorem 4. Informally, we will consider a bipartite graph $B = (V_0 \cup V_1, E)$ as obtained from two smaller intersection graphs G_0 and G_1, each having one side of the bipartition as its vertex-set. Our goal is to bound $\delta(B)$ depending on $\delta(G_i)$, for any $i \in \{0, 1\}$. In fact, since any side V_i is a dominating set of B, then it is not hard to prove that $\delta(B) \leq 2\delta(G_i) + 4$ (using the the 4-point Condition of Definition 1). The main difficulty is to obtain the sharp upper-bound $\delta(B) \leq 2\delta(G_i) + 2$, for which we will need far-apart pairs.

Theorem 4. *Let $B = (V_0 \cup V_1, E)$ be a bipartite graph. We have $\delta_B(V_i) \leq \delta(B) \leq \delta_B(V_i) + 2$, where $\delta_B(V_i) = \max_{u,v,x,y \in V_i} \delta_B(u, v, x, y)$ for every $i \in \{0, 1\}$, and these bounds are sharp.*

Proof. We will only need to consider the upper-bound $\delta(B) \leq \delta_B(V_i) + 2$, for the lower-bound $\delta_B(V_i) \leq \delta(B)$ trivially follows from the 4-points Condition of Definition 1. To prove the upper-bound, let (u, v) and (x, y) be two far-apart pairs of B such that $S_1 = \mathrm{d}(u, v) + \mathrm{d}(x, y) \geq \max\{\mathrm{d}(u, x) + \mathrm{d}(v, y), \mathrm{d}(u, y) + \mathrm{d}(v, x)\} = S_2$ and $\delta(u, v, x, y) = \delta(B)$, that exist by Lemma 3. Note that $\delta(B) = (S_1 - S_2)/2$.

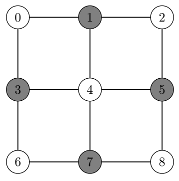


Figure 2: The bipartite graph $G_{3,3}$ with each side of the bipartition colored differently.

We claim that there are $u', v' \in V_i$ such that $\delta(u, v, x, y) \leq \delta(u', v', x, y) + 1$. To prove the claim assume $\delta(u, v, x, y) > 0$ (or else, it is trivial). The latter implies (by Definition 1) that u, v, x, y are pairwise different. There are three cases to be considered.

- If $u, v \in V_i$, then we are done by setting $u' = u$ and $v' = v$.
- If $u \in V_i$ and $v \notin V_i$ (resp., $u \notin V_i$ and $v \in V_i$), let us set $u' = u$ and $v' \in N(v)$ (resp., $u' \in N(u)$ and $v' = v$). In such case let $S_1' = \mathrm{d}(u', v') + \mathrm{d}(x, y)$ and let $S_2' = \max\{\mathrm{d}(u', x) + \mathrm{d}(v', y), \mathrm{d}(u', y) + \mathrm{d}(v', x)\}$. By the triangular inequality $|S_1 - S_1'| \leq 1$ and similarly $|S_2 - S_2'| \leq 1$. Therefore, either $S_1' < S_2'$ and so, $\delta(u, v, x, y) = (S_1 - S_2)/2 \leq (S_1' - S_2' + 2)/2 < 1 \leq \delta(u', v', x, y) + 1$, or $S_1' \geq S_2'$ and so, $\delta(u', v', x, y) = (S_1' - S_2')/2 \geq (S_1 - S_2 - 2)/2 = \delta(u, v, x, y) - 1$.
- Else, $u, v \notin V_i$. In particular, $N(u) \subseteq V_i$ and $N(v) \subseteq V_i$ because B is bipartite by the hypothesis. We will prove as an intermediate subclaim that for every pair (u', v') with $u' \in N(u)$ and $v' \in N(v)$, we have either $\mathrm{d}(u', v') = \mathrm{d}(u, v)$ or $\mathrm{d}(u', v') = \mathrm{d}(u, v) - 2$. Indeed, $\mathrm{d}(u, v) - 2 \leq \mathrm{d}(u', v') \leq \mathrm{d}(u, v) + 2$ by the triangular inequality, and so, since the pairs (u, v) and (u', v') are in distinct sides of the bipartition of B, either $\mathrm{d}(u', v') = \mathrm{d}(u, v) - 2$ or $\mathrm{d}(u', v') = \mathrm{d}(u, v)$ or $\mathrm{d}(u', v') = \mathrm{d}(u, v) + 2$. The latter case, $\mathrm{d}(u', v') = \mathrm{d}(u, v) + 2$, would contradict the fact that (u, v) is far-apart. Hence either $\mathrm{d}(u', v') = \mathrm{d}(u, v)$ or $\mathrm{d}(u', v') = \mathrm{d}(u, v) - 2$, which proves the subclaim. Now there are two subcases to be considered.
  - Suppose there are $u' \in N(u)$ and $v' \in N(v)$ such that $\mathrm{d}(u', v') = \mathrm{d}(u, v)$. Let $S_1' = \mathrm{d}(u', v') + \mathrm{d}(x, y)$ and let $S_2' = \max\{\mathrm{d}(u', x) + \mathrm{d}(v', y), \mathrm{d}(u', y) + \mathrm{d}(v', x)\}$. By the choice of u' and v', we have $S_1' = S_1$ while $|S_2 - S_2'| \leq 2$ by the triangular inequality. As

a result, either $S'_1 < S'_2$ and so, $\delta(u,v,x,y) = (S_1 - S_2)/2 \leq (S'_1 - S'_2 + 2)/2 < 1 \leq \delta(u',v',x,y) + 1$, or $S'_1 \geq S'_2$ and so, $\delta(u',v',x,y) = (S'_1 - S'_2)/2 \geq (S_1 - S_2 - 2)/2 = \delta(u,v,x,y) - 1$.

– Else, for every $u' \in N(u)$ and $v' \in N(v)$, we have $\mathrm{d}(u',v') = \mathrm{d}(u,v) - 2$. Let $u' \in N(u)$ and $v' \in N(v)$ satisfy $\mathrm{d}(u,x) = 1 + \mathrm{d}(u',x)$ and $\mathrm{d}(v,x) = 1 + \mathrm{d}(v',x)$. We set as before $S'_1 = \mathrm{d}(u',v') + \mathrm{d}(x,y)$ and $S'_2 = \max\{\mathrm{d}(u',x) + \mathrm{d}(v',y), \mathrm{d}(u',y) + \mathrm{d}(v',x)\}$. By the choice of u' and v', we have $S'_1 = S_1 - 2$. Furthermore, $S_2 - 2 \leq S'_2 \leq S_2$ because $\mathrm{d}(u',x) = \mathrm{d}(u,x) - 1$, $\mathrm{d}(v',x) = \mathrm{d}(v,x) - 1$, and $|\,\mathrm{d}(u',y) - \mathrm{d}(u,y)| \leq 1$ and $|\,\mathrm{d}(v',y) - \mathrm{d}(v,y)| \leq 1$ by the triangular inequality. It follows that either $S'_1 < S'_2$ and so, $\delta(u,v,x,y) = (S_1 - S_2)/2 \leq (S'_1 - S'_2 + 2)/2 < 1 \leq \delta(u',v',x,y) + 1$, or $S'_1 \geq S'_2$, and so $\delta(u',v',x,y) = (S'_1 - S'_2)/2 \geq (S_1 - S_2 - 2)/2 \geq \delta(u,v,x,y) - 1$, that achieves proving the claim.

Finally, since the pair (x,y) is also far-apart, there exist $x',y' \in V_i$ such that $\delta(u',v',x,y) \leq \delta(u',v',x',y') + 1$. As a result, $\delta(B) = \delta(u,v,x,y) \leq \delta(u',v',x,y) + 1 \leq \delta(u',v',x',y') + 2 \leq \delta_B(V_i) + 2$.

To show that the bounds are sharp, let us consider the square grid $G_{3,3}$ of side length two as drawn in Figure 2. This bipartite graph has vertex-set $V = V_0 \cup V_1$, with $V_0 = \{0,2,4,6,8\}$ and $V_1 = \{1,3,5,7\}$. We have $\delta(G_{3,3}) = 2$, that is reached with the four corners 0, 2, 6 and 8 (i.e., $\delta(0,2,6,8) = 2$). On the one hand, side V_0 contains the four corners and so $\delta_{G_{3,3}}(V_0) = \delta(G_{3,3}) = 2$. On the other hand, vertices on the other side V_1 are exactly the four neighbors of vertex 4, and so $\delta_{G_{3,3}}(V_1) = 0 = \delta(G_{3,3}) - 2$. □

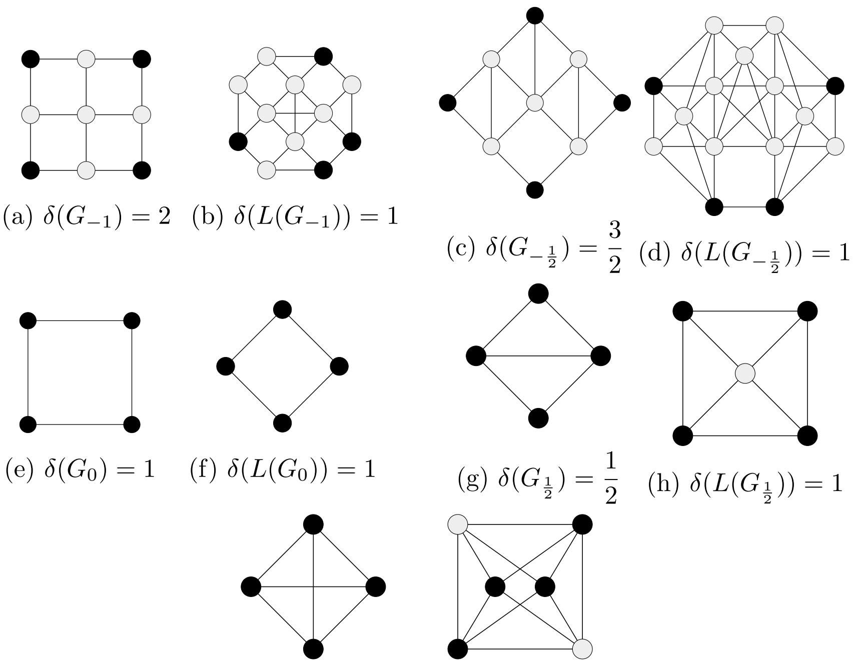
4. Applications to intersection graphs

Our main results in this section are (sharp) lower and upper-bounds on the hyperbolicity of intersection graphs that have been considered in the literature. These comprise the two well-known families of line graphs and clique graphs (we refer to [1, 29] for surveys), along with biclique graphs that have been introduced more recently as extensions of line graphs.

4.1. Line graph

Definition 5. *Given $G = (V,E)$, the line-graph of G, denoted by $L(G)$, is the intersection graph of E. That is, it has vertex-set E and for every $e,e' \in E$ there is an edge $\{e,e'\}$ in $L(G)$ if and only if e and e' share an end in G.*

Theorem 6. *For every graph G, $\delta(G)-1 \leq \delta(L(G)) \leq \delta(G)+1$, and these bounds are sharp.*


(a) $\delta(G_{-1}) = 2$ (b) $\delta(L(G_{-1})) = 1$ (c) $\delta(G_{-\frac{1}{2}}) = \frac{3}{2}$ (d) $\delta(L(G_{-\frac{1}{2}})) = 1$

(e) $\delta(G_0) = 1$ (f) $\delta(L(G_0)) = 1$ (g) $\delta(G_{\frac{1}{2}}) = \frac{1}{2}$ (h) $\delta(L(G_{\frac{1}{2}})) = 1$

(i) $\delta(G_1) = 0$ (j) $\delta(L(G_1)) = 1$

Figure 3: Examples of graphs G_i with $\delta(L(G_i)) = \delta(G_i) + i$ for every $i \in \{-1, -1/2, 0, +1/2, +1\}$. A 4-tuple with maximum hyperbolicity is drawn in bold on each graph.

Proof. Let B be the incidence graph of G, that is, it has vertex-set $V \cup E$ and there is an edge in B between $u \in V$ and $e \in E$ if and only if u is an end of e in G. By Theorem 4, $\delta_B(V) \leq \delta(B) \leq \delta_B(V)+2$ and similarly $\delta_B(E) \leq \delta(B) \leq \delta_B(E)+2$. Furthermore by construction $\mathrm{d}_B(u,v) = 2\,\mathrm{d}_G(u,v)$ for every $u,v \in V$ and in the same way $\mathrm{d}_B(e,e') = 2\,\mathrm{d}_{L(G)}(e,e')$ for every $e,e' \in E$. As a result, $\delta_B(V) = 2\delta(G)$, similarly $\delta_B(E) = 2\delta(L(G))$, and so,

$$2\delta(G) \leq \delta(B) \leq 2\delta(G) + 2,$$

$$2\delta(L(G)) \leq \delta(B) \leq 2\delta(L(G)) + 2.$$

By mixing up the two chains of inequality one obtains $2\delta(G) \leq 2\delta(L(G))+2$ and $2\delta(L(G)) \leq 2\delta(G)+2$, whence $\delta(G) \leq \delta(L(G))+1$ and $\delta(L(G)) \leq \delta(G)+1$, as desired.

To show that the bounds are sharp, consider the graphs G_{-1} and G_1 as drawn respectively in Figures 3a and 3i. We have $\delta(L(G_{-1})) = \delta(G_{-1})-1$ and $\delta(L(G_1)) = \delta(G_1)+1$. □

In Figure 3 we show that all possible cases of Theorem 6 (with defect between -1 and $+1$) are realized by some graphs. By taking the incidence graphs of G_{-1} and G_1, one obtains a new proof that the bounds of Theorem 4 are sharp.

4.2. Clique graph

Definition 7. *Given $G = (V,E)$, let Ω be the set of all maximal cliques of G. The clique-graph of G, denoted by $K(G)$, is the intersection graph of Ω. That is, it has vertex-set Ω and for every $S, S' \in \Omega$ there is an edge $\{S,S'\}$ in $K(G)$ if and only if the two cliques S and S' intersect.*

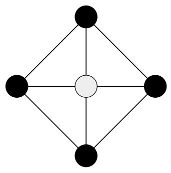
Theorem 8. *For every graph G, $\delta(G)-1 \leq \delta(K(G)) \leq \delta(G)+1$, and these bounds are sharp.*

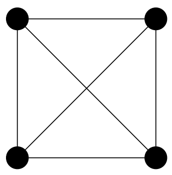
Proof. Let B be the bipartite graph defined as follows. It has vertex-set $V \cup \Omega$ and there is an edge between $u \in V$ and $S \in \Omega$ if and only if $u \in S$. By Theorem 4, $\delta_B(V) \leq \delta(B) \leq \delta_B(V)+2$ and similarly $\delta_B(\Omega) \leq \delta(B) \leq \delta_B(\Omega)+2$. Furthermore, $\mathrm{d}_B(S,S') = 2\,\mathrm{d}_{K(G)}(S,S')$ for every $S,S' \in \Omega$ by construction, so, $\delta_B(\Omega) = 2\delta(K(G))$. We claim in addition that $\mathrm{d}_B(u,v) = 2\,\mathrm{d}_G(u,v)$ for every $u,v \in V$. To prove the claim it is enough to prove $\mathrm{d}_B(u,v) = 2$ if and only if u and v are adjacent in G. By construction, $\mathrm{d}_B(u,v) = 2$ if and only if there is $S \in \Omega$ such that $u,v \in S$. If $u,v \in S$ for some $S \in \Omega$ then u and v are adjacent in G because S is a clique of G, conversely if u and v are adjacent in G then $u,v \in S$ with S being any maximal clique containing the edge $\{u,v\}$. Therefore, the claim is proved, and so, since $\mathrm{d}_B(u,v) = 2\,\mathrm{d}_G(u,v)$ for every $u,v \in V$, $\delta_B(V) = 2\delta(G)$. As a result:

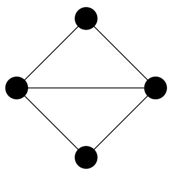
$$2\delta(G) \leq \delta(B) \leq 2\delta(G)+2,$$

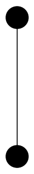
$$2\delta(K(G)) \leq \delta(B) \leq 2\delta(K(G))+2.$$

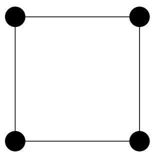
By mixing up the two chains of inequality one obtains $2\delta(G) \leq 2\delta(K(G))+2$ and $2\delta(K(G)) \leq 2\delta(G)+2$, whence $\delta(G) \leq \delta(K(G))+1$ and $\delta(K(G)) \leq \delta(G)+1$, as desired.

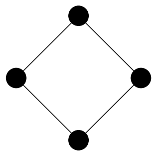

(a) $\delta(H_{-1}) = 1$

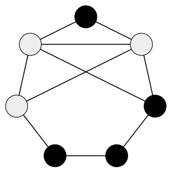

(b) $\delta(K(H_{-1})) = 0$

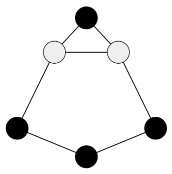

(c) $\delta(H_{-\frac{1}{2}}) = \dfrac{1}{2}$

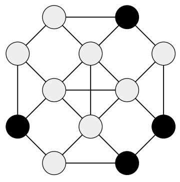

(d) $\delta(K(H_{-\frac{1}{2}})) = 0$


(e) $\delta(H_0) = 1$


(f) $\delta(K(H_0)) = 1$


(g) $\delta(H_{\frac{1}{2}}) = \dfrac{1}{2}$


(h) $\delta(K(H_{\frac{1}{2}})) = 1$


(i) $\delta(H_1) = 1$

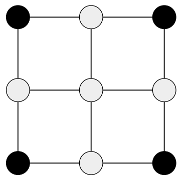

(j) $\delta(K(H_1)) = 2$

Figure 4: Examples of graphs H_i with $\delta(K(H_i)) = \delta(H_i) + i$ for every $i \in \{-1, -1/2, 0, +1/2, +1\}$. A 4-tuple with maximum hyperbolicity is drawn in bold on each graph.

To show that the bounds are sharp, consider the graphs H_{-1} and H_1 as drawn respectively in Figures 4a and 4i. We have $\delta(K(H_{-1})) = \delta(H_{-1}) - 1$ and $\delta(K(H_1)) = \delta(H_1) + 1$. □

In Figure 4 we show that all possible cases of Theorem 8 (with defect between -1 and $+1$) are realized by some graphs. Note that $H_{-1} = L(G_{\frac{1}{2}})$, $H_{-\frac{1}{2}} = G_{\frac{1}{2}}$, $H_0 = G_0$ and $H_1 = L(G_{-1})$.

4.3. Biclique graph

The above two examples of line graphs and clique graphs are intersection graphs of *cliques*. However, there are interesting graph families that are defined as the intersection graphs of some subgraphs of diameter larger than one. As a general method to overcome this difficulty, we now introduce graph powers in our framework.

Definition 9. *Given $G = (V, E)$ and $k \geq 1$, the k^{th}-power of G, denoted by G^k, is defined as follows. It has vertex-set V and for every $u, v \in V$ there is an edge $\{u, v\}$ in G^k if and only if $\mathrm{d}_G(u, v) \leq k$.*

Pushing further a previous result from [14], let us bound the hyperbolicity of graph powers (Proposition 11). We will need the following intermediate lemma.

Lemma 10 ([3])**.** *Given $G = (V, E)$ and $k \geq 1$, $\mathrm{d}_{G^k}(u, v) = \left\lceil \frac{\mathrm{d}_G(u, v)}{k} \right\rceil$ for every $u, v \in V$.*

Proposition 11. *For every graph G and $k \geq 2$, $\frac{\delta(G) + 1}{k} - 1 \leq \delta(G^k) \leq \frac{\delta(G) - 1}{k} + 1$, and these bounds are sharp.*

Proof. Let $u, v, x, y \in V$ be arbitrary. Assume w.l.o.g. $S_1 = \mathrm{d}_G(u, v) + \mathrm{d}_G(x, y) \geq S_2 = \mathrm{d}_G(u, x) + \mathrm{d}_G(v, y) \geq S_3 = \mathrm{d}_G(u, y) + \mathrm{d}_G(v, x)$. In order to prove Proposition 11, we will need to prove some relations between the hyperbolicity $\delta_G(u, v, x, y)$ of the 4-tuple in G and the hyperbolicity $\delta_{G^k}(u, v, x, y)$ of the 4-tuple in G^k. Let $S'_1 = \mathrm{d}_{G^k}(u, v) + \mathrm{d}_{G^k}(x, y)$, $S'_2 = \mathrm{d}_{G^k}(u, x) + \mathrm{d}_{G^k}(v, y)$ and $S'_3 = \mathrm{d}_{G^k}(u, y) + \mathrm{d}_{G^k}(v, x)$. By Lemma 10, we have:

$S'_1 = \left\lceil \frac{\mathrm{d}_G(u, v)}{k} \right\rceil + \left\lceil \frac{\mathrm{d}_G(x, y)}{k} \right\rceil$, $S'_2 = \left\lceil \frac{\mathrm{d}_G(u, x)}{k} \right\rceil + \left\lceil \frac{\mathrm{d}_G(v, y)}{k} \right\rceil$ and $S'_3 = \left\lceil \frac{\mathrm{d}_G(u, y)}{k} \right\rceil + \left\lceil \frac{\mathrm{d}_G(v, x)}{k} \right\rceil$.

In particular $S_i/k \leq S'_i \leq S_i/k + 2(1-1/k)$ for every $1 \leq i \leq 3$. Since $2(1-1/k) < 2$, there can be no more than two integers between S_i/k and $S_i/k + 2(1-1/k)$, that implies either $S'_i = \lceil S_i/k \rceil$ or $S'_i = \lceil S_i/k \rceil + 1$. Now there are two cases to be considered.

- Suppose $S'_1 < S'_j$ with $S'_j = \max\{S'_2, S'_3\}$. Then it must be the case that $S'_1 = \lceil S_1/k \rceil$ and $S'_j = \lceil S_j/k \rceil + 1$ because $\lceil S_1/k \rceil \geq \lceil S_j/k \rceil$. The latter implies

$$\begin{aligned}\delta_{G^k}(u,v,x,y) &\leq \frac{S'_j - S'_1}{2} \leq \frac{\left\lceil \frac{S_j}{k} \right\rceil + 1 - \left\lceil \frac{S_1}{k} \right\rceil}{2} \\ &\leq \frac{1}{2} \leq 1 - \frac{1}{k} \leq \frac{\delta_G(u,v,x,y) - 1}{k} + 1\end{aligned} \tag{1}$$

$$\begin{aligned}\delta_G(u,v,x,y) &\leq \frac{S_1 - S_j}{2} \leq k\frac{\frac{S_1}{k} - \frac{S_j}{k}}{2} \leq k\left[\frac{S'_1 - S'_j}{2} + 1 - \frac{1}{k}\right] \\ &\leq -\frac{k}{2} + k - 1 \leq \frac{k}{2} - 1\end{aligned} \tag{2}$$

  Furthermore if $\delta_G(u,v,x,y) \leq k/2 - 1$ then $(\delta_G(u,v,x,y)+1)/k - 1 < 0 \leq \delta_{G^k}(u,v,x,y)$.

- Else, $S'_1 \geq \max\{S'_2, S'_3\}$. In such case $\delta_{G^k}(u,v,x,y) = (S'_1 - \max\{S'_2, S'_3\})/2$. Moreover, $S_2/k \leq \max\{S'_2, S'_3\} \leq S_2/k + 2(1-1/k)$ because $S_2 \geq S_3$. Therefore,

$$\delta_{G^k}(u,v,x,y) \geq \frac{\frac{S_1}{k} - \frac{S_2}{k} - 2\left(1 - \frac{1}{k}\right)}{2} \geq \frac{\delta_G(u,v,x,y)}{k} - 1 + \frac{1}{k} \tag{3}$$

$$\delta_{G^k}(u,v,x,y) \leq \frac{\frac{S_1}{k} + 2\left(1 - \frac{1}{k}\right) - \frac{S_2}{k}}{2} \leq \frac{\delta_G(u,v,x,y)}{k} + 1 - \frac{1}{k} \tag{4}$$

It follows that $(\delta_G(u,v,x,y)+1)/k - 1 \leq \delta_{G^k}(u,v,x,y) \leq (\delta_G(u,v,x,y) - 1)/k + 1$ in both cases.

- When u,v,x,y maximizes δ_G the first inequality leads to $(\delta(G)+1)/k - 1 \leq \delta_{G^k}(u,v,x,y) \leq \delta(G^k)$.

- When it maximizes δ_{G^k} the second inequality leads to $\delta(G^k) \leq (\delta_G(u,v,x,y) - 1)/k + 1 \leq (\delta(G) - 1)/k + 1$.

Let us finally show that the bounds of Proposition 11 are sharp. Indeed, on the one hand the cycle C_4 with four vertices satisfies $\delta(C_4) = 1$ and $C_4^2 =$

K_4, the clique with four vertices. Therefore, $\delta(C_4^2) = 0 = (\delta(C_4)+1)/2 - 1$. On the other hand the rectangular grid $G_{2,3}$ (obtained from two C_4's sharing exactly one edge) satisfies $\delta(G_{2,3}) = 1$, and its four borders induce a C_4 in $G_{2,3}^2$. Consequently, $\delta(G_{2,3}^2) \geq 1 \geq (\delta(G_{2,3}) - 1)/2 + 1$. □

We will illustrate the benefit of using graph powers within our framework through the case of *biclique graphs*, that are defined as follows.

Definition 12. *Given $G = (V, E)$, the set $S \subseteq V$ is a biclique of G if it induces a complete bipartite subgraph of G. Let Σ be all maximal bicliques of G. The biclique graph of G, denoted by $BK(G)$, is the intersection graph of Σ. That is, it has vertex-set Σ and for every $S, S' \in \Sigma$ there is an edge $\{S, S'\}$ in $BK(G)$ if and only if the two bicliques S and S' intersect.*

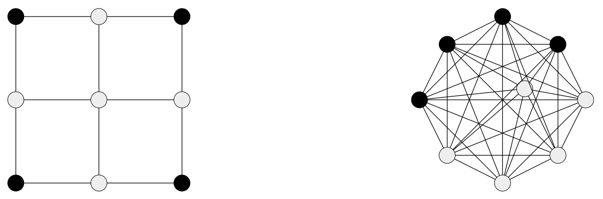

(a) $\delta(G_{3,3}) = 2$ (b) $\delta(BK(G_{3,3})) = 0$

Figure 5: The grid graph $G_{3,3}$ along with its biclique graph, that is the complete graph K_9 with nine vertices. A 4-tuple with maximum hyperbolicity is drawn in bold on each graph.

For instance, the biclique graph of a complete graph is exactly its line graph. In Figure 5 we consider the biclique graph of the grid $G_{3,3}$. The maximal bicliques of this grid comprise four cycles of length four, four stars with three branches each and one star with four branches. All of these pairwise intersect at the central vertex of the grid, therefore, $BK(G_{3,3}) = K_9$, the complete graph with nine vertices.

Theorem 13. *For every graph G, $(\delta(G)-3)/2 \leq \delta(BK(G)) \leq (\delta(G)+3)/2$.*

Proof. Let B be the bipartite graph defined as follows. It has vertex-set $V \cup \Sigma$ and there is an edge between $u \in V$ and $S \in \Sigma$ if and only if $u \in S$. By Theorem 4, $\delta_B(V) \leq \delta(B) \leq \delta_B(V) + 2$ and similarly $\delta_B(\Sigma) \leq \delta(B) \leq \delta_B(\Sigma) + 2$. Furthermore, $\mathrm{d}_B(S, S') = 2\,\mathrm{d}_{BK(G)}(S, S')$ for every $S, S' \in \Sigma$ by construction, so, $\delta_B(\Sigma) = 2\delta(BK(G))$. We claim in addition that $\mathrm{d}_B(u, v) = 2\,\mathrm{d}_{G^2}(u, v)$ for every $u, v \in V$, with G^2 be defined as in

Definition 9. To prove the claim it is enough to prove $\mathrm{d}_B(u,v) = 2$ if and only if $\mathrm{d}_G(u,v) \leq 2$. By construction, $\mathrm{d}_B(u,v) = 2$ if and only if there is $S \in \Sigma$ such that $u, v \in S$. If $u, v \in S$ for some $S \in \Sigma$ then $\mathrm{d}_G(u,v) \leq 2$ because S induces a complete bipartite subgraph of G, conversely if $\mathrm{d}_G(u,v) \leq 2$ then every uv-shortest-path P in G induces a complete bipartite subgraph of G (with one side containing one vertex and the other side containing one or two vertices) and so, $u, v \in S$ with S being any maximal biclique containing P. Therefore, the claim is proved, and since $\mathrm{d}_B(u,v) = 2\,\mathrm{d}_{G^2}(u,v)$ for every $u, v \in V$, we obtain $\delta_B(V) = 2\delta(G^2)$. As a result:

$$2\delta(G^2) \leq \delta(B) \leq 2\delta(G^2) + 2,$$

$$2\delta(BK(G)) \leq \delta(B) \leq 2\delta(BK(G)) + 2.$$

By mixing up the two chains of inequality one obtains $2\delta(G^2) \leq 2\delta(BK(G)) + 2$ and $2\delta(BK(G)) \leq 2\delta(G^2) + 2$, whence $\delta(G^2) \leq \delta(BK(G)) + 1$ and $\delta(BK(G)) \leq \delta(G^2) + 1$. Since by Proposition 11 $(\delta(G) - 1)/2 \leq \delta(G^2) \leq (\delta(G) + 1)/2$, one obtains $\delta(BK(G)) \geq \delta(G^2) - 1 \geq (\delta(G) - 3)/2$ and $\delta(BK(G)) \leq (\delta(G) + 1)/2 + 1 \leq (\delta(G) + 3)/2$, as desired. □

In fact, we prove the more precise inequalities $\delta(G^2) - 1 \leq \delta(BK(G)) \leq \delta(G^2) + 1$ for every graph G, and we claim these bounds are sharp.

Corollary 14. *For every graph G, $\delta(G^2) - 1 \leq \delta(BK(G)) \leq \delta(G^2) + 1$, and these bounds are sharp.*

Proof. The bounds are given by Theorem 13. Also, let us now show that they are sharp.

Consider first the grid graph $G_{3,3}$. We have $\delta(BK(G_{3,3})) = \delta(K_9) = 0$, while $\delta(G_{3,3}^2) \geq 1$ because the four corners of the grid induce a cycle of length four in the square graph $G_{3,3}^2$. As a result, $\delta(BK(G_{3,3})) = \delta(G_{3,3}^2) - 1$, and so the lower-bound is reached.

Now, recall that the biclique graph of a complete graph K_n is exactly the line graph $L(K_n)$. Therefore, consider the graph K_4 and its line graph (G_1 and $L(G_1)$ in Figures 3i and 3j). Since $K_4^2 = K_4$ then it is indeed the case that $\delta(BK(K_4)) = \delta(L(K_4)) = \delta(K_4) + 1 = \delta(K_4^2) + 1$, and so the upper-bound is also reached. □

4.4. Additional bounds

Before we conclude this paper, let us present a few other results that are obtained within our framework. More precisely, given a graph $G = (V, E)$

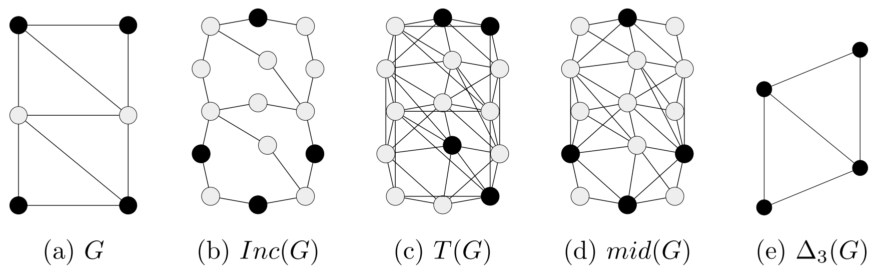


Figure 6: Some intersection graphs obtained from a triangular grid graph G. We have $\delta(G) = 1/2$, $\delta(Inc(G)) = 2$, $\delta(T(G)) = 1$, $\delta(mid(G)) = 1$, and $\delta(\Delta_3(G)) = 1/2$.

we consider the following extensions of line graphs (illustrations for each case are given in Figure 6).

The *incidence graph* of G, denoted by $Inc(G)$, has vertex set $V \cup E$ with an edge between every $u \in V$ and every $e \in E$ such that u is an end of e in G (see Figure 6b). It follows from the proof of Theorem 6 (for line graphs) that $2\delta(G) \leq \delta(Inc(G)) \leq 2\delta(G) + 2$ and the bounds are sharp.

The *total graph* of G [5], denoted by $T(G)$, is constructed from G and $L(G)$ by adding an edge between every $u \in V$ and every $e \in E$ such that u is an end of e in G (see Figure 6c). In fact, this implies $T(G) = (Inc(G))^2$, hence by Proposition 11 we have $(\delta(Inc(G)) - 1)/2 \leq \delta(T(G)) \leq (\delta(Inc(G)) + 1)/2$, and so, $\delta(G) - 1/2 \leq \delta(T(G)) \leq \delta(G) + 3/2$. One can sharpen the lower-bound and write $\delta(G) \leq \delta(T(G)) \leq \delta(G) + 3/2$ after noticing that G is an isometric subgraph (*i.e.*, a distance-preserving subgraph) of $T(G)$.

The *middle graph* of G [27], denoted by $mid(G)$, is constructed from $Inc(G)$ by adding an edge between every two "edge-vertices" $e, e' \in E$ sharing an end in G (see Figure 6d). Said differently, it is the intersection graph of all cliques of size two or less in G. Using a bipartite representation that is similar in spirit with those for line graphs (Theorem 6) and clique graphs (Theorem 8), one obtains $\delta(G) - 1 \leq \delta(mid(G)) \leq \delta(G) + 1$.

Last, the *k-edge graph* of G [26], denoted by $\Delta_k(G)$, is the intersection graph of all cliques of size k and maximal cliques of size at most $k-1$ in G (see Figure 6e). Note that if $k = 2$ then it is exactly the line graph, and if $k = n$ then it is exactly the clique graph. Again using a bipartite representation with similar properties as those for line graphs and clique graphs, one obtains $\delta(G) - 1 \leq \delta(\Delta_k(G)) \leq \delta(G) + 1$.

5. Conclusion

We have proved that the hyperbolicity of any bipartite graph can be approximated up to a small additive constant by only considering the smallest side of its bipartition. This means a decrease by half of the number of vertices to be considered, hence a speed-up in the computation of hyperbolicity. On a more theoretical side, we detailed a simple framework so as to bound the hyperbolicity of line graphs and several other intersection graphs. We let open the question whether our techniques could also be applied to more "exotic" generalizations of line graphs – say, edge clique graphs [10].

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Appendix E

Data center interconnection networks are not hyperbolic

Data center interconnection networks are not hyperbolic[*]

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Abstract

Topologies for data center interconnection networks have been proposed in the literature through various graph classes and operations. A common trait to most existing designs is that they enhance the symmetric properties of the underlying graphs. Indeed, symmetry is a desirable property for interconnection networks because it minimizes congestion problems and it allows each entity to run the same routing protocol. However, despite sharing similarities these topologies all come with their own routing protocol. Recently, generic routing schemes have been introduced which can be implemented for any interconnection network. The performances of such universal routing schemes are intimately related to the *hyperbolicity* of the topology. Roughly, graph hyperbolicity is a metric parameter which measures how close is the shortest-path metric of a graph from a tree metric (the smaller the gap the better). Motivated by the good performances in practice of these new routing schemes, we propose the first general study of the hyperbolicity of data center interconnection networks. Our findings are disappointingly negative: we prove that the hyperbolicity of most data center interconnection topologies scales linearly with their diameter, that it the worst-case possible for hyperbolicity. To obtain these results, we introduce original connection between hyperbolicity and the properties of the endomorphism monoid of a graph. In particular, our results extend to all vertex and edge-transitive graphs. Additional results are obtained for de Bruijn and Kautz graphs, grid-like graphs and networks from the so-called Cayley model.

Keywords. greedy routing scheme; metric embedding; graph endomorphism; Gromov hyperbolicity; Cayley graph; data center; interconnection network

1 Introduction

The network topologies that are used to interconnect the computing units of large-scale facilities (e.g., super computers, data centers hosting cloud applications, etc.) are designed to optimize various constraints such as equipment cost, deployment time, capacity and bandwidth, routing functionalities, reliability to equipment failures, power consumption, etc. This large variety of (conflicting) criteria has yielded numerous proposals of interconnection networks. See for instance [11, 12, 20, 47, 81] and [36, 38–40, 59] for the most recent ones. A common feature of the

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proposed constructions is to design network topologies offering a high-level of *symmetries*. Indeed, it is easier to balance the traffic load, and hence to minimize the congestion, on network topologies with a high-level of symmetry. Furthermore, it simplifies the initial wiring of the physical infrastructure and it ensures that each router node can run the protocol.

However, despite sharing properties, interconnection networks rely on specific routing algorithms that are optimized for each topology. As a novel step toward efficient and topology agnostic routing schemes, the authors in [64–66] proposed to use greedy routing schemes based on an embedding of the topology into certain metric space such as the hyperbolic metric space, and more recently the word metric space. This approach has been shown particularly efficient for Internet-like graphs [33, 42] where routes with low stretch are obtained. One explanation of this good behavior is that Internet-like graphs have low *hyperbolicity* [10, 74], a graph parameter providing sharp bounds on the stretch (or distortion) of the distances in a graph when it is embedded into an edge-weighted tree.

In this paper, we characterize or give upper and lower-bounds on the hyperbolicity of a broad range of interconnection network topologies. These bounds can be used to analyze the worst-case behavior of greedy routing schemes in these topologies. Before we present our results, let us further put in context the role they play in routing and in other distance-related problems.

Related work. Greedy routing schemes based on an embedding into the hyperbolic space have been introduced by Kleinberg in [33]. Since then, various authors explored further this approach [42, 45, 48]). In particular, they showed that the graphs of the Autonomous Systems of the Internet embed better into a hyperbolic space than into an Euclidean space[1]. It was only recently in [70] that a formal relationship between the performances of hyperbolic embeddings and the hyperbolicity was proved. Namely, the authors proved that the over-delay for such routing schemes, or equivalently the stretch of the routing, depends on the hyperbolicity. In [73], the authors proved that similar results hold for greedy routing schemes based on an embedding of the topology into some word metric space (*e.g.*, see [26] for more information). More precisely, they use hyperbolicity to upper-bound the complexity of their routings, as well as to bound the size of the automata that are involved in their routing schemes.

Their results add up to prior worst-case analysis of graph heuristics that already pointed out the important role played by the hyperbolicity. For instance, there are approximation algorithms for problems related to distances in graphs —like diameter and radius computation [37], and minimum ball covering [32]— whose approximation constant depends on the hyperbolicity. Sometimes the approximation factor is a universal constant but the algorithm relies on a data-structure whose size is proportional to the hyperbolicity of the network topology [31]. Geometric routing schemes in [42, 45, 48] do not make exception and so have a stretch *lower-bounded* by the hyperbolicity (the bound is reached by some of them).

There have been measurements to confirm that complex networks such as the graphs of the Autonomous Systems of the Internet, social networks and phylogenetic networks all have a low hyperbolicity. We refer to [60,62,63,71,74,77] for the most important studies in this area. Additional related work in [50,57] shows that the low hyperbolicity of complex networks may be a consequence

[1]In fact, it follows from [23] that for any n-vertex graph G there is an embedding φ of G into the Euclidean space (with unbounded dimension) such that for every $u, v \in V(G)$ we have $\mathrm{d}(\varphi(u), \varphi(v)) \leq \mathcal{O}(\sqrt{\log\log n}) \cdot \mathrm{d}_G(u, v) + \hat{\mathcal{O}}(\delta(G) \cdot \log n)$, with $\delta(G)$ being the hyperbolicity (the $\hat{\mathcal{O}}$-notation suppresses the polyloglog factors). However, it does not seem that hyperbolicity is the most relevant parameter in the study of Euclidean embeddings.

of some preferential attachment mechanisms. However, we are not informed of any study on the hyperbolicity of data center interconnection networks. In this paper, we aim to fill in this gap through a theoretical study of their underlying graphs.

Our contributions. In an attempt to confront with the diversity of interconnection network topologies proposed in the literature, we relate hyperbolicity with a few graph properties that are frequently encountered in these topologies. Indeed, we do not aim to provide a —long and non-exhaustive— listing of unrelated results for each network, but rather to exhibit a small number of their characteristics that are strongly related with their metric invariants. In particular, we relate hyperbolicity with the symmetries of a graph.

- We prove in Section 3 that for graphs whose center is a k-distance dominating set for some small value of k, the hyperbolicity scales linearly with the diameter. This class of graphs strictly contains graphs whose diameter equals the radius, *a.k.a.* the *self-centered graphs* [9, 14]. In particular, it comprises all vertex-transitive graphs (a strict subclass of self-centered graphs), as well as edge-transitive graphs. A main consequence of our result is that every interconnection network whose topology is based on a *Cayley graph* has large hyperbolicity[2].

- In addition, we prove that similar results hold for graphs admitting an *endomorphism* such that the distance between any vertex and its symmetric image is large. On the way to prove these results, we define a new graph invariant which is called *weak mobility*, that generalizes the so-called graph mobility (*e.g.*, see [22, 34]). We use these new results to improve our lower-bounds on the hyperbolicity of several interconnection networks.

- For completeness, we also characterize the hyperbolicity of other "symmetric" networks such as de Bruijn, Kautz and grid-like graphs. More precisely, we apply different techniques that are based on their shortest-paths distribution so that we can prove in Section 4 that they also have a large hyperbolicity. The techniques that are involved in the proofs have been introduced in previous papers [16, 41], but to the best of our knowledge the way we use them in this work is new.

  All of the above results are summarized in Table 1.

- Last, we extend our results in Section 5 to *heterogenous* data center interconnection networks. That is, we relate hyperbolicity with several graph operations, most of them being introduced in the Cayley model of [59] in order to enhance some desirable properties of data center interconnection networks.

Our main message is that existing designs in the literature yield graphs with the highest possible value for the hyperbolicity —w.r.t. their diameter. On the negative side, it means that any greedy routing scheme whose stretch depends on the hyperbolicity is not scalable enough to cope with large data centers. But on a more positive side, it also implies that any routing scheme relying on

[2] Independently from this work, the authors in [54] proved that for any vertex-transitive graph, the hyperbolicity scales linearly with the diameter. However, their proof relies on another definition of hyperbolicity, and it is unclear whether the proof can be extended to other graph classes. By contrast, our proof yields a tighter lower-bound for hyperbolicity, and it relies on a much simpler and more general argument (*i.e.*, see Theorem 4). Especially, it also applies to edge-transitive graphs.

a data-structure with size proportional to the hyperbolicity solely requires *sublogarithmic* space in the number of servers. Indeed, it is well-known that the data center interconnection networks often have a diameter that is logarithmic or sublogarithmic in their size.

We start this paper providing useful notations and definitions in Section 2, and we conclude it in Section 6 with open questions. Especially, can we infer a formal relationship between network congestion and graph hyperbolicity ?

2 Preliminaries

A data center is a facility that is used to house resources such as computer systems, servers, etc. Data center resources are interconnected using communication networks, that are called data center interconnection networks. They are modeled as a graph where the vertices are the data center resources (*e.g.*, computing units) and there is an edge between two resources if they are directly connected in the network. Different graph classes have been proposed in order to design data center interconnection networks [11, 12, 20, 36, 38–40, 47, 59, 81]. In what follows, our results apply to general graphs, but they are aimed at providing good lower-bounds on the hyperbolicity for these specific topologies.

We refer to [80, 82] for the usual graph terminology. Graphs in this study are finite, simple (hence, without loop nor multiple edges), connected and unweighted.

2.1 Metric graph theory

Given a connected graph $G = (V, E)$, the *distance* between any two vertices $u, v \in V$ is defined as the minimum number of edges on a uv-path. We will denote it by $\mathrm{d}_G(u, v)$, or by $\mathrm{d}(u, v)$ whenever G is clear from the context. For any subset $S \subseteq V$, the *eccentricity* of vertex $v \in S$, denoted $\mathrm{ecc}_G(v, S)$, is defined as the maximum distance in G between v and any other vertex in S. The *radius* of S is defined as the least eccentricity of vertices in S and is denoted by $\mathrm{rad}_G(S)$, while the *diameter* of S is defined as the largest eccentricity of vertices in S and is denoted by $\mathrm{diam}_G(S)$. Observe that it always holds $\mathrm{rad}_G(S) \leq \mathrm{diam}_G(S) \leq 2 \cdot \mathrm{rad}_G(S)$. In particular, for any vertex $v \in V$, we denote by $\mathrm{ecc}(v) = \mathrm{ecc}_G(v, V)$, $\mathrm{rad}(G) = \mathrm{rad}_G(V)$ and $\mathrm{diam}(G) = \mathrm{diam}_G(V)$. The *center* $\mathcal{C}(G)$ of the graph is the subset of all vertices with minimum eccentricity $\mathrm{rad}(G)$. We call the graph G *self-centered* if it holds $\mathrm{diam}(G) = \mathrm{rad}(G)$ *i.e.*, every vertex of G is in the center.

Last, we define graph hyperbolicity as follows.

Definition 1 (4-points Condition, [10]). Let G be a connected graph.

For every 4-tuple u, v, x, y of G, we define $\delta(u, v, x, y)$ as half of the difference between the two largest sums amongst:

$$S_1 = \mathrm{d}(u, v) + \mathrm{d}(x, y),\ S_2 = \mathrm{d}(u, x) + \mathrm{d}(v, y),\ \text{and}\ S_3 = \mathrm{d}(u, y) + \mathrm{d}(v, x).$$

The graph hyperbolicity, denoted by $\delta(G)$, is equal to $\max_{u,v,x,y} \delta(u, v, x, y)$.

Moreover, we say that G is *δ-hyperbolic*, for every $\delta \geq \delta(G)$.

Other definitions exist for the hyperbolicity, but they are pairwise equivalent up to a constant-factor (*e.g.*, see [10] for details). So far, the hyperbolicity of a few graph classes has been characterized such as: random graphs [56, 61, 69], chordal graphs [25], k-chordal graphs [53], outerplanar

Name	Degree max.	Diameter	Order	δ	Proof
de Bruijn graph, $UB(d,D)$	$2d$	D	d^D	$\frac{1}{2}\left\lfloor \frac{D}{2} \right\rfloor \leq \delta \leq \left\lfloor \frac{D}{2} \right\rfloor$	Prop. 37
Kautz graph, $UK(d,D)$	$2d$	D	$d^D(d+1)$	$\left\lfloor \frac{D}{4} \right\rfloor + \varepsilon \leq \delta \leq \left\lfloor \frac{D}{2} \right\rfloor, \varepsilon \in \{0,1\}$	Prop. 40
Shuffle exchange, $SE(n)$	3	$2n-1$	2^n	$\frac{1}{2}\left\lfloor \frac{n}{2} \right\rfloor \leq \delta \leq n-1$	Prop. 42
(n,m)-grid	4	$n+m-2$	nm	$\min\{n,m\}-1$	Cor. 48
d-dimensional grid of size s	$2d$	$d(s-1)$	s^d	$(s-1)\left\lfloor \frac{d}{2} \right\rfloor$	Cor. 49
Triangular (n,m)-grid	6	$n+m-2$	nm	$\frac{\min\{n,m\}-1}{2}$	Lem. 51
Hexagonal (n,m)-grid	6	$\begin{cases} n-1+\left\lceil \frac{m-1}{2} \right\rceil & \text{when } m \leq 2n-1 \\ m-1 & \text{otherwise} \end{cases}$	nm	$\frac{\min\{n,m\}-1}{2}$	Lem. 53
Cylinder (n,m)-grid	4	$\left\lfloor \frac{n}{2} \right\rfloor + m - 1$	nm	$\min\left\{\left\lfloor \frac{n}{2} \right\rfloor, \frac{1}{2}\left(\left\lfloor \frac{n}{2} \right\rfloor + m\right) - \varepsilon\right\}, \varepsilon \in \left\{\frac{1}{2}, 1\right\}$	Lem. 55
Torus (n,m)-grid	4	$\left\lfloor \frac{n}{2} \right\rfloor + \left\lfloor \frac{m}{2} \right\rfloor$	nm	$\left\lfloor \frac{1}{2}\left(\left\lfloor \frac{n}{2} \right\rfloor + \left\lfloor \frac{m}{2} \right\rfloor\right)\right\rfloor - 1 \leq \delta \leq \left\lfloor \frac{1}{2}\left(\left\lfloor \frac{n}{2} \right\rfloor + \left\lfloor \frac{m}{2} \right\rfloor\right)\right\rfloor$	Lem. 11
Gen. hypercube, $G(m_1,\ldots,m_r)$	$\sum_{i=1}^{r} m_i - r$	r	$\prod_{i=1}^{r} m_i$	$\left\lfloor \frac{r}{2} \right\rfloor$	Lem. 13
Cube Connected Cycle, $CCC(n)$	3	$2n-2+\max\left\{2, \left\lfloor \frac{n}{2} \right\rfloor\right\}$	$n2^n$	$n \leq \delta \leq n-1+\left\lfloor \frac{\max\{2,\lfloor \frac{n}{2} \rfloor\}}{2} \right\rfloor$	Lem. 15
BCube$_k(n)$	$\max\{n,k+1\}$	$2(k+1)$	$2^k(n+k+1)$	$k+1$	Lem. 17
Fat-Tree$_k$	k	6	$\frac{k^2}{4}(k+5)$	2	Lem. 19
Butterfly graph, $BF(n)$	4	$2n$	$2^n(n+1)$	n	Lem. 21
Wrapped Butterfly graph, $WBF(n)$	4	$n+\left\lfloor \frac{n}{2} \right\rfloor$	$2^n(n+1)$	$\left\lfloor \frac{n}{2} \right\rfloor \leq \delta \leq \left\lfloor \frac{1}{2}\left(n+\left\lfloor \frac{n}{2} \right\rfloor\right)\right\rfloor$	Lem. 21
k-ary n-fly	$2k$	$2n$	$k^n(n+1)$	n	Lem. 23
k-ary n-tree	$3k$	$2n$	$k^{n-1}(n+k)$	$n-1$	Lem. 25
d-ary tree grid, $MT(d,h)$	$d+1$	$4h$	$d^h\left(d^h+2\frac{d^h-1}{d-1}\right)$	$2h$	Lem. 27
Bubble-sort graph, $BS(n)$	$n-1$	$\binom{n}{2}$	$n!$	$\left\lfloor \frac{n(n-1)}{4} \right\rfloor$	Lem. 30
Transposition graph, $T(n)$	$\binom{n}{2}$	$n-1$	$n!$	$\frac{1}{2}\left\lfloor \frac{n-1}{2} \right\rfloor \leq \delta \leq \left\lfloor \frac{n-1}{2} \right\rfloor$	Lem. 32
Star graph, $S(n)$	$n-1$	$\left\lfloor \frac{3(n-1)}{2} \right\rfloor$	$n!$	$\left\lfloor \frac{1}{2}\left\lfloor \frac{3(n-1)}{2} \right\rfloor - \frac{1}{2} \right\rfloor \leq \delta \leq \left\lfloor \frac{1}{2}\left\lfloor \frac{3(n-1)}{2} \right\rfloor \right\rfloor$	Lem. 34
Cayley graph, $G(\Gamma,S)$	$2\lvert S\rvert$	$\operatorname{diam}(G(\Gamma,S))$	$\lvert\Gamma\rvert$	$\frac{1}{2}\left\lfloor \frac{\operatorname{diam}(G(\Gamma,S))}{2} \right\rfloor \leq \delta \leq \left\lfloor \frac{\operatorname{diam}(G(\Gamma,S))}{2} \right\rfloor$	Cor. 5

Table 1: Summary of results

graphs [67] and other geometrical graph classes [37]. Lower and upper-bounds for the hyperbolicity are obtained in [58] using graph invariants, and also in [52, 67] using graph decompositions. We refer to [44] for a compelling of many well-known facts about hyperbolicity. In particular, we will make use of the following upper-bound for hyperbolicity:

Lemma 2 ([10, 44, 74]). *For every connected graph G, it holds that $\delta(G) \leq \left\lfloor \frac{\operatorname{diam}(G)}{2} \right\rfloor$.*

Based on Lemma 2, the authors in [71] have proposed the following classification of finite graphs. A graph G is *strongly hyperbolic* if $\delta(G) = \mathcal{O}(\log(\log(diam(G))))$, *hyperbolic* if $\delta(G) = \mathcal{O}(\log(diam(G)))$, and *non hyperbolic* otherwise. We follow their terminology and we aim at proving that some graph classes are non hyperbolic. This is in contrast with many graph classes in the literature that have a constant upper-bound on their hyperbolicity, and so, that are strongly hyperbolic [53]. By Lemma 2, in order to prove that a graph is non hyperbolic, and more precisely that its hyperbolicity scales linearly with its diameter, it suffices to prove that one can *lower-bound* the hyperbolicity with the diameter —up to a constant-factor. This line of work was followed in [21, 76] to prove that expander graphs are non hyperbolic. Our proofs will make use of the notion of *isometric subgraphs*, the latter denoting a subgraph H of a graph G such that $\mathrm{d}_H(u,v) = \mathrm{d}_G(u,v)$ for any two vertices $u, v \in H$.

2.2 Algebraic graph theory

A graph *endomorphism* is a mapping σ from the vertex-set of a graph G to itself which preserves the adjacency relations, *i.e.*, for every $\{u,v\} \in E(G)$ we have that $\{\sigma(u), \sigma(v)\} \in E(G)$.

Definition 3. Let $G = (V, E)$ be a graph. Given an endomorphism σ of G, the *mobility* of σ is equal to $\min_{v \in V} \mathrm{d}(v, \sigma(v))$. The *weak mobility* of G is the largest integer l such that it admits an endomorphism with mobility l.

We note that a graph endomorphism might fail to preserve the *non-adjacency* relations, but it does so if it is a graph *automorphism*, *i.e.*, a one-to-one endomorphism. In particular a graph endomorphism σ is called *idempotent* if for every $v \in V(G)$ it holds that $\sigma^2(v) = v$, and in such a case it is an automorphism.

A graph is called *vertex-transitive* if for every $u, v \in V(G)$, there is an automorphism σ such that $\sigma(u) = v$. Similarly, we call a graph *edge-transitive* if for every $e = \{u,v\}, e' = \{u',v'\} \in E(G)$, there is an automorphism σ such that $\{\sigma(u), \sigma(v)\} = \{u', v'\}$. We emphasize that every vertex-transitive graph is self-centered. We will use this property in the following sections. Finally, let $(\Gamma, \cdot)$ be a group and let S be a generating set of Γ that is symmetric and that does not contain the neutral element of group Γ, *i.e.*, $S = S^{-1}$ and $S \cap S^{-1} = \emptyset$. The *Cayley graph* $G(\Gamma, S)$ of group Γ w.r.t. S has vertex-set Γ and edge-set $\{\{g, g \cdot s\} \mid g \in \Gamma, s \in S\}$. It is well-known that every Cayley graph is vertex-transitive [12].

3 The metric properties of the endomorphism monoid of a graph

Our belief is that any method to lower-bound the value of hyperbolicity needs to rely *as few as possible* on the shortest-path distribution of the graphs so as to be of practical use. Indeed, in most cases there is no good characterization of this distribution. There even exist interconnection networks topologies the diameter of which is still unknown [3,46]. In a need of more robust methods, we introduce new lower-bounds on the hyperbolicity that are based on non-trivial symmetries of the graphs. For clarity, our results are presented separately from their applications to interconnection networks topologies.

3.1 Main results

We first introduce a very generic argument to obtain lower-bounds on the hyperbolicity. In particular, we will show that it applies to highly symmetric graphs such as transitive graphs.

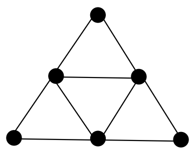


Figure 1: A self-centered graph G with $diam(G) = rad(G) = 2$, while $\delta(G) = 1/2 = diam(G)/4$.

Theorem 4. *Let G be a connected graph, and let $k \geq 0$ be such that all vertices are at distance at most k from the center of G. Then, $\delta(G) \geq \frac{1}{2} \cdot \left\lfloor \frac{\text{diam}(G)}{2} \right\rfloor - \frac{k}{2}$ and this bound is sharp.*

Proof. Let $\mathcal{C}(G)$ be the center of G. By the hypothesis every node in G is at distance at most k from $\mathcal{C}(G)$, therefore $\text{diam}_G(\mathcal{C}(G)) \geq \text{diam}(G) - 2k$. Moreover, by [37, Proposition 5] $\text{diam}_G(\mathcal{C}(G)) \leq 4\delta(G) + 1$. Consequently, it holds $\delta(G) \geq \lfloor \text{diam}_G(\mathcal{C}(G))/2 \rfloor /2 \geq \lfloor \text{diam}(G)/2 \rfloor /2 - k/2$.

The lower-bound is sharp, as shown with the example of Figure 1 where $diam(G) = rad(G) = 2$ while $\delta(G) = 1/2 = diam(G)/4$. □

Unlike all other techniques that we will discuss next, we can use the lower-bound of Theorem 4 to prove that all graphs studied in this work are non hyperbolic. However, the bounds obtained with this first method are usually loose, and they never outmatch the bounds obtained with the other techniques — when they apply. We will illustrate this point in what follows.

It is straightforward that Theorem 4 applies to self-centered graphs (with $k = 0$). Especially, it applies to vertex-transitive graphs.

Corollary 5. *Let G be a connected vertex-transitive graph. Then, $\delta(G) \geq \frac{1}{2} \cdot \left\lfloor \frac{\text{diam}(G)}{2} \right\rfloor$ and this bound is sharp.*

The lower-bound of Corollary 5 is sharp, as shown by any clique (that has diameter one and null hyperbolicity).

On the practical side, most of the interconnection networks topologies are based on vertex-transitive graphs. This comprises hypercube-based networks [8], generalized Petersen graphs [1,18], generalized Heawood graphs [30,68] and Cayley graphs [12]. For some of these topologies such as the Pancake graph [3], a well-known Cayley graph, Corollary 5 is the best lower-bound on the hyperbolicity we know so far.

Corollary 6. *Let G be a connected edge-transitive graph. Then, $\delta(G) \geq \frac{1}{2} \cdot \left\lfloor \frac{\text{diam}(G)}{2} \right\rfloor - \frac{1}{2}$ and this bound is sharp.*

Proof. We first claim that the center $\mathcal{C}(G)$ is a dominating set of G. Indeed, let $u \in V(G)$ and $v \in \mathcal{C}(G)$, and let $x \in N_G(u)$ and $y \in N_G(v)$. Since G is edge-symmetric by the hypothesis, there exists an automorphism σ such that $\{\sigma(v), \sigma(y)\} = \{u, x\}$. Furthermore $\sigma(v) \in \mathcal{C}(G)$ because σ is an automorphism and so, $\mathrm{d}_G(u, \mathcal{C}(G)) \leq \mathrm{d}_G(u, \sigma(v)) \leq 1$ which proves the claim. As a result, we can apply Theorem 4 by setting $k = 1$.

The lower-bound is sharp, as shown by any star (that has diameter two and null hyperbolicity). □

3.1.1 Improved lower-bounds using graph endomorphisms

However, despite its wide applicability to interconnection networks, the above Corollaries 5 and 6 require graphs to have an automorphism group with constrained properties. A natural question is whether we can weaken the requirements by considering endomorphisms instead of automorphisms. To answer this question, we use weakly vertex-transitive graphs that have been defined in [29] in a similar fashion to vertex-transitive graphs. Namely, a graph G is weakly vertex-transitive if, for any two vertices $u, v \in V(G)$ there exists a graph *endomorphism* σ satisfying $\sigma(u) = v$. Unlike vertex-transitive graphs, the gap between hyperbolicity and diameter may be arbitrarily large for weakly vertex-transitive graphs. Indeed, on the one hand it was proved in [29] that bipartite graphs are weakly vertex-transitive. On the other hand, trees are bipartite 0-hyperbolic graphs, whereas they may have a diameter that is arbitrarily large. We now show that surprisingly, some lower-bounds on the hyperbolicity can still be deduced from graph endomorphisms.

Theorem 7. *Let G be a connected graph of weak mobility $l \geq 2$. Then it holds $\delta(G) \geq \frac{1}{2} \cdot \left\lceil \frac{l}{2} \right\rceil$.*

Proof. We will consider a graph game which is a slight variation of the well-known 'Cop and Robber' game (*e.g.* see [5–7]). There are two players in this game that are playing alternatively on a (connected) graph, by moving along a path of length at most s, for some positive integer s. The first player to position herself on the graph is the Cop, and the second player is called the Robber. Last a graph is said *Cop-win* for this game if the Cop always has a winning-strategy *i.e.*, she can always reach the position of the Robber in a finite number of moves, and hence eventually catch the Robber. In [49] the authors proved that every connected graph G is Cop-win whenever $s \geq 4\delta(G)$. So, to prove the theorem we claim that it suffices to show that G is not Cop-win if $s \leq l - 1$. Indeed, in such a case it holds $4\delta(G) \geq l$, hence $2\delta(G) \geq l/2$ that implies $2\delta(G) \geq \lceil l/2 \rceil$ and so, $\delta(G) \geq \lceil l/2 \rceil / 2$. Equivalently, we will exhibit a winning-strategy for the Robber in such a case.

Let σ be an endomorphism of G with mobility l, that exists by the hypothesis. One can observe that if at each turn of the Cop the Robber is onto the image by σ of her current position, then it is a winning strategy for the Robber because by the hypothesis, both vertices are at distance at least l, and the maximum speed of the Cop is $l-1$. To achieve the result, let us proceed as follows. First if the Cop picks vertex u as her initial position then the Robber starts the game at vertex $\sigma(u)$. Then, if the Cop moves along a path $(u = x_0, x_1, \ldots, x_i, \ldots, x_k = v)$, $k \leq l - 1$, then the Robber moves along the path $(\sigma(u), \sigma(x_1), \ldots, \sigma(x_i), \ldots, \sigma(v))$ which exists because σ is a graph endomorphism. Such a move for the Robber is valid as long as $v \notin \{\sigma(u), \sigma(x_1), \ldots, \sigma(x_i), \ldots, \sigma(v)\}$, and that is always the case since $\sigma(x_i) = v$ would imply $\mathrm{d}(x_i, \sigma(x_i)) \leq l - 1$. □

We are particularly interested in the special case of the graphs G with weak mobility equal to their diameter $diam(G)$. These graphs are self-centered, and so, their hyperbolicity is at least

$\lfloor diam(G)/2 \rfloor/2$ by Theorem 4. The lower-bound is slightly improved by Theorem 7 in this situation. However, not all self-centered graphs have their weak mobility equal to the diameter [34].

In what follows, we will mostly rely upon the below refinement of Theorem 7 in our proofs. This way, we will obtain almost tight bounds on the hyperbolicity of data center interconnection networks. However, note that the following results require stronger constrictions on the endomorphism monoid than Theorem 7.

Theorem 8. *Let G be a connected graph, and l, l' be two non-negative integers. Suppose there exists an endomorphism σ of G with mobility l and such that for every $v \in V(G)$, $\mathrm{d}(v, \sigma^2(v)) \le l'$. Then, it holds $\delta(G) \ge \lfloor \frac{l}{2} \rfloor - \frac{l'}{2}$.*

Proof. Clearly, if $l \le l'$ then $\delta(G) \ge 0 \ge \lfloor l/2 \rfloor - l'/2$. Therefore, we will assume w.l.o.g. that $l \ge l' + 1$. Let $u \in V(G)$ minimizing $\mathrm{d}_G(u, \sigma(u))$ and let v be on a $u\sigma(u)$-shortest-path such that $\mathrm{d}_G(u, v) = \lfloor \mathrm{d}_G(u, \sigma(u))/2 \rfloor$. Then, we deduce from the endomorphism σ the following inequalities:

$$\begin{aligned}
S_1 &= \mathrm{d}(u, \sigma(u)) + \mathrm{d}(v, \sigma(v)) \ge 2 \cdot \mathrm{d}(u, \sigma(u)) \ge 2l; \\
S_2 &= \mathrm{d}(u, v) + \mathrm{d}(\sigma(u), \sigma(v)) \le 2 \cdot \mathrm{d}(u, v) \le 2 \lfloor \mathrm{d}(u, \sigma(u))/2 \rfloor; \\
S_3 &= \mathrm{d}(u, \sigma(v)) + \mathrm{d}(v, \sigma(u)) \le \mathrm{d}(u, \sigma^2(u)) + \mathrm{d}(\sigma^2(u), \sigma(v)) + \mathrm{d}(v, \sigma(u)) \le l' + 2 \cdot \mathrm{d}(v, \sigma(u)) \\
&\le 2 \lceil \mathrm{d}(u, \sigma(u))/2 \rceil + l' \le \mathrm{d}(u, \sigma(u)) + 1 + l'.
\end{aligned}$$

In such a case, $S_1 \ge \max\{S_2, S_3\}$ and as a result:

$$\delta(G) \ge \delta(u, v, \sigma(u), \sigma(v)) \ge \min\left(\left\lceil \frac{\mathrm{d}(u, \sigma(u))}{2} \right\rceil, \left\lfloor \frac{\mathrm{d}(u, \sigma(u))}{2} \right\rfloor - \frac{l'}{2} \right) \ge \left\lfloor \frac{l}{2} \right\rfloor - \frac{l'}{2}.$$

□

The lower-bound of Theorem 8 outmatches the one of Theorem 7 when $l' \le \lfloor l/2 \rfloor - 1$. Furthermore, in practice, we will use Theorem 8 with $l = diam(G)$ and $l' \in \{0, 1\}$. This way, we will improve by a factor two all previous lower-bounds.

It can be noticed that the lower-bound of Theorem 8 is sharp for almost every cycle. Indeed, let $\mathbb{Z}_n$ be the vertex set of the n-cycle C_n, and let σ be the automorphism mapping any vertex i to the vertex $i + \lfloor n/2 \rfloor \pmod n$. Applying Theorem 8 to σ, we obtain a lower-bound $\lfloor n/4 \rfloor$ for the hyperbolicity of even-length cycles, which is exact, and a lower-bound $\lfloor n/4 \rfloor - 1/2$ for odd-length cycles, which is exact when $n \equiv 1 \pmod 4$ and below $1/2$ of the true hyperbolicity when $n \equiv 3 \pmod 4$ [28, 53].

We emphasize on the following consequence of Theorem 8.

Corollary 9. *Let G be a connected graph and σ be an idempotent endomorphism with mobility l. Then, it holds $\delta(G) \ge \lfloor \frac{l}{2} \rfloor$.*

Proof. By the hypothesis, the endomorphism σ is idempotent and so, we can apply Theorem 8 by setting $l' = 0$. □

In the special case when $l = diam(G)$, the lower-bound of Corollary 9 is best possible. Indeed, it coincides with the upper-bound of Lemma 2, thereby giving the exact value for hyperbolicity.

It is natural to ask whether Theorems 7 and 8 can be further improved by using bounds on the distances $\mathrm{d}(v, \sigma^3(v)), \mathrm{d}(v, \sigma^4(v))$ and so on. However, answering this question is nontrivial since the techniques used for Theorems 7 and 8 are already quite different. We leave it as an interesting open question.

3.2 Applications

Equipped with Theorems 7, 8 and Corollary 9, we subsequently apply them on a broad range of topologies studied in the literature. We will combine the lower-bounds that we obtain with a slight variation of the well-known upper-bound of Lemma 2. Indeed it is folklore that the hyperbolicity of a graph is the maximum hyperbolicity taken over all of its biconnected components. So, $\delta(G) \leq \lfloor \mathrm{effdiam}(G)/2 \rfloor$, where the so-called *efficient diameter* $\mathrm{effdiam}(G)$ denotes the largest diameter amongst the biconnected components of the graph. This way, we will show that for most graphs found in the literature, their hyperbolicity scales linearly with the efficient diameter —that is the worst-case possible for hyperbolicity.

3.2.1 Torus

Let us first consider the torus, a well-known grid-like graph which is highly symmetrical. Other grid-like graphs will be considered in Section 4.2 using a different approach.

Definition 10. The *torus* (n, m)-grid has vertex-set $\mathbb{Z}_n \times \mathbb{Z}_m$; any two vertices $(i, j), (i', j')$ are adjacent if either $i' = i, j' \equiv j + 1 \pmod m$, or $i' \equiv i + 1 \pmod n, j' = j$.

Lemma 11. *Let $n = 2p + r,\ m = 2q + s$, with $r, s \in \{0, 1\}$. Then, the hyperbolicity $\delta_{n,m}$ of the torus (n, m)-grid satisfies:*

$$\left\lfloor \frac{1}{2} \cdot \left(\left\lfloor \frac{n}{2} \right\rfloor + \left\lfloor \frac{m}{2} \right\rfloor \right) \right\rfloor - \frac{r+s}{2} \leq \delta_{n,m} \leq \left\lfloor \frac{1}{2} \cdot \left(\left\lfloor \frac{n}{2} \right\rfloor + \left\lfloor \frac{m}{2} \right\rfloor \right) \right\rfloor .$$

Proof. For any two vertices $u = (i_u, j_u), v = (i_v, j_v)$:

$$\mathrm{d}(u, v) = \min\{|i_u - i_v|, n - |i_u - i_v|\} + \min\{|j_u - j_v|, m - |j_u - j_v|\}.$$

It implies that the diameter of the torus grid is $\lfloor n/2 \rfloor + \lfloor m/2 \rfloor$ and so, $\delta_{n,m} \leq \lfloor (\lfloor n/2 \rfloor + \lfloor m/2 \rfloor)/2 \rfloor$ by Lemma 2. Finally, let σ be the automorphism of the torus grid which maps any vertex (i, j) to the vertex $(i + \lfloor n/2 \rfloor \pmod n, j + \lfloor m/2 \rfloor \pmod m)$. Since for any vertex v, $\mathrm{d}(v, \sigma(v)) = \lfloor n/2 \rfloor + \lfloor m/2 \rfloor$ and $\mathrm{d}(v, \sigma^2(v)) = r + s$, then it follows from Theorem 8 that $\delta_{n,m} \geq \lfloor (\lfloor n/2 \rfloor + \lfloor m/2 \rfloor)/2 \rfloor - \frac{r+s}{2} \geq \lfloor (\lfloor n/2 \rfloor + \lfloor m/2 \rfloor)/2 \rfloor - 1$. □

3.2.2 Hybercube-like networks

Definition 12 ([8, 11])**.** Let $m_1, m_2, \ldots, m_r$ be positive integers with for every i, $m_i \geq 2$ and $r \geq 1$. The generalized hypercube $G(m_1, m_2, \ldots, m_r)$ has vertex-set $\{(x_1, x_2, \ldots, x_r) \mid \forall i, 0 \leq x_i \leq m_i - 1\}$, and two vertices $(x_1, x_2, \ldots, x_r), (y_1, y_2, \ldots, y_r)$ are adjacent in the graph if and only if their Hamming distance $\sum_i \mathbb{I}_{\{x_i \neq y_i\}}$ is equal to 1.

In particular, the k-ary hypercube $H_k(n)$ is the generalized hypercube $G(m_1, m_2, \ldots, m_n)$ with for every i, $m_i = k$.

Lemma 13. $\delta\left(G(m_1, m_2, \ldots, m_r)\right) = \left\lfloor \frac{r}{2} \right\rfloor$.

Proof. The diameter of $G(m_1, m_2, \ldots, m_r)$ is r and so, $\delta\left(G(m_1, m_2, \ldots, m_r)\right) \leq \lfloor r/2 \rfloor$ by Lemma 2. To prove the lower-bound, we first make the observation that the binary hypercube $H_2(r)$ is an isometric subgraph of $G(m_1, m_2, \ldots, m_r)$. Let σ be the automorphism mapping any vertex

$(x_1, x_2, \ldots, x_r) \in V(H_2(r))$ to its *complementary* vertex $(1-x_1, 1-x_2, \ldots, 1-x_r)$. Note that σ has mobility r and it is idempotent. As a result, we conclude by Corollary 9 that $\delta(G(m_1, m_2, \ldots, m_r)) \geq \delta(H_2(r)) \geq \lfloor r/2 \rfloor$. □

As we will show later, Lemma 13 also follows from Corollary 49 and the fact that the n-dimensional grid of size 2 is exactly the hypercube $H_2(n)$.

Definition 14 ([4]). The cube-connected-cycle $CCC(n)$ has vertex-set the pairs $\langle i, w\rangle$, for $0 \leq i \leq n-1$ and for w any binary word of length n; two vertices $\langle i, x_1x_2\ldots x_n\rangle$ and $\langle j, y_1y_2\ldots y_n\rangle$ are adjacent in the graph if and only if either $i = j$, $x_i = 1 - y_i$ and for every $k \neq i$, $x_k = y_k$; or $i \equiv j+1 \pmod n$ and for every k, $x_k = y_k$.

Lemma 15. $n \leq \delta(CCC(n)) \leq n - 1 + \left\lfloor \max\left\{1, \frac{1}{2} \cdot \left\lfloor \frac{n}{2} \right\rfloor\right\}\right\rfloor$.

Proof. By [19], $\mathrm{diam}(CCC(n)) = 2n-2+\max\{2, \lfloor n/2\rfloor\}$ and so, $\delta(CCC(n)) \leq n-1+\lfloor(\max\{2, \lfloor n/2\rfloor\})/2\rfloor$ by Lemma 2. Furthermore, the mapping $\sigma : \langle i, w\rangle \to \langle i, \bar{w}\rangle$ is an idempotent endomorphism and it has mobility $2n$ by [19]. We conclude by Corollary 9 that $\delta(CCC(n)) \geq n$. □

Definition 16 ([39]). Let $\mathbb{Z}_n^l$ be the set of words of length l over the alphabet $\{0, 1, \ldots, n-1\}$. The graph $\mathrm{BCube}_k(n)$ has vertex-set $\mathbb{Z}_n^{k+1} \cup \left(\{0, 1, \ldots, k\} \times \mathbb{Z}_n^k\right)$ and edge-set $\{\{\langle l, s_ks_{k-1}\ldots s_{l+1}s_{l-1}\ldots s_0\rangle, s_ks_{k-1}\ldots s_{l+1}s_ls_{l-1}\ldots s_0\} \mid 0 \leq l \leq k$ and for every $i, 0 \leq s_i \leq n-1\}$.

Lemma 17. $\delta(\mathrm{BCube}_k(n)) = k+1$.

Proof. By [43] $\mathrm{diam}(\mathrm{BCube}_k(n)) = 2(k+1)$ and so, $\delta(\mathrm{BCube}_k(n)) \leq k+1$ by Lemma 2. Then, let us assume that $n = 2$ because we have by [43] that $\mathrm{BCube}_k(2)$ is an isometric subgraph of $\mathrm{BCube}_k(n)$. We define the automorphism σ satisfying that for all binary word $w \in \mathbb{Z}_2^{k+1}$, $\sigma(w) = \bar{w}$, and for every pair $< l, w > \in \{0, 1, \ldots, k\} \times \mathbb{Z}_2^k$, $\sigma(< l, w >) = < l, \bar{w} >$. By [39, 43] σ has mobility $2(k+1)$ and so, by noticing that σ is idempotent we can conclude by Corollary 9 that $\delta(\mathrm{BCube}_k(n)) \geq \delta(\mathrm{BCube}_k(2)) \geq k+1$. □

3.2.3 Tree-like networks

Definition 18 ([36]). Let $k \geq 4$ be even. The Fat-Tree$_k$ is a graph with vertex-set that is partitioned into four layers:

1. a *core layer*, labeled with $\{0\} \times \mathbb{Z}_{(k/2)^2}$;
2. an *aggregation layer*, labeled with $\{1\} \times \mathbb{Z}_k \times \mathbb{Z}_{k/2}$. For every $0 \leq i \leq (k/2)^2 - 1$ the vertex labeled $\langle 0, i\rangle$ in the core layer is adjacent to all the vertices labeled $\langle 1, j, i \pmod k/2\rangle$ in the aggregation layer, with $0 \leq j \leq k-1$;
3. an *edge layer*, labeled with $\{2\} \times \mathbb{Z}_k \times \mathbb{Z}_{k/2}$. For every $0 \leq i \leq k-1$ there is a complete join between the subsets of vertices $\{\langle 1, i, j\rangle \mid 0 \leq j \leq k/2 - 1\}$ and $\{\langle 2, i, j\rangle \mid 0 \leq j \leq k/2 - 1\}$;
4. finally, a *server layer* labeled with $\{3\} \times \mathbb{Z}_k \times \mathbb{Z}_{(k/2)^2}$. For any $0 \leq q, r < k/2$ the vertex labeled $\langle 3, k, (k/2)q + r\rangle$ in the server layer is adjacent to the vertex labeled $\langle 2, k, q\rangle$ in the edge layer.

An example of a Fat-Tree$_4$ is given in Figure 2.

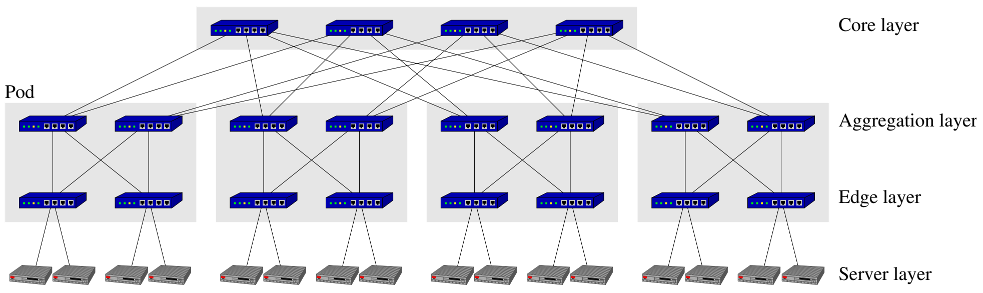


Figure 2: The graph Fat-Tree$_4$.

Lemma 19. $\delta\left(\text{Fat-Tree}_k\right) = 2$.

Proof. By construction, every vertex in the server layer is a pending vertex, that is a vertex of degree one. As a result, it can be ignored for the computation of hyperbolicity because the hyperbolicity of a graph is equal to the maximum hyperbolicity taken over all its biconnected components. It follows that the efficient diameter of Fat-Tree$_k$ is 4, hence $\delta\left(\text{Fat-Tree}_k\right) \leq 2$.

Furthermore, by construction Fat-Tree$_4$ is an isometric subgraph of Fat-Tree$_k$. So, let σ be the idempotent endomorphism of Fat-Tree$_4$ mapping: any vertex $\langle 0, i\rangle$ to the vertex $\langle 0, 3-i\rangle$ in the core layer; any vertex $\langle 1, i, j\rangle$ to the vertex $\langle 1, 3-i, 1-j\rangle$ in the aggregation layer, and in the same way any vertex $\langle 2, i, j\rangle$ to the vertex $\langle 2, 3-i, 1-j\rangle$ in the edge layer; last, any vertex $\langle 3, i, j\rangle$ to the vertex $\langle 3, 3-i, 3-j\rangle$ in the server layer. It can be hand-checked that σ has mobility 4 and so, by Corollary 9 $\delta\left(\text{Fat-Tree}_k\right) \geq \delta\left(\text{Fat-Tree}_4\right) \geq 2$. □

Definition 20 ([47]). The Butterfly graph $BF(n)$ has vertex-set $\{0, 1, \ldots, n\} \times \mathbb{Z}_2^n$; two vertices $\langle i, w\rangle, \langle i', w'\rangle$ are adjacent if $i' = i + 1$ and for every $j \neq i,\ w_j = w'_j$.

Lemma 21. $\delta\left(BF(n)\right) = n$.

Proof. Let w and w' be two binary words of length n and let i_1 and i_l be respectively the least and the largest index in which they differ. Then, it can be checked that for every integer i, $\mathrm{d}_{BF(n)}(\langle i, w\rangle, \langle i, w'\rangle) = 2(i_l - i_1)$. As a result, the endomorphism σ mapping any vertex $\langle i, w\rangle$ to the vertex $\langle i, \bar{w}\rangle$ has mobility $2n$. Since σ is idempotent then it follows from Corollary 9 that $\delta\left(BF(n)\right) \geq n$. Last, we also have that $\operatorname{diam}\left(BF(n)\right) = 2n$, hence $\delta\left(BF(n)\right) \leq n$ by Lemma 2. □

In the literature, the edge-set of the Butterfly network is sometimes defined as $\{\{\langle i, w\rangle, \langle i+1 \pmod n, w'\rangle\} \mid 0 \leq i \leq n \text{ and for every } j \neq i, w_j = w'_j\}$ [81], and this definition is also known as the wrapped Butterfly network. It modifies the diameter of the topology from $2n$ to $n + \lfloor n/2 \rfloor$, and the distance between any two vertices $\langle i, w\rangle, \langle i, \bar{w}\rangle$ from $2n$ to n. As a result, using the same arguments as for Lemma 21 one obtains that the hyperbolicity of the wrapped Butterfly graph is comprised between $\lfloor n/2 \rfloor$ and $\lfloor (n + \lfloor n/2 \rfloor)/2 \rfloor$.

Definition 22 ([20]). The k-ary n-fly has vertex-set $\{0, 1, \ldots, n\} \times \mathbb{Z}_k^n$; two vertices $\langle i, w\rangle, \langle i', w'\rangle$ are adjacent if $i' = i + 1$ and for every $j \neq i,\ w_j = w'_j$.

Observe that the Butterfly graph $BF(n)$ is isomorphic to the 2-ary n-fly.

Lemma 23. *The k-ary n-fly is n-hyperbolic.*

Proof. By [20], the diameter of the k-ary n-fly is $2n$ and so, it has hyperbolicity bounded from above by n by Lemma 2. Moreover, by construction it contains the Butterfly graph $BF(n)$ as an isometric subgraph and so, it has hyperbolicity at least n by Lemma 21. □

Definition 24 ([20]). The k-ary n-tree is the graph with vertex-set $\mathbb{Z}_k^n \cup \left(\{0,1,\ldots,n-1\} \times \mathbb{Z}_k^{n-1}\right)$ such that any two vertices $\langle i,w\rangle, \langle i',w'\rangle$ are adjacent if $i' = i+1$ and for every $j \neq i$, $w_j = w'_j$; any two vertices $\langle i,w\rangle, w'$ are adjacent if $i = n-1$ and $w' = w \cdot b$ for some $b \in \mathbb{Z}_k$.

Lemma 25. *The k-ary n-tree is $(n-1)$-hyperbolic.*

Proof. By construction, the biconnected components of the k-ary n-tree are composed of one single-vertex graph for each vertex $w \in \mathbb{Z}_k^n$, and of the k-ary $(n-1)$-fly. Since the hyperbolicity of the graph is equal to the maximum hyperbolicity taken over its biconnected components, then it follows from Lemma 23 that the k-ary n-tree is $(n-1)$-hyperbolic. □

Definition 26 ([81]). The d-ary tree grid $MT(d,h)$ is a graph whose vertices are labeled with the pairs of words $< u, v >$ over an alphabet of size d and such that $\max\{|u|,|v|\} = h$. Any two vertices $\langle u,v\rangle$ and $\langle u',v'\rangle$ are adjacent in $MT(d,h)$ if and only if there is some letter λ such that: either $|u| = h$, $u = u'$ and $v = v' \cdot \lambda$; or $|v| = h$, $v = v'$ and $u' = u \cdot \lambda$.

Lemma 27. $\delta\left(MT(d,h)\right) = 2h$.

Proof. By [81] $\operatorname{diam}\left(MT(d,h)\right) = 4h$ and so, $\delta\left(MT(d,h)\right) \leq 2h$. Furthermore, $MT(2,h)$ is an isometric subgraph of $MT(d,h)$ by construction. Let σ be the idempotent endomorphism of $MT(2,h)$ mapping any vertex $\langle u,v\rangle$ to the vertex $\langle \bar{u},\bar{v}\rangle$. By construction σ has mobility $4h$ and so, we conclude by Corollary 9 that $\delta\left(MT(d,h)\right) \geq \delta\left(MT(2,h)\right) \geq 2h$. □

3.2.4 Symmetric networks and Cayley graphs

Let $(\Gamma,\cdot)$ be a group and let S be a generating set of Γ that is symmetric and that does not contain the neutral element of Γ. We remind that the *Cayley graph* $G(\Gamma,S)$ —of group Γ w.r.t. S— has vertex-set Γ and edge-set $\{\{g, g\cdot s\} \mid g \in \Gamma, s \in S\}$. It is well-known that every Cayley graph is vertex-transitive [12]. Furthermore, it has been shown (see for instance Exercise 2.4.14 in [81]) that the cube connected cycle $CCC(n)$ and the Butterfly graph $BF(n)$ are Cayley graphs.

Lemma 28. *Let $(\Gamma,\cdot)$ be a commutative group and S be a symmetric generating set that does not contain the neutral element of Γ. If $G(\Gamma,S)$ is not a clique, then $\delta\left(G(\Gamma,S)\right) \geq \frac{1}{2}\left\lceil\frac{\operatorname{diam}(G(\Gamma,S))}{2}\right\rceil$.*

Proof. Let $id_\Gamma, g \in \Gamma$ be such that id_Γ is the neutral element of group Γ and $\mathrm{d}(id_\Gamma, g) = \operatorname{diam}\left(G(\Gamma,S)\right) = D > 1$. The mapping $\sigma : v \to g\cdot v$ is an automorphism satisfying that for every $v \in \Gamma$, $\mathrm{d}(v,\sigma(v)) = \mathrm{d}(id_\Gamma, v^{-1}\cdot g\cdot v) = \mathrm{d}(id_\Gamma, g) = D$. Therefore, we can conclude by Theorem 7 that $\delta\left(G(\Gamma,S)\right) \geq \lceil D/2\rceil/2$. □

Definition 29 ([12]). The Bubble-sort graph $BS(n)$ has vertex-set the n-element permutations, that is $\{\phi_1\phi_2\ldots\phi_i\ldots\phi_n \mid \{\phi_1,\ldots,\phi_n\} = \{1,\ldots,n\}\}$. Any two vertices ϕ,ψ are adjacent if and only if there is some index $i < n$ such that $\phi_i = \psi_{i+1}, \phi_{i+1} = \psi_i$ and for every $j \notin \{i, i+1\}$, $\phi_j = \psi_j$.

Lemma 30. $\delta(BS(n)) = \left\lfloor\frac{n(n-1)}{4}\right\rfloor$.

Proof. By [12] $\mathrm{diam}(BS(n)) = \binom{n}{2}$, hence $\delta(BS(n)) \leq \lfloor \mathrm{diam}(BS(n))/2 \rfloor$ by Lemma 2. Now, let σ be the idempotent endomorphism mapping any vertex $\phi_1\phi_2\ldots\phi_i\ldots\phi_n$ to $\phi_n\ldots\phi_{n-i+1}\ldots\phi_2\phi_1$. By [12] all pairs $(u,\sigma(u))$ are diametral pairs and so, we can conclude by Corollary 9 that $\delta(BS(n)) \geq \lfloor \mathrm{diam}(BS(n))/2 \rfloor$. $\square$

Definition 31 ([17]). The Transposition graph $T(n)$ has vertex-set the n-element permutations. Any two vertices ϕ, ψ are adjacent if and only if there are $i, j,\ i \neq j$ such that $\phi_i = \psi_j, \phi_j = \psi_i$ and for every $k \notin \{i,j\},\ \phi_k = \psi_k$.

Lemma 32. $\frac{1}{2}\left\lceil \frac{n-1}{2} \right\rceil \leq \delta\left(T(n)\right) \leq \left\lfloor \frac{n-1}{2} \right\rfloor$.

Proof. By [17] the diameter of $T(n)$ is $n-1$ and so, by Lemma 2 $\delta\left(T(n)\right) \leq \lfloor (n-1)/2 \rfloor$. Moreover, let σ be the endomorphism mapping any vertex $\phi_1\phi_2\ldots\phi_i\ldots\phi_{n-1}\phi_n$ to $\phi_2\phi_3\ldots\phi_{i+1}\ldots\phi_n\phi_1$. Again by [17] all pairs $(u,\sigma(u))$ are diametral pairs and so, we can conclude by Theorem 7 that $\delta\left(S(n)\right) \geq \lceil n-1/2 \rceil /2$. $\square$

Definition 33 ([12]). The star graph $S(n)$ has vertex-set the n-element permutations and edge-set $\{\{\phi_1\ldots\phi_{i-1}\phi_i\phi_{i+1}\ldots\phi_n, \phi_i\ldots\phi_{i-1}\phi_1\phi_{i+1}\ldots\phi_n\} \mid 2 \leq i \leq n\}$.

Lemma 34. $\left\lfloor \frac{1}{2}\left\lfloor \frac{3(n-1)}{2} \right\rfloor - \frac{1}{2} \right\rfloor \leq \delta\left(S(n)\right) \leq \left\lfloor \frac{1}{2}\left\lfloor \frac{3(n-1)}{2} \right\rfloor \right\rfloor$.

Proof. By [12] the diameter of $S(n)$ is $\lfloor 3(n-1)/2 \rfloor$ and so, $\delta\left(S(n)\right) \leq \lfloor \lfloor 3(n-1)/2 \rfloor /2 \rfloor$ by Lemma 2. Then, given $\phi = \phi_1\phi_2\ldots\phi_i\ldots\phi_{n-1}\phi_n$, let ψ be the unique n-element permutation satisfying that $\psi_{n-2j} = \phi_{n-2j-1}, \psi_{n-2j-1} = \phi_{n-2j}$, for every $0 \leq j \leq \lfloor (n-1)/2 \rfloor - 1$. Again by [12], $\mathrm{d}(\psi,\phi) \geq \lfloor 3(n-1)/2 \rfloor - \varepsilon \geq \lfloor 3(n-1)/2 \rfloor - 1$, with $\varepsilon = n+1 \pmod 2$. Moreover it can be checked that the mapping $\sigma : \psi \to \phi$ is an idempotent endomorphism of $S(n)$. Therefore, by Corollary 9 $\delta\left(S(n)\right) \geq \lfloor \lfloor 3(n-1)/2 \rfloor /2 - 1/2 \rfloor$. $\square$

4 Using the shortest-path distribution

It turns out that for "simple" topologies that are commonly found in the literature, desirable symmetries such as those in use in Section 3 might fail to exist. For instance, the infinite rectangular grid is vertex-symmetric, but finite rectangular grids are not. As we will show next, the more generic Theorem 4 could still be applied in order to obtain loose lower-bounds in these situations. However, since the shortest-path distributions of the "simplest" topologies are well-known and characterized, that allows us to lower-bound their hyperbolicity using more involved techniques. In particular, our proofs for grid-like graphs introduce a novel way to make use of the maximal shortest-paths in the study of graph hyperbolicity.

4.1 The fellow traveler property for graphs defined on an alphabet

As a warm up, we will lower-bound the hyperbolicity of some graph classes defined on alphabets, starting with the undirected de Bruijn graph.

Definition 35 ([13]). The undirected de Bruijn graph $UB(d,D)$ has vertex-set the words of length D taken over an alphabet Σ of size d. The 2-set $\{u,v\}$ is an edge of $UB(d,D)$ if and only if $u = u_{d-1}u_{d-2}\ldots u_1u_0$ and $v = u_{d-2}\ldots u_1u_0v_0$ for some letters $u_{d-1}, u_{d-2}, \ldots, u_1, u_0, v_0 \in \Sigma$.

De Bruijn graphs have been extensively studied in the literature [15, 24, 27, 81]. In particular, $UB(d,D)$ has diameter D, maximum degree $2d$, and d^D vertices. Shortest-path routing and shortest-path distances in $UB(d,D)$ are characterized as follows.

Lemma 36 ([24]). *Let u,v be two words of length D taken over some alphabet Σ of size d, and write $u = u_L \cdot x \cdot u_R$ and $v = v_L \cdot x \cdot v_R$ so that $D - |x| + \min\{|u_L| + |v_R|, |v_L| + |u_R|\}$ is minimized. Then it holds $\mathrm{d}_{UB(d,D)}(u,v) = D - |x| + \min\{|u_L| + |v_R|, |v_L| + |u_R|\}$.*

We say that a graph G falsifies the *k-fellow traveler property* if there are two shortest-paths $\mathcal{P}_1, \mathcal{P}_2$ with same endpoints $u,v \in V(G)$, and there are two vertices $x \in \mathcal{P}_1, y \in \mathcal{P}_2$ such that $\mathrm{d}_G(u,x) = \mathrm{d}_G(u,y)$ and $\mathrm{d}_G(x,y) > k$. By a straightforward calculation we obtain that in such a case $\delta(u,v,x,y) = \mathrm{d}_G(x,y)/2 > k/2$. So, we can lower-bound the hyperbolicity of G with the least k such that it *satisfies* the $2k$-fellow traveler property. This standard argument will be the one in use throughout the remaining of Section 4.1.

Proposition 37. *For any positive integers d and D, $\delta(UB(d,D)) \geq \frac{1}{2} \cdot \left\lfloor \frac{D}{2} \right\rfloor$.*

Proof. We prove that $UB(d,D)$ cannot satisfy the k-fellow traveler property for some range of k. W.l.o.g. the vertices of $UB(d,D)$ are labeled with the words of length D taken over the alphabet $\Sigma = \{0,1,\ldots,d-1\}$. Let $u = 0^D$, $v = 1^D$, $x = 0^{\lfloor D/2 \rfloor} \cdot 1^{\lceil D/2 \rceil}$, and $y = 1^{\lceil D/2 \rceil} \cdot 0^{\lfloor D/2 \rfloor}$. By Lemma 36 it comes that $\mathrm{d}(u,v) = D = \lceil D/2 \rceil + \lfloor D/2 \rfloor = \mathrm{d}(u,x) + \mathrm{d}(x,v) = \mathrm{d}(u,y) + \mathrm{d}(y,v)$. As a result, the graph $UB(d,D)$ cannot satisfy the k-fellow traveler property for $k < \mathrm{d}(x,y) = \lfloor D/2 \rfloor$ and so, $\delta(UB(d,D)) \geq \lfloor D/2 \rfloor / 2$. □

To compare the bounds of Theorem 4 and Proposition 37, we note that it has been proved in [79] that de Bruijn graphs with maximum degree $d \geq 3$ are self-centered. Therefore, if $d \geq 3$ then Proposition 37 follows from Theorem 4 (with $k = 0$), but it is not the case if $d = 2$. Furthermore, the lower-bound of Proposition 37 is reached for $d = D = 2$, *a.k.a.* the diamond graph. It can be computer-checked that is also holds for $d = 2, D = 4$. However, $\delta(UB(2,D)) = \left\lfloor \frac{D}{2} \right\rfloor$ for every odd $D \leq 11$. Based on computer experiments (for $d = 2, D \leq 12$), we made the following stronger conjecture:

Conjecture 38. *For every $D \geq 7, \delta(UB(d,D)) = \left\lfloor \frac{D}{2} \right\rfloor$.*

A closely related graph class that has been extensively studied in the literature is the class of undirected Kautz graphs $UK(d,D)$ [2, 13]. The graph $UK(d,D)$ has diameter D, maximum degree $2d$, and $d^D(d+1)$ vertices. Furthermore, it can be checked that the Kautz graph $UK(d,D)$ is an induced subgraph of the de Bruijn graph $UB(d+1,D)$.

Definition 39 ([2, 13]). The undirected Kautz graph $UK(d,D)$ has vertex-set the words of length D taken over an alphabet Σ of size $d+1$ and satisfying that no two adjacent letters are equal. The 2-set $\{u,v\}$ is an edge of $UK(d,D)$ if and only if $u = u_{d-1}u_{d-2}\ldots u_1u_0$ and $v = u_{d-2}\ldots u_1u_0v_0$ for some letters $u_{d-1}, u_{d-2}, \ldots, u_1, u_0, v_0 \in \Sigma$.

Proposition 40. *For any positive integers d and D, $\delta(UK(d,D)) \geq \left\lfloor \frac{D}{4} \right\rfloor + \left\lfloor \frac{D \pmod 4}{3} \right\rfloor$.*

Proof. As for the proof of Proposition 37, we prove that $UK(d,D)$ cannot satisfy the k-fellow traveler property for some range of k. W.l.o.g. the vertices of $UK(d,D)$ are labeled with the words of length D taken over the alphabet $\{0,1,2,\ldots,d\}$. Let $D = 2D' + r$, $r \in \{0,1\}$, let

$u = (01)^{D'} \cdot 0^r, v = (21)^{D'} \cdot 2^r$. Note that 0^r (resp. 2^r) is either the empty word or it is equal to 0 (resp. to 2). By Lemma 36 $\mathrm{d}_{UK(d,D)}(u,v) \geq \mathrm{d}_{UB(d+1,D)}(u,v) = D$ and so, $\mathrm{d}_{UK(d,D)}(u,v) = D$ because $\mathrm{diam}\,(UK(d,D)) = D$. In particular, let $\mathcal{P}_1$ be the uv-shortest-path in $UK(d,D)$ that one obtains by applying "right shiftings" on u until one obtains vertex v *i.e.*,

$$\mathcal{P}_1 = (01)^{D'} \cdot 0^r \to 1 \cdot (01)^{D'-1} \cdot 0^r \cdot 2 \to (01)^{D'-1} \cdot 0^r \cdot 21 \to \cdots \to (21)^{D'} \cdot 2^r$$

Similarly, let $\mathcal{P}_2$ be the vu-shortest-path in $UK(d,D)$ that one obtains by applying "right shiftings" on v until one obtains vertex u. That is,

$$\mathcal{P}_2 = (21)^{D'} \cdot 2^r \to 1 \cdot (21)^{D'-1} \cdot 2^r \cdot 0 \to (21)^{D'-1} \cdot 2^r \cdot 01 \to \ldots \to (01)^{D'} \cdot 0^r$$

Let now

$$\begin{aligned} x =& (01)^{\lfloor D'/2 \rfloor} \cdot 0^r \cdot (21)^{\lceil D'/2 \rceil} \in \mathcal{P}_1 \\ \text{and } y =& 1^r \cdot (21)^{\lceil D'/2 \rceil - r} \cdot 2^r \cdot (01)^{\lfloor D'/2 \rfloor} \cdot 0^r \in \mathcal{P}_2 \end{aligned}$$

be such that $\mathrm{d}(u,x) = \mathrm{d}(u,y)$.

The graph $UK(d,D)$ falsifies the k-fellow traveler property for all $k < \mathrm{d}_{UK(d,D)}(x,y)$, and we have by Lemma 36 that $\mathrm{d}_{UK(d,D)}(x,y) \geq \mathrm{d}_{UB(d+1,D)}(x,y) \geq 2\left(\lfloor D/4 \rfloor + \lfloor (D \pmod 4)/3 \rfloor\right)$.

As a result, it holds $\delta\left(UK(d,D)\right) \geq \lfloor D/4 \rfloor + \lfloor (D \pmod 4)/3 \rfloor$. □

The lower-bound of Proposition 40 is reached for $d = 2, D = 3$. Again to compare with Theorem 4, we note that it was also proved in [79] that Kautz graphs are self-centered, for every $d \geq 2$. Therefore, applying Theorem 4 (with $k = 0$) gives us a lower-bound $\lfloor D/2 \rfloor / 2$ for the hyperbolicity of $UK(d,D)$, that is of the same order of magnitude as the one of Proposition 40 (Proposition 40 is slightly better if $D \equiv 3 \pmod 4$, and slightly worse if $D \equiv 2 \pmod 4$). We last define another topology that is related to the de Bruijn graph:

Definition 41 ([81]). The shuffle-exchange graph $SE(n)$ has vertex-set the binary words of length n. The 2-set $\{u,v\}$ is an edge of $SE(n)$ if and only if $u = u_{n-1}u_{n-2}\ldots u_1u_0$ and: either $v = u_0u_{n-1}u_{n-2}\ldots u_1$, or $v = u_{n-2}\ldots u_1u_0u_{n-1}$, or $v = u_{n-1}u_{n-2}\ldots u_1\bar{u_0}$, for some booleans $u_{n-1}, u_{n-2}, \ldots, u_1, u_0$.

It was proved in [81] that the diameter of $SE(n)$ is $2n-1$, and that the pair of vertices $(0^n, 1^n)$ is a diametral pair. Furthermore, it can be checked that one can obtain the de Bruijn graph $UB(2, n-1)$ from $SE(n)$ as follows: for each edge $\{u_{n-1}u_{n-2}\ldots u_1u_0, u_{n-1}u_{n-2}\ldots u_1\bar{u_0}\}$, we contract the edge and we label $u_{n-1}u_{n-2}\ldots u_1$ the resulting vertex. This defines a *contraction mapping* σ, mapping any vertex $u_{n-1}u_{n-2}\ldots u_1u_0$ of $SE(n)$ to the vertex $u_{n-1}u_{n-2}\ldots u_1$ of $UB(2, n-1)$. In the following, it will be useful to observe that by construction, for every two vertices u, v of $SE(n)$ it holds $\mathrm{d}_{SE(n)}(u,v) \geq \mathrm{d}_{UB(2,n-1)}(\sigma(u), \sigma(v))$.

Proposition 42. *For any positive integer n, $\delta\left(SE(n)\right) \geq \frac{1}{2} \cdot \left\lfloor \frac{n}{2} \right\rfloor$.*

Proof. As for the proof of Proposition 37, we prove that $SE(n)$ cannot satisfy the k-fellow traveler property for some range of k. Let $u = 0^n$, $v = 1^n$ be a diametral pair of $SE(n)$, with $\mathrm{d}(u,v) = 2n-1$. Let $\mathcal{P}_1$ be the uv-shortest-path:

$$0^n \to 0^{n-1} \cdot 1 \to 1 \cdot 0^{n-1} \to 1 \cdot 0^{n-2} \cdot 1 \to 11 \cdot 0^{n-2} \to \ldots \to 1^{n-1} \cdot 0 \to 1^n$$

Similarly, let $\mathcal{P}_2$ be the vu-shortest-path:

$$1^n \to 1^{n-1} \cdot 0 \to 0 \cdot 1^{n-1} \to 0 \cdot 1^{n-2} \cdot 0 \to 00 \cdot 1^{n-2} \to \ldots \to 0^{n-1} \cdot 1 \to 0^n.$$

Finally, let $x = 1^{\lfloor n/2 \rfloor} \cdot 0^{\lceil n/2 \rceil} \in \mathcal{P}_1$, $y = 0^{\lceil n/2 \rceil - 1} \cdot 1^{\lfloor n/2 \rfloor} \cdot 0 \in \mathcal{P}_2$ be such that $\mathrm{d}(u,x) = \mathrm{d}(u,y)$. By using the above contraction mapping from $SE(n)$ to $UB(2, n-1)$ one obtains $\mathrm{d}_{UB(2,n-1)}(x', y') \leq \mathrm{d}_{SE(n)}(x,y)$ with $x' = 1^{\lfloor n/2 \rfloor} \cdot 0^{\lceil n/2 \rceil - 1}$, $y' = 0^{\lceil n/2 \rceil - 1} \cdot 1^{\lfloor n/2 \rfloor}$. As a result, we have by Lemma 36 that the shuffle-exchange graph falsifies the k-fellow traveler property for every $k < \mathrm{d}_{UB(2,n-1)}(x', y') = \lfloor \frac{n}{2} \rfloor$ and so, it holds $\delta\left(SE(n)\right) \geq \frac{1}{2} \cdot \lfloor \frac{n}{2} \rfloor$. □

4.2 The maximal shortest-paths in grid-like topologies

In this section, we name grid-like graphs some slight variations of the 2-dimensional grid. As a reminder, an (n,m)-grid is the Cartesian product of the path P_n, with n vertices, with the path P_m, with m vertices. That is, the vertex-set is $\{0, \ldots, n-1\} \times \{0, \ldots, m-1\}$, and the edge-set is $\{\{(i,j),(i',j')\} \mid |i - i'| + |j - j'| = 1\}$. Grid-like networks are used for modeling interconnection networks and other computational applications. We now propose to compute their hyperbolicity. Our main tool in this section is the notion of *far-apart pairs*, first introduced in [41, 52]:

Definition 43 (Far-apart pair [41, 52]). Given $G = (V,E)$, the pair (u,v) is far-apart if for every $w \in V \setminus \{u,v\}$, $\mathrm{d}(w,u) + \mathrm{d}(u,v) > \mathrm{d}(w,v)$ and $\mathrm{d}(w,v) + \mathrm{d}(u,v) > \mathrm{d}(w,u)$.

Said differently, far-apart pairs are the endpoints of *maximal* shortest-paths in the graph. The main motivation for introducing far-apart pairs was to speed-up the computation of hyperbolicity, via the following pre-processing method.

Lemma 44 ([41, 52]). *Let G be a connected graph. There exist two far-apart pairs (u,v) and (x,y) satisfying:*

- $\mathrm{d}_G(u,v) + \mathrm{d}_G(x,y) \geq \max\{\mathrm{d}_G(u,x) + \mathrm{d}_G(v,y), \mathrm{d}_G(u,y) + \mathrm{d}_G(v,x)\}$*;*
- $\delta(u,v,x,y) = \delta(G)$*.*

We here propose a novel application of this result in order to simplify proofs for the hyperbolicity of grid-like topologies.

Definition 45. The $(s_1, s_2, \ldots, s_d)$-grid is a graph with vertex set $\Pi_{i=1}^{d}\{0, \ldots, s_i - 1\}$ such that any two vertices $\langle u_1, u_2, \ldots, u_d \rangle, \langle v_1, v_2, \ldots, v_d \rangle$ are adjacent only if $\sum_{i=1}^{d} |u_i - v_i| = 1$.

Definition 46. The d-dimensional grid of size s is the $(s_1, s_2, \ldots, s_d)$-grid with for every i, $s_i = s$.

Let us determine the hyperbolicity of the above graphs. By doing so, we answer an open question of the literature [44, Remark 7].

Proposition 47. *The $(s_1, s_2, \ldots, s_d)$-grid has hyperbolicity:*

$$h_d(s_1, s_2, \ldots, s_d) = \max_{\mathcal{E} \subseteq \{1, \ldots, d\}} \min\left\{ \sum_{i \in \mathcal{E}} s_i - 1, \sum_{i \notin \mathcal{E}} s_i - 1 \right\}.$$

Proof. The 2^{d-1} far-apart pairs of the grid are the diametral pairs $\{(\langle u_1,\ldots,u_d\rangle, \langle v_1,\ldots,v_d\rangle) \mid \forall i, \{u_i,v_i\} = \{0, s_i - 1\}\}$. Let $(\langle u_1,\ldots,u_d\rangle, \langle v_1,\ldots,v_d\rangle)$ and $(\langle x_1,\ldots,x_d\rangle, \langle y_1,\ldots,y_d\rangle)$ be two such pairs, denoted with $(\overrightarrow{u}, \overrightarrow{v})$ and $(\overrightarrow{x}, \overrightarrow{y})$ for short. Finally, let $D = \sum_i s_i - 1$ be the diameter of the grid and let $l = \sum_{i|u_i \neq x_i} s_i - 1$. Then it comes:

$$\begin{aligned}
S_1 &= \mathrm{d}(\overrightarrow{u}, \overrightarrow{v}) + \mathrm{d}(\overrightarrow{x}, \overrightarrow{y}) = 2D \\
S_2 &= \mathrm{d}(\overrightarrow{u}, \overrightarrow{x}) + \mathrm{d}(\overrightarrow{v}, \overrightarrow{y}) = 2l \\
S_3 &= \mathrm{d}(\overrightarrow{u}, \overrightarrow{y}) + \mathrm{d}(\overrightarrow{v}, \overrightarrow{x}) = 2(D-l).
\end{aligned}$$

As a result, $\delta(\overrightarrow{x}, \overrightarrow{y}, \overrightarrow{u}, \overrightarrow{v}) = \min\{l, D-l\}$ which is maximum for $l = h_d(s_1, s_2, \ldots, s_d)$. We conclude that $h_d(s_1, s_2, \ldots, s_d)$ is the hyperbolicity by Lemma 44. □

We highlight two particular cases of Proposition 47 that were already known in the literature.

Corollary 48 ([44,55]). *The (n,m)-grid is $(\min\{n,m\}-1)$-hyperbolic.*

Corollary 49 ([55]). *The d-dimensional grid of size s is $(s-1) \cdot \left\lfloor \frac{d}{2} \right\rfloor$-hyperbolic.*

Similar results can be obtained for other grid-like graphs which can be found in the literature. We prove some of these results before concluding this section.

Definition 50. The triangular (n,m)-grid is a supergraph of the (n,m)-grid with same vertex-set and with additional edges $\{(i,j),(i+1,j+1)\}$ for every $0 \leq i \leq n-2$ and $0 \leq j \leq m-2$.

An example of a triangular $(6,7)$-grid is given in Figure 3a.

Lemma 51. *The triangular (n,m)-grid is $\frac{\min\{n,m\}-1}{2}$-hyperbolic.*

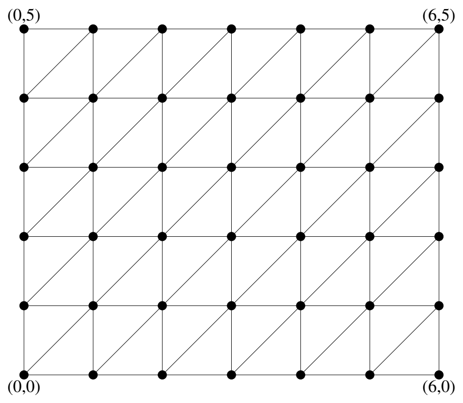
Proof. Let $u = (i_u, j_u)$ and $v = (i_v, j_v)$ be two vertices of the grid. We can assume w.l.o.g. that $i_u \geq i_v$. In such a case, either $j_u \geq j_v$ and so, $\mathrm{d}(u,v) = \max\{i_u - i_v, j_u - j_v\}$; or $j_u < j_v$ and so, $\mathrm{d}(u,v) = (i_u - i_v) + (j_v - j_u)$. We deduce from the above characterization that there is only one far-apart pair (u,v) such that $\mathrm{d}(u,v) \neq \max\{|i_u - i_v|, |j_u - j_v|\}$ namely, $u = (n-1, 0)$ and $v = (0, m-1)$ for which $\mathrm{d}(u,v) = n+m-2$. Furthermore, for any other far-apart pair (x,y) either $\mathrm{d}(x,y) = n-1$ or $\mathrm{d}(x,y) = m-1$.

Let (u,v) and (x,y) be two far-apart pairs satisfying the conditions of the above Lemma 44. We assume w.l.o.g. that $\mathrm{d}(u,v) \geq \mathrm{d}(x,y)$, and we claim that $2\delta(u,v,x,y) \leq \min\{n,m\} - 1$. First, by [74] $2\delta(u,v,x,y) \leq \min\{\mathrm{d}(u,v), \mathrm{d}(x,y)\} \leq \mathrm{d}(x,y)$. Note that $\mathrm{d}(x,y) = k \in \{n-1, m-1\}$ by the above characterization of the far-apart pairs in the grid. As a result, if $n = m$ then we are done because $\mathrm{d}(x,y) = \min\{n,m\} - 1$.

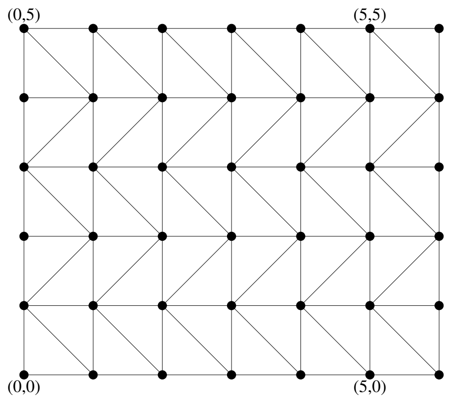
For the remaining of the proof, we will suppose that $n \neq m$ and $\mathrm{d}(x,y) = \max\{n,m\} - 1 = k$ (else we are done because $\mathrm{d}(x,y) = \min\{n,m\}-1$). If $k = n-1$, it implies that $\mathrm{d}(u,v) \geq |i_u - i_v| = |i_x - i_y| = \mathrm{d}(x,y) = n-1$; else, it implies $\mathrm{d}(u,v) \geq |j_u - j_v| = |j_x - j_y| = \mathrm{d}(x,y) = m-1$. Therefore, we always have that $\max\{\mathrm{d}(u,x) + \mathrm{d}(v,y), \mathrm{d}(u,y) + \mathrm{d}(v,x)\} \geq 2k$. It follows by Lemma 44 that the hyperbolicity of the triangular grid is:

$$\begin{aligned}
2\delta(u,v,x,y) &= \mathrm{d}(u,v) + \mathrm{d}(x,y) - \max\{\mathrm{d}(u,x) + \mathrm{d}(v,y), \mathrm{d}(u,y) + \mathrm{d}(v,x)\} \\
&\leq n+m-2+k-2k = n+m-2-\max\{n-1, m-1\} = \min\{n,m\} - 1
\end{aligned}$$

The bound is reached by setting $u = (n-1, 0)$, $v = (0, m-1)$, $x = (0,0)$, $y = (n-1, m-1)$. □



(a) The triangular $(7, 6)$-grid has hyperbolicity $\delta = \frac{5}{2} = \delta(u, v, x, y)$ with $u = (6, 0)$, $v = (0, 5)$, $x = (0, 0)$, $y = (6, 5)$.



(b) The hexagonal $(7, 6)$-grid has hyperbolicity $\delta = \frac{5}{2} = \delta(u, v, x, y)$ with $u = (0, 5)$, $v = (5, 0)$, $x = (0, 0)$, $y = (5, 5)$.

Figure 3: Examples of grid-like graphs.

In the example of Figure 3a, the hyperbolicity of the graph is given by the 4-tuple $u = (6, 0)$, $v = (0, 5)$, $x = (0, 0)$, $y = (6, 5)$.

Definition 52. The hexagonal (n, m)-grid is a supergraph of the (n, m)-grid with same vertex-set and with additional edges $\{\{(i, m - 2j - 1), (i + 1, m - 2j - 2)\} \mid 0 \leq i \leq n - 2 \text{ and } 0 \leq j \leq \lfloor \frac{m}{2} \rfloor - 1\} \cup \{\{(i, m - 2j - 3), (i + 1, m - 2j - 2)\} \mid 0 \leq i \leq n - 2 \text{ and } 0 \leq j \leq \lfloor \frac{m-1}{2} \rfloor - 1\}$.
The additional edges are called *diagonal* edges.

Informally, the difference between the triangular grid and the hexagonal grid is that in the hexagonal grid, the direction of diagonal edges alternate at each row. We refer to Figure 3b for an illustration. The hyperbolicity of hexagonal grids has already received some attention in [28]. In fact, they showed using the hexagonal grid that the gap between hyperbolicity of a graph and the length of its longest isometric cycle can be arbitrarily large (see also [78] for more explanations). However, to the best of our knowledge there was no formal bound so far established for the hyperbolicity of hexagonal grids.

Lemma 53. *The hexagonal (n, m)-grid is $\frac{\min\{n,m\}-1}{2}$-hyperbolic.*

Proof. We will first characterize the distances in the grid. Let $u = (i_u, j_u)$, $v = (i_v, j_v)$ be two vertices of the hexagonal grid. W.l.o.g., $i_u \geq i_v$. Let us observe that in order to obtain an uv-shortest-path, it suffices to maximize the number of *diagonal* edges used in the path, that is $\min\{k, |i_u - i_v|\}$ with:

- $k = \lfloor |j_u - j_v|/2 \rfloor$ if both $j_u - j_v$ and $2\,[m - j_v \pmod 2] - 1$ have the same sign;
- $k = \lceil |j_u - j_v|/2 \rceil$ otherwise.

As a result $\mathrm{d}(u, v) = |i_u - i_v| + |j_u - j_v| - \min\{k, |i_u - i_v|\}$ for some k depending on j_u and j_v, $k \in \{\lfloor |j_u - j_v|/2 \rfloor, \lceil |j_u - j_v|/2 \rceil\}$.

Suppose in addition that (u, v) is a far-apart pair. There are two cases. If $\mathrm{d}(u, v) = |j_u - j_v|$ then it is monotonically increasing with $|j_u - j_v|$ and so, $|j_u - j_v| = m - 1$. Else, $\mathrm{d}(u, v) =$

$|i_u - i_v| + |j_u - j_v| - k$ for some k *only* depending on j_u and j_v, that is monotonically increasing with $|i_u - i_v|$ and so, $|i_u - i_v| = n - 1$.

Finally, let (u, v), (x, y) be two far-apart pairs satisfying the conditions of the above Lemma 44. We will prove that $2\delta(u, v, x, y) \leq \min\{n, m\} - 1$.

Case $\mathbf{m \leq n}$. If $\min\{\mathrm{d}(u, v), \mathrm{d}(x, y)\} \leq m - 1$ then we are done because by [74] we have that $\delta(u, v, x, y) \leq \min\{\mathrm{d}(u, v), \mathrm{d}(x, y)\}/2 \leq (m - 1)/2$. Else, we must have that $|i_u - i_v| = |i_x - i_y| = n - 1$ and so, $\max\{\mathrm{d}(u, x) + \mathrm{d}(v, y), \mathrm{d}(u, y) + \mathrm{d}(v, x)\} \geq 2(n - 1)$. Since in such a case $\mathrm{d}(u, v) + \mathrm{d}(x, y) \leq (n - 1 + \lceil (m - 1)/2 \rceil) + (n - 1 + \lfloor (m - 1)/2 \rfloor) = 2(n - 1) + m - 1$ then it follows once again that $\delta(u, v, x, y) \leq (m - 1)/2$.

Case $\mathbf{m > n}$. There are three subcases to be considered.

- Suppose $\mathrm{d}(u, v) = |j_u - j_v| = m - 1$, $\mathrm{d}(x, y) = |j_x - j_y| = m - 1$. Then it comes that $\max\{\mathrm{d}(u, x) + \mathrm{d}(v, y), \mathrm{d}(u, y) + \mathrm{d}(v, x)\} \geq 2(m - 1)$ and so, $\delta(u, v, x, y) = 0$.

- Suppose $\mathrm{d}(u, v) = j_u - j_v = m - 1$ and $n - 1 + \lfloor (j_x - j_y)/2 \rfloor \leq \mathrm{d}(x, y) \leq n - 1 + \lceil (j_x - j_y)/2 \rceil$. Then it holds that $\mathrm{d}(u, y) + \mathrm{d}(v, x) \geq (j_u - j_y) + (j_x - j_v) = (j_u - j_x) + (j_x - j_y) + (j_x - j_v) = m - 1 + (j_x - j_y)$. As a result,

  $$2\delta(u, v, x, y) \leq (n - 1 + \lceil (j_x - j_y)/2 \rceil + m - 1) - (m - 1 + j_x - j_y) = n - 1 - \lfloor (j_x - j_y)/2 \rfloor \leq n - 1.$$

- Else, we consider the smallest hexagonal grid of dimensions (n', m') for which there exists two far-apart pairs (u', v') and (x', y') that satisfy the conditions of the above Lemma 44 and such that $\delta(u', v', x', y') \geq \delta(u, v, x, y)$. We assume w.l.o.g. that $n' < m'$ and $\mathrm{d}(u', v') \neq |j_{u'} - j_{v'}|$, $\mathrm{d}(x', y') \neq |j_{x'} - j_{y'}|$ (otherwise we fall in one of the above cases). Note that it implies that $|i_{u'} - i_{v'}| = |i_{x'} - i_{y'}| = n' - 1$ by our above characterization of the far-apart pairs.

  If the two far-apart pairs are $((0, 0), (n' - 1, m' - 1))$ and $((0, m' - 1), (n' - 1, 0))$, then we obtain by the computation that $2\delta(u', v', x', y') = n' - 1 + (n' - m') < n' - 1 \leq n - 1$.

  Else, by minimality of the subgrid there is some vertex in the 4-tuple, say u', which is contained amongst $\{(0, 0), (n' - 1, m' - 1), (n' - 1, 0), (0, m' - 1)\}$ and such that no other vertex $z \in \{v', x', y'\}$ satisfies that $j_{u'} = j_z$. By symmetry, we will assume that $u' \in \{(0, m' - 1), (n' - 1, m' - 1)\}$. Then, using the above characterization of the distances in the hexagonal grid, it can be checked that for any $0 \leq i \leq n' - 1$ and for any $0 \leq j \leq m' - 2$:

  $$\begin{aligned} &\mathrm{d}\big((n' - 1, m' - 2), (i, j)\big) = \mathrm{d}\big((n' - 1, m' - 1), (i, j)\big) - 1 \\ \text{and } &\mathrm{d}\big((1, m' - 2), (i, j)\big) = \mathrm{d}\big((0, m' - 1), (i, j)\big) - 1 \text{ unless } (i, j) = (0, m' - 2) \end{aligned}$$

  Therefore, by the 4-point condition $\delta(u', v', x', y') = \delta((n' - 1, m' - 2), v', x', y')$ when $u' = (n' - 1, m' - 1)$; $\delta(u', v', x', y') \leq \max\{\mathrm{d}((0, m' - 1), (0, m' - 2)), \delta((n' - 1, m' - 2), v', x', y')\} \leq \max\{1, \delta((n' - 1, m' - 2), v', x', y')\}$ when $u' = (0, m' - 1)$. In both cases, it contradicts the minimality of (n', m').

To conclude, let $l = \min\{n, m\} - 1$. The upper-bound $l/2$ for the hyperbolicity is reached by setting $u = (0, m - 1), v = (l, m - 1 - l), x = (0, m - 1 - l), y = (l, m - 1)$. □

In the example of Figure 3b for an illustration, the hyperbolicity of the graph is given by the 4-tuple $u = (0,5)$, $v = (5,0)$, $x = (0,0)$, $y = (5,5)$.

Definition 54. The cylinder (n,m)-grid is the supergraph of the (n,m)-grid with the same vertex-set and with additional edge-set $\{\{(0,j),(n-1,j)\} \mid 0 \leq j \leq m-1\}$.

In particular, when $m = 1$, then the cylinder (n,m)-grid is the n-cycle C_n. More generally, each row induces a cycle instead of inducing a path.

Lemma 55. *The cylinder (n,m)-grid is*

$$\begin{cases} \left\lfloor \frac{n}{2} \right\rfloor \textit{-hyperbolic} & \textit{when } m > \left\lfloor \frac{n}{2} \right\rfloor \\ \left(\frac{\left\lfloor \frac{n}{2} \right\rfloor + m}{2} - 1 \right) \textit{-hyperbolic} & \textit{when } m \leq \left\lfloor \frac{n}{2} \right\rfloor \textit{ and } (n \textit{ is odd or } \left\lceil \frac{n}{2} \right\rceil - m + 1 \textit{ is odd}) \\ \left(\frac{\left\lfloor \frac{n}{2} \right\rfloor + m}{2} - \frac{1}{2} \right) \textit{-hyperbolic} & \textit{otherwise.} \end{cases}$$

Proof. Let $u = (i_u, j_u), v = (i_v, j_v)$ be two vertices of the grid. We have:

$$\mathrm{d}(u,v) = \min\{|i_u - i_v|, n - |i_u - i_v|\} + |j_u - j_v|.$$

As a result, the far-apart pairs of the cylinder (n,m)-grid are exactly the pairs $\{(i,0),(i + \lfloor n/2 \rfloor \pmod n), m-1)\}$, and the pairs $\{(i,0),(i + \lceil n/2 \rceil \pmod n), m-1)\}$, with $0 \leq i \leq n-1$. Equivalently, these are the pairs $\{(u',0),(v',m-1)\}$ with (u',v') an arbitrary far-apart pair of the n-cycle C_n.

Let (u,v) and (x,y) be two far-apart pairs of the cylinder (n,m)-grid satisfying the conditions of the above Lemma 44. Write $u = (u',0)$, $v = (v',m-1)$, $x = (x',0)$, $y = (y',m-1)$. Furthermore, let $S_1 = \mathrm{d}(u,v) + \mathrm{d}(x,y)$, $S_2 = \mathrm{d}(u,x) + \mathrm{d}(v,y)$, and $S_3 = \mathrm{d}(u,y) + \mathrm{d}(v,x)$. Similarly, let $S_1' = \mathrm{d}_{C_n}(u',v') + \mathrm{d}_{C_n}(x',y')$, $S_2' = \mathrm{d}_{C_n}(u',x') + \mathrm{d}_{C_n}(v',y')$, and $S_3' = \mathrm{d}_{C_n}(u',y') + \mathrm{d}_{C_n}(v',x')$. Note that it holds: $S_1' = 2\lfloor n/2 \rfloor = \max\{S_1', S_2', S_3'\}$; $S_1 = S_1' + 2(m-1) = 2(\lfloor n/2 \rfloor + m - 1)$, $S_2' = S_2$, and $S_3 = S_3' + 2(m-1)$.
There are two cases to be considered.

- Suppose that $m > \lfloor n/2 \rfloor$. We have that $\delta(u,v,x,y) \leq (S_1 - S_3)/2 \leq (S_1' - S_3')/2 \leq S_1'/2 \leq \lfloor n/2 \rfloor$. The bound is reached by setting $u' = y'$ and $v' = x'$.

- Suppose that $m \leq \lfloor n/2 \rfloor$. If $(u',v') = (y',x')$ then we obtain by the calculation that $\delta(u,v,x,y) = (m-1)/2$. Otherwise, $S_2' + S_3' = n$ and hence

  $$2\delta(u,v,x,y) = S_1' - \max\{S_3', S_2' - 2(m-1)\} = S_1' - \max\{S_3', (n - 2(m-1)) - S_3'\},$$

  this is maximum when $\lfloor n/2 \rfloor - (m-1) \leq S_3' \leq \lceil n/2 \rceil - (m-1)$. In the following, let $\lceil n/2 \rceil - (m-1) = 2q + r$ with $0 \leq r \leq 1$. There are two subcases to be considered.

  (i) Assume that n is odd and let us set $u' = 0$, $v' = \lfloor n/2 \rfloor$, $x' = \lfloor n/2 \rfloor - q$, and $y' = n - q - r$. In such a case, $S_3' = (q+r) + q = 2q + r$. As a result, $\delta(u,v,x,y) = (\lfloor n/2 \rfloor + m)/2 - 1$ and so, the above upper-bound is always reached when n is odd.

(ii) Assume that n is even. Then, $S'_3 = 2\,\mathrm{d}(u',y')$ cannot be odd. It implies that the hyperbolicity is bounded from above by $n/4 + (m-1-r)/2$. We set $u' = 0$, $v' = n/2$, $x' = n/2 - q$, and $y' = n - q$. In such a case, $S'_3 = 2q$, hence $(n - 2(m-1)) - S'_3 = 4q + 2r - 2q = 2q + 2r$ and so, $\delta(u,v,x,y) = n/4 + (m-1-r)/2$ that is maximum.

□

Before concluding this section, let us compare the techniques employed for grids with Theorem 4. It is easy to see that for all grid-like graphs considered (cf. Definitions 10, 50, 52 and 54), there is either a row or a column contained in the center. Therefore, the diameter of the center is at least $\min\{n,m\} - 1$, and so, by [37, Proposition 5] one obtains the lower-bound $\lfloor(\min\{n,m\}-1)/2\rfloor/2$ on the hyperbolicity for all these graphs. In this section, we have conducted an in-depth analysis of their shortest-path distribution in order to establish the exact hyperbolicity of these grid-like graphs.

5 Relations between hyperbolicity and some graph operations

Our results so far are heavily focused on the so-called *homogeneous* data center interconnection networks. By contrast, heterogeneous data centers are based on the composition of homogeneous data center interconnection topologies through graph operations. We survey a few of these operations so that we can study the impact that they may have on the hyperbolicity of the network.

5.1 Biswap operation and biswapped networks

Definition 56 ([35]). Let G be a graph. The biswapped graph $Bsw(G)$ has vertex set $\{0,1\} \times V(G) \times V(G)$. Two vertices (b,u,v) and (b',u',v') are adjacent if, and only if either $b = b'$, $u = u'$ and $\{v,v'\} \in E(G)$, or $b = \bar{b'} = 1 - b'$, $u = v'$, and $u' = v$.

Lemma 57. *For any connected graph G, $\delta(Bsw(G)) = \mathrm{diam}(G) + 1$.*

Proof. By [35] $\mathrm{diam}(Bsw(G)) = 2\cdot\mathrm{diam}(G)+2$ and so, by Lemma 2 $\delta(Bsw(G)) \le \mathrm{diam}(G)+1$. To prove the lower-bound, let $u,v \in V(G)$ be such that $\mathrm{diam}(G) = \mathrm{d}_G(u,v)$. We define $\overrightarrow{x_1} = (0,u,v)$, $\overrightarrow{x_2} = (0,v,u)$, $\overrightarrow{x_3} = (1,u,u)$ and $\overrightarrow{x_4} = (1,v,v)$. We deduce from [35] that:

$$\begin{aligned}
S_1 &= \mathrm{d}(\overrightarrow{x_1},\overrightarrow{x_2}) + \mathrm{d}(\overrightarrow{x_3},\overrightarrow{x_4}) = 2(2\,\mathrm{d}_G(u,v)+2)\\
S_2 &= \mathrm{d}(\overrightarrow{x_1},\overrightarrow{x_3}) + \mathrm{d}(\overrightarrow{x_2},\overrightarrow{x_4}) = 2(\mathrm{d}_G(u,v)+1)\\
S_3 &= \mathrm{d}(\overrightarrow{x_1},\overrightarrow{x_4}) + \mathrm{d}(\overrightarrow{x_2},\overrightarrow{x_3}) = 2(\mathrm{d}_G(u,v)+1)
\end{aligned}$$

As a result, $\delta(Bsw(G)) \ge \delta(\overrightarrow{x_1},\overrightarrow{x_2},\overrightarrow{x_3},\overrightarrow{x_4}) = \mathrm{d}_G(u,v) + 1 = \mathrm{diam}(G) + 1$. □

It follows from Lemma 57 that the hyperbolicity of a biswap network always scales with its diameter, *regardless of the topology that is used for the operation.*

5.2 Generic Cayley construction

Let us finally consider the following transformation of a Hamiltonian graph, and the consequences of it on the hyperbolicity.

Lemma 58. *Let G be a Hamiltonian graph and c be a positive integer. We construct a graph G' from G by replacing every edge in some Hamilton cycle of G with a path of length c. Then, it holds $\delta(G') \geq \frac{1}{2}\left\lceil\frac{c-1}{2}\right\rceil$.*

Proof. Let P be a path of length c added by the construction, let x and y be the endpoints of P, and let P' be a xy-shortest-path in $G' \setminus (P \setminus \{x,y\})$. The union of P with P' is an isometric cycle and so, it has length upper-bounded by $4 \cdot \delta(G') + 3$ by [78]. Moreover, the length of P' is at least 2 because $\{x,y\}$ is an edge of G by the hypothesis. Thus it comes that the length of the cycle is at least $c+2$ and so, $c \leq 4 \cdot \delta(G') + 1$. □

The Cayley model in [59] aims to apply the construction defined in Lemma 58 to some Hamiltonian graph G of order N, with $c = \Omega(\log N)$ and so that the diameter of the resulting graph G' is $O(\log N)$. Summarizing, we get.

Theorem 59. *Graphs in the Cayley model have hyperbolicity $\Theta(\log N)$, which scales linearly with their diameter.*

6 Conclusion

We proved in this work that the topologies of various interconnection networks have their hyperbolicity that scales linearly with their diameter. This property is inherent to any graph having desired properties for data centers such as a high-level of symmetry. Interestingly, symmetries are a common way to minimize network congestion whereas it was shown in [51], using a simplified model, that a bounded hyperbolicity might explain the congestion phenomenon observed in some real-life networks. This was formally proved in [75] for shortest-path routing, but to the best of our knowledge no relation is known between hyperbolicity and congestion in *general*. Therefore, we let open whether a more general relationship between congestion and hyperbolicity can be determined.

Finally, our results imply that in any greedy routing scheme based on an embedding into the hyperbolic space —and in some cases, on an embedding into some word metric space— there is a *linear* number of routing paths for which the stretch is arbitrarily bad. However, this does not preclude the possibility that for most other routing paths, the stretch is bounded by a small constant. We thus believe that it might be of interest to compute the *average hyperbolicity* [63,72] of the data center interconnection topologies so as to verify whether it is the case.

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Papers on tree decompositions

Appendix F

Clique-decomposition revisited

Clique-decomposition revisited*

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Abstract

The decomposition of graphs by clique-minimal separators is a common algorithmic tool, first introduced by Tarjan. Since it allows to cut a graph into smaller pieces, it can be applied to preprocess the graphs in the computation of many optimization problems. However, the best known clique-decomposition algorithms have respective $\mathcal{O}(nm)$-time and $\mathcal{O}(n^{2.69})$-time complexity, that is prohibitive for large graphs. Here we prove that for every graph G, the decomposition can be computed in $\mathcal{O}\left(T(G) + \min\{n^{2.3729},\ \omega^2 n\}\right)$-time with $T(G)$ and ω being respectively the time needed to compute a minimal triangulation of G and the clique-number of G. In particular, it implies that every graph can be clique-decomposed in $\tilde{\mathcal{O}}(n^{2.3729})$-time. Based on prior work from Kratsch et al., we prove in addition that computing the clique-decomposition is at least as hard as triangle detection. Therefore, the existence of any $o(n^{2.3729})$-time clique-decomposition algorithm would be a significant breakthrough in the field of algorithmic. Finally, our main result implies that planar graphs, bounded-treewidth graphs and bounded-degree graphs can be clique-decomposed in linear or quasi-linear time.

Keywords: clique-decomposition; minimal triangulation; clique-number; treewidth; planar graphs; bounded-degree graphs.

1 Introduction

Our purpose in this work is to study the complexity of separating a graph with all its minimal separators that are cliques. In the literature, such minimal separators are called *clique-minimal separators*, and the decomposition process is called *clique-decomposition*. We refer to [6] for a survey. The clique-decomposition has been introduced by Tarjan in [32], where it is studied for its algorithmic applications. Indeed, it is often the case that hard problems on graphs (theoretically or in practice) can be solved on each subgraph of the clique-decomposition separately. See for instance [4, 9, 14, 15, 18, 19, 26, 34]. In particular, there are NP-hard problems that can be solved on graphs when the subgraphs obtained with the clique-decomposition are "simple enough" w.r.t. the problem. This was first noted by Gavril in [22] for the so-called clique-separable graphs. Other classes of graphs with a "simple" clique-decomposition comprise the chordal graphs (that can be clique-decomposed into complete subgraphs), the EPT graphs [23] and the P_6-free graphs [12, 13]. Note that general graphs may fail to contain a clique-minimal separator (we will call them *prime graphs* in the following), however in practice the biological networks, the graph of the autonomous systems of the Internet and some other complex networks do contain clique-minimal separators — as supported by some experimentations [1, 15].

With the exception of an $\mathcal{O}(n^{2.69})$-time algorithm in [28], all the best known algorithms for computing clique-decomposition have an $\mathcal{O}(nm)$-time complexity [2, 30, 32], that is cubic for dense graphs. Therefore,

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it becomes too prohibitive to run them on large graphs with thousands of vertices and sometimes billions of edges. Following a recent trend in algorithmic [11], we here investigate on the optimal time for computing the clique-decomposition.

Related work. To the best of our knowledge, the time complexity of clique-decomposition has received little attention in the literature. We are only aware of a recent article [7] introducing a generic framework to compute the clique-decomposition of graphs. This framework applies to all the best-known algorithms to compute the clique-decomposition. Indeed, all these algorithms follow the same three steps:

1. Compute a minimal triangulation of the graph;
2. Find the clique-minimal separators of the graphs (using the minimal triangulation);
3. Finally, recursively disconnect the graph with its clique-minimal separators.

We emphasize that the first step: computing a minimal triangulation, has been extensively studied (see [24] for a survey). So far, the best-known algorithm to compute a minimal triangulation of a graph has an $\tilde{\mathcal{O}}(n^{2.3729})$-time complexity. Note that it is less than $\mathcal{O}(n^{2.69})$, that has been the best-known complexity for computing the clique-decomposition of a graph — until this note.

Furthermore, new clique-decomposition algorithms are proposed in [7] that are provably faster than the classical approach in some cases, that is, they run in $\mathcal{O}(nm_0)$-time for some $m_0 < m$. In order to compare these algorithms with our work, let us note that the authors in [7] claim that bounded-treewidth graphs can be clique-decomposed in *quadratic-time*, whereas we will show that it can be done in quasi *linear-time*. Fast (quadratic-time) algorithms to compute the clique-decomposition can also be found in [3, 8] for some specific graph classes, but the latter algorithms deeply rely upon the structural properties of these graphs.

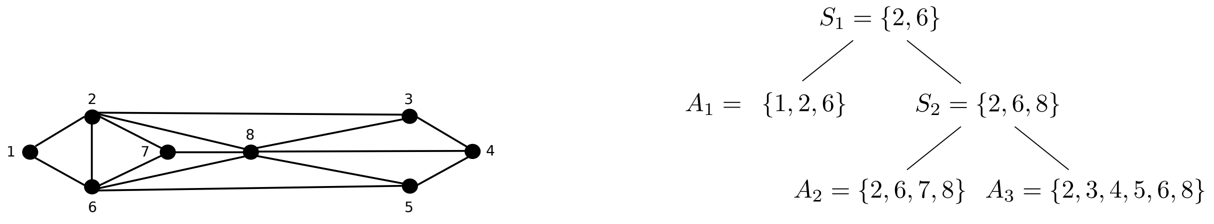
Closest to our work are two papers from Kratsch and Spinrad [27, 28]. In [28], they describe what has been, until this note, the best-known algorithm to compute the clique-decomposition. The latter algorithm has running time $\mathcal{O}(n^{2.69})$, that follows from an algorithm to compute a minimal triangulation of the graph within the same time bounds. We will generalize their result in our work, proving that the clique-decomposition can be computed in $\mathcal{O}(n^{2.3729})$-time if *any* minimal triangulation of the graph is given[1]. Furthermore, lower-bounds on the complexity of computing the clique-decomposition can be deduced from some results in [27]. In particular, they show that finding a clique-minimal separator in a graph is at least as hard as finding a simplicial vertex, *even if a minimal elimination ordering is given as part of the input.* The latter implies that computing a minimal triangulation is not the only complexity bottleneck of clique-decomposition algorithms.

Our contributions. On the negative side, we first prove a lower-bound on the complexity of computing the clique-decomposition. More precisely, we will build upon a result in [27] in order to prove that clique-decomposition is at least as hard as triangle detection (Theorem 4).

We next focus on the two last steps of clique-decomposition algorithms, that is, we ignore the first step of computing a minimal triangulation. Our main result is that the clique-minimal separators of a graph G can be computed in $\mathcal{O}(T(G) + \min\{n^{2.3729}, \omega^2 n\})$-time, with $T(G)$ and ω being respectively the time needed to compute a minimal triangulation of G and the *clique-number* of G (let us remind that the clique-number of G is the size of a largest clique in G). The latter result follows from two simple algorithms that respectively run in $\mathcal{O}(T(G) + n^{2.3729})$-time (Proposition 5) and in $\mathcal{O}(T(G) + \omega^2 n)$-time (Proposition 6). Furthermore, whereas the first algorithm (in $\mathcal{O}(T(G) + n^{2.3729})$-time) relies upon fast matrix multiplication, the second one is purely combinatorial and can be easily implemented.

We finally notice that any graph G can be clique-decomposed within the same time bound $\mathcal{O}(T(G) + \min\{n^{2.3729}, \omega^2 n\})$ (Theorem 7). Since a minimal triangulation can be computed in $T(G) = \tilde{\mathcal{O}}(n^{2.3729})$-time for any graph G, our main result implies that any graph can be clique-decomposed in $\tilde{\mathcal{O}}(n^{2.3729})$-time. Furthermore, faster and practical algorithms can be obtained in some cases — whenever the graphs have bounded clique-number and a minimal triangulation can be computed efficiently. We will show it is the case

[1]It seems to us that the techniques in [28] could also be applied to any minimal triangulation. Nonetheless, we will propose a method that is, to our opinion, slightly simpler than theirs.



(a) G (b) Atom tree of G

Figure 1: A connected graph G (Figure 1a), an atom tree of the graph (Figure 1b).

for interesting graph classes such as planar graphs, bounded-treewidth graphs and bounded-degree graphs (see Section 5.1 for details).

Altogether, this is hint that our $\tilde{\mathcal{O}}(n^{2.3729})$-time clique-decomposition algorithm is optimal up to polylogarithmic factors — due to the well-know equivalence between triangle detection and matrix multiplication [33].

Definitions and useful notations are given in Section 2. Last, we will conclude this paper with an open conjecture in Section 6.

2 Definitions and preliminaries

We will use standard graph terminology from [10]. Graphs in this study are finite, simple (hence without loops nor multiple edges) connected and unweighted, unless stated otherwise. Given a graph $G = (V, E)$ and a set $S \subseteq V$, we will denote by $G[S]$ the subgraph of G that is induced by S. The open neighbourhood of S, denoted by $N(S)$, is the set of all vertices in $G[V \setminus S]$ that are adjacent to at least one vertex in S. The closed neighbourhood of S is denoted by $N[S] = N(S) \cup S$.

Clique-minimal separators. A set $S \subseteq V$ is a *separator* in G if there are at least two connected components in $G[V \setminus S]$. In particular, a *full component* in $G[V \setminus S]$ is any connected component C in $G[V \setminus S]$ satisfying that $N(C) = S$ (note that a full component might fail to exist). The set S is called a *minimal separator* in G if it is a separator and there are at least two full components in $G[V \setminus S]$. In particular, S is a *clique-minimal separator* if it is a minimal separator and $G[S]$ is a complete subgraph.

Clique-decomposition and atom tree. A graph is *prime* if it does not contain any clique-minimal separator. Examples of prime graphs are the complete graph K_n and the cycle graph C_n. The *clique-decomposition* of a graph G is the family of all inclusionwise maximal subsets A_i such that $G[A_i]$ is prime, and it is unique [30]. The subsets A_i are called the *atoms* of G.

Usually, we represent the clique-decomposition with a binary rooted tree, that is called an *atom tree* and is recursively defined as follows (see Figure 1 for an illustration).

- If G is a prime graph then it has a unique atom tree, that is a single node labeled with V.
- Else, an atom tree of G is any binary rooted tree such that: its root is labeled with a clique-minimal separator S in G, the left child of the root is a leaf-node that is labelled with $A = S \cup C$ where C is a full component of $G[V \setminus S]$ and $G[A]$ is prime, furthermore the subtree that is rooted at the right child of the root is an atom tree of $G[V \setminus C]$.

Informally, an atom tree can be seen as the trace of some execution of a clique-decomposition algorithm (*e.g.*, a decomposition ordering). Note that the atom tree of a graph may not be unique. Furthermore, any atom tree has linear-size (defined as the sum of the label cardinalities) $\mathcal{O}(n + m)$ [5].

Lemma 1 ([30]). *Let $G = (V, E)$ and T be an atom tree of G. Each leaf-node of T is labeled with an atom of G, and each atom of G appears exactly once as a leaf-node label in T.*

Since any atom tree has linear-size, we have by Lemma 1 that $\sum_i |A_i| = \mathcal{O}(n+m)$, where the sets A_i denote the atoms of G. In contrast with the above result, we observe that there may be $\Omega(\omega^2 n)$ edges in the subgraphs that are induced by the atoms of G, with ω being the clique-number of G, that is, the size of a largest complete subgraph in G (*e.g.*, see Figure 2).

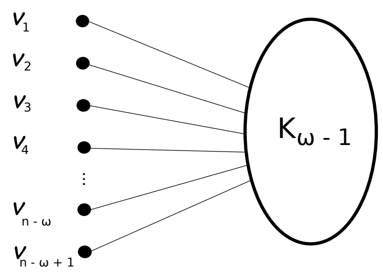


Figure 2: A split graph G with clique-number ω. The atoms of G are the sets $N[v_i]$ for $1 \leq i \leq n-\omega+1$. Hence, there are $\omega(\omega-1)(n-\omega+1)/2$ edges in the subgraphs $G[N[v_i]]$ that are induced by the atoms of G.

Minimal triangulation. A *triangulation* of $G=(V,E)$ is any supergraph $H=(V,E\cup F)$ such that H does not contain any induced cycle of length at least four. In particular, H is a *minimal triangulation* of G if for any strict subset $F' \subset F$, the supergraph $H'=(V,E\cup F')$ is not a triangulation of G.

There exist strong relationships between minimal triangulations and clique-minimal separators. Namely, we will use the following lemma.

Lemma 2 ([6]). *For any minimal triangulation H of a graph G, the clique-minimal separators in G are exactly the minimal separators in H that induce complete subgraphs of G.*

3 Time complexity lower-bound

Let us start proving the hardness of clique-decomposition by reducing this problem from triangle detection. In the following, recall that a simplicial vertex is one whose closed neighbourhood induces a complete subgraph. We will need the following lemma.

Lemma 3 ([27]). *The problem of counting the number of simplicial vertices in a graph with $3n+2$ vertices is at least as hard as determining whether a graph on n vertices has a triangle.*

Theorem 4. *The problem of computing the clique-decomposition of a graph with $3n+2$ vertices is at least as hard as determining whether a graph on n vertices has a triangle.*

Proof. Let $G=(V,E)$ be any graph with $3n+2$ vertices. In order to prove the theorem, by Lemma 3 it is sufficient to prove that counting the number of simplicial vertices in G can be done in $\mathcal{O}(n+m)$-time if the clique-decomposition of G is given (encoded as an atom tree).

We claim that for every simplicial vertex $v \in V$, its closed neighbourhood $N[v]$ is an atom, and in particular it is the unique atom containing v. Indeed, since $G[N[v]]$ is complete, we have that $G[N[v]]$ is prime, and so, the subset $N[v]$ must be contained in *any* atom A containing v. Furthermore, if it were the case that there exists $u \in A \setminus N[v]$ then the clique $N(v)$ would be a uv-separator, thus contradicting the fact that $G[A]$ is prime. As a result, we have that $A = N[v]$, that proves the claim.

Recall that using an atom tree of G, every atom A_i of G can be written $A_i = C_i \cup S_i$ with S_i being a clique-minimal separator and $S_i \subseteq N(C_i)$. In particular, let $M_i \subseteq C_i$ contain every vertex in the atom that is not contained in any other atom A_j, with $j \neq i$. Note that all the subsets M_i can be computed by visiting the atoms sequentially, which takes $\mathcal{O}(\sum_i |A_i|) = \mathcal{O}(n+m)$-time. Furthermore, we have by the above claim that in order to count the number of simplicial vertices in G, it is sufficient to sum together the cardinalities

$|M_i|$ of the subsets M_i such that the atom A_i is a clique. Here is a way to achieve the goal in linear-time. Since the subsets C_i are pairwise disjoint, let us reorder the vertices in G so that in any adjacency list, it first appears the neighbours in C_1, then those in C_2, and so on. In such case, the atom A_i is a clique if and only if each vertex in C_i has $|A_i| - 1$ neighbours in A_i, that is, $|A_i| - 1$ neighbours that are not contained in any C_j, with $j < i$. The latter can be verified by visiting the subsets C_i sequentially, while removing the vertices in C_i from all adjacency lists at the i^{th} step. Since the adjacency lists have been reordered, it can be done in $\mathcal{O}(m + \sum_i |C_i|) = \mathcal{O}(n + m)$-time. So, overall, finding the atoms A_i that are cliques can be done in $\mathcal{O}(n + m)$-time, which implies that counting the number of simplicial vertices in G can be done within the same time complexity. □

4 Computing the clique-minimal separators

This section is devoted to fast computation of the clique-minimal separators in a graph. We will introduce two methods which both make use of Lemma 2.

Proposition 5. *Let $G = (V, E)$. Suppose that a minimal triangulation of G can be computed in time $T(G)$. Then, the clique-minimal separators of G can be computed in $\mathcal{O}(T(G) + n^{2.3729})$-time.*

Proof. Let $H = (V, E \cup F)$ be a minimal triangulation of G, with $f = |F|$ fill edges. By the hypothesis it can be computed in time $T(G)$. Let $\Xi = (S_1, S_2, \ldots, S_l)$ be the minimal separators of H, with $l \leq n$. By [21], the family Ξ can be computed in $\mathcal{O}(n + m + f) = \mathcal{O}(n^2)$-time. Furthermore, recall that by Lemma 2 the clique-minimal separators of G are exactly the separators in Ξ that are cliques of G. In order to compute them, let $V = (v_1, v_2, \ldots, v_n)$ be totally ordered. Let $\mathcal{A}_G$ be the adjacency matrix of G, and let $\mathcal{B}_H$ be the *clique matrix* of H (of dimensions $n \times l$) defined as follows. For every $1 \leq i \leq n$ and for every $1 \leq j \leq n$, we have $b_{ij} = 1$ if $v_i \in S_j$ and $b_{ij} = 0$ otherwise. Then, $\mathcal{C} = \mathcal{A}_G \mathcal{B}_H$ is a matrix of dimensions $n \times l$. It can be computed in $\mathcal{O}(n^{2.3729})$-time by using fast matrix multiplication since $l \leq n$ [29]. Furthermore, for every $1 \leq i \leq n$ and for every $1 \leq j \leq n$, we have $c_{ij} = |N_G(v_i) \cap S_j|$. Therefore, $S_j \in \Xi$ is a clique-minimal separator of G if and only if we have $c_{ij} = |S_j| - 1$ for every $v_i \in S_j$. As a result, the clique-minimal separators of G are obtained from the matrix $\mathcal{C}$ in time $\mathcal{O}(\sum_{j=1}^{l} |S_j|)$, that is $\mathcal{O}(n + m + f) = \mathcal{O}(n^2)$. □

Proposition 6. *Let $G = (V, E)$. Suppose that a minimal triangulation of G can be computed in time $T(G)$. Then, the clique-minimal separators of G can be computed in $\mathcal{O}(T(G) + \omega^2 n)$-time.*

Proof. Let $H = (V, E \cup F)$ be a minimal triangulation of G, with $f = |F|$ fill edges. By the hypothesis it can be computed in time $T(G)$. Let us compute the set Ξ of all minimal separators of H. By [21], the family Ξ can be computed in $\mathcal{O}(n + m + f) = \mathcal{O}(T(G))$-time.

Let $\mathcal{S} = \Xi$. Our aim is to remove separators of H from $\mathcal{S}$ until it only contains the clique-minimal separators of G. In order to achieve the result, let $V = (v_1, v_2, \ldots, v_n)$ be totally ordered. We consider the vertices sequentially. For every $1 \leq i \leq n$, let $\mathcal{S}_i \subseteq \mathcal{S}$ contain every $S \in \mathcal{S}$ such that $v_i \in S$. Furthermore, let $S_{<i} := S \cap \{v_1, \ldots, v_{i-1}\}$ for every $S \in \mathcal{S}_i$. If $S_{<i} \not\subseteq N_G(v_i)$ then S is not a clique and it is discarded from $\mathcal{S}$. Therefore, once the algorithm has terminated, subsets in $\mathcal{S}$ are exactly the minimal separators of H that are cliques of G. By Lemma 2, these are exactly the clique-minimal separators of G. Hence the above algorithm is correct.

Let us focus on the time complexity. Assume for ease of computation that we maintain an "incidence graph" $\mathcal{I}_{\mathcal{S}}$: with vertex set $V \cup \mathcal{S}$ and an edge between every vertex $v_i \in V$ and every separator $S \in \mathcal{S}_i$. Note that $\mathcal{I}_{\mathcal{S}}$ can be constructed at the initialization step (when $\Xi = \mathcal{S}$) in $\mathcal{O}(|V| + \sum_{S \in \Xi} |S|) = \mathcal{O}(n+m+f)$-time, that is $\mathcal{O}(T(G))$. Furthermore, for every $1 \leq i \leq n$ the separators in $\mathcal{S}_i$ are exactly the neighbours of vertex v_i in $\mathcal{I}_{\mathcal{S}}$, hence it takes $\mathcal{O}(|\mathcal{S}_i|)$-time to access to each of the separators in $\mathcal{S}_i$. Discarding a separator $S \in \mathcal{S}_i$ from $\mathcal{S}$ is equivalent to deleting the vertex corresponding to S in $\mathcal{I}_{\mathcal{S}}$, which can be done in $\mathcal{O}(|S|)$-time. Overall, these two types of operations (accessing and discarding) take $\mathcal{O}(\sum_{i=1}^{n} |\mathcal{S}_i| + \sum_{S \in \Xi} |S|)$-time, that is $\mathcal{O}(\sum_{S \in \Xi} |S|) = \mathcal{O}(T(G))$-time.

Finally, deciding whether $S_{<i} \not\subseteq N_G(v_i)$ for every $S \in \mathcal{S}_i$ takes time $\mathcal{O}(|N_G(v_i)| + \sum_{S \in \mathcal{S}_i} |S_{<i}|)$. Furthermore, since the vertices are considered sequentially, we have that $S_{<i}$ is a clique for every $S \in \mathcal{S}_i$ (or else, S would have been discarded from $\mathcal{S}$ at some step $j < i$ of the algorithm). This implies that $\sum_{i | S \in \mathcal{S}_i} |S_{<i}| \leq \sum_{j=1}^{\omega} j = \omega(\omega+1)/2 = \mathcal{O}(\omega^2)$ for every $S \in \Xi$. Hence, since H is triangulated, and so, $|\Xi| \leq n$, we have:

$$\sum_{i=1}^{n} \sum_{S \in \mathcal{S}_i} |S_{<i}| = \sum_{S \in \Xi} \sum_{i | S \in \mathcal{S}_i} |S_{<i}| = \mathcal{O}(\omega^2 n).$$

□

5 Faster computation of clique-decomposition

In Section 4, we proved that if a minimal triangulation of a graph G can be computed in time $T(G)$, then the clique-minimal separators of G can be computed in $\mathcal{O}(T(G) + \min\{n^{2.3729}, \omega^2 n\})$-time. We now prove that an atom tree of G can be computed within the same time bounds.

Theorem 7. *Let $G = (V, E)$. Suppose that a minimal triangulation of G can be computed in time $T(G)$. Then, the clique-decomposition of G can be computed in $\mathcal{O}(T(G) + \min\{n^{2.3729}, \omega^2 n\})$-time.*

Proof. Let $H = (V, E \cup F)$ be a minimal triangulation of G, with $f = |F|$ fill edges. By the hypothesis it can be computed in time $T(G)$. Furthermore, the clique-decomposition of G can be computed in $\mathcal{O}(n+m+f) = \mathcal{O}(T(G))$-time if H and the clique-minimal separators of G are given [7]. By Propositions 5 and 6, the clique-minimal separators of G can be computed in $\mathcal{O}(T(G) + \min\{n^{2.3729}, \omega^2 n\})$-time. So, overall it takes $\mathcal{O}(T(G) + \min\{n^{2.3729}, \omega^2 n\})$-time to compute the clique-decomposition of G. □

On the combinatorial side, our approach for computing the clique-decomposition (Theorem 7) is at least as good as the state-of-the-art $\mathcal{O}(nm)$-time algorithm. Indeed, for any graph G, a minimal triangulation of G can be computed in time $T(G) = \mathcal{O}(nm)$ [31]. Furthermore if G has clique-number ω then it has number of edges $m \geq \omega(\omega-1)/2 = \Omega(\omega^2)$.

Corollary 8. *The clique-decomposition of a graph G can be computed in $\tilde{\mathcal{O}}(n^{2.3729})$-time.*

Proof. Since a minimal triangulation of a graph G can be computed in $\tilde{\mathcal{O}}(n^{2.3729})$-time [25], the result follows from Theorem 7 by replacing $T(G)$ with $\tilde{\mathcal{O}}(n^{2.3729})$. □

5.1 Applications

By Theorem 7, the clique-decomposition of a graph G can be computed in quasi linear-time if `i)` G has bounded clique-number and `ii)` a minimal triangulation of G can be computed efficiently. Below, we list a few graph classes for which it is the case.

- A graph G has *tree-width* at most k if there exists a triangulation of G with clique-number at most k. Note that the clique-number ω of G is a lower-bound on its tree-width. Furthermore, if G has tree-width k then a minimal triangulation of G can be computed in $\mathcal{O}(k^7 \cdot n \log n)$-time [20]. Therefore, by Theorem 7 the clique-decomposition of bounded tree-width graphs can be computed in $\mathcal{O}(n \log n)$-time.
- A graph G is *planar* if it can be drawn in the Euclidean plane so that edges may only intersect at their endpoints. By Kuratowski Theorem, G is planar if and only if G is $\{K_{3,3}, K_5\}$-minor-free. So, a planar graph G has bounded clique-number $\omega \leq 4$. Furthermore, if G is planar then a minimal triangulation of G can be computed in $\mathcal{O}(n)$-time [16]. As a result, by Theorem 7 the clique-decomposition of planar graphs can be computed in linear-time.

- Finally, let us consider bounded-degree graphs. Indeed, for every graph G, $\omega \leq \Delta + 1$ with ω and Δ being respectively the clique-number and the maximum degree of G. Therefore, bounded-degree graphs have bounded clique-number. Furthermore, if G has maximum degree Δ then a minimal triangulation of G can be computed in $\mathcal{O}(n \cdot (\Delta^3 + \alpha(n)))$-time where $\alpha(n)$ here denotes the inverse of Ackerman's function [17]. Hence by Theorem 7 the clique-decomposition of bounded-degree graphs can be computed in $\mathcal{O}(n \cdot \alpha(n))$-time.

6 Conclusion

By Corollary 8, the time complexity of computing the clique-decomposition of an n-vertex graph G is $\tilde{\mathcal{O}}(n^{2.3759})$. It is unlikely that the problem can be solved in $o(n^{2.3759})$-time by Theorem 4 (recall that the two problems of triangle detection and matrix multiplication are equivalent [33]).

Finally, we proved in Theorem 7 that for every graph G with bounded clique-number ω, the clique-decomposition of G can be computed in $\mathcal{O}(T(G) + \omega^2 n)$-time where $T(G)$ here denotes the time needed to compute a minimal triangulation of G. We conjecture that in fact, it can be computed in $\mathcal{O}(\omega^2 n)$-time.

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Appendix G

On the complexity of computing tree decompositions with metric constraints on the bags

On computing tree and path decompositions with metric constraints on the bags*

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Project-Teams COATI

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Abstract: We here investigate on the complexity of computing the *tree-length* and the *tree-breadth* of any graph G, that are respectively the best possible upper-bounds on the diameter and the radius of the bags in a tree decomposition of G. *Path-length* and *path-breadth* are similarly defined and studied for path decompositions. So far, it was already known that tree-length is NP-hard to compute. We here prove it is also the case for tree-breadth, path-length and path-breadth. Furthermore, we provide a more detailed analysis on the complexity of computing the tree-breadth. In particular, we show that graphs with tree-breadth one are in some sense the hardest instances for the problem of computing the tree-breadth. We give new properties of graphs with tree-breadth one. Then we use these properties in order to recognize in polynomial-time all graphs with tree-breadth one that are planar or bipartite graphs. On the way, we relate tree-breadth with the notion of k-*good* tree decompositions (for $k = 1$), that have been introduced in former work for routing. As a byproduct of the above relation, we prove that deciding on the existence of a k-good tree decomposition is NP-complete (even if $k = 1$). All this answers open questions from the literature.

Key-words: Tree-length; Tree-breadth; Path-length; Path-breadth; k-good tree decompositions;

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Sur la complexité du calcul de décompositions arborescentes ou linéaires avec des contraintes sur les distances dans les sacs

Résumé : Nous étudions la complexité du calcul de la *tree-length* et de la *tree-breadth* pour tout graphe G, qui sont respectivement les meilleures bornes supérieures possibles sur le diamètre et le rayon des sacs dans une décomposition arborescente de G. La *path-length* et la *path-breadth* sont définies (et étudiées) de manière identique pour les décompositions linéaires. Il était connu jusqu''à présent que le calcul de la tree-length est NP-difficile. Nous prouvons dans ce rapport qu'il en va de même pour les paramètres tree-breadth, path-length et path-breadth. Par ailleurs, nous analysons plus en détails la complexité du calcul de la tree-breadth. En particulier, nous montrons que les graphes de tree-breadth 1 sont, en un sens que nous préciserons par la suite, les instances les plus difficiles pour le problème du calcul de la tree-breadth. Nous démontrons de nouvelles propriétés des graphes de tree-breadth 1. Puis nous utilisons ces propriétés afin de reconnaître en temps polynomial si un graphe planaire ou biparti a sa tree-breadth égale à 1. En chemin dans la preuve des résultats ci-dessus, nous établissons une relation entre la tree-breadth d'un graphe et l'existence d'une décomposition arborescente "k-good" (avec $k = 1$), un problème qui avait été introduit dans la littérature sur le routage compact. Comme conséquence directe de cette relation, nous prouvons que décider de l'existence d'une décomposition arborescente "k-good" est un problème NP-complet (même si $k = 1$). Nous répondons ainsi à des questions ouvertes de la littérature.

Mots-clés : Tree-length; Tree-breadth; Path-length; Path-breadth; Décomposition k-good;

1 Introduction

Context. It is a fundamental problem in metric graph theory [5] to embed a graph into a simpler metric space while minimizing the (multiplicative) distortion of the distances in the graph. In particular, minimum distortion embeddings of a graph into a tree or a path have practical applications in computer vision [45], computational chemistry and biology [35] as well as in network design and distributed protocols [33]. The two problems to embed a graph into a tree or a path with minimum distortion are NP-hard [2, 6, 40]. However, there exists a nice setting in order to approximate these two problems. More precisely, a series of graph parameters has been introduced in recent work in order to measure how much the *distance distribution* of a graph is close to a tree metric or a path metric [24, 26, 27]. We refer to [25, 27] for details about the relationships between these parameters and the two above-mentioned embedding problems. Here we study the complexity of computing these parameters, thereby solving open problems in the literature.

The parameters that are considered in this note can be defined using the terminology of Robertson and Seymour tree decompositions [43]. Informally, a tree decomposition is a dividing of a graph G into "bags": that are overlapping subgraphs that can be pieced together in a tree-like manner (formal definitions will be given in the technical sections of the paper). The shortest-path metric of G is "tree-like" when each bag of the tree decomposition has bounded diameter and bounded radius, where the distance taken between two vertices in a same bag is their distance in G. The *tree-length* [24] and the *tree-breadth* [26] of G are respectively the best possible upper-bounds on the diameter and the radius of the bags in a tree decomposition of G. *Path-length* [46] and *path-breadth* [27] are defined in the same fashion as tree-length and tree-breadth for path decompositions. In this paper, we focus on the complexity of computing the four parameters tree-length, tree-breadth, path-length and path-breadth.

Recent studies suggest that some classes of real-life networks – including biological networks and social networks – have bounded tree-length and tree-breadth [1]. This metric tree-likeness can be exploited in algorithms. For instance, bounded tree-length graphs admit compact distance labeling scheme [23] as well as a PTAS for the well-known Traveling Salesman problem [38]. Furthermore, the diameter and the radius of bounded tree-length graphs can be approximated up to an additive constant in linear-time [17]. In contrast to the above result, we emphasize that under classical complexity assumptions the diameter of general graphs *cannot* be approximated up to an additive constant in subquadratic-time, that is prohibitive for very large graphs [15].

Note that a large amount of the literature about tree decompositions rather seeks to minimize the *size* of the bags than their diameter. The *tree-width* [43] of a graph G is the best possible upper-bound on the size of the bags in a tree decomposition of G. However, tree-length and the other parameters that are considered in this paper can differ arbitrarily from tree-width; we refer to [20] for a global picture on the relations between tree-length and tree-width. Furthermore, one aim of this paper is to complete the comparison between tree-width and path-width on one side, and tree-length, tree-breadth, path-length and path-breadth on the other side, from the complexity point of view. Let us remind that computing the tree-width (resp. the path-width) is NP-hard [3, 36], however for every fixed $k \geq 1$ there is a linear-time algorithm to decide whether a graph has tree-width at most k (resp., path-width at most k) [8, 12].

Related work. The complexity of computing tree-length, tree-breadth, path-length and path-breadth has been left open in several works [24, 26, 27]. So far, it has been solved only for tree-length, that is NP-hard to compute.

Tree-length and tree-breadth. It is NP-complete to decide whether a graph has tree-length at most k for every constant $k \geq 2$ [39]. However, the reduction used for tree-length goes through weighted graphs and then goes back to unweighted graphs using rather elegant gadgets. It does not seem to us these gadgets can be easily generalized in order to apply to the other parameters that are considered in this note. On a more positive side, there exists a 3-approximation algorithm for tree-length [24]. In this aspect, it looks natural to investigate on the complexity of computing the tree-breadth, since any polynomial-time algorithm would imply an improved 2-approximation algorithm for tree-length.

Path-length and path-breadth. There exist constant-factor approximation algorithms for path-length and path-breadth [27]. Recently, the minimum eccentricity shortest-path problem – that is close to the computation of path-length and path-breadth – has been proved NP-hard [28]. Let us point out that for every fixed k, it can be decided in polynomial-time whether a graph admits a shortest-path with eccentricity at most k [28]. Our results will show the situation is different for path-length and path-breadth than for the minimum eccentricity shortest-path.

Our contributions. On the negative side, we prove that tree-breadth, path-length and path-breadth are NP-hard to compute. More precisely:

- recognizing graphs with tree-breadth one is NP-complete;
- recognizing graphs with path-length two is NP-complete;
- recognizing graphs with path-breadth one is NP-complete.

It is remarkable the last two results (for path-length and path-breadth) are obtained using *the same reduction.* Our reductions have distant similarities with the reduction that was used for tree-length. However, they do not need any detour through weighted graphs.

We next focus our work on tree-breadth (although part of the results may extend to the three other parameters that are considered in this note). We give a more in-depth analysis on the complexity of computing this parameter. In particular, we prove it is equally hard to compute tree-breadth as to recognize graphs with tree-breadth one. Therefore, graphs with tree-breadth one are in some sense the hardest instances for the problem of computing the tree-breadth. The latter partly answers an open question from [26], where it was asked for a characterization of graphs with tree-breadth one. We also prove a few properties of graphs with tree-breadth one. In particular, graphs with tree-breadth one are exactly those graphs admitting a 1-*good tree decomposition*, that is a tree decomposition whose each bag has a spanning star. The more general notion of k-good tree decompositions was introduced in [37] to obtain new compact routing schemes. Note that as a byproduct of the above relation between 1-good tree decompositions and graphs with tree-breadth one, we obtain that deciding on the existence of a k-good tree decomposition is an NP-complete problem even when $k = 1$.

Finally, on the algorithmic side, we show how to recognize in polynomial time all graphs of tree-breadth one that are planar or bipartite. In particular, our recognition algorithm for planar graphs of tree-breadth one relies upon deep structural properties of these graphs.

Definitions and useful notations are given in Section 2. All our results of NP-completeness are listed and proved in Section 3. Sections 4 and 5 are devoted to the computation of tree-breadth. In particular, in Section 5 we present and we prove correctness of an algorithm to recognize planar graphs with tree-breadth one. Finally, we discuss about some open questions in the conclusion (Section 6).

2 Definitions and preliminary results

We refer to [22] for a survey on graph theory. Graphs in this study are finite, simple, connected and unweighted. Let $G = (V, E)$ be a graph. For any $X \subseteq V$, let $G[X]$ denote the subgraph of G induced by X. For any subgraph H of G, let $N_H(v)$ denote the set of neighbors of $v \in V$ in H, and let $N_H[v] = N_H(v) \cup \{v\}$. The distance $dist_H(u, v)$ between two vertices $u, v \in V$ in H is the minimum length (number of edges) of a path between u and v in a subgraph H of G. In what follows, we will omit the subscript when no ambiguity occurs. A set $S \subseteq V$ is a dominating set of G if any vertex of $V \setminus S$ has a neighbor in S. The *dominating number* $\gamma(G)$ of a graph G is the minimum size of a dominating set of G.

Tree decompositions and path decompositions of a graph. A *tree decomposition* $(T, \mathcal{X})$ of G is a pair consisting of a tree T and of a family $\mathcal{X} = (X_t)_{t \in V(T)}$ of subsets of V indexed by the nodes of T and satisfying:

- $\bigcup_{t \in V(T)} X_t = V$;
- for any edge $e = \{u, v\} \in E$, there exists $t \in V(T)$ such that $u, v \in X_t$;
- for any $v \in V$, the set of nodes $t \in V(T)$ such that $v \in X_t$ induces a subtree, denoted by T_v, of T.

The sets X_t are called *the bags* of the decomposition. If no bag is contained into another one, then the tree decomposition is called *reduced*. Starting from any tree decomposition, a reduced tree decomposition can be obtained in polynomial-time by contracting any two adjacent bags with one contained into the other until it is no more possible to do that.

In the following we will make use of the *Helly property* in our proofs:

Lemma 1 *[4, Helly property] Let T be a tree and let $T_1, T_2, \ldots, T_k$ be a finite family of pairwise intersecting subtrees. Then, $\bigcap_{i=1}^k T_i \neq \emptyset$, or equivalently there is a node contained in all the k subtrees.*

Finally, let $(T, \mathcal{X})$ be a tree decomposition, it is called a *path decomposition* if T induces a path.

Metric tree-likeness and path-likeness. All graph invariants that we consider in the paper can be defined in terms of tree decompositions and path decompositions. Let $(T, \mathcal{X})$ be any tree decomposition of a graph G. For any $t \in V(T)$,

- the *diameter* of bag X_t equals $\max_{v,w \in X_t} dist_G(v, w)$;
- the *radius* $\rho(t)$ of a bag X_t equals $\min_{v \in V} \max_{w \in X_t} dist_G(v, w)$.

The *length* of $(T, \mathcal{X})$ is the maximum diameter of its bags, while the *breadth* of $(T, \mathcal{X})$ is the maximum radius of its bags. The *tree-length* and the *tree-breadth* of G, respectively denoted by $tl(G)$ and $tb(G)$, are the minimum length and breadth of its tree decomposition, respectively.

Let k be a positive integer, the tree decomposition $(T, \mathcal{X})$ is called *k-good* when each bag contains a dominating induced path of length at most $k - 1$. It is proved in [37] every graph G has a k-good tree decomposition for $k = ch(G) - 1$, with $ch(G)$ denoting the size of a longest induced cycle of G. Finally, path-length, path-breadth and k-good path decompositions are similarly defined and studied for the path decompositions as tree-length, tree-breadth and k-good tree decompositions are defined and studied for the tree decompositions. The path-length and path-breadth of G are respectively denoted by $pl(G)$ and $pb(G)$.

It has been observed in [26, 27] that the four parameters tree-length, tree-breadth and path-length, path-breadth are contraction-closed invariants. We will use the latter property in our proofs.

Lemma 2 ([26, 27]) *For every $G = (V, E)$ and for any edge $e \in E$:*

$$tl(G/e) \leq tl(G),\ tb(G/e) \leq tb(G) \text{ and } pl(G/e) \leq pl(G),\ pb(G/e) \leq pb(G).$$

Furthermore, it can be observed that for any graph G, $tb(G) \leq tl(G) \leq 2 \cdot tb(G)$ and similarly $pb(G) \leq pl(G) \leq 2 \cdot pb(G)$. Moreover, if a graph G admits a k-good tree decomposition, then $tb(G) \leq \lfloor k/2 \rfloor + 1$ and $tl(G) \leq k + 1$. Before we end this section, let us prove the stronger equivalence, $tb(G) = 1$ if and only if G admits a 1-good tree decomposition. This result will be of importance in the following. Since a tree decomposition is 1-good if and only if each bag contains a spanning star, we will name the 1-good tree decompositions *star-decompositions* in the following.

Definition 1 *Let $G = (V, E)$ be a connected graph, a star-decomposition is a tree decomposition $(T, \mathcal{X})$ of G whose each bag induces a subgraph of dominating number one, i.e., for any $t \in V(T)$, $\gamma(G[X_t]) = 1$.*

Clearly, if a graph admits a star-decomposition, then it has tree-breadth at most one. Let us prove that the converse also holds.

Lemma 3 *For any graph G with $tb(G) \leq 1$, every* reduced *tree decomposition of G of breadth one is a star-decomposition. In particular:*

- *any tree decomposition of G of breadth one can be transformed into a star-decomposition in polynomial-time;*
- *similarly, any path decomposition of G of breadth one can be transformed into a 1-good path decomposition in polynomial-time.*

Proof. Let $(T, \mathcal{X})$ be any reduced tree decomposition of G of breadth one. We will prove it is a star-decomposition. To prove it, let $X_t \in \mathcal{X}$ be arbitrary and let $v \in V$ be such that $\max_{w \in X_t} dist_G(v, w) = 1$, which exists because X_t has radius one. We now show that $v \in X_t$. Indeed, since the subtree T_v and the subtrees $T_w, w \in X_t$, pairwise intersect, then it comes by the Helly Property (Lemma 1) that $T_v \cap \left(\bigcap_{w \in X_t} T_w\right) \neq \emptyset$ *i.e.*, there is some bag containing $\{v\} \cup X_t$. As a result, we have that $v \in X_t$ because $(T, \mathcal{X})$ is a reduced tree decomposition, hence $\gamma(G[X_t]) = 1$. The latter implies that $(T, \mathcal{X})$ is a star-decomposition because X_t is arbitrary.

Now let $(T, \mathcal{X})$ be any tree decomposition of G of breadth one. It can be transformed in polynomial-time into a reduced tree decomposition $(T', \mathcal{X}')$ so that $\mathcal{X}' \subseteq \mathcal{X}$. Furthermore, $(T', \mathcal{X}')$ has breadth one because it is the case for $(T, \mathcal{X})$, therefore $(T', \mathcal{X}')$ is a star-decomposition. In particular, if $(T, \mathcal{X})$ is a path decomposition then so is $(T', \mathcal{X}')$. ■

Corollary 1 *For any graph G, $tb(G) \leq 1$ if and only if G admits a star-decomposition.*

3 Intractability results

3.1 Path-length and path-breadth

This section is devoted to the complexity of all path-like invariants that we consider in this paper.

Theorem 1 *Deciding whether a graph has path-length at most k is NP-complete even if $k = 2$.*

In contrast to Theorem 1, graphs with path-length one are exactly the interval graphs [27], *i.e.*, they can be recognized in linear-time.

Theorem 2 *Deciding whether a graph has path-breadth at most k is NP-complete even if $k = 1$.*

From the complexity result of Theorem 2, we will also prove the hardness of deciding on the existence of k-good path decompositions.

Theorem 3 *Deciding whether a graph admits a k-good path decomposition is NP-complete even if $k = 1$.*

Proof. The problem is in NP. By Lemma 3, a graph G admits a 1-good path decomposition if and only if $pb(G) \leq 1$, therefore it is NP-hard to decide whether a graph admits a 1-good path decomposition by Theorem 2. ■

All of the NP-hardness proofs in this section will rely upon the same reduction from the Betweenness problem, defined below. The Betweenness problem, sometimes called the Total Ordering problem, is NP-complete [41]. In [31], it was used to show that the Interval Sandwich problem is NP-complete. What we here prove is that the Interval Sandwich problem remains NP-complete even if the second graph is a *power* of the first one, where the k^{th} power G^k of any graph G is obtained from G by adding an edge between every two distinct vertices that are at distance at most k in G for every integer $k \geq 1$. Indeed, a graph G has path-length at most k if and only if there is an Interval Sandwich between G and G^k (we refer to [39] for the proof of a similar equivalence between tree-length and the Chordal Sandwich problem).

Problem 1 (Betweenness)

Input: *a set $\mathcal{S}$ of n elements, a set $\mathcal{T}$ of m ordered triples of elements in $\mathcal{S}$.*

Question: *Is there a total ordering of $\mathcal{S}$ such that for every triple $t = (s_i, s_j, s_k) \in \mathcal{T}$, either $s_i < s_j < s_k$ or $s_k < s_j < s_i$?*

Now, given an instance $(\mathcal{S}, \mathcal{T})$ of the Betweenness problem, we will construct from $\mathcal{S}$ and $\mathcal{T}$ a graph $G_{\mathcal{S},\mathcal{T}}$ as defined below. We will then prove that $pl(G_{\mathcal{S},\mathcal{T}}) \leq 2$ (resp. $pb(G_{\mathcal{S},\mathcal{T}}) \leq 1$) if and only if $(\mathcal{S}, \mathcal{T})$ is a yes-instance of the Betweenness problem.

Definition 2 *Let $\mathcal{S}$ be a set of n elements, let $\mathcal{T}$ be a set of m ordered triples of elements in $\mathcal{S}$. The graph $G_{\mathcal{S},\mathcal{T}}$ is constructed as follows:*

- *For every element $s_i \in \mathcal{S}$, $1 \leq i \leq n$, there are two adjacent vertices u_i, v_i in $G_{\mathcal{S},\mathcal{T}}$. The vertices u_i are pairwise adjacent i.e., the set $U = \{u_i \mid 1 \leq i \leq n\}$ is a clique.*
- *For every triple $t = (s_i, s_j, s_k) \in \mathcal{T}$, let us add in $G_{\mathcal{S},\mathcal{T}}$ the v_iv_j-path (v_i, a_t, b_t, v_j) of length 3, and the v_jv_k-path (v_j, c_t, d_t, v_k) of length 3.*

- *Finally, for every triple $t = (s_i, s_j, s_k) \in \mathcal{T}$ let us make adjacent a_t, b_t with every u_l such that $l \neq k$, similarly let us make adjacent c_t, b_t with every u_l such that $l \neq i$.*

It can be noticed from Definition 2 that for any $1 \leq i \leq n$, the vertex u_i is adjacent to any vertex but those v_j such that $j \neq i$, those a_t, b_t such that s_i is the last element of triple t and those c_t, b_t such that s_i is the first element of triple t. We refer to Figure 1 for an illustration (see also Figure 2). Observe that $G_{\mathcal{S},\mathcal{T}}$ has diameter 3 because the clique U dominates $G_{\mathcal{S},\mathcal{T}}$, therefore $pl(G_{\mathcal{S},\mathcal{T}}) \leq 3$ and we will show that it is hard to distinguish graphs with path-length two from graphs with path-length three. Similarly, the clique U dominates $G_{\mathcal{S},\mathcal{T}}$ hence $pb(G_{\mathcal{S},\mathcal{T}}) \leq 2$, thus we will show that it is hard to distinguish graphs with path-breadth one from graphs with path-breadth two.

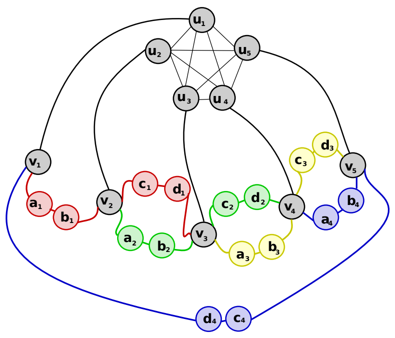

Figure 1: The graph $G_{\mathcal{S},\mathcal{T}}$ for $\mathcal{S} = [|1,5|]$ and $\mathcal{T} = \{(i, i+1, i+2) \mid 1 \leq i \leq 4\}$. Each colour corresponds to a given triple of $\mathcal{T}$. For ease of reading, the adjacency relations between the vertices u_i and the colored vertices a_t, b_t, c_t, d_t are not drawn.

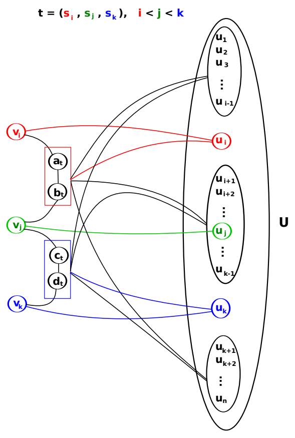

Figure 2: Adjacency relations in $G_{\mathcal{S},\mathcal{T}}$ for one given triple $t = (s_i, s_j, s_k)$.

Lemma 4 *Let $\mathcal{S}$ be a set of n elements, let $\mathcal{T}$ be a set of m ordered triples of elements in $\mathcal{S}$. If $(\mathcal{S}, \mathcal{T})$ is a yes-instance of the Betweenness problem then $pb(G_{\mathcal{S},\mathcal{T}}) \leq 1$ and $pl(G_{\mathcal{S},\mathcal{T}}) \leq 2$, where $G_{\mathcal{S},\mathcal{T}}$ is the graph that is defined in Definition 2.*

Proof. Since $pl(G_{\mathcal{S},\mathcal{T}}) \leq 2 \cdot pb(G_{\mathcal{S},\mathcal{T}})$ then we only need to prove that $pb(G_{\mathcal{S},\mathcal{T}}) \leq 1$. For convenience, let us reorder the elements of $\mathcal{S}$ so that for every triple $(s_i, s_j, s_k) \in \mathcal{T}$ either $i < j < k$ or $k < j < i$. It is possible to do that because by the hypothesis $(\mathcal{S}, \mathcal{T})$ is a yes-instance of the Betweenness problem. If furthermore $k < j < i$, let us also replace (s_i, s_j, s_k) with the inverse triple (s_k, s_j, s_i). This way, we have a total ordering of $\mathcal{S}$ such that $s_i < s_j < s_k$ for every triple $(s_i, s_j, s_k) \in \mathcal{T}$. Then, let us construct a path decomposition $(P, \mathcal{X})$ with n bags, denoted $X_1, X_2, \ldots, X_n$, as follows. For every $1 \leq i \leq n$, $U \subseteq X_i$ and $v_i \in X_i$. For every $t = (s_i, s_j, s_k) \in \mathcal{T}$, we add both a_t, b_t into the bags X_l with $i \leq l \leq j$, similarly we add both c_t, d_t into the bags X_l with $j \leq l \leq k$. By construction, the clique U is contained in any bag of P and for every triple $t = (s_i, s_j, s_k) \in \mathcal{T}$ we have $a_t, b_t, v_i \in X_i$ and $a_t, b_t, c_t, d_t, v_j \in X_j$ and $c_t, d_t, v_k \in X_k$, therefore $(P, \mathcal{X})$ is indeed a path decomposition of $G_{\mathcal{S},\mathcal{T}}$.

We claim that for every i, $X_i \subseteq N[u_i]$, that will prove the lemma. Indeed if it were not the case for some i then by Definition 2 there should exist $t \in \mathcal{T}, j, k$ such that: either $t = (s_i, s_j, s_k) \in \mathcal{T}$ and $c_t, d_t \in X_i$; or $t = (s_k, s_j, s_i) \in \mathcal{T}$ and $a_t, b_t \in X_i$. But then by construction either a_t, b_t

are only contained in the bags X_l for $k \leq l \leq j$, or c_t, d_t are only contained in the bags X_l for $j \leq l \leq k$, thus contradicting the fact that either $a_t, b_t \in X_i$ or $c_t, d_t \in X_i$. ■

Lemma 5 *Let $\mathcal{S}$ be a set of n elements, let $\mathcal{T}$ be a set of m ordered triples of elements in $\mathcal{S}$. If $pb(G_{\mathcal{S},\mathcal{T}}) \leq 1$ or $pl(G_{\mathcal{S},\mathcal{T}}) \leq 2$ then $(\mathcal{S},\mathcal{T})$ is a yes-instance of the Betweenness problem, where $G_{\mathcal{S},\mathcal{T}}$ is the graph that is defined in Definition 2.*

Proof. Since $pl(G_{\mathcal{S},\mathcal{T}}) \leq 2 \cdot pb(G_{\mathcal{S},\mathcal{T}})$ then we only need to consider the case when $pl(G_{\mathcal{S},\mathcal{T}}) \leq 2$. Let $(P, \mathcal{X})$ be a path decomposition of length two, that exists by the hypothesis. Since the vertices v_i are pairwise at distance 3 then the subpaths P_{v_i} that are induced by the bags containing vertex v_i are pairwise disjoint. Therefore, starting from an arbitrary endpoint of P and considering each vertex v_i in the order that it appears in the path decomposition, this defines a total ordering over $\mathcal{S}$. Let us reorder the set $\mathcal{S}$ so that vertex v_i is the i^{th} vertex to appear in the path-decomposition. We claim that for every triple $t = (s_i, s_j, s_k) \in \mathcal{T}$, either $i < j < k$ or $k < j < i$, that will prove the lemma.

By way of contradiction, let $t = (s_i, s_j, s_k) \in \mathcal{T}$ such that either $j < \min\{i,k\}$ or $j > \max\{i,k\}$. By symmetry, we only need to consider the case when $j < i < k$. In such case by construction the path between P_{v_j} and P_{v_k} in P contains P_{v_i}. Let $B \in P_{v_i}$, by the properties of a tree decomposition it is a $v_j v_k$-separator, so it must contain one of c_t, d_t. However, vertex $v_i \in B$ is at distance 3 from both vertices c_t, d_t, thus contradicting the fact that $(P, \mathcal{X})$ has length 2. ■

We are now able to prove Theorems 1 and 2.

Proof of Theorem 1. To prove that a graph G satisfies $pl(G) \leq k$, it suffices to give as a certificate a tree decomposition of G with length at most k. Indeed, the all-pairs-shortest-paths in G can be computed in polynomial-time. Therefore, the problem of deciding whether a graph has path-length at most k is in NP. Given an instance $(\mathcal{S},\mathcal{T})$ of the Betweenness problem, let $G_{\mathcal{S},\mathcal{T}}$ be as defined in Definition 2. We claim that $pl(G_{\mathcal{S},\mathcal{T}}) \leq 2$ if and only if the pair $(\mathcal{S},\mathcal{T})$ is a yes-instance of the Betweenness problem. This will prove the NP-hardness because our reduction is polynomial and the Betweenness problem is NP-complete. To prove the claim in one direction, if $(\mathcal{S},\mathcal{T})$ is a yes-instance then by Lemma 4 $pl(G_{\mathcal{S},\mathcal{T}}) \leq 2$. Conversely, if $pl(G_{\mathcal{S},\mathcal{T}}) \leq 2$ then $(\mathcal{S},\mathcal{T})$ is a yes-instance by Lemma 5, that proves the claim in the other direction. ■

Proof of Theorem 2. To prove that a graph G satisfies $pb(G) \leq k$, it suffices to give as a certificate a tree decomposition of G with breadth at most k. Indeed, the all-pairs-shortest-paths in G can be computed in polynomial-time. Therefore, the problem of deciding whether a graph has path-breadth at most k is in NP. Given an instance $(\mathcal{S},\mathcal{T})$ of the Betweenness problem, let $G_{\mathcal{S},\mathcal{T}}$ be as defined in Definition 2. We claim that $pb(G_{\mathcal{S},\mathcal{T}}) \leq 1$ if and only if the pair $(\mathcal{S},\mathcal{T})$ is a yes-instance of the Betweenness problem. This will prove the NP-hardness because our reduction is polynomial and the Betweenness problem is NP-complete. To prove the claim in one direction, if $(\mathcal{S},\mathcal{T})$ is a yes-instance then by Lemma 4 $pb(G_{\mathcal{S},\mathcal{T}}) \leq 1$. Conversely, if $pb(G_{\mathcal{S},\mathcal{T}}) \leq 1$ then $(\mathcal{S},\mathcal{T})$ is a yes-instance by Lemma 5, that proves the claim in the other direction. ■

To conclude this section, we strenghten the above hardness results with two inapproximability results. Indeed, it has to be noticed that for any graph parameter *param*, an α-approximation algorithm for *param* with $\alpha < 1 + \frac{1}{k}$ is enough to separate the graphs G such that $param(G) \leq k$ from those such that $param(G) \geq k+1$. Therefore, the two following corollaries follow from our polynomial-time reduction.

Corollary 2 *For every $\varepsilon > 0$, the path-length of a graph cannot be approximated within a factor $\frac{3}{2} - \varepsilon$ unless P=NP.*

Proof. Let $G_{\mathcal{S},\mathcal{T}}$ be the graph of the reduction in Theorem 1. By Definition 2, it has diameter at most 3 and so $pl(G_{\mathcal{S},\mathcal{T}}) \leq 3$. Since it is NP-hard to decide whether $pl(G_{\mathcal{S},\mathcal{T}}) \leq 2$, therefore it does not exist a $\left(\frac{3}{2} - \varepsilon\right)$-approximation algorithm for path-length unless P=NP. ■

Corollary 3 *For every $\varepsilon > 0$, the path-breadth of a graph cannot be approximated within a factor $2 - \varepsilon$ unless P=NP.*

Proof. Let $G_{\mathcal{S},\mathcal{T}}$ be the graph of the reduction in Theorem 2. By Definition 2, the set U is a dominating clique and so $pb(G_{\mathcal{S},\mathcal{T}}) \leq 2$. Since it is NP-hard to decide whether $pb(G_{\mathcal{S},\mathcal{T}}) \leq 1$, therefore it does not exist a $(2 - \varepsilon)$-approximation algorithm for path-breadth unless P=NP. ■

So far, there exists a 2-approximation algorithm for path-length and a 3-approximation algorithm for path-breadth [27]. Therefore, we let open whether there exist $\frac{3}{2}$-approximation algorithms for path-length and 2-approximation algorithms for path-breadth.

3.2 Tree-breadth

We prove next that computing the tree-breadth is NP-hard.

Theorem 4 *Deciding whether a graph has tree-breadth at most k is NP-complete even if $k = 1$.*

Theorem 5 *Deciding whether a graph admits a k-good tree decomposition is NP-complete even if $k = 1$.*

Proof. The problem is in NP. By Corollary 1, a graph G admits a star-decomposition if and only if $tb(G) \leq 1$, therefore it is NP-hard to decide whether a graph admits a 1-good path decomposition by Theorem 4. ■

In order to prove Theorem 4, we will reduce from the Chordal Sandwich problem (defined below). In [39], the author also proposed a reduction from the Chordal Sandwich problem in order to prove that computing tree-length is NP-hard. However, we will need different gadgets than in [39], and we will need different arguments to prove correctness of the reduction.

Problem 2 (Chordal Sandwich)

Input: *graphs $G_1 = (V, E_1)$ and $G_2 = (V, E_2)$ such that $E_1 \subseteq E_2$.*

Question: *Is there a chordal graph $H = (V, E)$ such that $E_1 \subseteq E \subseteq E_2$?*

The Chordal Sandwich problem is NP-complete even when the $2n = |V|$ vertices induce a perfect matching in $\bar{G_2}$ (the complementary of G_2) [11, 32]. Perhaps surprisingly, the later constriction on the structure of $\bar{G_2}$ is a key element in our reduction. Indeed, we will need the following technical lemma.

Lemma 6 *Let $G_1 = (V, E_1)$, $G_2 = (V, E_2)$ such that $E_1 \subseteq E_2$ and $\bar{G_2}$ (the complementary of G_2) is a perfect matching. Suppose that $\langle G_1, G_2 \rangle$ is a yes-instance of the Chordal Sandwich problem.*

Then, there exists a reduced tree decomposition $(T, \mathcal{X})$ of G_1 such that for every forbidden edge $\{u, v\} \notin E_2$: $T_u \cap T_v = \emptyset$, $T_u \cup T_v = T$, furthermore there are two adjacent bags $B_u \in T_u$ and $B_v \in T_v$ such that $B_u \setminus u = B_v \setminus v$.

Proof. Let $H = (V, E)$ be any chordal graph such that $E_1 \subseteq E \subseteq E_2$ (that exists because $\langle G_1, G_2 \rangle$ is a yes-instance of the Chordal Sandwich problem by the hypothesis) and the number $|E|$ of edges is maximized. We will prove that any clique-tree $(T, \mathcal{X})$ of H satisfies the above properties (given in the statement of the lemma). To prove it, let $\{u, v\} \notin E_2$ be arbitrary. Observe that $T_u \cap T_v = \emptyset$ (else, $\{u, v\} \in E$, that would contradict that $E \subseteq E_2$).

Furthermore, let $B_u \in T_u$ minimize the distance in T to the subtree T_v, let B be the unique bag that is adjacent to B_u on a shortest-path between B_u and T_v in T. Note that $B \notin T_u$ by the minimality of $dist_T(B_u, T_v)$, however B may belong to T_v. Removing the edge $\{B_u, B\}$ in T yields two subtrees T_1, T_2 with $T_u \subseteq T_1$ and $T_v \subseteq T_2$. In addition, we have that for every $x \in V \setminus u$ such that $T_x \cap T_1 \neq \emptyset$, $\{u, x\} \in E_2$ since $x \neq v$ and $\bar{G_2}$ is a perfect matching by the hypothesis. Similarly, we have that for every $y \in V \setminus v$ such that $T_y \cap T_2 \neq \emptyset$, $\{v, y\} \in E_2$. Therefore, by maximality of the number $|E|$ of edges, it follows that $T_1 = T_u$ and $T_2 = T_v$, and so, $T_u \cup T_v = T$. In particular, $B = B_v \in T_v$.

Finally, let us prove that $B_u \setminus u = B_v \setminus v$. Indeed, assume for the sake of contradiction that $B_u \setminus u \neq B_v \setminus v$. In particular, $(B_u \setminus B_v) \setminus u \neq \emptyset$ or $(B_v \setminus B_u) \setminus v \neq \emptyset$. Suppose w.l.o.g. that $(B_u \setminus B_v) \setminus u \neq \emptyset$. Let $H' = (V, E')$ be obtained from H by adding an edge between vertex v and every vertex of $(B_u \setminus B_v) \setminus u$. By construction $|E'| > |E|$. Furthermore, H' is chordal since a clique-tree of H' can be obtained from $(T, \mathcal{X})$ by adding a new bag $(B_u \setminus u) \cup \{v\}$ in-between B_u and B_v. However, for every $x \in (B_u \setminus B_v) \setminus u$ we have that $\{x, v\} \in E_2$ since $x \neq u$ and $\bar{G_2}$ is a perfect matching by the hypothesis. As a result, $E' \subseteq E_2$, thus contradicting the maximality of the number $|E|$ of edges in H. ■

Proof of Theorem 4. The problem is in NP. To prove the NP-hardness,let $\langle G_1, G_2 \rangle$ be any input of the Chordal Sandwich problem such that $\bar{G_2}$ is a perfect matching. The graph G' is constructed from G_1 as follows. First we add a clique V' of $2n = |V|$ vertices in G'. Vertices $v \in V$ are in one-to-one correspondance with vertices $v' \in V'$. Then, for every forbidden edge $\{u, v\} \notin E_2$, vertices u, v are respectively made adjacent to all vertices in $V' \setminus v'$ and $V' \setminus u'$. Finally, we add a distinct copy of the gadget F_{uv} in Figure 3, and we make adjacent s_{uv} and t_{uv} to the two vertices u', v' (see also Figure 4 for an illustration). We will prove $tb(G') = 1$ if and only if $\langle G_1, G_2 \rangle$ is a yes-instance of the Chordal Sandwich problem. This will prove the NP-hardness because our reduction is polynomial and the Chordal Sandwich problem is NP-complete even when the $2n = |V|$ vertices induce a perfect matching in $\bar{G_2}$ (the complementary of G_2) [11, 32].

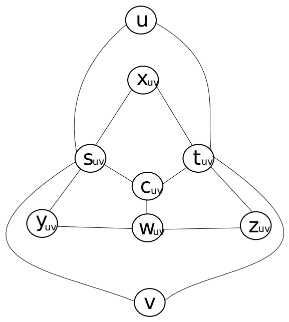

Figure 3: The gadget F_{uv}.

In one direction, assume $tb(G') = 1$, let $(T, \mathcal{X})$ be a star-decomposition of G'. Let $H = (V, \{\{u, v\} \mid T_u \cap T_v \neq \emptyset\})$, that is a chordal graph such that $E_1 \subseteq E(H)$. To prove that $\langle G_1, G_2 \rangle$ is a yes-instance of the Chordal Sandwich problem, it suffices to prove that $T_u \cap T_v = \emptyset$ for every forbidden edge $\{u, v\} \notin E_2$. More precisely, we will prove that $T_{s_{uv}} \cap T_{t_{uv}} \neq \emptyset$, for we claim that the latter implies $T_u \cap T_v = \emptyset$. Indeed, assume $T_{s_{uv}} \cap T_{t_{uv}} \neq \emptyset$ and $T_u \cap T_v \neq \emptyset$. Since s_{uv} and t_{uv} are both adjacent to u and v, therefore the four subtrees $T_u, T_v, T_{s_{uv}}, T_{t_{uv}}$ pairwise intersect. By the Helly property (Lemma 1) $T_u \cap T_v \cap T_{s_{uv}} \cap T_{t_{uv}} \neq \emptyset$, hence there is a bag containing u, v, s_{uv}, t_{uv} but then it contradicts the fact that $(T, \mathcal{X})$ is a star-decomposition because no vertex dominates the four vertices. Therefore, $T_{s_{uv}} \cap T_{t_{uv}} \neq \emptyset$ implies $T_u \cap T_v = \emptyset$. Let us prove that $T_{s_{uv}} \cap T_{t_{uv}} \neq \emptyset$. By contradiction, assume $T_{s_{uv}} \cap T_{t_{uv}} = \emptyset$. Every bag B onto the path between $T_{s_{uv}}$ and $T_{t_{uv}}$ must contain c_{uv}, x_{uv}, furthermore $N[c_{uv}] \cap N[x_{uv}] = \{s_{uv}, t_{uv}\}$. Since, $(T, \mathcal{X})$ is a star-decomposition, the latter implies either $s_{uv} \in B$ and $B \subseteq N[s_{uv}]$ or $t_{uv} \in B$ and $B \subseteq N[t_{uv}]$. Consequently, there exist two adjacent bags $B_s \in T_{s_{uv}}, B_t \in T_{t_{uv}}$ such that $B_s \subseteq N[s_{uv}]$ and $B_t \subseteq N[t_{uv}]$. Furthermore, $B_s \cap B_t$ is an $s_{uv}t_{uv}$-separator by the properties of a tree decomposition. In particular, $B_s \cap B_t$ must intersect the path (y_{uv}, w_{uv}, z_{uv}) because $y_{uv} \in N(s_{uv})$ and $z_{uv} \in N(t_{uv})$. However, $B_s \subseteq N[s_{uv}], B_t \subseteq N[t_{uv}]$ but $N[s_{uv}] \cap N[t_{uv}] \cap \{y_{uv}, w_{uv}, z_{uv}\} = \emptyset$, hence $B_s \cap B_t \cap \{y_{uv}, w_{uv}, z_{uv}\} = \emptyset$, that is a contradiction. As a result, $T_{s_{uv}} \cap T_{t_{uv}} \neq \emptyset$ and so, $T_u \cap T_v = \emptyset$.

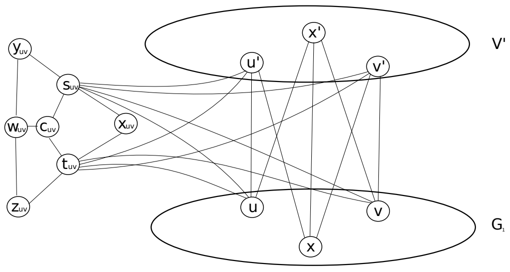

Figure 4: The graph G' (simplified view).

Conversely, assume that $\langle G_1, G_2 \rangle$ is a yes-instance of the Chordal Sandwich problem. Since $\bar{G_2}$ is a perfect matching by the hypothesis, by Lemma 6 there exists a reduced tree decomposition $(T, \mathcal{X})$ of G_1 such that for every forbidden edge $\{u, v\} \notin E_2$: $T_u \cap T_v = \emptyset, T_u \cup T_v = T$ and there are two adjacent bags $B_u \in T_u, B_v \in T_v$ so that $B_u \setminus u = B_v \setminus v$. Let us modify $(T, \mathcal{X})$ in order to obtain a star-decomposition of G'.

In order to achieve the result, we first claim that for every edge $\{t, t'\} \in E(T)$, the bags $X_t, X_{t'}$ differ in exactly one vertex, that is, $|X_t \setminus X_{t'}| = 1$ and similarly $|X_{t'} \setminus X_t| = 1$. Indeed, $X_t \setminus X_{t'} \neq \emptyset$ because $(T, \mathcal{X})$ is reduced, so, let $u_{tt'} \in X_t \setminus X_{t'}$. Let $v_{tt'} \in V$ be the unique vertex satisfying $\{u_{tt'}, v_{tt'}\} \notin E_2$, that is well-defined because $\bar{G_2}$ is a perfect matching by the hypothesis. Note that $v_{tt'} \in X_{t'}$ because $u_{tt'} \notin X_{t'}$ and $T_{u_{tt'}} \cup T_{v_{tt'}} = T$. Furthermore, $v_{tt'} \notin X_t$ because $u_{tt'} \in X_t$ and $T_{u_{tt'}} \cap T_{v_{tt'}} = \emptyset$. By construction of $(T, \mathcal{X})$, there are two adjacent bags $B_{u_{tt'}} \in T_{u_{tt'}}, B_{v_{tt'}} \in T_{v_{tt'}}$ such that $B_{u_{tt'}} \setminus u_{tt'} = B_{v_{tt'}} \setminus v_{tt'}$. Since $u_{tt'} \in X_t \setminus X_{t'}$ and $v_{tt'} \in X_{t'} \setminus X_t$, therefore, $X_t = B_{u_{tt'}}$ and $X_{t'} = B_{v_{tt'}}$, and so, $X_t \setminus X_{t'} = \{u_{tt'}\}$ and $X_{t'} \setminus X_t = \{v_{tt'}\}$. In the following, we will keep the above notations $u_{tt'}, v_{tt'}$ for every edge $\{t, t'\} \in E(T)$ (in particular, $u_{tt'} = v_{t't}$ and $v_{tt'} = u_{t't}$).

Let us construct the star-decomposition $(T', \mathcal{X}')$ of G' as follows.

- For every node $t \in V(T)$, let $S_t = X_t \cup V' \cup (\bigcup_{t' \in N_T(t)} \{s_{u_{tt'}v_{tt'}}, t_{u_{tt'}v_{tt'}}\})$ (in particular, $|S_t| = 2n + |X_t| + 2 \cdot deg_T(t)$). We will first construct a path decomposition of $G'[S_t]$ whose bags are the sets $Y_{tt'} = X_t \cup V' \cup \{s_{u_{tt'}v_{tt'}}, t_{u_{tt'}v_{tt'}}\}$ for every edge $\{t, t'\} \in E(T)$ (note that the bags can be linearly ordered in an arbitrary way in the path decomposition). Furthermore, for every edge $\{t, t'\} \in E(T)$, $Y_{tt'} \subseteq N[u'_{tt'}]$, where $u'_{tt'} \in V'$ is the corresponding vertex to $u_{tt'} \in V$ in the clique V' (see Figure 5 for an illustration). Therefore, the above constructed path decomposition is a 1-good path decomposition.

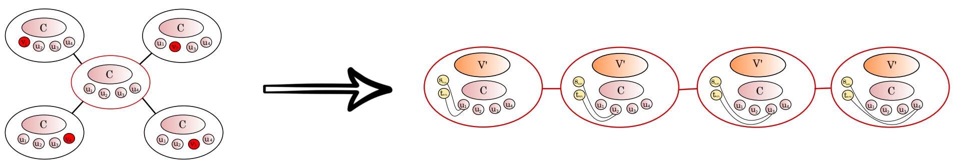

Figure 5: The 1-good path decomposition (right) obtained from the central bag with degree four (left).

- Then, we will connect the 1-good path decompositions together. More precisely, let us add an edge between the two bags $Y_{tt'}$ and $Y_{t't}$ for every edge $\{t,t'\} \in E(T)$ (see Figure 6 for an illustration).

  In so doing, we claim that one obtains a star-decomposition of $G'[\bigcup_{t \in V(T)} S_t]$. Indeed, it is a tree decomposition since:

  - the clique V' is contained in all bags;
  - for every $\{t,t'\} \in E(T)$ the two vertices $s_{u_{tt'}v_{tt'}}, t_{u_{tt'}v_{tt'}}$ are only contained in the two adjacent bags $Y_{tt'}$ and $Y_{t't}$, furthermore $u_{tt'}, u'_{tt'}, v'_{tt'} \in Y_{tt'}$ and $v_{tt'}, u'_{tt'}, v'_{tt'} \in Y_{t't}$;
  - last, each vertex $v \in V$ is contained in $\{Y_{tt'} \mid v \in X_t \text{ and } t' \in N_T(t)\}$ which induces a subtree since $(T, \mathcal{X})$ is a tree decomposition of G_1.

  Since in addition every bag $Y_{tt'}$, with $\{t,t'\} \in E(T)$, is dominated by $u'_{tt'} \in V'$, this proves the claim that one obtains a star-decomposition.

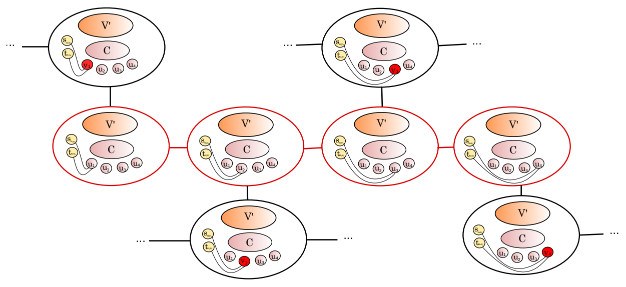

Figure 6: Connection of the 1-good path decomposition in Figure 5 to the neighbouring 1-good path decompositions.

- In order to complete the construction, let us observe that for every forbidden edge $\{u,v\} \notin E_2$, there is a star-decomposition of $F_{uv} \setminus \{u,v\}$ with three leaf-bags $\{x_{uv}, s_{uv}, t_{uv}\}$, $\{y_{uv}, s_{uv}, w_{uv}\}$ and $\{z_{uv}, s_{uv}, w_{uv}\}$ and one internal bag of degree three $B_{uv} = \{c_{uv}, s_{uv}, t_{uv}, w_{uv}\}$. For every $\{t,t'\} \in E(T)$, we simply connect the above star-decomposition of $F_{u_{tt'}v_{tt'}} \setminus \{u_{tt'}, v_{tt'}\}$ by making the internal bag $B_{u_{tt'}v_{tt'}}$ adjacent to one of $Y_{tt'}$ or $Y_{t't}$ (see Figure 7 for an illustration).

By construction, the resulting tree decomposition $(T', \mathcal{X}')$ of G' is a star-decomposition, hence $tb(G') = 1$.

■

Recall that we can use our reduction from Definition 2 in order to prove that computing path-length and path-breadth is NP-hard. By contrast, our reduction from Theorem 4 cannot

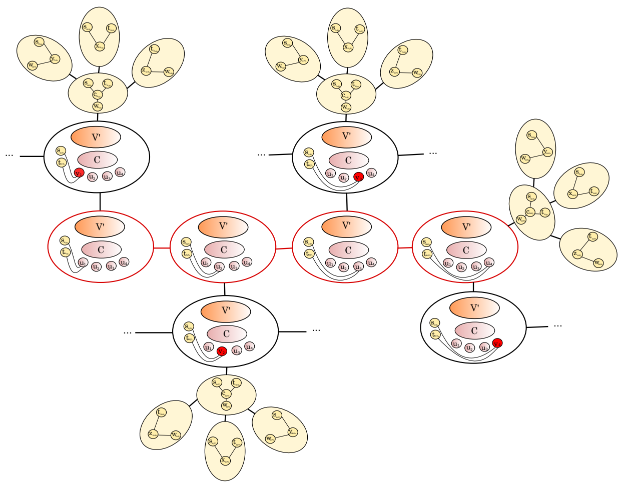

Figure 7: The respective star-decompositions of the gadgets $F_{u_i v_i}$ are connected to the other bags.

be used to prove that tree-length is NP-hard to compute (in fact, the graph G' resulting from the reduction has tree-length two).

Finally, as in the previous Section 3.1, let us strenghten Theorem 4 with an inapproximability result.

Corollary 4 *For every $\varepsilon > 0$, the tree-breadth of a graph cannot be approximated within a factor $2 - \varepsilon$ unless P=NP.*

4 General properties of graphs with tree-breadth one

In Section 3.2, we prove that computing the tree-breadth is NP-hard. In particular, the recognition of graphs with tree-breadth one is NP-complete. In light of this result, we focus on graphs with tree-breadth one (in order to obtain a better understanding of what makes the problem difficult)

Problem 3 (1-tree-breadth)

Input: *a connected graph $G = (V, E)$*

Question: $tb(G) \leq 1$ *?*

In Lemma 7, we show that the problem of recognizing graphs with tree-breadth at most one is equivalent to the problem of computing tree-breadth. This further motivates our study of these graphs. Then, we will prove necessary conditions for a graph to be of tree-breadth one.

- One is that all graphs with a star-decomposition have a *domination elimination ordering* (see Section 4.1). We will outline a few implications of this property.
- Second, we will prove in Lemma 9 that if a graph G admits a star-decomposition then so do all the *blocks* of G, where the blocks here denote a particular case of induced subgraphs of G (*e.g.*, see Definition 4).

Finally, we will obtain from the latter result a polynomial-time algorithm to decide whether a bipartite graph has tree-breadth at most one (*e.g.*, see Section 4.3).

Definition 3 *Let G be a graph with n vertices, denoted by $v_1, v_2, \ldots, v_n$, and let r be a positive integer. The graph G'_r is obtained from G by adding a clique with n vertices, denoted by $U = \{u_1, u_2, \ldots, u_n\}$, so that for every $1 \leq i \leq n$, vertex u_i is adjacent to $B_G(v_i, r) = \{x \in V(G) \mid dist_G(v_i, x) \leq r\}$.*

Lemma 7 *For every graph G, for every positive integer r, let G'_r be as defined in Definition 3, $tb(G) \leq r$ if and only if $tb(G'_r) \leq 1$.*

Proof. If $tb(G) \leq r$ then we claim that starting from any tree decomposition $(T, \mathcal{X})$ of G with breadth at most r, one obtains a star-decomposition of G'_r by adding the clique U in every bag X_t, $t \in V(T)$. Indeed, in such case for every bag X_t, $t \in V(T)$, by the hypothesis there is $v_i \in V(G)$ such that $\max_{x \in X_t} dist_G(v_i, x) \leq r$, whence $X_t \cup U \subseteq N_{G'_r}[u_i]$. Conversely, if $tb(G'_r) \leq 1$ then we claim that starting from any tree decomposition $(T', \mathcal{X}')$ of G'_r with breadth at most one, one obtains a tree decomposition of G with breadth at most r by removing every vertex of the clique U from every bag X'_t, $t \in V(T')$. Indeed, in such case for every bag X'_t, $t \in V(T')$, by the hypothesis there is $y \in V(G'_r)$ such that $X'_t \subseteq N_{G'_r}[y]$. Furthermore, $y \in \{u_i, v_i\}$ for some $1 \leq i \leq n$, and so, since $N_{G'_r}[v_i] \subseteq N_{G'_r}[u_i]$ by construction, therefore $X'_t \setminus U \subseteq N_{G'_r}(u_i) \setminus U = \{x \in V(G) \mid dist_G(v_i, x) \leq r\}$. ■

4.1 Existence of specific elimination orderings

Independently from the remaining of the section, let us prove some interesting properties of graphs with tree-breadth one in terms of *elimination orderings*. More precisely, a *domination elimination ordering* [21] of a graph G is a total ordering of its vertex-set, denoted by $v_1, v_2, \ldots, v_n$, so that for every $1 \leq i < n$, there is $j > i$ satisfying that $N_G(v_i) \cap \{v_{i+1}, v_{i+2}, \ldots, v_n\} \subseteq N_G[v_j]$. The existence of domination elimination orderings in some graph classes and their algorithmic applications has been studied in [16]. Let us prove that graphs with tree-breadth one all admit a domination elimination ordering.

Lemma 8 *Let G be such that $tb(G) \leq 1$, G admits a domination elimination ordering.*

Proof. Assume G has at least two vertices (or else, the lemma is trivial). To prove the lemma, it suffices to prove the existence of $u, v \in V(G)$ distinct such that $N(v) \subseteq N[u]$ and $tb(G \setminus v) \leq 1$ (then, the lemma follows by induction on the order of the graph).

If G admits a universal vertex u, then one can pick $v \in V(G) \setminus u$ arbitrary, $N(v) \subseteq N[u]$ because u is universal in G, furthermore $tb(G \setminus v) \leq 1$ because $G \setminus v$ admits a universal vertex u.

Else, G does not admit any universal vertex, let $(T, \mathcal{X})$ be a reduced tree decomposition of G of breadth one, that is a star-decomposition by Lemma 3. Let X_t, $t \in V(T)$ be a leaf. Since the tree decomposition is reduced, there must be $v \in X_t$ satisfying $T_v = \{X_t\}$. Now there are two cases.

- Suppose there is $u \in X_t \setminus v$ such that $X_t \subseteq N[u]$. Then, $N(v) \subseteq X_t \subseteq N[u]$, and $tb(G \setminus v) \leq 1$ because $G \setminus v$ can be obtained from G by contracting the edge $\{u, v\}$ and tree-breadth is contraction-closed by Lemma 2.
- Else, $X_t \subseteq N[v]$, and for every $x \in X_t \setminus v$, $X_t \nsubseteq N[x]$. Let $t' \in V(T)$ be the unique node adjacent to node t in T, that exists because G does not admit any universal vertex

and so, T has at least two bags. Let us assume that for every $x \in X_t \setminus v$, $x \in X_t \cap X_{t'}$ (for otherwise, $N(x) \subseteq N[v]$ and $tb(G \setminus x) \leq 1$ because $G \setminus x$ can be obtained from G by contracting the edge $\{v, x\}$ to v and tree-breadth is contraction-closed by Lemma 2). In particular, let $u \in X_{t'}$ satisfy $X_{t'} \subseteq N[u]$. Then, $N(v) = X_t \cap X_{t'} \subseteq N[u]$, furthermore $tb(G \setminus v) \leq 1$ because $(T \setminus t, \mathcal{X} \setminus X_t)$ is a star-decomposition of $G \setminus v$. ■

Note that for a graph to have tree-breadth one, it must satisfy the necessary condition of Lemma 8 and this can be checked in polynomial-time. However, the existence of some domination elimination ordering is not a sufficient condition for the graph to have tree-breadth one. Indeed, every grid has a domination elimination ordering but the *tree-length* of the $n \times m$ grid is at least $\min\{n, m\} - 1$ [24] (recall that $tl(G) \leq 2tb(G)$ for any graph G).

The existence of a domination elimination ordering has some interesting consequences about the graph structure. Let us recall one such a consequence about the *cop-number* of the graph.

Corollary 5 *For any graph G with $tb(G) \leq 1$, G has cop-number ≤ 2 and the upper-bound is sharp.*

Proof. By Lemma 8, G admits a domination elimination ordering. Therefore, by [19, Theorem 4] G has cop-number ≤ 2. One can prove the sharpness of the upper-bound by setting $G := C_4$, the cycle with four vertices. ■

4.2 Properties of particular decompositions

In the following, it will be useful not only to constrain the properties of the star-decomposition whose existence we are interested in, but also to further constrain the properties of the graph G that we take as input. Let us first remind basic terminology about graph separators.

Definition 4 *Let $G = (V, E)$ be connected, a* separator *of G is any subset $S \subseteq V$ such that $G \setminus S$ has at least two connected components.*

In particular, a full component *for S is any connected component C of $G \setminus S$ satisfying $N(C) = S$. A* block *is any induced subgraph $G[C \cup S]$ with S being a separator and C being a full component for S.*

Finally, a minimal separator *is a separator with at least two full components.*

Our objective is to prove that if a graph G has tree-breadth one then so do all its blocks. In fact, we will prove a slightly more general result:

Lemma 9 *Let $G = (V, E)$ be a graph, $S \subseteq V$ be a separator, and $W \subseteq V \setminus S$ be the union of some connected components of $G \setminus S$. If $tb(G) = 1$ and W contains a full component for S, then $tb(G[W \cup S]) = 1$. More precisely if $(T, \mathcal{X})$ is a tree decomposition of G of breadth one, then $(T, \{X_t \cap (W \cup S) \mid X_t \in \mathcal{X}\})$ is a tree decomposition of $G[W \cup S]$ of breadth one.*

Proof. Let $(T, \mathcal{X})$ be a tree decomposition of breadth one of G. Let us remove all vertices in $V \setminus (W \cup S)$ from bags in $(T, \mathcal{X})$, which yields a tree decomposition $(T', \mathcal{X}')$ of the induced subgraph $G[W \cup S]$. To prove the lemma, we are left to prove that $(T', \mathcal{X}')$ has breadth one. Let X_t be a bag of $(T', \mathcal{X}')$. By construction, X_t is fully contained into some bag of $(T, \mathcal{X})$, so it has radius one in G. Let $v \in V$ be such that $X_t \subseteq N_G[v]$. If $v \in W \cup S$, then we are done. Else, since for all $x \notin S \cup W, N(x) \cap (S \cup W) \subseteq S$ (because S is a separator by the hypothesis), we must have that $X_t \subseteq S$. Let $A \subseteq W$ be a full component for S, that exists by the hypothesis, and let T_A be the subtree that is induced by the bags intersecting the component. Since we have that the subtree T_A and the subtrees $T_x, x \in X_t$ pairwise intersect — because for all $x \in X_t$, $x \in S$ and so, x has a neighbour in A —, then by the Helly property (Lemma 1) $T_A \cap \left(\bigcap_{x \in X_t} T_x\right) \neq \emptyset$ *i.e.*, there exists a bag in $(T, \mathcal{X})$ containing X_t and intersecting A. Moreover, any vertex dominating this bag must be either in S or in A, so in particular there exists $u \in A \cup S$ dominating X_t, which proves the lemma. ■

Lemma 9 implies that, under simple assumptions, a graph of tree-breadth one can be disconnected using any (minimal) separator, and the components must still induce subgraphs with tree-breadth one. The converse does not hold in general, yet there are interesting cases when it does.

Lemma 10 *Let $G = (V, E)$ be a graph, $S \subseteq V$ be a clique-minimal-separator and A be a full component for S. Then, $tb(G) = 1$ if and only if both $tb(G[A \cup S]) = 1$ and $tb(G[V \setminus A]) = 1$.*

Proof. By the hypothesis $V \setminus (A \cup S)$ contains a full component because S is a minimal separator. Therefore, if G has tree-breadth one, then so do $G[A \cup S]$ and $G[V \setminus A]$ by Lemma 9. Conversely, suppose that we have both $tb(G[A \cup S]) = 1$ and $tb(G[V \setminus A]) = 1$. Let $(T^1, \mathcal{X}^1)$ be a tree decomposition of $G[A \cup S]$ with breadth one, let $(T^2, \mathcal{X}^2)$ be a tree decomposition of $G[V \setminus A]$ with breadth one. Then for every $i \in \{1, 2\}$ we have that since S is a clique the subtrees T_s^i, $s \in S$, pairwise intersect, so by the Helly Property (Lemma 1) $\bigcap_{s \in S} T_s^i \neq \emptyset$ *i.e.*, S is fully contained into some bag of $(T^1, \mathcal{X}^1)$ and it is fully contained into some bag of $(T^2, \mathcal{X}^2)$. Moreover, $(A \cup S) \cap (V \setminus A) = S$, therefore a tree decomposition of G with breadth one can be obtained by adding an edge between some bag of $(T^1, \mathcal{X}^1)$ containing S and some bag of $(T^2, \mathcal{X}^2)$ containing S. ■

Recall that computing the clique-minimal-decomposition of a graph G can be done in $\mathcal{O}(nm)$-time, where m denotes the number of edges [7]. By doing so, one replaces a graph G with the maximal subgraphs of G that have no clique-separator, *a.k.a. atoms*. Therefore, we will assume in the remaining of the proofs that there is no clique-separator in the graphs that we will study, we will call them *prime graphs*.

4.3 Application to bipartite graphs

In this section, we describe an $\mathcal{O}(nm)$-time algorithm so as to decide whether a prime bipartite graph has tree-breadth one. This combined with Lemma 10 proves that it can be decided in polynomial-time whether a bipartite graph has tree-breadth one.

We will first describe a more general problem and how to solve it in polynomial-time.

Tree decompositions with constrained set of bags. Our algorithm for bipartite graphs makes use of the correspondance between tree decompositions and triangulations of a graph. Indeed, recall that any reduced tree decomposition $(T, \mathcal{X})$ of a graph G is a clique-tree for some chordal supergraph H of G whose maximal cliques are the bags of $\mathcal{X}$. Conversely, for any chordal supergraph H of G, every clique-tree of H is a tree decomposition of G whose bags are the maximal cliques of H [30]. Therefore as shown below, the following subproblem can be solved in polynomial-time:

Problem 4

Input: *a graph G, a family $\mathcal{X}$ of subsets of $V(G)$.*

Question: *Does there exist a tree T such that $(T, \mathcal{X})$ is a tree decomposition of G ?*

Let us assume w.l.o.g. that no subset of $\mathcal{X}$ is properly contained into another one. To solve Problem 4.3, it suffices to make every subset $X \in \mathcal{X}$ a clique in G, then to verify whether the resulting supergraph H of G is a chordal graph whose maximal cliques are exactly the sets in $\mathcal{X}$. Since chordal graphs can be recognized in linear-time, and so can be enumerated their maximal cliques [29], therefore Problem 4.3 can be solved in polynomial-time.

The algorithm for bipartite graphs. Now, given a bipartite graph G, we aim to exhibit a family $\mathcal{X}$ so that $tb(G) = 1$ if and only if there is a star-decomposition of G whose bags are $\mathcal{X}$. By doing so, we will reduce the recognition of bipartite graph with tree-breadth at most one to the more general Problem 4.3.

Lemma 11 *Let $G = (V_0 \cup V_1, E)$ be a prime bipartite graph with tree-breadth one. There is $(T, \mathcal{X})$ a star-decomposition of G such that either $\mathcal{X} = \{N[v_0] \mid v_0 \in V_0\}$, or $\mathcal{X} = \{N[v_1] \mid v_1 \in V_1\}$.*

Proof. Let $(T, \mathcal{X})$ be a star-decomposition of G, that exists by Lemma 3, minimizing the number $|\mathcal{X}|$ of bags. Suppose there is some $v_0 \in V_0$, there is $t \in V(T)$ such that $X_t \subseteq N_G[v_0]$ (the case when there is some $v_1 \in V_1$, there is $t \in V(T)$ such that $X_t \subseteq N_G[v_1]$ is symmetrical to this one). We claim that for every $t' \in V(T)$, there exists $v_0' \in V_0$ satisfying $X_{t'} \subseteq N_G[v_0']$. By contradiction, let $v_0 \in V_0, v_1 \in V_1$, let $t, t' \in V(T)$ be such that $X_t \subseteq N_G[v_0], X_{t'} \subseteq N_G[v_1]$. By connectivity of the tree T we may assume w.l.o.g. that $\{t, t'\} \in E(T)$. Moreover, $N_G(v_0) \cap N_G(v_1) = \emptyset$ because G is bipartite. Therefore, $X_t \cap X_{t'} \subseteq \{v_0, v_1\}$, and in particular if $X_t \cap X_{t'} = \{v_0, v_1\}$ then v_0, v_1 are adjacent in G. However, by the properties of a tree decomposition this implies that $X_t \cap X_{t'}$ is a clique-separator (either an edge or a single vertex), thus contradicting the fact that G is prime.

Now, let $v_0 \in V_0$ be arbitrary. We claim that there is a unique bag $X_t,\ t \in V(T)$, containing v_0. Indeed, any such bag X_t must satisfy $X_t \subseteq N_G[v_0]$, whence the subtree T_{v_0} can be contracted into a single bag $\bigcup_{t \in T_{v_0}} X_t$ without violating the property for the tree decomposition to be a star-decomposition. As a result, the unicity of the bag X_t follows from the minimality of $|\mathcal{X}|$. Finally, since X_t is unique and $X_t \subseteq N_G[v_0]$, therefore $X_t = N_G[v_0]$ and so, $\mathcal{X} = \{N[v_0] \mid v_0 \in V_0\}$. ■

We can easily deduce from Lemma 11 the following algorithm for deciding whether a prime bipartite graph G has tree-breadth one. Let (V_0, V_1) be the (unique) bipartition of the vertex-set of G into two stable sets. Let $\mathcal{X}_0 = \{N[v_0] \mid v_0 \in V_0\}$, let $\mathcal{X}_1 = \{N[v_1] \mid v_1 \in V_1\}$. By Lemma 11, $tb(G) = 1$ if and only if one of $(G, \mathcal{X}_0), (G, \mathcal{X}_1)$ is a yes-instance of Problem 4.3.

5 Algorithm for planar graphs

We are now ready to present our main result. In this section, we describe a quadratic-time algorithm for deciding whether a prime planar graph has tree-breadth one. Overall, we claim that it gives us a quadratic-time algorithm for deciding whether a general planar graph has tree-breadth one. Indeed, the clique-decomposition of a planar graph takes $\mathcal{O}(n^2)$-time to be computed, furthermore the disjoint union of the atoms has $\mathcal{O}(n + m)$ vertices [7], that is $\mathcal{O}(n)$ for planar graphs.

Roughly, we will construct a star-decomposition of the graph by increments. The main principle of the recursive algorithm is to find a particular vertex, called *leaf-vertex*. Informally, it extracts a new bag of the star-decomposition from some ball around the leaf-vertex. Then, depending on the case, either the leaf-vertex vertex is removed or some edge is added or contracted. In both cases, the resulting graph remains prime and planar and has tree-breadth one if and only if the initial one has tree-breadth one.

We prove that each inductive step takes a linear time. Moreover, we prove that there are at most a linear number of recursive iterations (Lemma 27).

There are three kinds of leaf-vertices (*e.g.*, see Figure 8).

Definition 5 *Let $G = (V, E)$ be a graph. A vertex v is a* leaf-vertex *if one of the following conditions hold.*

Type 1. *$N(v)$ induces an $a_v b_v$-path for some $a_v, b_v \in V \setminus \{v\}$, denoted by Π_v, of length at least 3 and there exists $d_v \in V \setminus \{v\}$ such that $N(v) \subseteq N(d_v)$, i.e., d_v dominates Π_v.*

Type 2. *$N(v)$ induces a path, denoted by $\Pi_v = (a_v, b_v, c_v)$, of length 2.*

Type 3. *$N(v)$ consists of two non adjacent vertices a_v and c_v, and there exists $b_v \in (N(a_v) \cap N(c_v)) \setminus \{v\}$.*

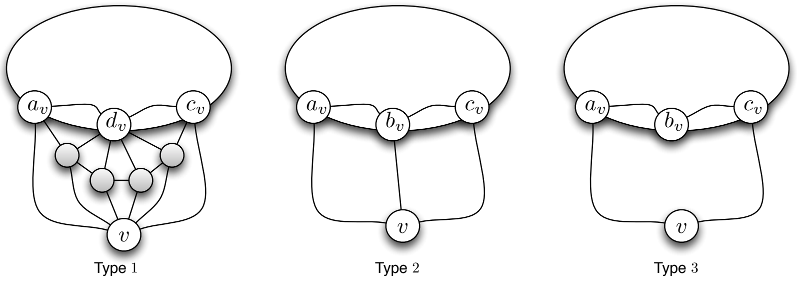

Figure 8: The three kinds of leaf-vertices.

We are now ready to describe the algorithm.

5.1 Algorithm `Leaf-BottomUp`

Let $G = (V, E)$ be prime planar graph. Assume G has at least 7 vertices (else, it is easy to conclude).

Step 1 The first step is to find a leaf-vertex in G. In Section 5.4.1, we describe how to decide whether G has a leaf-vertex in linear-time.

- if G has no leaf-vertex, then, by Theorem 7, no minimal separator of G induces a path of length 2. Therefore, by Lemma 20, $tb(G) = 1$ only if G has a star-decomposition with at most 2 bags. In that case, Algorithm `Leaf-BottomUp` checks whether it exists a star-decomposition with at most 2 bags, which can be done in quadratic time (see Lemma 26). If it exists, then $tb(G) = 1$. Otherwise, $tb(G) > 1$.

- otherwise, let v be a leaf-vertex of G and go to Step 2 if v is of Type 1 and go to Step 3 otherwise.

Step 2 **Case v is of Type 1.** Let Π_v and d_v be defined as in Definition 5. If $V = N[v] \cup \{d_v\}$ then trivially $tb(G) = 1$. Else by Theorem 8, G' is prime and planar, where G' is the graph obtained from $G \setminus v$ by contracting the internal nodes of Π_v to a single edge, and $tb(G) = 1$

if and only if $tb(G') = 1$. In that case, Algorithm `Leaf-BottomUp` is recursively applied on G'.

Step 3 **Case v is of Type 2 or 3.** Let a_v, b_v, c_v be defined as in Definition 5.

In that case, Algorithm `Leaf-BottomUp` checks whether $G \setminus v$ is prime. By Theorem 6, for any clique minimal separator S of $G \setminus v$ (if any), there exists $u_v \in V \setminus \{a_v, b_v, c_v, v\}$ such that $S = \{b_v, u_v\}$. Therefore, this can be checked in linear time (by checking with a Depth-First-Search whether there is a cut-vertex of $G \setminus \{a_v, b_v, c_v, v\}$ in the neighbors of b_v). If $G \setminus v$ is prime then go to Step 3.1, else go to Step 3.2.

Step 3.1 **Case v is of Type 2 or 3 and $G \setminus v$ is prime.** There are 4 cases that can be determined in linear-time.

(a) **Case $|N(a_v) \cap N(c_v)| \geq 3$ in $G \setminus v$, or there exists a minimal separator $S \subseteq (N(a_v) \cap N(c_v)) \cup \{a_v, c_v\}$ in $G \setminus v$ and $\{a_v, c_v\} \subseteq S$.**
By Theorem 9, $tb(G) = 1$ if and only if $tb(G \setminus v) = 1$. Since, moreover, $G \setminus v$ is planar and prime, then Algorithm `Leaf-BottomUp` is recursively applied on $G \setminus v$.

(b) **Case: $|N(a_v) \cap N(c_v)| < 3$ in $G \setminus v$ and there is no minimal separator $S \subseteq (N(a_v) \cap N(c_v)) \cup \{a_v, c_v\}$ in $G \setminus v$ such that $\{a_v, c_v\} \subseteq S$.**

i **Subcase: $|N(a_v) \cap N(c_v)| = 1$ in $G \setminus v$.** In that subcase, $N(a_v) \cap N(c_v) = \{v, b_v\}$ and, by Theorem 10, $tb(G) = 1$ if and only if $G = C_4$, a cycle with four vertices. Note that here it implies that $tb(G) > 1$ because G has at least 7 vertices.

ii **Subcase: $|N(a_v) \cap N(c_v)| = 2$ in $G \setminus v$.** In that subcase, let $N(a_v) \cap N(c_v) = \{v, b_v, u_v\}$. By Theorem 11, since G has more than 5 vertices, the graph G' obtained from G by adding edges $\{v, u_v\}$ and $\{b_v, v\}$ is planar and prime, and moreover $tb(G) = 1$ if and only if $tb(G') = 1$. In that case, Algorithm `Leaf-BottomUp` is recursively applied on G'.

Step 3.2 **Case v is of Type 2 or 3 and $G \setminus v$ has a clique separator.** As mentioned in Step 3, in that case, there exists $u_v \in V \setminus \{a_v, b_v, c_v, v\}$ such that $S = \{b_v, u_v\}$ is a minimal clique separator of $G \setminus v$. Moreover, by Theorem 6, $G \setminus \{a_v, b_v, c_v, v\}$ is connected.

By Theorem 12, $tb(G) = 1$ if and only if $tb(G') = 1$ where G' is obtained from G by adding the edge $\{v, b_v\}$ (if it were not already there). Moreover, G' is prime and planar. Hence, we may assume that $\{v, b_v\} \in E$ (if not Algorithm `Leaf-BottomUp` adds it).

Furthermore by Theorem 6, since G has more than 5 vertices, $u_v \notin N(a_v) \cap N(c_v)$. In the latter case, let us assume w.l.o.g. that $u_v \notin N(a_v)$, that is either $u_v \notin N(a_v) \cup N(c_v)$ or $u_v \in N(c_v) \setminus N(a_v)$. There are several cases to be considered.

(a) **Case $u_v \notin N(a_v) \cup N(c_v)$,**
or $(N(u_v) \cap N(a_v)) \cup \{v, c_v\}$ does not separate u_v and a_v in G.

By Theorem 13, G/va_v is prime and planar, and $tb(G) = 1$ if and only if $tb(G/va_v) = 1$. In that case, Algorithm `Leaf-BottomUp` is recursively applied on G/va_v, the graph obtained from G by contracting the edge $\{v, a_v\}$.

(b) **Case $u_v \in N(c_v) \setminus N(a_v)$,**
and $(N(u_v) \cap N(a_v)) \cup \{v, c_v\}$ separates u_v and a_v in G.

In that case, recall that G has at least 7 vertices. Again, Algorithm `Leaf-BottomUp` distinguishes several subcases.

i **Subcase $N(b_v) = \{v, a_v, c_v, u_v\}$.** In that subcase, by Theorem 14, we can find in linear-time a vertex $x \in (N(a_v) \cap N(u_v)) \setminus \{b_v\}$ such that G' is planar, where G' is obtained from G by adding the edge $\{b_v, x\}$. Moreover, by Theorem 15, G'/b_vx (obtained by contracting $\{b_v, x\}$) is prime and $tb(G) = 1$ if and only if $tb(G'/b_vx) = 1$. In that case, Algorithm `Leaf-BottomUp` is recursively applied on G'/b_vx.

ii **Subcase $\{v, a_v, c_v, u_v\} \subset N(b_v)$ and $N(b_v) \cap N(a_v) \cap N(u_v) \neq \emptyset$.** In that subcase, $|N(b_v) \cap N(a_v) \cap N(u_v)| = 1$ by Lemma 23 and let x be this common neighbor. By Theorem 15, G/b_vx (obtained by contracting $\{b_v, x\}$) is prime and $tb(G) = 1$ if and only if $tb(G/b_vx) = 1$. In that case, Algorithm `Leaf-BottomUp` is recursively applied on G/b_vx.

iii **Subcase $\{v, a_v, c_v, u_v\} \subset N(b)$ and $N(b_v) \cap N(a_v) \cap N(u_v) = \emptyset$.** In that subcase, by Theorem 16, there must be a unique $x \in (N(a_v) \cap N(u_v)) \setminus \{b_v\}$ such that $N(b_v) \cap N(x)$ is a b_vx-separator of G and $|N(b_v) \cap N(x)| \geq 3$ (or else, $tb(G) > 1$).

- **Suppose there is a leaf-vertex $\ell \in N(b_v) \cap N(x)$.** By Lemma 24, ℓ is of Type 1 or $G \setminus \ell$ is prime. In that case, go to Step 2 if ℓ is of Type 1, and go to Step 3.1 if ℓ has Type 2 or 3 (in both cases, ℓ takes the role of v). Note that we never go back to Step 3.2 in such case, so the algorithm cannot loop.
- Otherwise, by Theorem 17, there exist $y, z \in N(b_v) \cap N(x)$ two non-adjacent vertices, such that G' is prime and planar, and $tb(G) = 1$ if and only if $tb(G') = 1$, where G' is obtained from G by adding the edge $\{x, y\}$. In that case, Algorithm `Leaf-BottomUp` is recursively applied on G'.

5.2 Properties of prime planar graphs with tree-breadth one

5.2.1 General lemmas

We will first investigate on general properties of prime planar graphs. In particular, the following properties do not depend on the existence of a star-decomposition, therefore we do not use tree decompositions in our proofs. However, note that we refer to Definition 5 in Theorem 6. For clarity, we will separate the properties that hold for every *biconnected* planar graph from those that only hold for prime planar graphs.

Properties of biconnected planar graphs. In order to obtain these properties, we will mostly rely on the notion of *intermediate graphs*, defined below.

Definition 6 *[13, Definition 6] Let $G = (V, E)$ be a planar graph. We fix a plane embedding of G. Let F be the set of faces of this embedding. The* intermediate graph *$G_I = (V \cup F, E_I)$ has vertex-set $V \cup F$, furthermore $E \subseteq E_I$ and we add an edge in G_I between an original vertex $v \in V$ and a face-vertex $f \in F$ whenever the corresponding vertex and face are incident in G (see Figure 9).*

Note that an intermediate graph is planar. Furthermore, since a plane embedding can be constructed in linear-time [34], therefore so can be an intermediate graph. This is important for

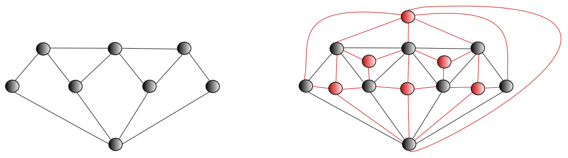

Figure 9: A plane embedding of some planar graph (left) and the corresponding intermediate graph (right). Face-vertices are coloured in red.

the quadratic-time complexity of Algorithm `Leaf-BottomUp`. To prove the correctness of Algorithm `Leaf-BottomUp` in the following, we will rely upon the following property of intermediate graphs.

Lemma 12 *[13, Proposition 9] Let S be a minimal separator of some biconnected planar graph $G = (V, E)$ and let C be a full component of $G \setminus S$. We fix a plane embedding of G. Then S corresponds to a cycle $v_S(C)$ of G_I, of length $2|S|$ and with $V \cap v_S(C) = S$, and such that $G_I \setminus v_S(C)$ has at least two connected components. Moreover, the original vertices of one of these components are exactly the vertices of C.*

In the following, we will rely upon two properties which both follow from Lemma 12. The first one is the following structural property of minimal separators of planar graphs.

Corollary 6 *Let S be a minimal separator of a biconnected planar graph $G = (V, E)$. Then, S either induces a cycle or a forest of paths.*

Proof. Let us fix a plane embedding of G, let G_I be the corresponding intermediate graph. Then, let C_S be a smallest cycle of G_I such that $V \cap C_S = S$, that exists by Lemma 12. To prove the corollary, it suffices to prove that C_S is an induced cycle of G_I. By contradiction, assume the existence of a chord xy of C_S. Note that $x \in S$ or $y \in S$ because face-vertices are pairwise non-adjacent in G_I. Therefore assume w.l.o.g. that $x \in S$. Let us divide C_S in two cycles C_1, C_2 such that $C_1 \cap C_2 = \{x, y\}$. By the minimality of C_S, S intersects both $C_1 \setminus C_2$ and $C_2 \setminus C_1$. Therefore, let $z_1, z_2 \in S$ such that $z_1 \in C_1 \setminus C_2$ and $z_2 \in C_2 \setminus C_1$. Finally, let A, B be two full components of $G \setminus S$. Observe that $(A \cup B) \cap (C_1 \cup C_2) = \emptyset$ because $V \cap C_S = S$. Let us contract C_1, C_2 in order to obtain the two triangles (z_1, x, y) and (z_2, x, y). In such case, there is a $K_{3,3}$-minor of G_I with $\{A, B, y\}$ and $\{x, z_1, z_2\}$ being the respective sides of the bipartition, thus contradicting the fact that G_I is planar. Therefore, C_S is an induced cycle of G_I and so, S induces a subgraph of a cycle in G, that is either a cycle or a forest of path. ■

On the algorithmic side, one can also deduce from Lemma 12 the following corollary.

Corollary 7 *Let G be a biconnected planar graph, let S be a minimal separator of G. There is a planar supergraph G_S of G with same vertex-set so that S either induces an edge (if $|S| = 2$) or a cycle of G_S, and it can be constructed in linear-time.*

Proof. Let us fix a plane embedding of G, let G_I be the corresponding intermediate graph. For every face-vertex f of G_I, let us consider $S_f = S \cap N_{G_I}(f)$. We first claim that $|S_f| \leq 2$. Indeed, let A, B be two full components of $G \setminus S$, let us contract them to any two vertices $a \in A, b \in B$. Then, there is a $K_{3,|S_f|}$-minor of G_I with $\{a, b, f\}$ and S_f being the respective parts of the bipartition. Since G_I is planar by construction, therefore, $|S_f| \leq 2$.

Now, the graph G_S is constructed from G as follows (we refer to Figure 10 for an illustration of the proof). For every face-vertex f of G_I, if $S_f = (x, y)$ then we add the edge $\{x, y\}$ in G_S.

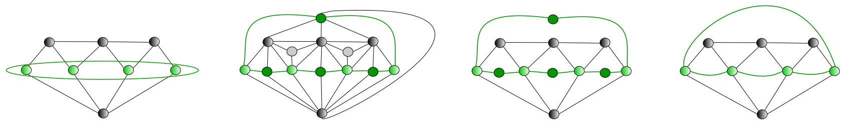

Figure 10: Addition of edges in a planar graph G so as to make a minimal separator of G induce a cycle.

Note that G_S is a minor of G_I and so, it is a planar graph. Moreover, by Lemma 12 there is a cycle of G_I whose original vertices are exactly S and so, S induces a connected subgraph of G_S. In particular if $|S| = 2$, then it must be an edge. Else, $|S| > 2$ and the connected subgraph $G_S[S]$ contains a cycle by construction. Since S is a minimal separator of G_S by construction and $G_S[S]$ is not acyclic, it follows from Corollary 6 that S induces a cycle of G_S. ■

We will often make use of the routine of Corollary 7 in order to prove the quadratic-time complexity of Algorithm `Leaf-BottomUp`.

Properties of prime planar graphs. Unlike the above Corollaries 6 and 7 (which hold for every biconnected planar graph), the following results only hold for prime planar graphs. We will make use of the following structural properties of prime planar graphs in order to prove the correctness of Algorithm `Leaf-BottomUp`.

Lemma 13 *Let $G = (V, E)$ be a prime graph that is $K_{3,3}$-minor-free. Let $v \in V$, for every minimal separator $S \subseteq N_G(v)$ of the subgraph $G \setminus v$, S consists of two non-adjacent vertices.*

Proof. Let $S \subseteq N_G(v)$ be a minimal separator of $G \setminus v$. There must exist two full components A and B of S in $G \setminus (S \cup \{v\})$. Let us remove all nodes of the components of $G \setminus (S \cup \{v\})$ but the ones in A or B. Then, let us contract A (resp., B) in a single vertex a (resp., b). We get a $K_{3,|S|}$ as a minor of G where $\{a, b, v\}$ is one part of the bipartition, and so $|S| \leq 2$. Finally, since $S \cup \{v\}$ is also a separator of G, then $|S| \geq 2$ because otherwise $S \cup \{v\}$ would be an edge-separator. Therefore, $|S| = 2$ and it is a stable set because otherwise there would be a clique-separator of size 3 in G. ■

Lemma 14 *Let G be a prime planar graph, let the path $\Pi = (a, b, c)$ be a separator of G, and let C be a component of $G \setminus \Pi$. Then, there is at most one common neighbour of a, b in C.*

Proof. First note that Π is induced or else it would be a clique-separator of G. Furthermore, $a, c \in N(C')$ for every component C' of $G \setminus (\Pi \cup C)$ or else $N(C')$ would be a clique-separator of G (either a vertex-separator or an edge-separator). In particular, it is always possible to make vertices a, c adjacent by contracting an arbitrary component of $G \setminus (\Pi \cup C)$.

By contradiction, let $u, u' \in N(a) \cap N(b) \cap C$ be distinct. We claim that there exists a uc-path Q in $C \cup \{c\}$ that does not contain u', because else the triangle a, b, u' would separate u from Π, that contradicts the fact that G is prime. By symmetry, there also exists a $u'c$-path Q' in $C \cup \{c\}$ that does not contain u. There are two cases.

- Q and Q' are internally vertex-disjoint paths (see Figure 11 for an illustration). Let us contract $Q \setminus c, Q' \setminus c$ to the vertices u, u', let us contract an arbitrary component of $G \setminus (\Pi \cup C)$ in order to make vertices a, c adjacent, then let us contract a path from Q to Q' in C (that exists, because C is connected by the hypothesis) in order to make vertices u, u' adjacent. Then one obtains from a, b, c, u, u' a K_5-minor, which contradicts the fact that G is planar.

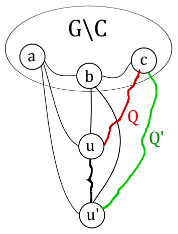

Figure 11: Case where the paths Q and Q' are internally vertex-disjoint paths.

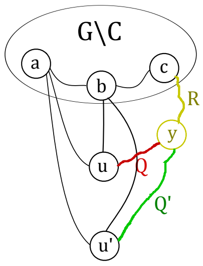

Figure 12: Case where the paths Q and Q' intersect.

- Q and Q' intersect (see Figure 12 for an illustration). Let $y \in (Q \cap Q') \setminus c$ be such that the uy-subpath of Q does not intersect Q'. Let R be the yc-subpath of Q'. We may assume w.l.o.g. that $R \subseteq Q \cap Q'$ for the remaining of the proof, whence $Q \cap Q' = R$. Let us contract $Q \setminus R, Q' \setminus R, R \setminus c$ in order to make vertices u, u', c adjacent to vertex y, then let us contract an arbitrary component of $G \setminus (P \cup C)$ in order to make vertices a, c adjacent. One obtains from a, b, c, u, u', y a $K_{3,3}$-minor with $\{a, b, y\}$ being one side of the bipartition, that contradicts the fact that G is planar.

■

Lemma 15 *Let G be a prime planar graph, let the path $\Pi = (a, b, c)$ be a separator of G, and let C be a component of $G \setminus \Pi$. Suppose there is some vertex $v \in C$ that is a common neighbour of a, b, c. Then, either C is reduced to v, or (a, v, c) is a separator of G. Furthermore, in the latter case, the path (a, v, c) separates vertex b from $C \setminus v$.*

Proof. Let us assume that $C \setminus v \neq \emptyset$. Let D be a connected component of $G[C \setminus v]$. Note that $v \in N(D)$ because C is a connected component of $G \setminus \Pi$ by the hypothesis. To prove the lemma, it suffices to prove that $b \notin N(D)$. By contradiction, suppose that $b \in N(D)$ (see Figure 13 for an illustration). Since v, b, a and v, b, c are pairwise adjacent and G has no clique-separator by the hypothesis, then necessarily $N(D) = \{a, b, c, v\}$.

Let us contract the component D to a single vertex x. Then, let C' be any component of $G \setminus (\Pi \cup C)$. We have that $a, c \in N(C')$ or else $N(C')$ would be a clique-separator of G (either a vertex-separator or an edge-separator). So, let us contract the component C' onto vertex a in order to make a and c adjacent. One obtains from a, b, c, v, x a K_5-minor, which contradicts the fact that G is planar. ■

We recall that the gist of Algorithm `Leaf-BottomUp` is (informally) to try to remove a leaf-vertex v from G then to apply recursively the algorithm on $G \setminus v$. Because the algorithm is strongly dependent on the fact that G is prime, it is important to characterize the cases when

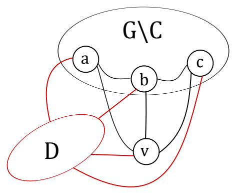

Figure 13: Existence of a component $D \subseteq C \setminus v$ that is adjacent to b.

$G \setminus v$ is also prime. Indeed, new clique-decompositions are needed when $G \setminus v$ is not prime, which may provoke a combinatorial explosion of the number of subgraphs to be considered. Therefore, before we conclude this section, let us characterize whenever there may be clique-separators in $G \setminus v$ with v being a leaf-vertex. This will first require the following lemma.

Lemma 16 *Let $G = (V, E)$ be a graph and let the path $\Pi = (a, b, c)$ be a separator of G. Let C be the union of some components of $G \setminus \Pi$ and let S be a separator of $G[C \cup \Pi]$. Then, S is a separator in G or S separates a and c in $G[C \cup \Pi]$.*

Moreover, in the latter case, $G[C \cup \Pi] \setminus S$ has exactly two components C_a and C_c containing a and c respectively.

Proof. There are two cases.

- Suppose there exists a component D of $G[C \cup \Pi] \setminus S$ such that $N_G(D) \subseteq C \cup \Pi$. Since $D \cap S = \emptyset$, $S \neq V \setminus D$ and $N_G(D) \subseteq S$ therefore S is a separator of G with D being a component of $G \setminus S$.

- Else, every component D of $G[C \cup \Pi] \setminus S$ has a neighbour in $V \setminus (C \cup \Pi)$. The latter implies that $D \cap \Pi \neq \emptyset$ for every component D of $G[C \cup \Pi] \setminus S$ because C is a union of components of $G \setminus \Pi$ by the hypothesis. In particular, since there exist at least two components of $G[C \cup \Pi] \setminus S$ then there must be one containing an endpoint of Π. W.l.o.g. assume there is a component C_a of $G[C \cup \Pi] \setminus S$ such that $a \in C_a$. Let C_c be any component of $G[C \cup \Pi] \setminus (S \cup C_a)$. We have that $C_c \cap N[C_a] = \emptyset$ because S separates C_a and C_c in $G[C \cup \Pi]$. Therefore, $a, b \notin C_c$ and so, $c \in C_c$ because $C_c \cap \Pi \neq \emptyset$. This finally proves that $G[C \cup \Pi] \setminus S$ has exactly two components C_a and C_c containing a and c respectively.

■

Theorem 6 *Let $G = (V, E)$ be a prime planar graph, let v be a leaf-vertex of Type either 2 or 3 and let $\Pi_v = (a_v, b_v, c_v)$ be as defined in Definition 5. Suppose that there exists a minimal separator S in $G \setminus v$ that is a clique. Then, $S = \{u_v, b_v\}, u_v \notin \Pi_v$ and the following hold:*

- *$V \setminus (\Pi_v \cup \{v\})$ is a full component of $G \setminus \Pi_v$.*
- *If $u_v \in N(a_v)$ (resp. $u_v \in N(c_v)$), then a_v (resp. c_v) is simplicial in $G \setminus v$ with neighbours $\{u_v, b_v\}$;*
- *Furthermore $u_v \notin N(a_v) \cap N(c_v)$ unless $V = \Pi_v \cup \{u_v, v\}$;*

Proof. Note that the subgraph $G \setminus v$ is planar and S is a minimal separator of $G \setminus v$ by the hypothesis, therefore by Corollary 6 either S induces a cycle or a forest of path. Since in addition S is a clique by the hypothesis, it follows that S either induces a singleton, an edge

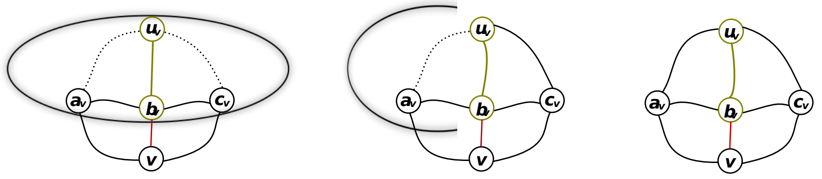

Figure 14: Existence of a clique-separator in $G \setminus v$.

or a triangle. Since S is a clique and G is prime, S is not a separator of G, so by Lemma 16 with $C = V \setminus (\Pi_v \cup \{v\})$, S is an a_vc_v-separator of $G \setminus v$. This both implies that $b_v \in S$ and $S' := S \cup \{v\}$ is a minimal a_vc_v-separator of G. In particular, S being a strict subset of some minimal separator of G it cannot induce a cycle (by Corollary 6), hence it must induce either a singleton or an edge. Furthermore, still by Lemma 16 with $C = V \setminus (\Pi_v \cup \{v\})$ there exist exactly two components C_a, C_c of $G \setminus (S \cup \{v\})$, with $a_v \in C_a, c_v \in C_c$. As a result, $S \setminus b_v \neq \emptyset$, or else $\{a_v, b_v\}, \{b_v, c_v\}$ would be edge-separators of G, thus contradicting the hypothesis. Let $S = \{u_v, b_v\}, u_v \notin \Pi_v \cup \{v\}$. If $u_v \in N(a_v)$, then $C_a \setminus a_v = \emptyset$ (and so, a_v is simplicial in $G \setminus v$), for otherwise (a_v, u_v, b_v) would be a clique-separator of G. Similarly, if $u_v \in N(c_v)$ then $C_c \setminus c_v = \emptyset$ (and so, c_v is simplicial in $G \setminus v$). In particular if $u_v \in N(a_v) \cap N(c_v)$ then $\Pi_v \cup \{u_v, v\} = V$. Last, as there exists an a_vc_v-path in every component C' of $G \setminus (\Pi_v \cup \{v\})$ because G has no clique-separator by the hypothesis, therefore $u_v \in C'$. This implies that $V \setminus (\Pi_v \cup \{v\})$ is a full component of $G \setminus \Pi_v$. ■

5.2.2 Constrained star-decompositions

In the following, it will be useful to impose additional structure on the star-decompositions. In order to do that, we will prove properties on some pairs of vertices in the graph. Namely, we will prove that when $x, y \in V$ satisfy a few technical conditions, then it can be assumed that $T_x \cup T_y$ is a subtree of the star-decomposition $(T, \mathcal{X})$.

Lemma 17 *Let G be a connected graph with $tb(G) = 1$, let $x, y \in V(G)$ be non-adjacent (and $x \neq y$).*

Suppose the pair (x, y) satisfies that for every xy-separator S of G, if there is $z \notin \{x, y\}$ that dominates S then $z \in N_G(x) \cap N_G(y)$.

Then, there is a star-decomposition $(T, \mathcal{X})$ of G with $B_x, B_y \in \mathcal{X}$, $x \in B_x, y \in B_y$ and either $B_x = B_y$ or B_x, B_y are adjacent in T. Moreover, in the latter case, $B_x \subseteq N[x], B_y \subseteq N[y]$.

Proof. Consider a star-decomposition $(T, \mathcal{X})$ of G, that exists by Lemma 3. If x and y are not in a same bag, let B_x and B_y be the bags containing respectively x and y and as close as possible in T. By the properties of a tree decomposition, $N(x) \cap N(y) \subseteq B_x \cap B_y$. Hence, for any bag B between B_x and B_y in T, $N(x) \cap N(y) \subseteq B$.

- **Case 1:** If B_x and B_y are not adjacent in T, let B be any bag in the path between B_x and B_y in T. By the properties of a tree decomposition, B is an xy-separator. Moreover, let $z \in B$ dominate the bag, by the hypothesis $z \in N(x) \cap N(y)$ because $x, y \notin B$. As a result, adding x and y in each bag B between B_x and B_y achieves a star-decomposition of G that has a bag containing both x, y.

- **Case 2:** Now, let us assume that B_x and B_y are adjacent in T. Note that, if $B_x \subseteq N[z]$ for some $z \in N(x) \cap N(y)$ (resp., if $B_y \subseteq N[z]$ for some $z \in N(x) \cap N(y)$) the result holds.

Indeed, adding y in B_x (resp., x in B_y) achieves a star-decomposition of G that has a bag containing both x, y.

So, let us consider the case when none of the two bags B_x, B_y is dominated by a vertex of $N(x) \cap N(y)$. Then, $B_x \setminus x$ and $B_y \setminus y$ are xy-separators by the properties of a tree decomposition. Let $z_x \in B_x, z_y \in B_y$ satisfy $B_x \subseteq N[z_x]$ and $B_y \subseteq N[z_y]$. By the hypothesis, $z_x \in \{x\} \cup (N(x) \cap N(y))$ and $z_y \in \{y\} \cup (N(x) \cap N(y))$. Thus it follows that $z_x = x$ and $z_y = y$ (or else, we are back to Case 1). Note that $B_x \cap B_y = N(x) \cap N(y)$ in such a case.

■

We will mostly use the following two weaker versions of Lemma 17 in our proofs.

Corollary 8 *Let G be a connected graph with $tb(G) = 1$, let $x, y \in V(G)$ be non-adjacent (and $x \neq y$).*

Suppose there exists a minimal separator $S \subseteq (N(x) \cap N(y)) \cup \{x, y\}$ in G and $\{x, y\} \subseteq S$.

Then, there is a star-decomposition $(T, \mathcal{X})$ of G with $B_x, B_y \in \mathcal{X}$, $x \in B_x, y \in B_y$ and either $B_x = B_y$ or B_x, B_y are adjacent in T. Moreover, in the latter case, $B_x \subseteq N[x], B_y \subseteq N[y]$.

Proof. We claim that for every xy-separator S' of G, if there is $z \notin \{x, y\}$ such that $S' \subseteq N[z]$ then $z \in N(x) \cap N(y)$. Observe that if the claim holds, then the corollary follows from Lemma 17. To prove the claim, let $S \subseteq (N(x) \cap N(y)) \cup \{x, y\}$ be a separator of G and $\{x, y\} \subseteq S$, that exists by the hypothesis. Note that for any full component C of $G \setminus S$, the xy-separator S' must contain some vertex in C. Since there are at least two full components of $G \setminus S$, then $z \in S \setminus (x, y) \subseteq N(x) \cap N(y)$, that finally proves the claim. ■

So far, the two above results in this section (Lemma 17 and Corollary 8) apply to *general* graphs with tree-breadth one. However, we will need the fact that the graph is planar for the following corollary.

Corollary 9 *Let G be a connected graph with $tb(G) = 1$, let $x, y \in V(G)$ be non-adjacent (and $x \neq y$).*

Suppose G is $K_{3,3}$-minor-free and $|N_G(x) \cap N_G(y)| \geq 3$.

Then, there is a star-decomposition $(T, \mathcal{X})$ of G with $B_x, B_y \in \mathcal{X}$, $x \in B_x, y \in B_y$ and either $B_x = B_y$ or B_x, B_y are adjacent in T. Moreover, in the latter case, $B_x \subseteq N[x], B_y \subseteq N[y]$.

Proof. We claim that for every xy-separator S of G, if there is $z \notin \{x, y\}$ such that $S \subseteq N[z]$ then $z \in N(x) \cap N(y)$. Observe that if the claim holds, then the corollary follows from Lemma 17. To prove the claim, first recall that $|N(x) \cap N(y)| \geq 3$. Since vertex z dominates S and S is an xy-separator, therefore, z dominates $N(x) \cap N(y)$ because $N(x) \cap N(y) \subseteq S$. In such case, $z \in N(x) \cap N(y)$, or else, G admits a $K_{3,|N(x) \cap N(y)|}$-minor with $\{x, y, z\}$ and $N(x) \cap N(y)$ being the respective of the bipartition, which contradicts the hypothesis. ■

Before we conclude this section, let us emphasize a useful consequence of Corollary 8 regarding minimal 2-separators.

Lemma 18 *Let $G = (V, E)$ with $tb(G) = 1$, let $x, y \in V$ be non-adjacent such that $S = \{x, y\}$ is a minimal separator of G ($x \neq y$). For every full component C of $G \setminus S$, we have that $N(x) \cap N(y) \cap C \neq \emptyset$.*

Proof. Let $(T, \mathcal{X})$ be a star-decomposition of G, that exists by Lemma 3, minimizing the distance in T between the subtrees T_x and T_y (respectively induced by the bags containing x and y). There are two cases.

- First, suppose that $T_x \cap T_y \neq \emptyset$. For any full component C of $G \setminus S$, let T_C be the subtree that is induced by all bags intersecting C. Because C is a full component, there must be an edge between x and a vertex of C, and this edge is in a bag of $T_x \cap T_C$. Similarly, there must be an edge between y and a vertex of C, and this edge is in a bag of $T_y \cap T_C$. As a result, the subtrees T_x, T_y, T_C are pairwise intersecting, and so by the Helly property (Lemma 1) $T_x \cap T_y \cap T_C \neq \emptyset$ *i.e.*, there exists a bag X_t which contains S and it intersects C. Let $z \in X_t$ dominate the bag. Note that $z \in C \cup S$ because it has to dominate some vertices in C and so, it cannot be in $V \setminus (C \cup S)$. Furthermore, recall that x, y are non-adjacent by the hypothesis. Therefore, $z \in C \cap N(x) \cap N(y)$, and the result holds for any full component C of $G \setminus S$.
- Else, since $S = \{x, y\}$ is a minimal separator and we assume $(T, \mathcal{X})$ to minimize the distance in T between T_x and T_y, by Corollary 8 there are two adjacent bags B_x, B_y such that $x \in B_x \setminus B_y$ dominates B_x, $y \in B_y \setminus B_x$ dominates B_y. Since $B_x \cap B_y$ is an xy-separator by the properties of a tree-decomposition, then $B_x \cap B_y \cap C \neq \emptyset$ for every full component C of $G \setminus S$, that is $N(x) \cap N(y) \cap C \neq \emptyset$.

■

5.2.3 Bounded Treewidth

Independently from Algorithm `Leaf-BottomUp`, let us introduce in this section another property of (not necessarily prime) planar graphs with tree-breadth one. More precisely, we prove these graphs have bounded treewidth. To prove this property, we will use the same terminology as for the previous subsections.

Lemma 19 *Let G be planar with $tb(G) \leq 1$. Then, $tw(G) \leq 4$ and the upper-bound is sharp.*

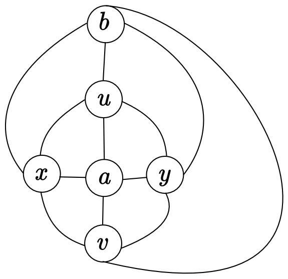

Figure 15: A planar graph G with $tb(G) = 1$ and $tw(G) = 4$.

Proof. The treewidth of G is the maximum treewidth of its atoms [10], so, let us assume G to be a prime planar graph. Let $(T, \mathcal{X})$ be any star-decomposition of G, the graph $H = (V, \{\{u, v\} \mid T_u \cap T_v \neq \emptyset\})$ is chordal. Furthermore, if H' is a chordal graph with same vertex-set V and such that $E(G) \subseteq E(H') \subseteq E(H)$ then any clique-tree of H' is still a star-decomposition of G. Therefore, we will assume w.l.o.g. that H is a minimal triangulation of G and $(T, \mathcal{X})$ is a clique-tree of H (in particular, $(T, \mathcal{X})$ is reduced). Additional properties of $(T, \mathcal{X})$ will be deduced from the latter assumption about H by using the results from [14]. Let us now prove the lemma by induction on $|V(G)|$ (the base-case of the graph with a single vertex is trivial).

- If $|\mathcal{X}| = 1$, then G has some universal vertex u. Furthermore, since G is planar therefore, $G \setminus u$ is outerplanar [44]. Consequently, $tw(G \setminus u) \leq 2$ [9], so, $tw(G) \leq 3$.

- Suppose $|\mathcal{X}| = 2$. Let $\mathcal{X} = \{B, B'\}$. Since $(T, \mathcal{X})$ is assumed to be a clique-tree of some minimal triangulation H of G, therefore, $B \cap B'$ is a minimal separator [14]. Let us remind that by Corollary 7 there is a planar supergraph G' of G with same vertex-set so that $B \cap B'$ induces either an edge or a cycle of G'. Furthermore $(T, \mathcal{X})$ is also a star-decomposition of G', so, $tb(G') \leq 1$. In addition, $tw(G) \leq tw(G')$. Recall that we can further assume G' to be prime (or else, we apply the induction hypothesis on the atoms of G'), hence $B \cap B'$ induces a cycle of G' of length at least four. Let $B \Delta B' = (B \setminus B') \cup (B' \setminus B)$. Since H is assumed to be a minimal triangulation and B, B' are leaves of a clique-tree of H, therefore, $B \setminus B'$ is a (nonempty) dominating clique of the subgraph $G[B]$, and similarly $B' \setminus B$ is a (nonempty) dominating clique of the subgraph $G[B']$ [14]. Thus, every vertex $u \in B \Delta B'$ satisfies $B \cap B' \in N(u)$. Since $|B \cap B'| \geq 4$ because $B \cap B'$ induces a cycle of G' of length at least four, therefore, $|B \Delta B'| \leq 2$ or else there would be a $K_{3,3}$-minor of G' with any three vertices of $B \cap B'$ being one part of the bipartition. As a result, since $B \cap B'$ induces a cycle, $tw(G) \leq tw(G') \leq 2 + |B \Delta B'| = 4$.

- Finally, suppose $|\mathcal{X}| \geq 3$. Let $t \in V(T)$ be an internal node, by the properties of a tree decomposition the bag X_t is a separator of G. Let $b \in X_t$ satisfy $X_t \subseteq N_G[b]$. Since G is prime and so, biconnected, therefore $X_t \setminus b$ is a separator of $G \setminus b$. In such case, let us remind by Lemma 13 that there exist $a, c \in X_t \setminus b$ non-adjacent such that $\{a, c\}$ is a minimal separator of $G \setminus b$. In particular, the path $\Pi = (a, b, c)$ is a separator of G. Let $C_1, C_2, \ldots, C_l$ be the components of $G \setminus \Pi$. For every $1 \leq i \leq l$, let G_i be obtained from $G[C_i \cup \Pi]$ by making the two endpoints a, c of Π adjacent. Note that G_i can be obtained from G by edge-contractions (because G is prime and so, $a, c \in N(C_j)$ for every $1 \leq j \leq l$), therefore, $tb(G_i) \leq 1$ because tree-breadth is stable under edge-contractions (Lemma 2). In addition, $tw(G) \leq \max_i tw(G_i)$ because Π induces a triangle in every graph G_i by construction. As a result, for every $1 \leq i \leq l$, since $|V(G_i)| < |V(G)|$ by construction, therefore $tw(G_i) \leq 4$ by the induction hypothesis, whence $tw(G) \leq 4$.

Let G be constructed from the cycle (u, v, x, y) of length four by adding two vertices a, b such that $N_G(a) = N_G(b) = \{u, x, v, y\}$ (see Figure 15 for an illustration). Since there exists a star-decomposition of G with two bags (respectively dominated by a, b), $tb(G) \leq 1$. Moreover, G is 4-regular by construction, therefore $tw(G) \geq 4$ [10]. This proves the sharpness of the upper-bound. ■

Note that since it is well-known that many difficult problems can be solved on bounded-treewidth graphs in linear-time, therefore, it may be the case that the recognition of planar graphs with tree-breadth at most one can be simplified by using Lemma 19. However, we were unable to find a way to use it in our proofs (actually, the star-decomposition that can be computed using our algorithm may have unbounded width — because of leaf-vertices of Type 1).

5.3 Correctness of Algorithm `Leaf-BottomUp`

5.3.1 Existence of a P_3-separator

As a first step to prove correctness of Algorithm `Leaf-BottomUp`, let us prove correctness of Step 1. That is, we will prove that for every planar graph G with $tb(G) = 1$, G contains a leaf-vertex or G admits a star-decomposition with at most two bags.

To prove this step, we will prove additional properties of the minimal separators of prime planar graphs with tree-breadth one. In the following, let $\mathcal{P}_3(G)$ be the set of (not necessarily minimal) separators of G that induce paths of length 2 (we will call them P_3-separators since they have three vertices). We will distinguish the case when $\mathcal{P}_3(G) \neq \emptyset$ from the case when $\mathcal{P}_3(G) = \emptyset$.

Theorem 7 *Let G be a prime planar graph with $tb(G) = 1$. If $\mathcal{P}_3(G) \neq \emptyset$, then G has a leaf-vertex.*

Proof. Let $\Pi = (a, b, c) \in \mathcal{P}_3(G)$ minimize the size of a smallest component of $G \setminus \Pi$. We recall that $\{a, c\} \notin E(G)$ because G is assumed to be prime by the hypothesis (the latter fact will be used in the following). Let C be any component of $G \setminus \Pi$ of minimum size. Our aim is to prove the existence of some leaf-vertex $v \in C$ (the latter dominating the component C), that will prove Theorem 7.

Claim 1 *There do not exist $\Pi' \subseteq \Pi \cup C$, $C' \subset C$ such that $\Pi' \in \mathcal{P}_3(G)$ and C' is a component of $G \setminus \Pi'$.*

Proof. The claim follows from the minimality of C. $\diamond$

We will often use Claim 1 in the remaining of the proof.

Let $(T, \mathcal{X})$ be a star-decomposition of G, that exists by Lemma 3. In particular, let T_a, T_c be the subtrees that are respectively induced by the bags containing a or c. Assume w.l.o.g. that $(T, \mathcal{X})$ minimizes the distance in T between the subtrees T_a and T_c. We will distinguish the case $T_a \cap T_c \neq \emptyset$ from the case $T_a \cap T_c = \emptyset$.

Case $T_a \cap T_c \neq \emptyset$. In such case, the subtrees T_a, T_b, T_c are pairwise intersecting and so, by the Helly property (Lemma 1) $T_a \cap T_b \cap T_c \neq \emptyset$. Let us remove all vertices in $V \setminus (\Pi \cup C)$ from bags in $(T, \mathcal{X})$. Let us call $(T, \mathcal{X}^C)$ the resulting tree decomposition of $G[\Pi \cup C]$.

Claim 2 $(T, \mathcal{X}^C)$ *has breadth one.*

Proof. There are two cases to be considered.

- If b has some neighbour in C, then C must be a full component of $G \setminus \Pi$, or else one of $\{a, b\}, \{b, c\}$ should be a clique-separator thus contradicting the fact that G is prime by the hypothesis. In such case, the claim follows from Lemma 9.

- Else, b has no neighbour in C, and let D be the connected component of b in $G \setminus (a, c)$. Let H be obtained from G by contracting D to b. By Lemma 2, $tb(H) = 1$. Let $(T, \mathcal{X}^H)$ be the tree decomposition of breadth one of H where for every $t \in V(T)$, $X_t^H = X_t$ if $X_t \cap D = \emptyset$, $X_t^H = (X_t \setminus D) \cup \{b\}$ else. Moreover, since b has no neighbour in C, $D \cap N_G[C] = \emptyset$ and so, $H[C \cup \Pi] = G[C \cup \Pi]$ by construction. Finally, since $\{b\}$ is a full component of $H \setminus (a, c)$, therefore, by Lemma 9 applied to H, the tree decomposition $(T, \mathcal{X}^C)$ is indeed a tree decomposition of breadth one of $G[C \cup \Pi]$.

$\diamond$

Let $(T', \mathcal{X}')$ be any reduced tree decomposition obtained from $(T, \mathcal{X}^C)$. We point out that $T'_a \cap T'_b \cap T'_c \neq \emptyset$ by construction (because $T_a \cap T_b \cap T_c \neq \emptyset$). Furthermore, since by Claim 2 $(T, \mathcal{X}^C)$ has breadth one, therefore $(T', \mathcal{X}')$ is a star-decomposition of $G[C \cup \Pi]$ by Lemma 3.

We will prove that C contains a leaf-vertex by contradiction. Informally, we will show, using the properties of the star-decomposition $(T', \mathcal{X}')$, that if it is not the case that C contains a leaf-vertex, then $\mathcal{P}_3(G[C \cup \Pi]) \cap \mathcal{P}_3(G) \neq \emptyset$ and the latter contradicts Claim 1.

In order to prove this, first note that a has at least one neighbour in C because G is prime by the hypothesis (indeed, (b, c) cannot be an edge-separator of G). We now distinguish between several subcases.

- **Case 1.** There is $u \in C$ such that $u \in N(a) \cap N(b) \cap N(c)$ (*e.g.*, see Figure 16). By Lemma 15, either C is reduced to u or there exist $\Pi' = (a, u, c) \in \mathcal{P}_3(G)$, $C' \subseteq C \setminus u$ and C' is a component of $G \setminus \Pi'$. The latter case contradicts Claim 1, therefore, C is reduced to u and so u is a leaf-vertex of Type 2.

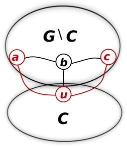

Figure 16: Case 1

Thus, from now on let us assume that no such vertex u exists.

- **Case 2.** By contradiction, assume $N(a) \cap C \subseteq N(b) \cap C$. By Lemma 14, $|N(a) \cap N(b) \cap C| \leq 1$, so, $|N(a) \cap C| = 1$. Let $u \in N(a) \cap N(b) \cap C$ be the unique neighbour of vertex a in C (see Figure 17). Since in such case we can assume that $u \notin N(c)$ (for otherwise, we are back to Case 1), and vertex c has some neighbour in C because G is prime (and so, (a, b) cannot be an edge-separator of G), therefore, C is not reduced to vertex u. Then, $\Pi' = (u, b, c) \in \mathcal{P}_3(G)$ because it separates a from $C \setminus u$, and so there is at least one component of $G \setminus \Pi'$ that is strictly contained into C by construction. This contradicts Claim 1, so, Case 2 cannot occur.

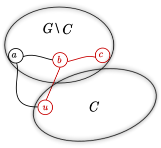

Figure 17: Case 2

- **Case 3.** There is $u \in C$ satisfying $u \in N(a) \setminus N(b)$. By the properties of a tree decomposition, there is some bag $B' \in T'_a \cap T'_u$. Let $v \in B'$ dominate the bag B'. By construction, $v \neq b$ because $u \in B' \setminus N(b)$, similarly $v \neq c$ because $a \in B' \setminus N(c)$. We will also prove later that $v \neq a$. Moreover, $\Pi \setminus N[v] \neq \emptyset$ (or else, we are back to Case 1), hence $\Pi \setminus B' \neq \emptyset$. So let B be the bag adjacent to B' onto the unique path in T' from B' to $T'_a \cap T'_b \cap T'_c$ (we remind that the latter subtree is nonempty by construction). By the properties of the tree decomposition $(T', \mathcal{X}')$, $B \cap B'$ is a separator of $G[C \cup \Pi]$. Furthermore, $a \in B \cap B'$. More generally $\Pi \cap B' \subseteq B \cap B'$ by construction, therefore $B \cap B'$ is also a separator of G by Lemma 16. Let $w \in B$ dominate this bag. Observe that $w \neq c$ because $a \in B \cap B'$.

  We will prove that $v \in C$ and v is a leaf-vertex. In order to prove these two results, we will need to prove that $C \cup \Pi$ is fully contained into the two adjacent bags B, B' (Claim 7). The latter will require intermediate claims.

  Claim 3 *$c \in B \cap B'$.*

Proof. Assume for the sake of contradiction that $c \notin B \cap B'$ (see Figure 18). Then, $c \notin B'$ because $\Pi \cap B' \subseteq B \cap B'$ by construction. We will prove that the latter contradicts Claim 1.

Indeed, first observe that $G \setminus w$ is connected because G is prime and so, biconnected, by the hypothesis. In addition $(B \cap B') \setminus w$ is a (not necessarily minimal) separator of $G \setminus w$ because it separates $B' \setminus B$ from c. Let $S \subseteq (B \cap B') \setminus w$ be a minimal separator of $G \setminus w$. By Lemma 13, there exist $x, y \in (B \cap B') \setminus w$ non-adjacent such that $S = \{x, y\}$, and so, $\Pi' = (x, w, y) \in \mathcal{P}_3(G)$. Note that $\Pi' \neq \Pi$, because we assume that $c \notin B \cap B'$ and so $c \notin \{x, y\}$. Moreover, since $(T', \mathcal{X}')$ is a star-decomposition of $G[C \cup \Pi]$ by construction we have that $\Pi' \subseteq \Pi \cup C$, therefore $x \in C$ or $y \in C$, because $c \notin \{x, y\}$ and a, b are adjacent whereas x, y are non-adjacent. W.l.o.g. let $x \in C$.

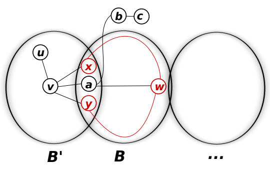

Figure 18: Case $c \notin B \cap B'$

Subclaim 3.1 Π' *is not an ac-separator.*

Proof. We refer to Figure 19 for an illustration of the proof. Let C' be any component of $G \setminus (\Pi \cup C)$. Observe that C' is fully contained into some component D of $G \setminus \Pi'$, because $\Pi' \subseteq \Pi \cup C$. In addition, $a, c \in N(C')$ because G is prime by the hypothesis (and so, neither a nor b nor c nor (a, b) nor (b, c) can be a separator of G). In particular, since we assume $c \notin B \cap B'$ and so, $c \notin \Pi'$, therefore, $c \in D$. As a result, either $a \in \Pi'$ or $a, c \in D$, that finally proves the subclaim. ◦

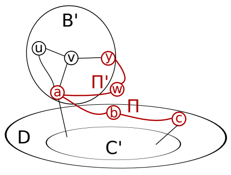

Figure 19: Π' is not an ac-separator.

Let D be the component of $G \setminus \Pi'$ such that $c \in D$, that exists because we assume $c \notin B \cap B'$ and so, $c \notin \Pi'$. Since b, c are adjacent and Π' is not an ac-separator by Claim 3.1, therefore, $\Pi \subseteq \Pi' \cup D$.

Moreover, let us show that Claim 3.1 implies the existence of some $D' \subset C$ being a component of $G \setminus \Pi'$, thus contradicting Claim 1. Indeed, let D' be any component of $G \setminus (\Pi' \cup D)$. Since G is prime by the hypothesis, x has some neighbour in D' and so, $D' \cap C \neq \emptyset$ because $x \in C$ and $\Pi \cap D' = \emptyset$ by construction. But then, $D' \subseteq C \setminus x$, for the existence of some $z \in D' \setminus C$ would imply that $D' \cap \Pi \neq \emptyset$.

To sum up, we conclude that it must be the case that $c \in B \cap B'$. ⋄

We will use Claim 3 to prove that $v \in C$, as follows:

Claim 4 *$v \in C$. Furthermore, the two vertices b, v are non-adjacent.*

Proof. Recall that $v \in C \cup \Pi$ because $(T', \mathcal{X}')$ is a star-decomposition of $G[C \cup \Pi]$ by construction. So we will only need to prove that $v \notin \Pi$. First, since $a \in B \cap B'$ by construction and $c \in B \cap B'$ by Claim 3, therefore, $a, c \in B' \subseteq N[v]$. The latter implies that $v \notin \{a, c\}$ because $a, c \in N[v]$ whereas a, c are non-adjacent. Furthermore, this implies $b \notin N[v]$ because we assume that $\Pi \not\subseteq N[v]$ (for otherwise, we are back to Case 1). As a result, $v \notin \Pi$, whence $v \in C$. ◇

Then, we will need the following technical claim in order to prove that $w = b$ (Claim 6).

Claim 5 *$G[C \cup \Pi]$ is prime.*

Proof. Suppose by contradiction there exists a clique-separator S of $G[C \cup \Pi]$. Then, S could not be a separator of G because G is prime by the hypothesis. By Lemma 16, the latter implies that S is an ac-separator of $G[C \cup \Pi]$. Therefore, the two vertices $b, v \in N(a) \cap N(c)$ must be in S, and so, since b, v are non-adjacent by Claim 4, the latter contradicts the fact that S is a clique. ◇

Claim 6 *$w = b$.*

Proof. Assume for the sake of contradiction $w \neq b$ (see Figure 20). We will prove that it contradicts Claim 1.

Indeed, the graph $G[C \cup \Pi] \setminus w$ is connected because $G[C \cup \Pi]$ is prime by Claim 5 and so, biconnected. In addition, $(B \cap B') \setminus w$ is a (not necessarily minimal) separator of $G[C \cup \Pi] \setminus w$ because it separates b from $B' \setminus B$ (recall that b, v are non-adjacent by Claim 3, and so, $b \notin B' \subseteq N[v]$). Let $S \subseteq (B \cap B') \setminus w$ be a minimal separator of $G[C \cup \Pi] \setminus w$. By Lemma 13, there exist $x, y \in (B \cap B') \setminus w$ non-adjacent such that $S = \{x, y\}$, and so, $\Pi' = (x, w, y) \in \mathcal{P}_3(G[C \cup \Pi])$. Furthermore, $b \notin \Pi' \subseteq (B \cap B') \cup \{w\} \subseteq N[v] \cup \{w\}$ and so, Π' cannot be an ac-separator of $G[C \cup \Pi]$, whence by Lemma 16 Π' is a separator of G, and so, $\Pi' \in \mathcal{P}_3(G)$.

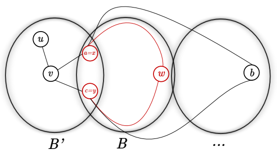

Figure 20: Case $c \in B \cap B'$ and $w \neq b$.

Let $D \subseteq C \cup \Pi$ be the component of $G[C \cup \Pi] \setminus \Pi'$ containing vertex b. Note that $\Pi \subseteq D \cup \Pi'$ because Π' is not an ac-separator of $G[C \cup \Pi]$. Let D' be any component of $G[C \cup \Pi] \setminus (\Pi' \cup D)$, that exists because $\Pi' \in \mathcal{P}_3(G[C \cup \Pi])$. Since $N(D') \subseteq C \cup \Pi$ by construction, $D' \cap \Pi = \emptyset$ by construction and D' is a component of $G[C \cup \Pi] \setminus \Pi'$, therefore, D' is also a component of $G \setminus \Pi'$. The latter contradicts Claim 1 because $D' \subset C$. ◇

Let $S = \{v, b\} \cup (B \cap B')$. We are now able to prove that $S = C \cup \Pi$ (Claim 7). That is, $C \cup \Pi$ is fully contained in the two adjacent bags B, B' (respectively dominated by b, v).

Claim 7 *$S = C \cup \Pi$.*

Proof. Assume by contradiction $S \neq C \cup \Pi$, let D be a component of $G[C \cup \Pi] \setminus S$ (see Figure 21). Note that $D \subset C$ because $\Pi \subset S$ by construction. Furthermore, $v, b \notin B \cap B'$ because $w = b$ by Claim 6 and $b \notin N(v)$ by Claim 3, so, $B \cap B'$ is a (minimal) vb-separator of $G[C \cup \Pi]$. The latter implies $v \notin N(D)$ or $b \notin N(D)$ because D induces a connected subgraph, $D \cap B \cap B' = \emptyset$ by construction, and $B \cap B'$ is a bv-separator of $G[C \cup \Pi]$. As a result, there exists $z \in \{v, b\}$ such that $N(D) \setminus z \subseteq B \cap B'$.

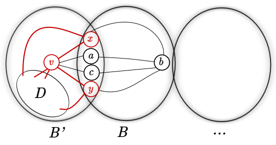

Figure 21: Case $z = v$.

Moreover let $\{z, z'\} = \{v, b\}$. $G[C \cup \Pi] \setminus z$ is connected because $G|C \cup \Pi]$ is prime by Claim 5, and so, biconnected. In addition, $N(D) \setminus z$ is a minimal separator of $G[C \cup \Pi] \setminus z$ because it separates D from z' and $N(D) \setminus z \subseteq B \cap B' \subseteq N(z')$ by construction. By Lemma 13, one obtains the existence of two non-adjacent vertices $x, y \in B \cap B'$ such that $N(D) \setminus z = \{x, y\}$, whence $N(D) \subseteq \{x, y, z\}$. Then, by construction $\Pi' = (x, z, y) \in \mathcal{P}_3(G)$ with $D \subset C$ being a component of $G \setminus \Pi'$, that contradicts Claim 1. $\diamond$

By Claim 7, $C \cup \Pi = S$ (see Figure 22). Note that it implies that $C \subseteq N[v]$ because $C \setminus v = (B \cap B') \setminus (a, c)$. In order to conclude that v is a leaf-vertex, we will finally prove in Claim 8 that either $B \cap B' = \{a, c\}$ or $B \cap B'$ induces a path.

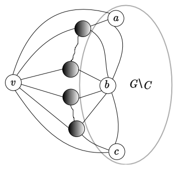

Figure 22: Case $c \in B \cap B'$, $w = b$ and $C \cup \Pi = \{v, b\} \cup (B \cap B')$.

Claim 8 *If $B \cap B' \neq \{a, c\}$, then $G[B \cap B']$ is a path.*

Proof. Recall that $b, v \notin B \cap B'$ because $w = b$ by Claim 6 and $b \notin N(v)$ by Claim 3. Hence by the properties of a tree decomposition, $B \cap B'$ is a bv-separator of $G[C \cup \Pi]$. Since $v \in C$ by Claim 4, $a \in B \cap B'$ by construction and $c \in B \cap B'$ by Claim 3, therefore $B \cap B'$ is also a vb-separator of G. In particular, $B \cap B'$ is a minimal bv-separator of G because $B \cap B' \subseteq N(v) \cap N(w) = N(v) \cap N(b)$ (indeed, recall that $w = b$ by Claim 6). By Corollary 6, $B \cap B'$ either induces a cycle or it induces a forest of paths.

Subclaim 8.1 *$B \cap B'$ does not induce a cycle.*

Proof. By contradiction, let $B \cap B'$ induce a cycle. Recall that $B \cap B'$ contains the pair of non-adjacent vertices a, c (because $a \in B \cap B'$ by construction and $c \in B \cap B'$ by Claim 3). Therefore, one can contract $B \cap B'$ until one obtains an induced quadrangle (a, x, c, y). Let us contract an arbitrary component of $G \setminus (\Pi \cup C)$ so as to obtain a vertex z. Note that $a, c \in N(z)$ because G is prime by the hypothesis (indeed, neither a nor b nor c nor (a, b)

nor (a, c) can be a separator of G). Then, let us contract the edge $\{a, z\}$ to a. By doing so, one obtains a $K_{3,3}$-minor with $\{a, b, v\}$ being one part of the bipartition and $\{x, y, c\}$ being the other part. This contradicts the fact that G is planar by the hypothesis, therefore $B \cap B'$ does not induce a cycle. $\circ$

It follows from Claim 8.1 that $B \cap B'$ induces a forest of paths. Suppose for the sake of contradiction that $B \cap B'$ induces a forest of at least two paths. Let $x \notin \{a, c\}$ be the endpoint of some path in the forest, that exists because we assume that $B \neq \{a, c\}$. Observe that $|N(x)| \geq 2$ because $b, v \in N(x)$, and $|N(x)| = |N(x) \cap (C \cup \Pi)| \leq 3$ because x is the endpoint of some path of $B \cap B'$ and $x \in C$. Furthermore, $N(x) \setminus (b, v) \subseteq B \cap B' \subseteq N(b) \cap N(v)$, and so, if $|N(x)| = 3$ then $N(x)$ induces a path. Let $\Pi' = N(x)$ if $|N(x)| = 3$, else $\Pi' = (b, a, v)$. By construction, $\Pi' \subseteq \Pi \cup C$ is a separator of G with $\{x\} \subset C$ being a component of $G \setminus \Pi'$, thus contradicting Claim 1. Consequently, $B \cap B'$ induces a path. $\diamond$

By Claim 8, either $B \cap B' = \{a, c\}$ or $B \cap B'$ induces a path. Furthermore, $B \cap B' = N(v)$ because $v \in C$ (Claim 4) and $C \cup \Pi = \{v, b\} \cup (B \cap B')$ (Claim 7). In particular, if $B \cap B' = \{a, c\}$ then v is a leaf-vertex of Type 3. Else, $B \cap B'$ induces a path and the latter implies that $|B \cap B'| \geq 4$ or else the path $B \cap B'$ would be a separator of G with $\{v\}$ being a component of $G \setminus (B \cap B')$, thus contradicting Claim 1. As a result, since we also have that $B \cap B' \subseteq N(b)$ and b, v are non-adjacent by Claim 4, therefore, v is a leaf-vertex of Type 1.

Case $T_a \cap T_c = \emptyset$. Since Π is a separator of G and G is prime by the hypothesis, one of Π or $\Pi \setminus b$ must be a minimal separator of G. Therefore, since $(T, \mathcal{X})$ is assumed to minimize the distance in T between T_a and T_c, by Corollary 8 there exist two bags B_a, B_c that are adjacent in T and such that $a \in B_a \setminus B_c$ and $c \in B_c \setminus B_a$. Furthermore, a dominates B_a while c dominates B_c. Note that $B_a \cap B_c = N(a) \cap N(c)$, so, $b \in B_a \cap B_c$. In particular, by the properties of a tree decomposition this implies that $S = N(a) \cap N(c)$ is a minimal ac-separator of G.

We will prove that C is reduced to a vertex (Claim 10), the latter being a leaf-vertex.

Claim 9 *$C \subseteq S$.*

Proof. Assume for the sake of contradiction that $C \not\subseteq B \cap B'$. By the properties of a tree decomposition it comes that some vertex $y \in C$ is separated from a or c by the set $S = B \cap B' = N(a) \cap N(c)$. Say w.l.o.g. that S is an yc-separator. Let $C' \subset C$ be the connected component containing y in $G \setminus (S \cup \{a\})$. Since we have that $G \setminus a$ is connected because G is prime by the hypothesis (and so, biconnected), that $c \notin C'$ and $N(C') \setminus a \subseteq S \cap (C \cup \Pi) \subseteq N(c) \cap (C \cup \Pi)$, then it comes that $N(C') \setminus a$ is a minimal yc-separator of $G \setminus a$. So, by Lemma 13 there exist $x', y' \in S$ such that $N(C') \setminus a = \{x', y'\}$. Therefore, $\Pi' = (x', a, y') \in \mathcal{P}_3(G)$ and $C' \subset C$ is a component of $G \setminus \Pi'$, that contradicts Claim 1. $\diamond$

By Claim 9, $C \subseteq S$ (see Figure 23 for an illustration). Since S is an ac-separator and for any component C' of $G \setminus (\Pi \cup C)$, $a, c \in N(C')$ because G is prime, therefore $S \cap C' \neq \emptyset$. One thus obtains the following chain of strict subset containment relations $C \subset C \cup \{b\} \subset S$. Furthermore, by Corollary 6, S either induces a cycle or a forest of paths, so, C being a strict connected subset of S, it must induce a path. In particular, $C \cup \{b\}$ also being a strict subset of S, either it induces a path or it is the union of the path induced by C with the isolated vertex b.

Claim 10 *$|C| = 1$.*

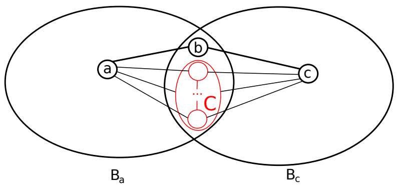

Figure 23: Case $T_a \cap T_c = \emptyset$.

Proof. Assume for the sake of contradiction that $|C| \geq 2$. Since C induces a path, let us pick an endpoint $v \in C$ that is not adjacent to vertex b (recall that $C \cup \{b\}$ being a strict subset of S, it does not induce a cycle). In such a case, $N(v)$ induces a path $\Pi' \in \mathcal{P}_3(G)$, with $a, c \in \Pi'$ and $\{v\} \subset C$ is a component of $G \setminus \Pi'$, thus contradicting Claim 1. $\diamond$

By Claim 10, C is reduced to a vertex v, that is either a leaf-vertex of Type 2 (if $v \in N(b)$) or of Type 3 (if $v \notin N(b)$). ∎

Note that in some cases, there may only exist leaf-vertices of only one Type (*i.e.*, see respectively Figure 24, 25 and 26 for Types 1,2 and 3). Therefore, there is none of the three Types of leaf-vertices that can be avoided in our algorithm.

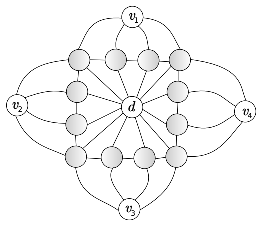

Figure 24: A planar graph G with $tb(G) = 1$ and all of its four leaf-vertices v_1, v_2, v_3, v_4 of Type 1.

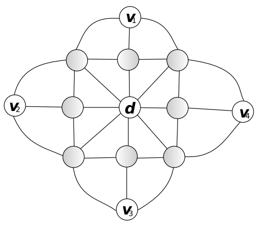

Figure 25: A planar graph G with $tb(G) = 1$ and all of its four leaf-vertices v_1, v_2, v_3, v_4 of Type 2.

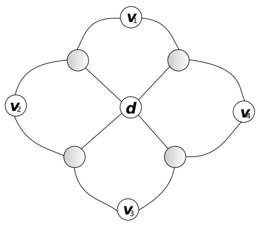

Figure 26: A planar graph G with $tb(G) = 1$ and all of its four leaf-vertices v_1, v_2, v_3, v_4 of Type 3.

Examples of planar graphs G with $tb(G) = 1$ and $\mathcal{P}_3(G) = \emptyset$ include C_4, the cycle with four vertices. To prove correctness of Step 1, it now suffices to prove that all these graphs (with $\mathcal{P}_3(G) = \emptyset$) admit a star-decomposition with at most two bags.

Lemma 20 *For any prime planar graph G, if $tb(G) = 1$ and $\mathcal{P}_3(G) = \emptyset$, then G admits a star-decomposition with at most 2 bags.*

Proof. By contradiction, let $(T, \mathcal{X})$ be a star-decomposition of G with at least three bags. Let $t \in V(T)$ be an internal node, by the properties of a tree decomposition the bag X_t is a separator of G. Let $u \in X_t$ satisfy $X_t \subseteq N_G[u]$. Since G is biconnected, therefore $X_t \setminus u$ is a separator of $G \setminus u$. By Lemma 13, there exist $x, y \in X_t \setminus u$ non-adjacent such that $\{x, y\}$ is a minimal separator of $G \setminus u$. In such case, $(x, u, y) \in \mathcal{P}_3(G)$, which contradicts the fact that $\mathcal{P}_3(G) = \emptyset$. ∎

5.3.2 Case of leaf-vertex v of Type 1

Lemma 21 *Let G be a prime planar graph and v be a leaf-vertex of Type 1. Let Π_v be the path induced by $N(v)$ and let a_v, c_v be the ends of Π_v. Suppose $V(G) \neq N[v] \cup \{d_v\}$.*

Then $\Pi' = (a_v, d_v, c_v) \in \mathcal{P}_3(G)$ and $N[v] \setminus \{a_v, c_v\}$ is a component of $G \setminus \Pi'$.

Proof. Let C be a component of $G\setminus(N[v]\cup\{d_v\})$, that exists by the hypothesis. By construction, $v \notin N[C]$, so, $N(C) \subseteq N(v) \cup \{d_v\}$ separates v from C. Furthermore, since G is prime by the hypothesis, there exist $x, y \in N(C)$ non-adjacent. Note that $d_v \notin \{x, y\}$ because $N(v) \subseteq N(d_v)$ by the hypothesis, hence $x, y \in N(v)$.

We claim that $\{x, y\} = \{a_v, c_v\}$. By contradiction, suppose $x \notin \{a_v, c_v\}$. Let us write $\Pi_v = (P, x, Q, y, R)$ with P, Q non-empty subpaths of Π_v and R a (possibly empty) subpath of Π_v. In such a case, the connected subsets $S_1 := \{v\} \cup P$, $S_2 := \{d_v\}$, $S_3 := \{x\}$, $S_4 := Q$ and $S_5 := \{y\} \cup C$ induce a K_5-minor of G, that contradicts the hypothesis that G is planar. Therefore, the claim is proved, that is, $\{x, y\} = \{a_v, c_v\}$.

To prove the lemma, it now suffices to prove that $N(C) \cap N(v) = \{a_v, c_v\}$ for in such a case the result will hold for any component C' of $G \setminus (N[v] \cup \{d_v\})$. By contradiction, let $x' \in (N(C) \cap N(v)) \setminus (a_v, c_v)$. Since $|N(v)| \geq 4$ because v is a leaf-vertex of Type 1 by the hypothesis, therefore, x' and a_v are non-adjacent or x' and c_v are non-adjacent. Let $y' \in \{a_v, c_v\}$ be non-adjacent to x'. Since $x', y' \in N(C) \cap N(v)$ are non-adjacent, therefore, by the same proof as for the above claim $\{x', y'\} = \{a_v, c_v\}$, that would contradict the assumption that $x' \notin \{a_v, c_v\}$. As a result, $N(C) \subseteq (a_v, d_v, c_v)$ and so, since the result holds for any component C' of $G \setminus (N[v] \cup \{d_v\})$, $\Pi' = (a_v, d_v, c_v) \in \mathcal{P}_3(G)$ with $N[v] \setminus \{a_v, c_v\}$ being a full component of $G \setminus \Pi'$. ■

Theorem 8 *Let G be a prime planar graph and v be a leaf-vertex of Type 1. Let Π_v be the path induced by $N(v)$ and let a_v, c_v be the ends of Π_v. Suppose $V(G) \neq N[v] \cup \{d_v\}$.*

Then, the graph G', obtained from $G \setminus v$ by contracting the internal vertices of Π_v to a single edge, is prime and planar, and $tb(G) = 1$ if and only if $tb(G') = 1$.

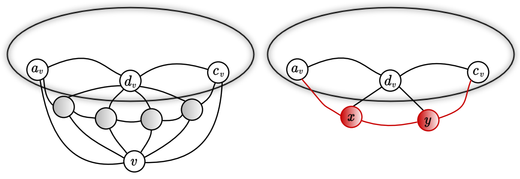

Figure 27: Contraction of the internal vertices of Π_v to a single edge and removal of v.

Proof. For the remaining of the proof, let $\Pi'_v = (a_v, x, y, c_v)$ be the path resulting from the contraction of the internal vertices of Π_v to the edge $\{x, y\}$ in G'. By Lemma 21 $(a_v, d_v, c_v) \in \mathcal{P}_3(G)$ with $(N[v] \setminus (a_v, c_v))$ being a full component of $G \setminus (a_v, d_v, c_v)$. Consequently, $N_{G'}(x) = \{a_v, d_v, y\}$ and $N_{G'}(y) = \{c_v, d_v, x\}$.

The graph G' is a minor of G, that is a planar graph by the hypothesis, so, G' is also planar. In order to prove that G' is prime, by contradiction, let S be a minimal clique-separator of G'. There are two cases to be considered.

- Suppose $x \in S$ or $y \in S$. In such case, $S \subseteq (a_v, x, d_v)$, or $S \subseteq (x, d_v, y)$, or $S \subseteq (y, d_v, c_v)$. By Lemma 21 $(a_v, d_v, c_v) \in \mathcal{P}_3(G)$ with$(N[v] \setminus (a_v, c_v))$ being a full component of $G \setminus (a_v, d_v, c_v)$, and so, for every component C of $G' \setminus (\Pi'_v \cup \{d_v\}) = G \setminus (N[v] \cup \{d_v\})$ $a_v, c_v \in N(C)$ because G is prime by the hypothesis. In such case, since $a_v \notin S$ or $c_v \notin S$, therefore, $G' \setminus S$ is connected, that contradicts the assumption that S is a clique-separator of G'.

- Else, $x, y \notin S$. Since $a_v \notin S$ or $c_v \notin S$ because a_v and c_v are non-adjacent in G', therefore, S must be a separator of $G' \setminus (x, y)$ or else $G' \setminus S$ would be connected because Π'_v induces a path of G' (thus contradicting the assumption that S is a separator of G'). In such a case, since by Lemma 21 $(a_v, d_v, c_v) \in \mathcal{P}_3(G)$ with$(N[v] \setminus (a_v, c_v))$ being a full component of $G \setminus (a_v, d_v, c_v)$, since S is a separator of $G' \setminus (x, y) = G \setminus (N[v] \setminus (a_v, c_v))$ and since S is not a separator of G because G is prime by the hypothesis, therefore, by Lemma 16 there are exactly two components C_a, C_c in $G' \setminus (S \cup \{x, y\})$ with $a_v \in C_a$ and $c_v \in C_c$. However, Π'_v is an $a_v c_v$-path of $G' \setminus S$, thus contradicting the assumption that S is a separator of G'.

As a result, G' is a prime planar graph.

Finally, let us prove $tb(G) = 1$ if and only if $tb(G') = 1$.

- If $tb(G) = 1$ then $tb(G \setminus v) = 1$ because $N(v) \subseteq N(d_v)$ by the hypothesis, and so, $tb(G') = 1$ because G' is obtained from $G \setminus v$ by edge-contractions and tree-breadth is contraction-closed (Lemma 2).

- Conversely, let us prove that $tb(G) = 1$ if $tb(G') = 1$. To prove this, let $(T', \mathcal{X}')$ be a reduced star-decomposition of G', that exists by Lemma 3, minimizing the distance in T' between the two subtrees T'_{a_v} and T'_{c_v}. In order to prove $tb(G) = 1$, it suffices to show how to construct a star-decomposition of G from $(T', \mathcal{X}')$.

  We will prove as an intermediate claim that $T'_{a_v} \cap T'_{c_v} \neq \emptyset$. By contradiction, suppose $T'_{a_v} \cap T'_{c_v} = \emptyset$. Since by Lemma 21 $(a_v, d_v, c_v) \in \mathcal{P}_3(G)$ with $(N[v] \setminus (a_v, c_v))$ being a full component of $G \setminus (a_v, d_v, c_v)$, therefore, $(a_v, d_v, c_v) \in \mathcal{P}_3(G')$ with $\{x, y\}$ being a full component of $G' \setminus (a_v, d_v, c_v)$. Since we proved that G' is prime, it follows that one of (a_v, c_v) or (a_v, d_v, c_v) is a minimal separator of G'. In such a situation, since $(T', \mathcal{X}')$ is assumed to minimize the distance in T' between T'_{a_v} and T'_{c_v}, therefore, by Corollary 8 there are two adjacent bags B'_{a_v}, B'_{c_v} such that $a_v \in B'_{a_v} \setminus B'_{c_v}$ and $c_v \in B'_{c_v} \setminus B'_{a_v}$ respectively dominate B'_{a_v} and B'_{c_v} in G'. However by the properties of a tree decomposition this implies that $B'_{a_v} \cap B'_{c_v} = N(a_v) \cap N(c_v)$ is an $a_v c_v$-separator of G', thus contradicting the existence of the $a_v c_v$-path Π'_v. Therefore, the claim is proved and $T'_{a_v} \cap T'_{c_v} \neq \emptyset$.

  Recall that $T'_{a_v} \cap T'_{d_v} \neq \emptyset$ and similarly $T'_{c_v} \cap T'_{d_v} \neq \emptyset$ by the properties of a tree decomposition. Hence, the subtrees $T'_{a_v}, T'_{c_v}, T'_{d_v}$ are pairwise intersecting, and so, by the Helly property (Lemma 1), $T'_{a_v} \cap T'_{d_v} \cap T'_{c_v} \neq \emptyset$. Let us now proceed as follows so as to obtain a star-decomposition of G. Let us remove x, y from all bags in $\mathcal{X}'$, that keeps the property for $(T', \mathcal{X}')$ to be a star-decomposition because x and y are dominated by d_v in G'. Then, let us add two new bags $B_1 = N[v]$, $B_2 = N(v) \cup \{d_v\}$, and finally let us make B_1, B_2 pairwise adjacent and let us make B_2 adjacent to some bag of $T'_{a_v} \cap T'_{d_v} \cap T'_{c_v}$. By construction, the resulting tree decomposition is indeed a star-decomposition of G, whence $tb(G) = 1$.

■

5.3.3 Proof of Step 3.1 (a)

In the following three subsections (5.3.3, 5.3.4 and 5.3.5) we will prove correctness of the algorithm for the case of a leaf-vertex v of Type 2 or 3 and $G \setminus v$ is prime (Step 3.1). Our proofs in these subsections will mostly rely on Lemma 17.

Let us first show how we can use Lemma 17 in order to prove correctness of Step 3.1 (a). Note that since we are in the case when $G \setminus v$ is prime, we needn't prove it in the following Theorem 9.

Theorem 9 *Let $G = (V, E)$ be a prime planar graph, let v be a leaf-vertex of Type 2 or 3, and let $\Pi_v = (a_v, b_v, c_v)$ be as in Definition 5.*

Suppose that $|N(a_v) \cap N(c_v)| \geq 3$ in $G \setminus v$, or there exists a minimal separator $S \subseteq (N(a_v) \cap N(c_v)) \cup \{a_v, c_v\}$ in $G \setminus v$ and $\{a_v, c_v\} \subseteq S$.

Then, $tb(G) = 1$ if and only if $tb(G \setminus v) = 1$.

Proof. First we prove that $tb(G) = 1$ implies that $tb(G \setminus v) = 1$, that is the easy part of the result. Let $(T, \mathcal{X})$ be a tree decomposition of G of breadth one, let $(T, \mathcal{X}')$ be such that for every node $t \in V(T)$, $X'_t = X_t \setminus v$. Observe that $(T, \mathcal{X}')$ is a tree decomposition of $G \setminus v$. Furthermore, we claim that it has breadth one, indeed, for every $t \in V(T)$ such that $X_t \subseteq N_G[v]$, $X'_t \subseteq N_G[b_v]$ because $N_G(v) \subseteq N_G[b_v]$. As a result, $tb(G \setminus v) = 1$.

Conversely, we prove that $tb(G \setminus v) = 1$ implies that $tb(G) = 1$. Let $(T', \mathcal{X}')$ be a star-decomposition of $G \setminus v$ minimizing the distance in T' between the subtrees T'_{a_v} and T'_{c_v}. There are two cases. If $T'_{a_v} \cap T'_{c_v} \neq \emptyset$, then the subtrees $T'_{a_v}, T'_{b_v}, T'_{c_v}$ are pairwise intersecting, hence by the Helly property (Lemma 1) $T'_{a_v} \cap T'_{b_v} \cap T'_{c_v} \neq \emptyset$, and so it suffices to make adjacent to any bag of $T'_{a_v} \cap T'_{b_v} \cap T'_{c_v}$ the new bag $N_G[v] \subseteq \{a_v, b_v, c_v, v\}$ so as to obtain a star-decomposition of G. Else $T'_{a_v} \cap T'_{c_v} = \emptyset$ and so, by Corollary 9 if $|N(a_v) \cap N(c_v)| \geq 3$ in $G \setminus v$ or by Corollary 8 else, there are two adjacent bags B'_{a_v}, B'_{c_v} such that $a_v \in B'_{a_v} \setminus B'_{c_v}$, $b_v \in B'_{a_v} \cap B'_{c_v} \subseteq N(a_v) \cap N(c_v)$ and $c_v \in B'_{c_v} \setminus B'_{a_v}$. Furthermore, a_v dominates B'_{a_v} while c_v dominates B'_{c_v}. One obtains a star-decomposition of G simply by adding vertex v into bags B'_{a_v} and B'_{c_v}. ■

5.3.4 Proof of Step 3.1 (b) i

The proof of this step is more involved than the proof of previous Step 3.1 (a). We will need the following intermediate lemma.

Lemma 22 *Let $G = (V, E)$ be a prime graph with $tb(G) = 1$, let v be a leaf-vertex of Type 2 or 3 and let $\Pi_v = (a_v, b_v, c_v)$ be as in Definition 5. Suppose that $N(a_v) \cap N(c_v) = \{v, b_v\}$ and $V \neq \Pi_v \cup \{v\}$. Then, $N_G[b_v] \setminus (a_v, c_v, v)$ is an $a_v c_v$-separator of $G \setminus v$.*

Proof. Let $(T, \mathcal{X})$ be a star-decomposition of G, that exists by Lemma 3, minimizing the distance in T between the subtrees T_{a_v} and T_{c_v}. We claim that $T_{a_v} \cap T_{c_v} \neq \emptyset$, *i.e.*, a_v, c_v are in a same bag of the decomposition. By contradiction, let $T_{a_v} \cap T_{c_v} = \emptyset$. Since G is prime and Π_v is a separator of G, therefore, one of Π_v or $\Pi_v \setminus b_v$ is a minimal separator of G. Since $(T, \mathcal{X})$ minimizes the distance in T between T_{a_v} and T_{c_v}, therefore, by Corollary 8 there exist two adjacent bags B_{a_v}, B_{c_v} such that $a_v \in B_{a_v} \setminus B_{c_v}$ and $c_v \in B_{c_v} \setminus B_{a_v}$. Furthermore, vertices a_v and c_v respectively dominate the bags B_{a_v} and B_{c_v}. This implies $B_{a_v} \cap B_{c_v} = N_G(a_v) \cap N_G(c_v)$ and so, $N_G(a_v) \cap N_G(c_v)$ is a minimal $a_v c_v$-separator of G by the properties of the tree decomposition. However, let C be any component of $G \setminus (\Pi_v \cup \{v\})$, that exists because $V \neq \Pi_v \cup \{v\}$ by the hypothesis. Since G is prime, therefore, $a_v, c_v \in N(C)$ (or else, one of the cliques a_v or b_v or c_v or (a_v, b_v) or (b_v, c_v) would be a clique-separator of G, thus contradicting the assumption that G is prime). Then, the $a_v c_v$-separator $N_G(a_v) \cap N_G(c_v)$ must contain some vertex of C, which contradicts the fact that $N_G(a_v) \cap N_G(c_v) = \{v, b_v\}$ by the hypothesis. As a result, we proved that $T_{a_v} \cap T_{c_v} \neq \emptyset$.

Let H be the chordal supergraph of G such that $(T, \mathcal{X})$ is a clique-tree of H. Equivalently, every two vertices $x, y \in V$ are adjacent in H if and only if they are in a same bag of $\mathcal{X}$. In particular, a_v, c_v are adjacent in H. Let $S := N_H(a_v) \cap N_H(c_v)$. We claim that S is an $a_v c_v$-separator of G. By contradiction, if it is not an $a_v c_v$-separator of G, then there exists an $a_v c_v$-path $P_{a_v c_v}$ of G which does not intersect S. Furthermore, $P_{a_v c_v}$ is a path of H because H is a supergraph of G, and it has length at least two because a_v, c_v are non-adjacent in G. So, let $Q_{a_v c_v}$ be taken of minimum length amongst all $a_v c_v$-paths of length at least two in H that do not intersect S (the existence of such a path follows from the existence of $P_{a_v c_v}$). Observe that

$Q_{a_vc_v}$ may be not a path in G. By minimality of $Q_{a_vc_v}$, the vertices of $Q_{a_vc_v}$ induce a cycle of H because a_v, c_v are adjacent in H. Therefore, the vertices of $Q_{a_vc_v}$ induce a triangle because H is chordal. However, this contradicts the fact that $Q_{a_vc_v}$ does not intersect $S = N_H(a_v) \cap N_H(c_v)$, so, the claim is proved.

Finally, let us prove that $S \setminus v \subseteq N_G[b_v] \setminus (a_v, c_v, v)$, that will conclude the proof that $N_G[b_v] \setminus (a_v, c_v, v)$ is an a_vc_v-separator of $G \setminus v$. For every vertex $x \in S \setminus v$, $x \in N_H(a_v) \cap N_H(c_v)$, therefore, $T_{a_v} \cap T_x \neq \emptyset$ and $T_{c_v} \cap T_x \neq \emptyset$ by construction of H. Since the subtrees T_{a_v}, T_{c_v}, T_x are pairwise intersecting, by the Helly property (Lemma 1) $T_{a_v} \cap T_{c_v} \cap T_x \neq \emptyset$, or equivalently there is some bag $B \in T_{a_v} \cap T_{c_v} \cap T_x$. Let $z \in B$ dominate the bag. Clearly, $x \in N_G[z]$. Furthermore, $z \in N_G(a_v) \cap N_G(c_v)$ because a_v, c_v are non-adjacent in G. As a result, either $z = b_v$ or $z = v$. Since $x \neq v$ and $N_G(v) \subseteq N_G[b_v]$, we have that $x \in N_G[b_v]$ in both cases. ■

Theorem 10 *Let $G = (V, E)$ be a prime planar graph with $tb(G) = 1$, v be a leaf-vertex of Type 2 or 3, and let $\Pi_v = (a_v, b_v, c_v)$ be as in Definition 5. Suppose $N(a_v) \cap N(c_v) = \{b_v, v\}$, and $G \setminus v$ is prime, and there is no minimal separator $S \subseteq (N(a_v) \cap N(c_v)) \cup \{a_v, c_v\}$ in $G \setminus v$ such that $\{a_v, c_v\} \subseteq S$. Then, $G = C_4$, a cycle with four vertices.*

Proof. By contradiction, assume $G \neq C_4$. Since G is prime by the hypothesis, G has at least five vertices (the single other graph with four vertices and a leaf-vertex of Type 2 or 3 is the diamond, which is not prime). Equivalently, $V \neq \Pi_v \cup \{v\}$. By Lemma 22, this implies that $N[b_v] \setminus (a_v, c_v, v)$ is an a_vc_v-separator of $G \setminus v$. Since $G \setminus v$ is prime by the hypothesis, and so, biconnected, therefore, $G \setminus (b_v, v)$ is connected, and so, $N(b_v) \setminus (a_v, c_v, v) \neq \emptyset$ is an a_vc_v-separator of $G \setminus (b_v, v)$. In particular, $a_v, b_v, c_v \in N(V \setminus (\Pi_v \cup \{v\}))$.

Moreover, we claim that $V \setminus (\Pi_v \cup \{v\})$ induces a connected subgraph (note that the latter implies that $V \setminus (\Pi_v \cup \{v\})$ is a full component of $G \setminus \Pi_v$). By contradiction, let C_1, C_2 be distinct components of $V \setminus (\Pi_v \cup \{v\})$. Since G is prime, $a_v, c_v \in N_G(C_1) \cap N_G(C_2)$ (or else, one of the cliques a_v or b_v or c_v or (a_v, b_v) or (b_v, c_v) would be a clique-separator of G, thus contradicting the assumption that G is prime). Therefore, $b_v \in N_G(C_1) \cap N_G(C_2)$ because $N[b_v] \setminus (a_v, c_v, v)$ is an a_vc_v-separator of $G \setminus v$. It follows that Π_v is a minimal separator of $G \setminus v$, that contradicts the hypothesis that there is no minimal separator $S \subseteq (N(a_v) \cap N(c_v)) \cup \{a_v, c_v\}$ in $G \setminus v$ and $\{a_v, c_v\} \subseteq S$. Consequently, $V \setminus (\Pi_v \cup \{v\})$ induces a connected subgraph.

Let $S' \subseteq N(b_v) \setminus (a_v, c_v, v)$ be a minimal a_vc_v-separator of $G \setminus (b_v, v)$. By Lemma 13, there exist $x, y \in N(b_v) \setminus (a_v, c_v, v)$ non-adjacent such that $S' = \{x, y\}$. Finally, let $\Pi' = (x, b_v, y)$ and let A, C be the respective components of a_v, c_v in $G \setminus (\Pi' \cup \{v\})$. Note that $x, y \in N(A) \cap N(C)$ because $G \setminus v$ is prime by the hypothesis (indeed, neither x nor b_v nor y nor (b_v, x) nor (b_v, y) can be a separator of $G \setminus v$). Let P be an xy-path of $V \setminus (\Pi_v \cup \{v\})$, that exists because $V \setminus (\Pi_v \cup \{v\})$ is connected. Also, let $A' \subseteq A$ and $C' \subseteq C$ be the respective components of a_v, c_v in $G \setminus (P \cup \Pi' \cup \{v\})$. Note that the subpath $P \setminus (x, y)$ lies onto a unique component of $G \setminus (\Pi' \cup \{v\})$ because it does not intersect $\Pi_v \cup \{v\}$ by construction, so, $A' = A$ or $C' = C$. By symmetry, assume that $C' = C$. There are two cases to consider.

- Assume $A' = A$ (see Figure 28 for an illustration). Let us contract the internal vertices of P so as to make vertices x, y adjacent. Then, let us contract the components A, C to the two vertices a_v, c_v, respectively. Finally, let us contract v to either a_v or c_v. By construction, the five vertices a_v, b_v, c_v, x, y now induce a K_5, that contradicts the fact that G is planar by the hypothesis.

- Else, $A' \neq A$. Equivalently, $P \subseteq A \cup \{x, y\}$ (see Figure 29 for an illustration). Since A is connected, $N(A') \cap (P \setminus (x, y)) \neq \emptyset$. Let $z \in N(A') \cap P$. Let us contract the internal vertices of P to vertex z. Then, let us contract the components A' and $C' = C$ to the two vertices

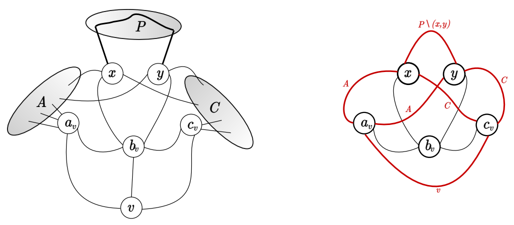

Figure 28: Case $A' = A$ (left). A K_5-minor is drawn (right), with edges resulting from contractions labeled in red.

a_v, c_v, respectively. Finally let us contract v to either a_v or c_v. By construction, there is a $K_{3,3}$-minor whose sides of the bipartition are $\{a_v, x, y\}$ and $\{b_v, c_v, z\}$, respectively, that contradicts the fact that G is planar by the hypothesis.

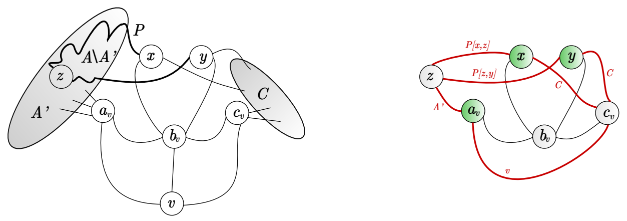

Figure 29: Case $A' \neq A$ (left). A $K_{3,3}$-minor is drawn (right), with each side of the bipartition being coloured differently. Edges resulting from contractions are labeled in red.

Since both cases contradict the hypothesis that G is planar, therefore, $G = C_4$. ■

5.3.5 Proof of Step 3.1 (b) ii

Theorem 11 *Let $G = (V, E)$ be a prime planar graph, let v be a leaf-vertex of Type 2 or 3, and let $\Pi_v = (a_v, b_v, c_v)$ be as in Definition 5.*

Suppose that all of the following statements hold:

- $N(a_v) \cap N(c_v) = \{v, b_v, u_v\}$ *with* $u_v \notin \{v\} \cup \Pi_v$*;*
- $V \neq \{a_v, b_v, c_v, u_v, v\}$*;*
- *there is no minimal separator* $S \subseteq (N(a_v) \cap N(c_v)) \cup \{a_v, c_v\}$ *in* $G \setminus v$ *and* $\{a_v, c_v\} \subseteq S$*.*

Let G' be the graph obtained from G by adding edges $\{v, u_v\}$ and $\{b_v, v\}$, then $tb(G) = 1$ if and only if $tb(G') = 1$. Moreover, G' is planar and prime.

Proof. We will first prove that $G \setminus v$ is prime. By contradiction, let S' be a minimal clique-separator of $G \setminus v$. By Theorem 6, there is $w_v \neq v$ such that $S' = \{b_v, w_v\}$, and by Lemma 16, S' must be an a_vc_v-separator of $G \setminus v$. Then, it follows that $w_v = u_v \in N(a_v) \cap N(c_v)$, whence $V = \{a_v, b_v, c_v, u_v, v\}$ by Theorem 6, that contradicts the hypothesis. Therefore, $G \setminus v$ is prime.

Let us prove that $tb(G) = 1$ implies that $tb(G') = 1$. Let $(T, \mathcal{X})$ be a star-decomposition of G, which exists by Lemma 3, minimizing the distance in T between the subtrees T_{a_v} and T_{c_v}. Since $N_G(v) \subseteq N_G[b_v]$ then removing v from all bags leaves a tree decomposition of $G \setminus v$ of breadth

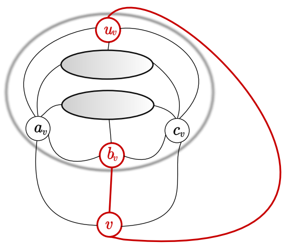

Figure 30: Case of a leaf-vertex v of Type 3 with $G \setminus v$ is prime and $N(a_v) \cap N(c_v) = \{u_v, b_v, v\}$. Red edges are those added by Algorithm `Leaf-BottomUp`.

one. Up to reducing the tree decomposition, let $(T', \mathcal{X}')$ be any reduced tree decomposition of $G \setminus v$ that is obtained from $(T, \mathcal{X})$ by first removing v from the bags. Note that $(T', \mathcal{X}')$ is a star-decomposition of $G \setminus v$ by Lemma 3. Now, there are two cases.

- Suppose $T'_{a_v} \cap T'_{c_v} \neq \emptyset$. We will need to prove in this case that the two subtrees $T'_{a_v} \cap T'_{b_v} \cap T'_{c_v}$ and $T'_{a_v} \cap T'_{u_v} \cap T'_{c_v}$ are nonempty and disjoint.

  Claim 11 *b_v, u_v are non-adjacent in G.*

  Proof. By contradiction, if it were the case that b_v, u_v are adjacent, then by Lemma 15, either u_v is an isolated vertex of $G \setminus (\Pi_v \cup \{v\})$ — in which case, $\Pi_v \in \mathcal{P}_3(G \setminus v)$ because we assume $V \neq \{a_v, b_v, c_v, u_v, v\}$ by the hypothesis —, or $(a_v, u_v, b_v) \in \mathcal{P}_3(G \setminus v)$. Since $G \setminus v$ is prime, it follows that one of Π_v or $\Pi_v \setminus b_v$ must be a minimal separator of $G \setminus v$, similarly one of (a_v, u_v, c_v) or (a_v, c_v) must be a minimal separator of $G \setminus v$. Therefore, both cases contradict the hypothesis that there is no minimal separator $S \subseteq (N(a_v) \cap N(c_v)) \cup \{a_v, c_v\}$ in $G \setminus v$ and $\{a_v, c_v\} \subseteq S$, which proves that b_v, u_v are non-adjacent. ◇

  Recall that we are in the case when $T'_{a_v} \cap T'_{c_v} \neq \emptyset$. The subtrees $T'_{a_v}, T'_{c_v}, T'_{u_v}$ are pairwise intersecting, similarly the subtrees $T'_{a_v}, T'_{c_v}, T'_{b_v}$ are pairwise intersecting. Therefore, by the Helly property (Lemma 1) $T'_{a_v} \cap T'_{b_v} \cap T'_{c_v} \neq \emptyset$ and $T'_{a_v} \cap T'_{u_v} \cap T'_{c_v} \neq \emptyset$. Furthermore, $T_{a_v} \cap T_{b_v} \cap T_{c_v} \cap T_{u_v} = \emptyset$, because since b_v, u_v are non-adjacent by Claim 11 no vertex dominates all of $\{a_v, b_v, c_v, u_v\}$ in G, and so, $T'_{a_v} \cap T'_{b_v} \cap T'_{c_v} \cap T'_{u_v} = \emptyset$.

  Claim 12 *The subtrees $T'_{a_v} \cap T'_{b_v} \cap T'_{c_v}$ and $T'_{a_v} \cap T'_{u_v} \cap T'_{c_v}$ are adjacent in T'.*

  Proof. By contradiction, let B be an internal bag onto the path between both subtrees in T', let $z \in B$ dominate the bag. Note that $a_v, c_v \in B$ by the properties of the tree decomposition, $z \notin \{a_v, c_v\}$ because a_v, c_v are non-adjacent, and so, $z \in N(a_v) \cap N(c_v) \setminus v = \{u_v, b_v\}$. This contradicts the fact that $B \notin T'_{a_v} \cap T'_{b_v} \cap T'_{c_v}$ and $B \notin T'_{a_v} \cap T'_{u_v} \cap T'_{c_v}$, therefore, the subtrees $T'_{a_v} \cap T'_{b_v} \cap T'_{c_v}$ and $T'_{a_v} \cap T'_{u_v} \cap T'_{c_v}$ are adjacent in T'. ◇

  Finally, let $B \in T'_{a_v} \cap T'_{b_v} \cap T'_{c_v}, B' \in T'_{a_v} \cap T'_{u_v} \cap T'_{c_v}$ be adjacent, that exist by Claim 12. Observe that b_v dominates B, u_v dominates B'. To obtain a star-decomposition of G' from $(T', \mathcal{X}')$, it now suffices to add vertex v in B and B', whence $tb(G') = 1$.

- Else, $T'_{a_v} \cap T'_{c_v} = \emptyset$. This implies $T_{a_v} \cap T_{c_v} = \emptyset$. Since the tree decomposition $(T, \mathcal{X})$ minimizes the distance in T between T_{a_v} and T_{c_v}, G is planar and $|N(a_v) \cap N(c_v)| \geq 3$, therefore by Corollary 9, the subtrees T_{a_v} and T_{c_v} are adjacent in T, whence the subtrees T'_{a_v}, T'_{c_v} are also adjacent in T'. In particular, by Corollary 9 there exist two adjacent bags

$B'_{a_v}, B'_{c_v} \in \mathcal{X}'$ such that $a_v \in B'_{a_v} \setminus B'_{c_v}, B'_{a_v} \cap B'_{c_v} = N_G(a_v) \cap N_G(c_v) \setminus v = \{u_v, b_v\}, c_v \in B'_{c_v} \setminus B'_{a_v}$. Furthermore, a_v dominates B'_{a_v} while c_v dominates B'_{c_v}. Therefore, in order to obtain a star-decomposition of G' from $(T', \mathcal{X}')$, it now suffices to add vertex v in B'_{a_v} and B'_{c_v} – that yields exactly $(T, \mathcal{X})$ –, whence $tb(G') = 1$.

Before we can prove the equivalence, *i.e.*, $tb(G) = 1$ if and only if $tb(G') = 1$, we need to prove first that G' is prime and planar.

Claim 13 *G' is prime.*

Proof. Let S' be a clique-separator of G'. Note that $v \in S'$ by construction of G'. Therefore, $S' \setminus v$ is a clique-separator of $G \setminus v$, that contradicts the fact that $G \setminus v$ is prime. Consequently, G' is prime. ◇

Claim 14 *G' is planar.*

Proof. Let us fix a plane embedding of G. By Jordan Theorem, the cycle induced by (a_v, b_v, c_v, u_v) separates the plane into two regions. Let G_1, G_2 be respectively the subgraphs of G that are induced by all the vertices in each region.

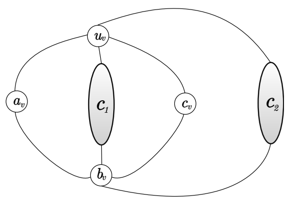

Figure 31: Proof that the graph G' of Theorem 11 is planar.

We claim that either $V \setminus (a_v, b_v, c_v, u_v, v) \subseteq V(G_1)$, or $V \setminus (a_v, b_v, c_v, u_v, v) \subseteq V(G_2)$. Note that it will prove that G' is planar, because then drawing vertex v onto the region that does not contain the set $V \setminus (a_v, b_v, c_v, u_v, v)$ yields a planar embedding of G'. By contradiction, let $C_1 \subseteq V(G_1), C_2 \subseteq V(G_2)$ be connected components of $V \setminus (a_v, b_v, c_v, u_v, v)$. Let $\Pi'_v = (a_v, u_v, c_v)$. If one of Π_v or Π'_v belongs to $\mathcal{P}_3(G \setminus v)$, then, there exists a minimal separator $S \subseteq (N(a_v) \cap N(c_v)) \cup \{a_v, c_v\}$ in $G \setminus v$ and since $G \setminus v$ is prime, $\{a_v, c_v\} \subseteq S$. This would contradict the hypothesis, so, $\Pi_v, \Pi'_v \notin \mathcal{P}_3(G \setminus v)$. As a result, since $(a_v, b_v, c_v, u_v) = \Pi_v \cup \Pi'_v$ separates C_1 from C_2, therefore, $u_v, b_v \in N(C_1) \cap N(C_2)$ (or else, $\Pi_v \in \mathcal{P}_3(G \setminus v)$ or $\Pi'_v \in \mathcal{P}_3(G \setminus v)$). Let us remove all other components of $V \setminus (a_v, b_v, c_v, u_v, v)$ but C_1 and C_2, and let us remove all edges between $\{a_v, c_v\}$ and $C_1 \cup C_2$ if any (see Figure 31). Finally, let us contract C_1, C_2 to the two vertices x_1, x_2. The cycle induced by (u_v, x_1, b_v, x_2) separates the plane into two regions with a_v, c_v being into different regions by construction. Vertex v must belong to one of the regions, but then it is a contradiction because $v \in N(a_v) \cap N(c_v)$ by the hypothesis. ◇

To conclude the proof, let us prove that conversely, $tb(G') = 1$ implies that $tb(G) = 1$. Let $(T', \mathcal{X}')$ be a star-decomposition of G' minimizing the distance in T' between the subtrees T'_{a_v} and T'_{c_v}. As an intermediate step, we claim that if removing vertex v from all bags of $\mathcal{X}'$ leaves a tree decomposition of $G \setminus v$ of breadth one, then it implies that $tb(G) = 1$. To prove the claim, there are two cases to be considered.

- If $T'_{a_v} \cap T'_{c_v} \neq \emptyset$, then the subtrees $T'_{a_v}, T'_{b_v}, T'_{c_v}$ are pairwise intersecting, hence by the Helly property (Lemma 1) $T'_{a_v} \cap T'_{b_v} \cap T'_{c_v} \neq \emptyset$. Equivalently there is bag containing Π_v, and so it suffices to remove v from all bags and then to make any bag containing Π_v adjacent to the new bag $N_G[v]$ in order to obtain a tree decomposition of G of breadth one.
- Else, $T'_{a_v} \cap T'_{c_v} = \emptyset$. Since $(T', \mathcal{X}')$ minimizes the distance in T' between the subtrees T'_{a_v} and T'_{c_v}, G' is planar by Claim 14 and a_v, c_v have three common neighbours in G', therefore, by Corollary 9 there must exist two adjacents bags B'_{a_v}, B'_{c_v} such that $a_v \in B'_{a_v} \setminus B'_{c_v}, B'_{a_v} \cap B'_{c_v} = N(a_v) \cap N(c_v)$ and $c_v \in B'_{c_v} \setminus B'_{a_v}$. Furthermore, vertex a_v dominates the bag B'_{a_v}, while vertex c_v dominates the bag B'_{c_v}. As a result, removing vertex v from all bags but B'_{a_v}, B'_{c_v} leads to a tree decomposition of G of breadth one.

Consequently, we are left to modify the tree decomposition $(T', \mathcal{X}')$ so as to ensure that none of the bags is only dominated by vertex v in G', for if it is the case then removing v from all bags does leave a tree decomposition of $G \setminus v$ of breadth one. We will call the latter property the *removal property*. Observe that if it is the case that $(T', \mathcal{X}')$ does not satisfy the removal property, then there must be a bag B fully containing $N_{G'}(v)$ because any strict subset of $N_{G'}(v)$ is dominated by some vertex of $G \setminus v$. In particular, $B = N_{G'}[v]$ because only vertex v dominates $N_{G'}(v)$ in G', and so we can further assume that $T'_v = \{B\}$ without violating the property for $(T', \mathcal{X}')$ to be a tree decomposition of G' of breadth one. Therefore in the following, assume that $(T', \mathcal{X}')$ is a reduced star-decomposition of G' and $T'_v = \{B\}$, that is always possible to achieve by Lemma 3 and above remarks.

Since $V \neq \{a_v, b_v, c_v, u_v, v\} = N_{G'}[v]$ by the hypothesis, therefore, $\mathcal{X}' \setminus B \neq \emptyset$. Let B' be adjacent to B in T'. Note that $B \cap B' \neq \{a_v, b_v, c_v, u_v\}$ because no other vertex than v dominates the subset $\{a_v, b_v, c_v, u_v\}$ in G'. By the properties of a tree decomposition, $B \cap B'$ is a separator of G'. Consequently, $B \cap B'$ is not a clique because G' is prime by Claim 13. Furthermore, since $B \cap B' \neq \{a_v, b_v, c_v, u_v\}$ it holds that $B \setminus (B' \cup \{v\}) \neq \emptyset$, consequently $B \cap B'$ is also a separator of $G \setminus v$. Since $G \setminus v$ is prime, $B \cap B'$ cannot be any of (a_v, c_v), Π_v or Π'_v because by the hypothesis there is no minimal separator $S \subseteq (N(a_v) \cap N(c_v)) \cup \{a_v, c_v\}$ in $G \setminus v$ and $\{a_v, c_v\} \subseteq S$. It follows that $B \cap B' \subseteq \{a_v, b_v, u_v\}$ or $B \cap B' \subseteq \{b_v, c_v, u_v\}$. Let us substitute the bag B with the two adjacent bags $B_1 = \{a_v, u_v, b_v, v\}, B_2 = \{b_v, c_v, u_v, v\}$, then we make adjacent all bags B'' that were formerly adjacent to B to some bag amongst B_1, B_2 containing $B \cap B''$. Note that $B_1 \subseteq N[a_v]$ and that $B_2 \subseteq N[c_v]$. Therefore, the resulting tree decomposition is a tree decomposition of G of breadth one such that v dominates no bag. ■

5.3.6 Case of leaf-vertex v of Type 2 or 3 and $G \setminus v$ not prime

The remaining subsections will be devoted to the proof of correctness of Step 3.2. In particular, this subsection is devoted to the proof that when $G \setminus v$ is not prime one can only consider the case when the leaf-vertex v is of Type 2, *i.e.*, v and b_v are adjacent in G. Note that when v is of Type 3, then in general one cannot add an edge between v and b_v without violating the property for the graph G to be planar, as shown in Figure 32. We will now prove that whenever we are in the conditions of Step 3.2, it is always possible to do so while preserving the planarity of the graph G and the property to be of tree-breadth one.

Theorem 12 *Let G be a prime planar graph. Let v be a leaf-vertex of Type 3 such that $G \setminus v$ is not prime. Finally, let $\Pi_v = (a_v, b_v, c_v)$ be as in Definition 5. Let G' be obtained from G by adding the edge $\{v, b_v\}$.*

Then, G' is prime and planar, and $tb(G) = 1$ if and only if $tb(G') = 1$.

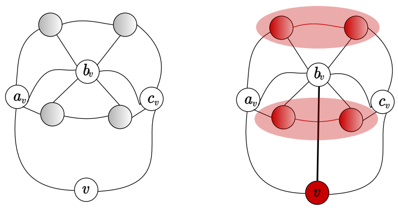

Figure 32: A planar graph G with $tb(G) = 1$ (left), and a leaf-vertex v of Type 3 so that adding an edge between v and b_v violates the property for the graph to be planar (right). In the latter case, one side of the bipartition of the $K_{3,3}$-minor is coloured red.

Proof. First, we prove that G' is prime and planar.

- In order to prove that G' is prime, by contradiction let S be a clique-separator of G'. Since G' is a supergraph of G, therefore S is a separator of G but it does not induce a clique in G. Hence, S contains the edge $\{v, b_v\}$, and so either $S \subseteq \{a_v, b_v, v\}$ or $S \subseteq \{b_v, c_v, v\}$. Let $C = V \setminus (\Pi_v \cup \{v\})$, by Theorem 6, C is a full component of $G \setminus \Pi_v$ because $G \setminus v$ is not prime. In particular, C is connected and $a_v, c_v \in N(C)$, that contradicts the fact that $G' \setminus S$ is unconnected.

- Then in order to prove that G' is planar, let us fix a plane embedding of G. The cycle induced by (a_v, b_v, c_v, v) separates the plane into two regions. To prove that G' is planar, we claim that it suffices to prove that all vertices in $C = V \setminus (\Pi_v \cup \{v\})$ are in the same region, for then drawing the edge $\{b_v, v\}$ in the other region leads to a plane embedding of G'. By contradiction, let $x, y \in C$ be in different regions. By [13, Proposition 8], the cycle (a_v, b_v, c_v, v) is an xy-separator of G, that contradicts the fact that C is connected.

Let us now prove that $tb(G) = 1$ implies that $tb(G') = 1$. Let $(T, \mathcal{X})$ be a star-decomposition of G, that exists by Lemma 3, minimizing the distance in T between the subtrees T_{a_v} and T_{c_v}. Let us remove vertex v from all bags, that leads to a tree decomposition $(T, \mathcal{X}_{-v})$ of $G \setminus v$ of breadth one because $N_G(v) \subseteq N_G(b_v)$. Then, let $(T', \mathcal{X}')$ be any reduced tree decomposition that is obtained from $(T, \mathcal{X}_{-v})$, that is a star-decomposition of $G \setminus v$ by Lemma 3. Now, there are two cases. If $T'_{a_v} \cap T'_{c_v} \neq \emptyset$, then the subtrees $T'_{a_v}, T'_{b_v}, T'_{c_v}$ are pairwise intersecting and so, by the Helly property (Lemma 1) $T'_{a_v} \cap T'_{b_v} \cap T'_{c_v} \neq \emptyset$. Hence one obtains a star-decomposition of G' simply by making some bag of $T'_{a_v} \cap T'_{b_v} \cap T'_{c_v}$ adjacent to the new bag $N_{G'}[v] = \{a_v, b_v, c_v, v\}$. Else, $T'_{a_v} \cap T'_{c_v} = \emptyset$, so, $T_{a_v} \cap T_{c_v} = \emptyset$. Since $\Pi_v \in \mathcal{P}_3(G)$ and G is prime by the hypothesis, therefore, one of Π_v or $\Pi_v \setminus b_v$ must be a minimal separator of G. As a result, since $(T, \mathcal{X})$ is assumed to minimize the distance in T between the subtrees T_{a_v} and T_{c_v}, by Corollary 8 there exist two adjacent bags $B_{a_v}, B_{c_v} \in \mathcal{X}$ so that $a_v \in B_{a_v} \setminus B_{c_v}$ and $c_v \in B_{c_v} \setminus B_{a_v}$ respectively dominate the bags B_{a_v} and B_{c_v}. In such case, $B_{a_v} \cap B_{c_v} = N_G(a_v) \cap N_G(c_v)$ and so, since $b_v, v \in B_{a_v} \cap B_{c_v}$, $(T, \mathcal{X})$ is also a star-decomposition of G'. So, in conclusion, $tb(G') = 1$ in both cases.

Conversely, let us prove that $tb(G') = 1$ implies that $tb(G) = 1$. Let $(T', \mathcal{X}')$ be a star-decomposition of G', that exists by Lemma 3, minimizing the distance in T' between the subtrees T'_{a_v} and T'_{c_v}. Let us remove vertex v from all bags, that leads to a tree decomposition $(T', \mathcal{X}'_{-v})$ of $G' \setminus v = G \setminus v$ of breadth one because $N_{G'}[v] \subseteq N_{G'}[b_v]$. Then, let $(T, \mathcal{X})$ be any reduced tree decomposition that is obtained from $(T', \mathcal{X}'_{-v})$, that is a star-decomposition of $G \setminus v$ by Lemma 3. There are two cases. If $T_{a_v} \cap T_{c_v} \neq \emptyset$, then one obtains a star-decomposition of G simply by making some bag of $T_{a_v} \cap T_{c_v}$ adjacent to the new bag $N_G[v] = \{a_v, c_v, v\}$. Else, $T_{a_v} \cap T_{c_v} = \emptyset$, so, $T'_{a_v} \cap T'_{c_v} = \emptyset$. Since $\Pi_v \in \mathcal{P}_3(G')$ and G' is also prime, therefore, one of Π_v or $\Pi_v \setminus b_v$ must be a minimal separator of G'. As a result, since $(T', \mathcal{X}')$ is assumed to minimize the distance in T' between the subtrees T'_{a_v} and T'_{c_v}, by Corollary 8 there exist two adjacent bags $B'_{a_v}, B'_{c_v} \in \mathcal{X}'$ so that $a_v \in B'_{a_v} \setminus B'_{c_v}$ and $c_v \in B'_{c_v} \setminus B'_{a_v}$ respectively dominate the bags B'_{a_v} and B'_{c_v}. In such case, one obtains a star-decomposition of G by adding v in the two bags B'_{a_v}, B'_{c_v}. So, in conclusion, $tb(G) = 1$ in both cases.

■

5.3.7 Proof of Step 3.2 (a)

Theorem 13 *Let G be a prime planar graph, let v be a leaf-vertex of Type 2, $\Pi_v = (a_v, b_v, c_v)$ be as in Definition 5, and let $u_v \notin \Pi_v \cup \{v\}$ be such that (b_v, u_v) is an edge-separator of $G \setminus v$.*

Suppose a_v and u_v are non-adjacent, and either c_v and u_v are non-adjacent or the subset $N_G(a_v) \cap N_G(u_v)$ is not *an $a_v u_v$-separator in the subgraph $G \setminus (c_v, v)$.*

Then, G/va_v (obtained by contracting $\{v, a_v\}$) is planar and prime and $tb(G) = 1$ if and only if $tb(G/va_v) = 1$.

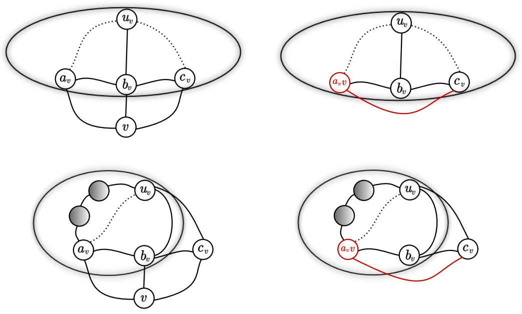

Figure 33: Cases when Theorem 13 applies and the edge $\{v, a_v\}$ can be contracted to a_v.

Proof. The graph G/va_v is a contraction of the planar graph G, therefore it is planar. Let us prove that G/va_v is prime. By contradiction, let S be a minimal clique-separator of G/va_v. Since G/va_v is a supergraph of $G \setminus v$, S is also a separator of $G \setminus v$. Furthermore, it is not an $a_v c_v$-separator because a_v, c_v are adjacent in G/va_v, therefore, by Lemma 16 S is a separator of G. Since G is prime by the hypothesis, S does not induce a clique of G, whence $a_v, c_v \in S$. However, since (b_v, u_v) is not a separator of G because G is prime by the hypothesis, therefore by Lemma 16 (u_v, b_v) is an $a_v c_v$-separator of $G \setminus v$. So, $N_G(a_v) \cap N_G(c_v) \subseteq \{v, b_v, u_v\}$, that implies $N_G(a_v) \cap N_G(c_v) = \{v, b_v\}$ because a_v and u_v are non-adjacent by the hypothesis. In such a case $S \subseteq \Pi_v$, but then $V \setminus (\Pi_v \cup \{v\})$ cannot be a full component of $G \setminus \Pi_v$, thus contradicting Theorem 6. As a result, the graph G/va_v is planar and prime.

If $tb(G) = 1$ then $tb(G/va_v) = 1$ because tree-breadth is contraction-closed by Lemma 2. Conversely, let us prove that $tb(G/va_v) = 1$ implies $tb(G) = 1$. To show this, let $(T, \mathcal{X})$ be a star-decomposition of G/va_v, that exists by Lemma 3, minimizing the number of bags $|\mathcal{X}|$ (in particular, $(T, \mathcal{X})$ is a reduced tree decomposition). Assume moreover $(T, \mathcal{X})$ to minimize the number of bags that are not contained into the closed neighbourhood of some vertex in G w.r.t. this property. Note that there is a bag of $(T, \mathcal{X})$ containing Π_v, because since it is a clique of G/va_v the subtrees $T_{a_v}, T_{b_v}, T_{c_v}$ are pairwise intersecting and so, by the Helly property (Lemma 1), $T_{a_v} \cap T_{b_v} \cap T_{c_v} \neq \emptyset$. So, we can add in $(T, \mathcal{X})$ a new bag $N_G[v]$, and by making this bag adjacent to any bag of $T_{a_v} \cap T_{b_v} \cap T_{c_v}$ one obtains a tree decomposition of G (not necessarily a star-decomposition). Consequently, we claim that to prove that $tb(G) = 1$, it suffices to prove that $(T, \mathcal{X})$ is a star-decomposition of $G \setminus v$, for then the above construction leads to a star-decomposition of G.

By contradiction, suppose it is not the case that $(T, \mathcal{X})$ is a star-decomposition of $G \setminus v$. Since G/va_v and $G \setminus v$ only differ in the edge $\{a_v, c_v\}$, there must be a bag B of $T_{a_v} \cap T_{c_v}$ that is only dominated by some of a_v, c_v. We make the stronger claim that the bag B has a unique dominator, that is either a_v or c_v. Since B is only dominated by some of a_v, c_v, then in order to prove the claim by contradiction we only need to consider the case when $B \subseteq N_{G/va_v}[a_v] \cap N_{G/va_v}[c_v]$. Recall that $N_{G/va_v}[a_v] \cap N_{G/va_v}[c_v] = \{a_v, b_v, c_v\}$ by the above remarks (because (u_v, b_v) is an a_vc_v-separator of $G \setminus v$), therefore either $B = \{a_v, b_v, c_v\}$ or $B = \{a_v, c_v\}$. In the first case ($B = \{a_v, b_v, c_v\}$) we have that $B \subseteq N[b_v]$, thus contradicting the fact that B is only dominated by some of a_v, c_v. However in the second case ($B = \{a_v, c_v\}$) the bag B is strictly contained in any bag of the nonempty subtree $T_{a_v} \cap T_{b_v} \cap T_{c_v}$, thus contradicting the fact that $(T, \mathcal{X})$ is a reduced tree decomposition by minimality of $|\mathcal{X}|$. Therefore, the claim is proved and so, the bag B has a unique dominator, that is either a_v or c_v. Note that if $B \subseteq N_{G/va_v}[c_v]$ then we may further assume that c_v, u_v are nonadjacent, or else by Theorem 6 $N_{G/va_v}[c_v] = \{a_v, b_v, c_v, u_v\} \subseteq N[b_v]$ and so, $B \subseteq N[b_v]$, that would contradict the claim that B is only dominated by some of a_v, c_v. In addition, since a_v and c_v play symmetrical roles in the case when u_v, c_v are nonadjacent, let us assume w.l.o.g. that vertex a_v is the sole dominator of the bag B.

In such a case, $N_{G/va_v}(a_v) \cap N_{G/va_v}(c_v) = \{b_v\}$ because (u_v, b_v) is an a_vc_v-separator of $G \setminus v$, so, since $N(c_v) \setminus (\Pi_v \cup \{v\}) \neq \emptyset$ because G is prime by the hypothesis, the existence of a bag B' containing vertex c_v and adjacent to B follows. By the properties of a tree decomposition, $B \cap B'$ is a separator of G/va_v Now, let C_a be the component of vertex a_v in $G \setminus (b_v, u_v, v)$. Observe that $c_v \notin C_a$ because (u_v, b_v) is an a_vc_v-separator of $G \setminus v$. Since $B \cap B' \subseteq N_{G/va_v}[a_v] \subseteq C_a \cup \Pi_v$, therefore, $B \cap B' \cap C_a \neq \emptyset$ or else $B \cap B'$ would be a clique-separator in G/va_v (impossible since it is a prime graph). There are several cases to be considered depending on the dominators of bag B'.

- If a_v dominates B' then B, B' can be merged into one, thus contradicting the minimality of $|\mathcal{X}|$;

- Else, B' must be dominated by one of b_v or u_v because $B \cap B' \cap C_a \neq \emptyset$, $c_v \in (B \cap B') \setminus C_a$ and (b_v, u_v) separates c_v from C_a. In fact, we claim that it cannot be dominated by vertex u_v. By contradiction, suppose that it is the case. Since a_v and u_v are non-adjacent, therefore, $a_v \in B \setminus B'$ and $u_v \in B' \setminus B$. So, it follows by the properties of a tree decomposition that $B \cap B'$ is an a_vu_v-separator of G/va_v. However, $B \cap B' \subseteq N(a_v) \cap N(u_v)$, that contradicts the hypothesis that $N_G(a_v) \cap N_G(u_v)$ is not an a_vu_v-separator in the subgraph $G \setminus (c_v, v)$.

  Therefore, $b_v \in B'$ dominate the bag. Observe that if it were the case that there are at least two bags that are both adjacent to B and dominated by b_v, then they could all be merged into one without violating the property for $(T, \mathcal{X})$ to be a star-decomposition. As a result, by minimality of $|\mathcal{X}|$, B' is the unique bag that is both adjacent to B and dominated by b_v, whence it is also the unique bag adjacent to B containing vertex c_v. Let us substitute the two bags B, B' with $B \setminus c_v, B' \cup \{a_v\}$. Since $N_{G/va_v}(a_v) \cap N_{G/va_v}(c_v) = \{b_v\}$, it is still a star-decomposition of G/va_v with equal number of bags $|\mathcal{X}|$. Furthermore, there is one less bag that is not contained in the closed neighbourhood of some vertex in G, thus contradicting the minimality of $(T, \mathcal{X})$.

■

5.3.8 Proof of Step 3.2 (b) i and Step 3.2 (b) ii

In order to deal with all remaining cases, it will require us to further study the neighbourhood of vertex b_v in the graph. Observe that in the following Theorem 14 we needn't prove that the resulting graph G' is prime because it will be proved in Theorem 15.

Theorem 14 *Let G be a prime planar graph, let v be a leaf-vertex of Type 2, $\Pi_v = (a_v, b_v, c_v)$ be as in Definition 5, and let $u_v \notin \Pi_v \cup \{v\}$ be such that (b_v, u_v) is an edge-separator of $G \setminus v$.*

Suppose $u_v \in N(c_v) \setminus N(a_v)$, $N(a_v) \cap N(u_v)$ is an $a_v u_v$-separator of $G \setminus (c_v, v)$, and $N(b_v) = \{a_v, c_v, u_v, v\}$.

Then, there exists $x \in (N(a_v) \cap N(u_v)) \setminus b_v$ such that the graph G', obtained from G by adding the edge $\{b_v, x\}$, is planar and satisfies $tb(G') = 1$ if $tb(G) = 1$. Moreover, the vertex x can be found in linear-time.

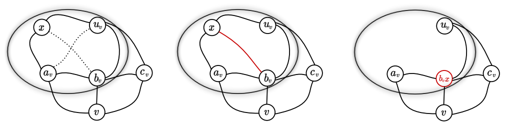

Figure 34: Cases when one of Theorem 14 or Theorem 15 applies and vertex b_v can be eventually contracted to another vertex.

Proof. First, we claim that (a_v, u_v) is a minimal 2-separator of G. Indeed, by the hypothesis c_v and u_v are adjacent, therefore, by Theorem 6 $N_G(c_v) = \{b_v, u_v, v\}$. In addition, $N(b_v) = \{a_v, c_v, u_v, v\}$ by the hypothesis. Last, since G is prime by the hypothesis, therefore, $N(a_v) \setminus (\Pi_v \cup \{v\}) \neq \emptyset$, and so, since a_v and u_v are non-adjacent by the hypothesis, $V(G) \setminus (a_v, b_v, c_v, u_v, v) \neq \emptyset$. As a result, (a_v, u_v) is a minimal 2-separator of G with $\{b_v, c_v, v\}$ being a full component of $G \setminus (a_v, u_v)$.

Since $N(a_v) \cap N(u_v)$ is an $a_v u_v$-separator of $G \setminus (c_v, v)$ by the hypothesis, therefore, $N(a_v) \cap N(u_v) \setminus b_v \neq \emptyset$, for it has to contain a vertex from every component of $G \setminus (a_v, b_v, c_v, u_v, v)$. For now, let $x \in N(a_v) \cap N(u_v) \setminus b_v$ be arbitrary. Let us prove that $tb(G) = 1$ implies that $tb(G') = 1$ where G' is obtained by adding an edge between b_v and x (for now, G' may not be planar, depending on the choice for x). To prove this, let $(T, \mathcal{X})$ be a star-decomposition of G, that exists by Lemma 3, minimizing the distance in T between the subtrees T_{a_v} and T_{u_v}. We claim that $T_{a_v} \cap T_{u_v} \neq \emptyset$. By contradiction, if $T_{a_v} \cap T_{u_v} = \emptyset$, then by Corollary 8, there are two bags B_{a_v}, B_{u_v} that are adjacent in T and such that $a_v \in B_{a_v} \setminus B_{u_v}, u_v \in B_{u_v} \setminus B_{a_v}$ respectively dominate B_{a_v}, B_{u_v}. However, this implies by the properties of a tree decomposition that $B_{a_v} \cap B_{u_v} \subseteq N(a_v) \cap N(u_v)$ is an $a_v u_v$-separator of G. Since the $a_v u_v$-path (a_v, v, c_v, u_v) does not intersect $N(a_v) \cap N(u_v)$, that is clearly a contradiction, and so, $T_{a_v} \cap T_{u_v} \neq \emptyset$.

Furthermore, since there is a full component of $G \setminus (a_v, u_v)$ in the subgraph $G \setminus (b_v, c_v, v)$, therefore, by Lemma 9 the removal of vertices b_v, c_v, v from all bags in $\mathcal{X}$ leads to a tree decomposition $(T, \mathcal{X}^-)$ of breadth one of $G \setminus (b_v, c_v, v)$. Let $(T', \mathcal{X}')$ be a reduced star-decomposition obtained from $(T, \mathcal{X}^-)$, thar exists by Lemma 3. Since the subtrees T'_{a_v}, T'_x, T'_{u_v} are pairwise intersecting (because $x \in N(a_v) \cap N(u_v)$ and $T_{a_v} \cap T_{u_v} \neq \emptyset$), therefore by the Helly property (Lemma 1) $T'_{a_v} \cap T'_x \cap T'_{u_v} \neq \emptyset$. Let $B \in T'_{a_v} \cap T'_x \cap T'_{u_v}$. To obtain a star-decomposition of G', it now suffices to make the bag B adjacent to the new bag $N_{G'}[b_v] = \{a_v, b_v, c_v, u_v, v, x\}$.

The above result holds for any choice of vertex $x \in (N_G(a_v) \cap N_G(u_v)) \setminus b_v$. Let us finally prove that one such a vertex x exists so that G' is planar. Indeed, since $N(a_v) \cap N(u_v)$ is an $a_v u_v$-separator of $G \setminus (c_v, v)$ by the hypothesis, therefore, $S := (N(a_v) \cap N(u_v)) \cup \{v\}$ is an a_vu_v-separator of G, and in particular it is a minimal a_vu_v-separator (because for every vertex $s \in S$, there is an a_vu_v-path that intersects S only in s). By Corollary 7, it can be computed in linear-time a planar supergraph G_S of G so that S induces a cycle of G_S. Then, let $N_{G_S}(b_v) \cap S = \{x, v\}$, by construction the graph G' is planar for such a choice of vertex x. ■

In Theorem 14, we show conditions so that vertex b_v can be made adjacent to some other vertex of $N_G(a_v) \cap N_G(u_v)$. Lemma 23 completes the picture by proving that if it is the case that $N_G(a_v) \cap N_G(u_v) \cap N_G(b_v) \neq \emptyset$, then $|N_G(a_v) \cap N_G(u_v) \cap N_G(b_v)| = 1$ and vertex b_v has exactly five neighbours.

Lemma 23 *Let G be a prime planar graph, let v be a leaf-vertex of Type 2, $\Pi_v = (a_v, b_v, c_v)$ be as in Definition 5, and let $u_v \notin \Pi_v \cup \{v\}$ be such that (b_v, u_v) is an edge-separator of $G \setminus v$.*

Suppose $u_v \in N_G(c_v) \setminus N_G(a_v)$ and there exists $x \in N_G(a_v) \cap N_G(u_v) \cap N_G(b_v)$.

Then, $N_G(b_v) = \{a_v, c_v, u_v, v, x\}$.

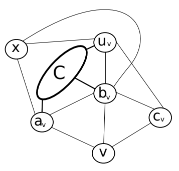

Figure 35: Case when $N_G(b_v) \neq \{a_v, c_v, u_v, v, x\}$.

Proof. By contradiction, let C be a component of $G \setminus (a_v, b_v, c_v, u_v, v, x)$ such that $b_v \in N(C)$ (see Figure 35 for an illustration). By Theorem 6 $N_G(c_v) = \{b_v, u_v, v\}$, therefore, $c_v, v \notin N(C)$. It follows that $N(C)$ is a separator of G. In particular, $N(C) \subseteq \{a_v, b_v, u_v, x\}$, so, $a_v, u_v \in N(C)$ or else $N(C)$ should be a clique-separator of the prime graph G. As a result, there is a $K_{3,3}$-minor with $\{a_v, b_v, u_v\}$ and $\{C, x, \{c_v, v\}\}$ being the two sides of the bipartition. It contradicts the fact that G is planar by the hypothesis. ■

Theorem 15 *Let G be a prime planar graph, let v be a leaf-vertex of Type 2, $\Pi_v = (a_v, b_v, c_v)$ be as in Definition 5, and let $u_v \notin \Pi_v \cup \{v\}$ be such that (b_v, u_v) is an edge-separator of $G \setminus v$.*

Suppose $u_v \in N(c_v) \setminus N(a_v)$, $N(a_v) \cap N(u_v)$ is an a_vu_v-separator of $G \setminus (c_v, v)$, and either $N(b_v) = \{a_v, c_v, u_v, v\}$ or $N(b_v) \cap N(a_v) \cap N(u_v) \neq \emptyset$.

Then, there is $x \in N(a_v) \cap N(u_v)$ such that one of the following must hold:

- *$V(G) = \{a_v, b_v, c_v, u_v, v, x\}$, and G admits a star-decomposition with two bags $N_G[b_v], N_G[x]$;*
- *or $\Pi' = (a_v, x, u_v) \in \mathcal{P}_3(G)$, and let G' be obtained from G by adding the edge $\{b_v, x\}$ (if it is not already present) then contracting this edge. The graph G' is planar and prime, furthermore $tb(G) = 1$ if and only if $tb(G') = 1$.*

Moreover, vertex x can be computed in linear-time.

Proof. There are two cases. If $N_G(b_v) = \{a_v, c_v, u_v, v\}$, then let x be set as in the statement of Theorem 14. Else, let x be the unique vertex of $N(b_v) \cap N(a_v) \cap N(u_v)$, that is well-defined by Lemma 23. Note that in both cases, vertex x can be computed in linear-time. In addition, $N(b_v) \subseteq \{a_v, c_v, u_v, v, x\}$ (the latter property following from Lemma 23 when b_v and x are adjacent, and being trivial else). Suppose for the proof that $V(G) \neq \{a_v, b_v, c_v, u_v, v, x\}$ (else, Theorem 15 is trivial). We claim that $\{b_v, c_v, v\}$ is a component of $G \setminus \Pi'$. Indeed, $N(b_v) \subseteq \Pi' \cup \{c_v, v\}$

by the hypothesis, and by Theorem 6 $N_G(c_v) = \{b_v, u_v, v\}$. Since $V(G) \neq \{a_v, b_v, c_v, u_v, v, x\}$, then it indeed follows that $\Pi' \in \mathcal{P}_3(G)$, with $\{b_v, c_v, v\}$ being a component of $G \setminus \Pi'$.

Let us prove that G' is prime and planar. By Theorem 14, adding an edge between b_v and x if it is not already present does not violate the property for the graph G to be planar. Therefore, G' is planar because it is obtained by an edge-contraction from some planar graph. To prove that G' is prime, by contradiction suppose the existence of a minimal clique-separator S' of G'.

Let us denote by x' the vertex resulting from the contraction of the edge $\{b_v, x\}$. Let $S := S'$ if $x' \notin S'$, $S := (S' \setminus x') \cup \{b_v, x\}$ else. By construction, S is a separator of G. In particular, S is not a clique because G is prime by the hypothesis. Therefore, $S \neq S'$, whence $x' \in S'$ or equivalently, $x, b_v \in S$. We now claim that $c_v \in S \cap S'$ or $v \in S \cap S'$ (possibly, $v, c_v \in S \cap S'$). There are two cases.

- Suppose that $S \setminus b_v$ is a separator of G. Then, $S \setminus b_v$ is not a clique because G is prime by the hypothesis. Since $S \setminus (b_v, x) = S' \setminus x'$ is a clique, there must be some vertex of $S \setminus (b_v, x) = S \cap S'$ that is adjacent to x' in G' but non-adjacent to x in G. Consequently, $v \in S \cap S'$ or $c_v \in S \cap S'$.

- Else, $S \setminus b_v$ is not a separator of G. Recall that by construction, S is a separator of G. In particular, there must be two neighbours of b_v in G that are separated by S in G. Since $N_G(b_v) \setminus x$ induces the path (a_v, v, c_v, u_v), it follows that S must contain an internal node of the path, whence $c_v \in S \cap S'$ or $v \in S \cap S'$.

However, in such case S' must be contained in one of (a_v, x', v), (v, x', c_v) or (c_v, x', u_v), for it is a clique of G'. In particular, let $z \in \{a_v, u_v\} \setminus S'$. Since z has a neighbour in every component C' of $G \setminus \Pi'$, $\{z\} \cup C'$ is not disconnected by S' in G'. Furthermore, let us contract C' to z so as to make a_v and u_v adjacent, S' intersects the resulting cycle (a_v, u_v, c_v, v) either in an edge (different from $\{a_v, u_v\}$) or a single vertex because it is a clique of G', therefore, $(a_v, u_v, c_v, v) \setminus S'$ is not disconnected by S'. Altogether, this contradicts the fact that S' is a separator of G', and so, G' is prime.

Finally, let us prove that $tb(G') = 1$ if and only if $tb(G) = 1$. If $tb(G) = 1$, then let us assume b_v and x to be adjacent (if they are not, then Theorem 14 ensures we can add the edge without violating the property for the graph to be of tree-breadth one). Then, $tb(G') = 1$ because it is obtained by an edge-contraction from some graph with tree-breadth one and that tree-breadth is contraction-closed by Lemma 2.

Conversely, let us prove that $tb(G') = 1$ implies that $tb(G) = 1$. To prove this, let $(T, \mathcal{X})$ be a star-decomposition of G', that exists by Lemma 3, minimizing the distance in T between the subtrees T_{a_v} and T_{u_v}. We claim that $T_{a_v} \cap T_{u_v} \neq \emptyset$. By contradiction, suppose $T_{a_v} \cap T_{u_v} = \emptyset$. Recall that $(a_v, x', u_v) \in \mathcal{P}_3(G')$ (because $\Pi' \in \mathcal{P}_3(G)$) and G' is prime, therefore one of (a_v, x', u_v) or (a_v, u_v) is a minimal separator of G'. Since we assume the distance in T between T_{a_v} and T_{u_v} to be minimized, by Corollary 8, there are two bags B_{a_v}, B_{u_v} that are adjacent in T so that $a_v \in B_{a_v} \setminus B_{u_v}, u_v \in B_{u_v} \setminus B_{a_v}$ respectively dominate B_{a_v}, B_{u_v}. However, by the properties of a tree decomposition $B_{a_v} \cap B_{u_v} \subseteq N(a_v) \cap N(u_v)$ is an $a_v u_v$-separator of G', that is impossible due to the existence of the path (a_v, v, c_v, u_v) in G' that does not intersect $N(a_v) \cap N(u_v)$. Therefore, $T_{a_v} \cap T_{u_v} \neq \emptyset$. Hence the subtrees $T_{a_v}, T_{x'}, T_{u_v}$ are pairwise intersecting and so, by the Helly Property (Lemma 1), $T_{a_v} \cap T_{x'} \cap T_{u_v} \neq \emptyset$. Furthermore, $N_{G'}[c_v] \cup N_{G'}[v] \subseteq N_{G'}[x']$ by construction. So, let us construct a tree decomposition of G of breadth one as follows. First, let us remove c_v and v from all bags in $\mathcal{X}$. Since $N_{G'}[c_v] \cup N_{G'}[v] \subseteq N_{G'}[x']$, one obtains a tree decomposition of $G' \setminus (c_v, v)$ of breadth one. Then let us replace x' with x in all bags. Note that in so doing, one obtains a tree decomposition of $G \setminus (b_v, c_v, v)$ of breadth one. Finally, let us make adjacent the new bag $N_G[b_v]$ with any bag of $T_{a_v} \cap T_x \cap T_{u_v}$. The result is indeed a tree decomposition of G' because $N_G[b_v] \subseteq \{a_v, b_v, c_v, u_v, v, x\}$ and $N_G[c_v] \cup N_G[v] \subseteq N_G[b_v]$. ■

5.3.9 Proof of Step 3.2 (b) iii

Theorem 16 *Let G be a prime planar graph, let v be a leaf-vertex of Type 2, $\Pi_v = (a_v, b_v, c_v)$ be as in Definition 5, and let $u_v \notin \Pi_v \cup \{v\}$ be such that (b_v, u_v) is an edge-separator of $G \setminus v$.*

Suppose $u_v \in N(c_v) \setminus N(a_v)$, $N(a_v) \cap N(u_v)$ is an a_vu_v-separator in the subgraph $G \setminus (c_v, v)$, $N(b_v) \neq \{a_v, c_v, u_v, v\}$ and $N(a_v) \cap N(b_v) \cap N(u_v) = \emptyset$.

Then it can be computed in linear-time (a unique) $x \in N(a_v) \cap N(u_v)$ such that if $tb(G) = 1$, $N(b_v) \cap N(x)$ is a b_vx-separator and $|N(b_v) \cap N(x)| \geq 3$.

Proof. Let $W = (N(a_v) \cap N(u_v)) \cup \{a_v, c_v, u_v, v\}$. By the hypothesis, $N(b_v) \neq \{a_v, c_v, u_v, v\}$ and $N(a_v) \cap N(b_v) \cap N(u_v) = \emptyset$, therefore, it exists a component C_0 of $G \setminus W$ such that $b_v \in N(C_0)$. We claim that there is $x \in N(a_v) \cap N(u_v) \cap N(C_0)$ satisfying that $N(C_0) \subseteq (a_v, b_v, x)$ or $N(C_0) \subseteq (u_v, b_v, x)$. Indeed, first observe that $v, c_v \notin N(C_0)$ because by Theorem 6 $N_G(c_v) = \{b_v, u_v, v\}$. Furthermore, $a_v \notin N(C_0)$ or $u_v \notin N(C_0)$ because $N(a_v) \cap N(u_v)$ is an a_vu_v-separator of $G \setminus (c_v, v)$ by the hypothesis. So, let $\{z, z'\} = \{a_v, u_v\}$ satisfy $z' \notin N(C_0)$. Since G is prime by the hypothesis, and so, biconnected, $G \setminus z$ is connected. Furthermore, $N(C_0) \setminus z \subseteq N(z')$ (by the definition of W), therefore, $N(C_0) \setminus z$ is a minimal separator of $G \setminus z$. By Lemma 13 there exist $s, t \in N(a_v) \cap N(u_v)$ non-adjacent such that $N(C_0) \setminus z = \{s, t\}$. Since $b_v \in N(C_0)$ by construction, therefore, let us set $\{s, t\} = \{b_v, x\}$, that finally proves the claim.

We claim in addition that x does not depend on the choice of the component C_0. By contradiction, let C, C' be two components of $G \setminus W$ such that $b_v \in N(C) \cap N(C')$ and let $x, x' \in N(a_v) \cap N_G(u_v)$ be distinct and such that $x \in N(C)$, $x' \in N(C')$. Then, there exists a $K_{3,3}$-minor with $\{a_v, b_v, u_v\}$ and $\{\{c_v, v\}, C \cup \{x\}, C' \cup \{x'\}\}$ being the sides of the bipartition, that contradicts the hypothesis that G is planar. Thus from now on, let $x \in N(a_v) \cap N(u_v) \setminus b_v$ be the unique vertex satisfying that for every component C of $G \setminus W$, if $b_v \in N(C)$ then $x \in N(C)$.

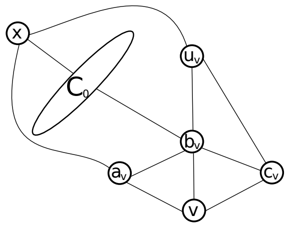

Figure 36: Component C_0 such that $b_v, x \in N(C_0)$.

Recall that C_0 is a fixed component of $G \setminus W$ such that $b_v, x \in N(C_0)$ (see Figure 36 for an illustration). Finally, assume for the remaining of the proof that $tb(G) = 1$ and let us prove that $N(b_v) \cap N(x)$ is a b_vx-separator and $|N(b_v) \cap N(x)| \geq 3$. To prove it, we will only need to prove that $N(b_v) \cap N(x)$ is a b_vx-separator of G. Indeed, in such a case $N(b_v) \cap N(x) \cap C_0 \neq \emptyset$, and so, $|N(b_v) \cap N(x)| \geq 3$ because $a_v, u_v \in N(b_v) \cap N(x)$ and $a_v, u_v \notin C_0$.

Let $(T, \mathcal{X})$ be star-decomposition of G, that exists by Lemma 3, minimizing the distance in T between the subtrees T_{b_v} and T_x. We claim that $T_{b_v} \cap T_x = \emptyset$. By contradiction, suppose $T_{b_v} \cap T_x \neq \emptyset$. Let us prove as an intermediate subclaim that $T_{a_v} \cap T_{u_v} \neq \emptyset$. By contradiction, let $T_{a_v} \cap T_{u_v} = \emptyset$. By the properties of a tree decomposition, every bag B onto the path in T between T_{a_v} and T_{u_v} must contain $N(a_v) \cap N(u_v)$ and at least one of v or c_v. If $c_v \in B$ then $B \subseteq N[u_v]$ since $N(c_v) = \{b_v, u_v, v\}$ and $x \in B$. Similarly if $v \in B$ then $B \subseteq N[a_v]$ since $N(v) = \{a_v, b_v, c_v\}$

and $x \in B$. Consequently, there are two adjacent bags B_{a_v}, B_{u_v} such that $a_v \in B_{a_v} \setminus B_{u_v}$ and $u_v \in B_{u_v} \setminus B_{a_v}$ respectively dominate B_{a_v} and B_{u_v}. However, by the properties of a tree decomposition, $B_{a_v} \cap B_{u_v} = N(a_v) \cap N(u_v)$ is an $a_v u_v$-separator of G, thus contradicting the existence of the path (a_v, v, c_v, u_v) in G. Therefore, it follows that $T_{a_v} \cap T_{u_v} \neq \emptyset$, that proves the subclaim.

If $T_{a_v} \cap T_{u_v} \neq \emptyset$ and $T_{b_v} \cap T_x \neq \emptyset$ then the subtrees $T_{a_v}, T_{b_v}, T_{u_v}, T_x$ are pairwise intersecting and so, it implies $T_{a_v} \cap T_{u_v} \cap T_{b_v} \cap T_x \neq \emptyset$ by the Helly property (Lemma 1). However, let $B' \in T_{a_v} \cap T_{u_v} \cap T_{b_v} \cap T_x$, no vertex in G can dominate B' because $N(b_v) \cap N(a_v) \cap N(u_v) = \emptyset$ by the hypothesis, thus contradicting the fact that $(T, \mathcal{X})$ is a star-decomposition. As a result, we proved the claim that $T_{b_v} \cap T_x = \emptyset$.

Finally, since there exists $S \subseteq (N(b_v) \cap N(x)) \cup \{b_v, x\}$ a minimal separator of G such that $b_v, x \in S$ (namely, $S := N(C_0)$), and $(T, \mathcal{X})$ is assumed to minimize the distance in T between T_{b_v} and T_x, by Corollary 8 there exist two adjacent bags B_{b_v}, B_x such that $b_v \in B_{b_v} \setminus B_x$, $x \in B_x \setminus B_{b_v}$ respectively dominate B_{b_v} and B_x. By the properties of a tree decomposition, $B_{b_v} \cap B_x = N(b_v) \cap N(x)$ is indeed a $b_v x$-separator of G. ■

Lemma 24 *Let G be a prime planar graph, let v be a leaf-vertex of Type 2, $\Pi_v = (a_v, b_v, c_v)$ be as in Definition 5, and let $u_v \notin \Pi_v \cup \{v\}$ be such that (b_v, u_v) is an edge-separator of $G \setminus v$.*

Suppose $u_v \in N(c_v) \setminus N(a_v)$, $N(a_v) \cap N(u_v)$ is an $a_v u_v$-separator in the subgraph $G \setminus (c_v, v)$, $N(b_v) \neq \{a_v, c_v, u_v, v\}$ and $N(a_v) \cap N(b_v) \cap N(u_v) = \emptyset$. Assume furthermore that there is $x \in N(a_v) \cap N(u_v)$, and there exists a leaf-vertex $l \in N(b_v) \cap N(x)$.

Then, l is a leaf-vertex of Type 1, or l is a leaf-vertex of Type 2 or 3 and $G \setminus l$ is prime.

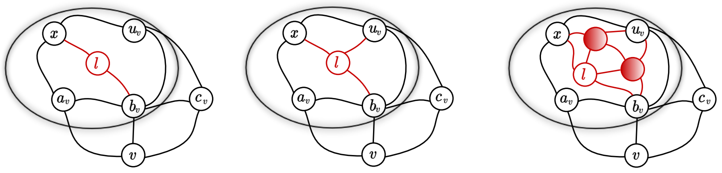

Figure 37: Existence of a leaf-vertex in $N(b_v) \cap N(x)$.

Proof. Suppose for the proof that l is not of Type 1 (else, Lemma 24 is trivial). Then, l is of Type 2 or 3, let Π_l be as in Definition 5. Note that $l \neq a_v$ because $v, b_v, x \in N(a_v)$ do not induce a path, similarly $l \neq u_v$ because $b_v, c_v, x \in N(u_v)$ do not induce a path. Furthermore by the hypothesis, b_v and x are the two endpoints of Π_l. Suppose by way of contradiction that there is a minimal clique-separator S of $G \setminus l$. Since G is prime by the hypothesis, by Lemma 16 S is a $b_v x$-separator of $G \setminus l$. However, it implies that $a_v, u_v \in S$, that contradicts the fact that S is a clique. As a result, $G \setminus l$ is prime. ■

Equipped with Lemma 24, we can assume from now on that there is no leaf-vertex that is adjacent to both vertices b_v, x, or else it could be immediately processed by the algorithm.

Theorem 17 *Let G be a prime planar graph, let v be a leaf-vertex of Type 2, $\Pi_v = (a_v, b_v, c_v)$ be as in Definition 5, and let $u_v \notin \Pi_v \cup \{v\}$ be such that (b_v, u_v) is an edge-separator of $G \setminus v$.*

Suppose $u_v \in N(c_v) \setminus N(a_v)$, $N(a_v) \cap N(u_v)$ is an $a_v u_v$-separator in the subgraph $G \setminus (c_v, v)$, $N(b_v) \neq \{a_v, c_v, u_v, v\}$ and $N(a_v) \cap N(b_v) \cap N(u_v) = \emptyset$. Assume furthermore that there is $x \in N(a_v) \cap N(u_v)$ such that $N(b_v) \cap N(x)$ is a $b_v x$-separator, $|N(b_v) \cap N(x)| \geq 3$, and there is no leaf-vertex in $N(b_v) \cap N(x)$.

Then, there exist $y, z \in N(b_v) \cap N(x)$ non-adjacent such that the graph G', obtained from G by making y, z adjacent, is planar and prime, and it holds $tb(G) = 1$ if and only if $tb(G') = 1$. Furthermore, the pair y, z can be computed in linear-time.

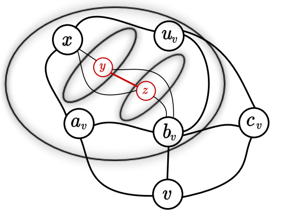

Figure 38: Illustration of Theorem 17.

Proof. Let us first show how to find the pair y, z. Let $W = \{a_v, c_v, v, u_v\} \cup (N(a_v) \cap N(u_v))$. Choose any component C_0 of $G \setminus W$ such that $b_v, x \in N(C_0)$ and $N(C_0) \subseteq (a_v, b_v, x)$ or $N(C_0) \subseteq (u_v, b_v, x)$ (the existence of such a component has been proved in Theorem 16). Note that $N(b_v) \cap N(x) \cap C_0 \neq \emptyset$ since $N(b_v) \cap N(x)$ is a $b_v x$-separator of G by the hypothesis. Then, let $S := N(b_v) \cap N(x)$. By the hypothesis S is a minimal separator of G and $|S| \geq 3$, therefore, by Corollary 7 there is a planar supergraph G_S of G so that S induces a cycle of G_S. Furthermore, G_S can be computed in linear-time. Let P be an $a_v u_v$-path of the cycle $G_S[S]$ that intersects C_0. Since by the above claim $a_v \notin N_G(C_0)$ or $u_v \notin N_G(C_0)$, therefore, there is $y \in C_0 \cap V(P)$, there is z adjacent to vertex y in P so that either $z \in C_1$ for some component C_1 of $G \setminus (W \cup C_0)$ or $z \in \{a_v, u_v\} \setminus N_G(C_0)$. In particular, $z \notin N_G[C_0] = C_0 \cup N_G(C_0)$. Moreover, the graph G', obtained from G by adding an edge between y and z, is planar by construction.

Claim 15 *G' is prime.*

Proof. By contradiction, let X be a minimal clique-separator of G'. Since G' is a supergraph of G, X is a separator of G. As a result, $y, z \in X$ because G is prime by the hypothesis. Let us prove as an intermediate step that $N(y) \cap N(z) = \{b_v, x\}$. There are two cases. If $z \in \{a_v, u_v\}$, then let $\{z, z'\} = \{a_v, u_v\}$. Since $N(C_0) \subseteq (z', b_v, x)$ (because $z \notin N_G(C_0)$) and z, z' are non-adjacent by the hypothesis, therefore, the claim immediately follows in this case. Else, $z \notin \{a_v, u_v\}$. Let C_1 be the component of $G \setminus (W \cup C_0)$ containing z. In such case, $b_v, x \in N(C_1)$ because $z \in S$ by construction. Therefore, $N(C_1) \subseteq (a_v, b_v, x)$ or $N(C_1) \subseteq (u_v, b_v, x)$ because the respective roles of components C_0, C_1 are symmetrical in this case. Suppose by way of contradiction $N(C_0) = N(C_1) = \{s, b_v, x\}$ for some $s \in \{a_v, u_v\}$ and let $\{s, t\} = \{a_v, u_v\}$. Then, there is a $K_{3,3}$-minor of G with $\{b_v, x, s\}$ and $\{C_0, C_1, \{c_v, v, t\}\}$ being the sides of the bipartition, that contradicts the hypothesis that G is planar. As a result, $N(C_0) \cap N(C_1) = \{b_v, x\}$, that finally proves the claim.

Since X is assumed to be a clique of G' and $y, z \in X$, it follows $X \subseteq \{b_v, y, z\}$ or $X \subseteq \{x, y, z\}$. Consequently, $G[W \setminus X]$ is connected because $a_v, u_v \notin X$ is a dominating pair of W, $b_v, x \in N(a_v) \cap N(u_v)$ and $b_v \notin X$ or $x \notin X$. However, since $y, z \in X$ and $N_G(y) \subseteq W \cup C_0$, then in such case there must be a component A of $G \setminus X$ so that $A \subset C_0$. Since $z \notin N_G[C_0]$ by construction, $N_G(A) \subseteq X \setminus z$ is a clique-separator of G, thus contradicting the hypothesis that G is prime. As a result, G' is prime. $\diamond$

Now, let us prove $tb(G) = 1$ if and only if $tb(G') = 1$.

If $tb(G) = 1$, then let $(T, \mathcal{X})$ be star-decomposition of G, that exists by Lemma 3, minimizing the distance in T between T_{a_v} and T_{u_v}. Let us prove that $(T, \mathcal{X})$ is a star-decomposition of

G', whence $tb(G') = 1$. To prove it, it is sufficient to prove $T_y \cap T_z \neq \emptyset$. We will prove as an intermediate claim that $T_{a_v} \cap T_{u_v} \neq \emptyset$. By contradiction, assume $T_{a_v} \cap T_{u_v} = \emptyset$. Observe that $\Pi' = (a_v, b_v, u_v) \in \mathcal{P}_3(G)$ with $\{c_v, v\}$ being a full component of $G \setminus \Pi'$. Therefore, since G is prime by the hypothesis, one of Π' or $\Pi' \setminus b_v$ is a minimal separator of G. Since $(T, \mathcal{X})$ is assumed to minimize the distance in T between T_{a_v} and T_{u_v}, therefore, by Corollary 8 there are two adjacent bags B_{a_v}, B_{u_v} such that $a_v \in B_{a_v} \setminus B_{u_v}$ and $u_v \in B_{u_v} \setminus B_{a_v}$ respectively dominate B_{a_v} and B_{u_v}. However, by the properties of a tree decomposition $B_{a_v} \cap B_{u_v} = N(a_v) \cap N(u_v)$ is an $a_v u_v$-separator of G, that contradicts the existence of the path (a_v, v, c_v, u_v) in G. Consequently the claim is proved, hence $T_{a_v} \cap T_{u_v} \neq \emptyset$. The latter claim implies $T_{b_v} \cap T_x = \emptyset$, for if $T_{b_v} \cap T_x \neq \emptyset$ then the subtrees $T_{a_v}, T_{b_v}, T_{u_v}, T_x$ are pairwise intersecting, hence $T_{a_v} \cap T_{b_v} \cap T_x \cap T_{u_v} \neq \emptyset$ by the Helly property (Lemma 1), that would contradict the fact that $(T, \mathcal{X})$ is a star-decomposition because $N(a_v) \cap N(u_v) \cap N(b_v) = \emptyset$ by the hypothesis. Finally, since (x, y, b_v, z) induces a cycle of G and $T_{b_v} \cap T_x = \emptyset$, therefore, by the properties of a tree decomposition $T_y \cap T_z \neq \emptyset$, and so, $(T, \mathcal{X})$ is indeed a star-decomposition of G'.

Conversely, let us prove $tb(G') = 1$ implies $tb(G) = 1$. To prove it, let $(T', \mathcal{X}')$ be a star-decomposition of G', that exists by Lemma 3, minimizing the number $|\mathcal{X}'|$ of bags. Assume furthermore $(T', \mathcal{X}')$ to minimize the number of bags $B \in \mathcal{X}'$ that are not contained into the closed neighbourhood of some vertex in G w.r.t. the minimality of $|\mathcal{X}'|$. In order to prove $tb(G) = 1$, it suffices to prove that $(T', \mathcal{X}')$ is a star-decomposition of G. We will start proving intermediate claims.

Claim 16 *$a_v, u_v \notin N_G(y)$.*

Proof. By contradiction, assume the existence of $z' \in \{a_v, u_v\}$ so that z' and y are adjacent in G. In particular, $z' \neq z$ (since $z \notin N_G[C_0]$) and $N_G(C_0) = \{b_v, x, z'\}$ since either $N_G(C_0) \subseteq \{b_v, x, a_v\}$ or $N_G(C_0) \subseteq \{b_v, x, u_v\}$. Hence, the path (b_v, z', x) is a separator of G. Since $y \in N_G(b_v) \cap N_G(z') \cap N_G(x)$, by Lemma 15 either C_0 is reduced to y or $(b_v, y, x) \in \mathcal{P}_3(G)$ separates z' from $C_0 \setminus y$. The case $C_0 \setminus y = \emptyset$ implies that y is a leaf-vertex of Type 2, that contradicts the hypothesis that there is no leaf-vertex in $N_G(b_v) \cap N_G(x)$. Therefore, let $(b_v, y, x) \in \mathcal{P}_3(G)$ separates z' from $C_0 \setminus y$ in G, and let $C_0' \subseteq C_0 \setminus y$ be a component of $G \setminus (b_v, y, x)$ (such a component C_0' exists because $N_G(C_0) = \{z', b_v, x\}$). Since G is prime, $b_v, x \in N_G(C_0')$ (indeed, neither b_v nor y nor x nor (b_v, y) nor (y, x) can be a separator of G). Therefore, $N_G(b_v) \cap N_G(x) \cap C_0' \neq \emptyset$ because $N_G(b_v) \cap N_G(x)$ is a $b_v x$-separator of G by the hypothesis. Furthermore, $y \in N_G(C_0')$ because C_0 is connected. However in such case, there is a $K_{3,3}$-minor of G' with $\{b_v, x, y\}$ and $\{a_v, C_0', u_v\}$ being the sides of the bipartition, that contradicts the fact that G' is planar. ◇

Claim 17 *There is no vertex dominating the cycle (a_v, b_v, u_v, x) in G'.*

Proof. By contradiction, if it were the case that such a vertex exists, then, since $N_G(b_v) \cap N_G(a_v) \cap N_G(u_v) = \emptyset$ by the hypothesis, the dominator should be y and furthermore $z \in \{a_v, u_v\}$. In particular, $y \in N_G(b_v) \cap N_G(x) \cap N_G(z')$ with $\{z, z'\} = \{a_v, u_v\}$, thus contradicting Claim 16. ◇

Claim 18 *$T'_{a_v} \cap T'_{u_v} \neq \emptyset$.*

Proof. By contradiction, let $T'_{a_v} \cap T'_{u_v} = \emptyset$. By the properties of a tree decomposition, every bag B onto the path in T' between T'_{a_v} and T'_{u_v} (including the endpoints) must contain $N_{G'}(a_v) \cap N_{G'}(u_v)$ and at least one of v or c_v. Then, if $c_v \in B$ then $B \subseteq N_{G'}[u_v]$ and so, $B \in T'_{u_v}$, since $N_{G'}(c_v) = \{b_v, u_v, v\}$ and $x \in B$. Similarly if $v \in B$ then $B \subseteq N_{G'}[a_v]$ and so, $B \in T'_{a_v}$, since

$N_{G'}(v) = \{a_v, b_v, c_v\}$ and $x \in B$. Consequently, there are two adjacent bags B_{a_v}, B_{u_v} such that $a_v \in B_{a_v} \setminus B_{u_v}$ and $u_v \in B_{u_v} \setminus B_{a_v}$ respectively dominate B_{a_v} and B_{u_v} in G'. However, by the properties of a tree decomposition, $B_{a_v} \cap B_{u_v} = N_{G'}(a_v) \cap N_{G'}(u_v)$ is an $a_v u_v$-separator of G', thus contradicting the existence of the path (a_v, v, c_v, u_v) in G'. Therefore, it follows that $T'_{a_v} \cap T'_{u_v} \neq \emptyset$, that proves the claim. $\diamond$

Claim 19 $T'_{b_v} \cap T'_x = \emptyset$

Proof. Suppose for the sake of contradiction that $T'_{b_v} \cap T'_x \neq \emptyset$. By Claim 18, $T'_{a_v} \cap T'_{u_v} \neq \emptyset$, and so, the subtrees $T'_{a_v}, T'_{b_v}, T'_{u_v}, T'_x$ are pairwise intersecting. Hence by the Helly property (Lemma 1), $T'_{a_v} \cap T'_{b_v} \cap T'_{u_v} \cap T'_x \neq \emptyset$. However in such case, since $(T', \mathcal{X}')$ is a star-decomposition of G' there must be a vertex dominating the cycle (a_v, b_v, u_v, x) in G', thereby contradicting Claim 17. $\diamond$

As a result, $T'_{a_v} \cap T'_{u_v} \neq \emptyset$ by Claim 18 and $T'_{b_v} \cap T'_x = \emptyset$ by Claim 19.

Finally, suppose by way of contradiction $(T', \mathcal{X}')$ is not a star-decomposition of G. In such case, since G and G' only differ in the edge $\{y, z\}$, there must exist $B \in T'_y \cap T'_z$ that is uniquely dominated by some of y, z in G'. More precisely, let us prove that only one of y, z can dominate B. By contradiction, suppose $B \subseteq N_{G'}[y] \cap N_{G'}[z] = \{b_v, x, y, z\}$ (indeed, $y \in C_0$ whereas $z \notin N_G[C_0]$). Since $T'_{b_v} \cap T'_x = \emptyset$ by Claim 19, $B \subseteq \{b_v, y, z\}$ or $B \subseteq \{x, y, z, \}$. Therefore, B is a clique of G'. However, since $B \neq V(G')$, there is a bag B' adjacent to B and by the properties of a tree decomposition $B \cap B'$ is a clique-separator of G', thus contradicting the fact that G' is prime by Claim 15. Consequently, either $B \subseteq N_{G'}[y]$ or $B \subseteq N_{G'}[z]$, and either $B \not\subseteq N_{G'}[y]$ or $B \not\subseteq N_{G'}[z]$. In the following, let $\{s, t\} = \{y, z\}$ satisfy $B \subseteq N_{G'}[s]$, that is well-defined. Let B' be any bag adjacent to B so that $t \in B'$ (such bag exists because $y, z \in N(b_v) \cap N(x)$, and $b_v \notin B$ or $x \notin B$ because $T'_{b_v} \cap T'_x = \emptyset$). There are three cases.

- Suppose no vertex of b_v, x, y, z dominates B' in G' (see Figure 39 for an illustration). Since $b_v \notin B$ or $x \notin B$ because $T'_{b_v} \cap T'_x = \emptyset$, therefore, $(B \cap B') \setminus (b_v, x, y, z) \neq \emptyset$, or else by the properties of a tree decomposition that would be a clique-separator of G', thus contradicting the fact that G' is prime by Claim 15. Let $t' \in (B \cap B') \setminus (b_v, x, y, z)$. Note that t' and t are non-adjacent in G' because $t' \in N_{G'}[s]$ and $N_{G'}[y] \cap N_{G'}[z] = \{b_v, x, y, z\}$. Let $s' \in B'$ dominate this bag. Note that s' and s are non-adjacent in G' because we assume $s' \notin \{b_v, x, y, z\}$, $t \in N_{G'}(s')$ and $N_{G'}[y] \cap N_{G'}[z] = \{b_v, x, y, z\}$. In particular, $s' \neq t'$ and (s, t', s', t) induces a path in G. By construction, $y \in C_0$ and $z \notin N_G[C_0]$, hence there must be some of s', t' in $N_G(C_0)$. Since $N_G(C_0) \subseteq \{a_v, b_v, u_v, x\}$ and $s', t' \notin \{b_v, x, y, z\}$, therefore the pairs $\{s', t'\}$ and $\{a_v, u_v\}$ intersect. However, by Claim 16 $a_v, u_v \notin N_G(y)$, similarly $a_v, u_v \notin N_G(z)$, that contradicts the existence of the path (s, t', s', t) in G. Consequently, assume in the remaining cases that there is some vertex of b_v, x, y, z dominating B' in G'.

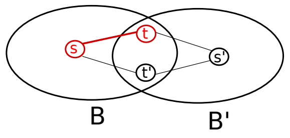

Figure 39: $B \subseteq N_{G'}[s]$, $B' \subseteq N_{G'}[s']$.

- Suppose B' is dominated by one of y, z in G'. We claim that B and B' are dominated by the same vertex of y, z, for if it were not the case $B \cap B' \subseteq N_{G'}[y] \cap N_{G'}[z] = \{b_v, x, y, z\}$, and so, since by the properties of a tree decomposition $B \cap B'$ is a separator of G', and $b_v \notin B$ or $x \notin B$ because $T'_{b_v} \cap T'_x = \emptyset$, $B \cap B'$ should be a clique-separator of G', thus contradicting the fact that G' is prime by Claim 15. However, in such a case bags B, B' could be merged into one while preserving the property for the tree decomposition to be a star-decomposition of G', that would contradict the minimality of $|\mathcal{X}'|$.

- Therefore, B' is dominated by some of b_v, x. We claim that there is a unique such bag B' that is adjacent to B. By contradiction, let $B'' \neq B'$ be adjacent to B and such that B'' is also dominated by some of b_v, x. In particular, if $B'' \cup B' \subseteq N[b_v]$ or $B'' \cup B' \subseteq N[x]$ then both bags B', B'' could be merged into one without violating the property for the tree decomposition to be a star-decomposition of G', that would contradict the minimality of $|\mathcal{X}'|$. Else, w.l.o.g. $B' \subseteq N[b_v]$ and $B'' \subseteq N[x]$. Since $T'_{b_v} \cap T'_x = \emptyset$, $a_v, u_v \in N(b_v) \cap N(x)$ and B', B'' are adjacent to B, therefore, by the properties of the tree decomposition $a_v, u_v \in B$. However, $a_v, u_v \notin N_G[y]$ by Claim 16, a_v and u_v are non-adjacent, and either $z \in \{a_v, u_v\}$ or $a_v, u_v \notin N_G[z]$ (by the same proof as for Claim 16), thus contradicting the fact that either $B \subseteq N_{G'}[y]$ or $B \subseteq N_{G'}[z]$. Hence, the claim is proved and B' is assumed to be the unique bag adjacent to B such that $B \subseteq N[b_v]$ or $B \subseteq N[x]$. In particular, B' is the unique bag adjacent to B containing vertex t (recall that $\{s, t\} = \{y, z\}$ and $B \subseteq N_{G'}[s]$, $B \nsubseteq N_{G'}[t]$).

  Let us substitute the bags B, B' with $B \setminus t, B' \cup \{s\}$. We claim that this operation keeps the property for $(T', \mathcal{X}')$ to be a star-decomposition of G'. To prove the claim, first note that the operation only modifies bags B and B', furthermore $B \setminus t \subseteq N[s]$ and $B' \cup \{s\} \subseteq N[b_v]$ or $B' \cup \{s\} \subseteq N[x]$. Consequently, to prove the claim, it suffices to prove that the operation keeps the property for $(T', \mathcal{X}')$ to be a tree decomposition of G' (for in such a case, it is always a star-decomposition). Since $T'_t \setminus B$ is connected because B' is the only bag containing vertex t that is adjacent to the bag B, therefore, we are left to prove that there is no $w \in N_{G'}(t) \setminus s$ such that $T'_w \cap T'_t = \{B\}$. By contradiction, let $w \in N_{G'}(t) \setminus s$ satisfy $T'_w \cap T'_t = \{B\}$. Since $w \in B \subseteq N_{G'}[s]$, therefore $w \in N_{G'}(s) \cap N_{G'}(t) = N_G(y) \cap N_G(z) = \{b_v, x\}$. Moreover, $w \notin B'$ because $t \in B'$ and we assume that $T'_w \cap T'_t = \{B\}$. In such a case, since it is assumed that $B' \subseteq N[b_v]$ or $B' \subseteq N[x]$, and in addition $T'_x \cap T'_{b_v} = \emptyset$, let us write $\{w, w'\} = \{b_v, x\}$ such that $w \in B \setminus B'$, $w' \in B' \setminus B$ and $B' \subseteq N_{G'}[w']$. By the properties of a tree decomposition, $B \cap B'$ is a $b_v x$-separator of G', so, $a_v, u_v \in B \cap B'$. However, $a_v, u_v \notin N_G(y)$ by Claim 16 and similarly $a_v, u_v \notin N_G(z)$, that contradicts the fact that $B \subseteq N_{G'}[s]$ for some $s \in \{y, z\}$. This finally proves the claim that substituting the bags B, B' with $B \setminus t, B' \cup \{s\}$ keeps the property for $(T', \mathcal{X}')$ to be a star-decomposition of G'.

  However, the above operation does not increase the number of bags $|\mathcal{X}'|$, furthermore there is one less bag that is not contained in the closed neighbourhood of some vertex in G. This contradicts the minimality of $(T', \mathcal{X}')$ w.r.t. these two properties.

As a result, we proved by contradiction that $(T', \mathcal{X}')$ is a star-decomposition of G, hence $tb(G) = 1$. ■

5.4 Complexity of Algorithm `Leaf-BottomUp`

To complete this section, let us emphasize on some computational aspects of Algorithm `Leaf-BottomUp`, that will ensure the quadratic-time complexity of the algorithm. We here assume that the planar graph G is encoded with adjacency lists. Note that the adjacency lists can be updated in linear-time before each recursive call to the algorithm.

We will need as a routine to test whether two vertices are adjacent in *constant-time.* In order to achieve the goal, the following result (relying upon the bounded degeneracy of planar graphs) will be used:

Lemma 25 ([18]) *There exists a data structure such that each entry in the adjacency matrix of a planar graph can be looked up in constant time. The data structure uses linear storage, and can be constructed in linear time.*

5.4.1 Finding a leaf-vertex

At each call to the algorithm, it is first required to decide whether a leaf-vertex exists. If that is the case, then one such a vertex must be computed. Here is a way to achieve the goal in linear-time. Let us start computing the degree sequence of G, then let us order the vertices of the graph G by increasing degree.

Finding a leaf-vertex of Type 1. Let v be any vertex of degree at least four. We claim that a necessary condition for v to be a leaf-vertex of Type 1 is that all but at most two neighbours of v have degree four. Indeed, if v is a leaf-vertex of Type 1, then let Π_v, d_v be defined as in Definition 5. By Lemma 21, either $V(G) = N[v] \cup \{d_v\}$ or $\Pi' = (a_v, d_v, c_v) \in \mathcal{P}_3(G)$ and $N[v] \setminus (a_v, c_v)$ is a full component of $G \setminus \Pi'$. In both cases, all neighbours in $N(v) \setminus (a_v, c_v)$ have degree four.

- Therefore, let us count the number of neighbours of degree four in $N(v)$, that can be done in $\mathcal{O}(deg(v))$-time simply by traversing the adjacency list of vertex v (recall that the degree sequence of G has been computed).
- If there are all but at most two neighbours in $N(v)$ that have degree four, then we claim that one can construct the induced subgraph $G[N(v)]$ in $\mathcal{O}(deg(v))$-time. Indeed, for every neighbour $u \in N(v)$ that has degree four, let us test in constant-time for each of its four neighbours whether they are adjacent to vertex v — we only keep those for which it is the case in the adjacency list of u in $G[N(v)]$. Then, for every $u \in N(v)$ that does not have degree four (there are at most two such vertices), let us construct the adjacency list of u in $G[N(v)]$ simply by testing to which vertices in $N(v) \setminus u$ it is adjacent — the latter takes constant-time by neighbour.
- Once $G[N(v)]$ has been computed, it is easy to check whether it is a path in $\mathcal{O}(|N(v)|) = \mathcal{O}(deg(v))$-time.
- Finally, let $u \in N(v)$ have degree four. Let us pick in constant-time any neighbour $d_v \in N(u) \setminus N(v)$ (note that such a vertex is unique if $G[N(v)]$ induces a path). In order to decide whether v is a leaf-vertex of Type 1, it is now sufficient to test whether vertex d_v is adjacent to every vertex in $N(v)$ — that takes constant-time by neighbour.

Finding a leaf-vertex of Type 2. Recall that a vertex is a leaf-vertex of Type 2 if and only if it has degree three and its three neighbours induce a path. Given any vertex of degree three, three adjacency tests are enough in order to determine whether its three neighbours induce a path — and each adjacency tests takes constant-time. Therefore, it can be checked in constant-time whether a vertex is a leaf-vertex of Type 2.

Finding a leaf-vertex of Type 3. By Definition 5, a vertex v is a leaf-vertex of Type 3 if and only if it has degree two and its two neighbours are non-adjacent and they have at least two common neighbours (including v). Note that given a degree-two vertex, it can be checked whether its two neighbours are non-adjacent in constant-time. We now distinguish three cases.

1. First, suppose there is a vertex v such that $N(v) = \{x, y\}$ and neighbour x is a degree-two vertex. In such case, let $N(x) = \{v, z\}$, in order to decide whether v is a leaf-vertex of Type 3, it is sufficient to test in constant-time whether y, z are adjacent.

2. Second, suppose there are two degree-two vertices v, v' that share the same two non-adjacent neighbours (*i.e.*, $N(v) = N(v') = \{x, y\}$ and x, y are non-adjacent). In such case, both vertices v, v' are leaf-vertices of Type 3 (this case may happen if for instance, $G = K_{2,q}$ with $q \geq 2$). In order to check whether this case happens, it is sufficient to sort the pairs $N(v)$ with v being a degree-two vertex in linear-time (for instance, using a bucket-sort).

3. Else, let V' contain every degree-two vertex v with two non-adjacent neighbours of degree at least three (if one of the two neighbours of v has degree two, we fall in the first case) W.l.o.g., every vertex $v \in V'$ is uniquely determined by the pair $N(v)$ composed of its two neighbours (or else, we fall in the second case). In such case, let us contract every $v \in V'$ to one of its two neighbours. By doing so, we remove v and we make the two vertices in $N(v)$ adjacent. Note that all these edge-contractions are pairwise independent. Let us call G' the graph resulting from all edge-contractions, and let us call "virtual edges" any new edge resulting from an edge-contraction. Then, let us list all triangles in the resulting graph G', it can be done in linear-time [42]. By construction, $v \in V'$ is a leaf-vertex of Type 3 if and only if the virtual edge resulting from its contraction belongs to a triangle in which it is the unique virtual edge.

Overall, finding a leaf-vertex in G takes $\mathcal{O}(\sum_{v \in V} deg(v))$-time, that is $\mathcal{O}(n)$-time because G is planar.

5.4.2 Existence of a star-decomposition with two bags

Lemma 26 *Let G be a planar graph, it can be decided in quadratic-time whether G admits a star-decomposition with one or two bags.*

Proof. G admits a star-decomposition with one bag if and only if there is a universal vertex in G, hence it can be decided in linear-time. Assume for the remaining of the proof that G does not admit a star-decomposition with less than two bags. We will consider two necessary conditions for some fixed pair x, y to be the dominators of the only two bags in some star-decomposition of G. For each of the two conditions, we will prove that all pairs satisfying the condition can be computed in quadratic-time. Then, we will conclude the proof by showing that the two conditions are sufficient to ensure the existence of a star-decomposition of G with two bags.

1. Recall that if it exists a star-decomposition of G with two bags, then by the properties of a tree decomposition every vertex of G must be contained in at least one bag. Therefore, if x, y are the only two dominators of the bags in some star-decomposition of G, they must be a dominating pair of G. It can be decided in $\mathcal{O}(deg(x) + deg(y))$-time whether a fixed pair x, y is a dominating pair. So, overall, it takes $\mathcal{O}(n^2)$-time to compute all dominating pairs of G with n being the order of the graph, for the graph is planar and so, it is a sparse graph.

2. Furthermore, recall that if it exists a star-decomposition of G with two bags, then by the properties of a tree decomposition every edge of G must be contained in at least one bag. Therefore, if there is a star-decomposition of G with two bags that are respectively dominated by x and y, then it must be the case that there does not exist any edge $e = \{u, v\}$ so that $u \in N[x] \setminus N[y]$ and $v \in N[y] \setminus N[x]$ (else, such an edge could not be contained in any of the two bags). In order to decide whether the latter condition holds for some fixed pair x, y, it suffices to test whether every vertex of $N[x] \setminus N[y]$ is non-adjacent to all vertices in $N[y] \setminus N[x]$ — it takes constant-time per test and so, $\mathcal{O}(deg(x) \cdot deg(y))$-time in total. As a result, computing all pairs x, y satisfying the condition requires $\mathcal{O}(\sum_{x,y} deg(x) \cdot deg(y)) = \mathcal{O}([\sum_x deg(x)][\sum_y deg(y)]) = \mathcal{O}(n^2)$-time because the graph G is planar and so, it is a sparse graph.

Finally, let x, y satisfy the two above necessary conditions. We claim that $(T, \mathcal{X})$ with T being an edge and $\mathcal{X} = \{N[x], N[y]\}$ is a star-decomposition of G. Indeed, every vertex is contained into a bag because the pair x, y satisfies the first necessary condition. Furthermore, every edge has its both ends contained into a common bag because the pair x, y satisfies the second necessary condition. Last, all the bags containing a common vertex induce a subtree because there are only two bags. As a result, $(T, \mathcal{X})$ is a tree decomposition of G. Since each bag of $\mathcal{X}$ is respectively dominated by x or y, therefore $(T, \mathcal{X})$ is indeed a star-decomposition of G, that proves the claim, hence the lemma. ■

Note that in any execution of Algorithm `Leaf-BottomUp`, it is verified at most once whether some planar graph admits a star-decomposition with one or two bags.

5.4.3 Upper-bound on the number of steps in the algorithm

Lemma 27 *Let G be a prime planar graph with n vertices and m edges. Then, there are at most $5n - m$ recursive calls to the Algorithm `Leaf-BottomUp`, that is $\mathcal{O}(n)$.*

Proof. First note that since G is planar by the hypothesis, $5n - m \geq 0$ and $5n - m = \mathcal{O}(n)$. Let G' with n' vertices and m' edges so that Algorithm `Leaf-BottomUp` is recursively applied on G' when G is the input. Since there is at most one such a graph G' (*i.e.*, there is no more than one recursive call at each call of the algorithm), furthermore G' is prime and planar, therefore, in order to prove the lemma it suffices to prove that $5n' - m' < 5n - m$. To prove it, let us consider at which step of the algorithm the recursive call occurs.

- If it is at Step 2, then G' is obtained by removing a leaf-vertex of Type 1, denoted by v, and then contracting all the internal vertices in the path Π_v (induced by $N(v)$) to a single edge. Therefore, $n' = n - deg(v) + 3$, $m' = m - 3deg(v) + 8$ and so, $5n' - m' = 5n - m - (2deg(v) - 7) < 5n - m$ because $deg(v) \geq 4$.

  Thus, from now on let us assume we fall in Step 3, *i.e.*, a leaf-vertex of Type 2 or 3 is considered, denoted by v.

- If the recursion happens at Step 3.1 (a), then G' is obtained by removing v. Therefore, $n' = n - 1$ and either $m' = m - 3$ (if v is of Type 2) or $m' = m - 2$ (if v is of Type 3), hence $m' \geq m - 3$ and so, $5n' - m' \leq 5n - m - 2 < 5n - m$.

- If it is at Step 3.1 (b), then we fall in Step 3.1 (b) ii (no recursion occurs in Step 3.1 (b) i), thus G' is obtained by making v adjacent to the two vertices in $(N(a_v) \cap N(c_v)) \setminus v$ (including b_v in the case when v is of Type 3). Therefore, $n' = n$ and either $m' = m+1$ (if v is of Type 2) or $m' = m+2$ (if v is of Type 3), hence $m' \geq m+1$ and so, $5n' - m' \leq 5n - m - 1 < 5n - m$.

- Else, the recursion happens at Step 3.2. Recall that in such case, there exists a vertex u_v such that (b_v, u_v) is a clique-separator of $G \setminus v$. Adding an edge between v and b_v if it does not exist, decreases $5n - m$ by 1, therefore from now on let us assume that v is a leaf-vertex of Type 2.
  - if it is at Step 3.2 (a), then G' is obtained by contracting the edge $\{v, a_v\}$. Therefore, $n' = n - 1$, $m' = m - 2$, hence $5n' - m' = 5n - m - 3 < 5n - m$.
  - If it is at Step 3.2 (b) i, then G' is obtained by adding an edge between b_v and some vertex $x \in (N(a_v) \cap N(u_v)) \setminus b_v$ then contracting this edge. Furthermore, $N(b_v) = \{a_v, c_v, u_v, v\}$ in such case and $c_v, v \notin N(x)$. Therefore, $n' = n-1$, $m' = m-2$ and so, $5n' - m' = 5n - m - 3 < 5n - m$.
  - If it is at Step 3.2 (b) ii, then G' is obtained by contracting the edge $\{b_v, x\}$ where $x \in N(a_v) \cap N(u_v) \cap N(b_v)$. Furthermore, $N(b_v) = \{a_v, c_v, u_v, v, x\}$ in such case and $c_v, v \notin N(x)$. Therefore, $n' = n-1$, $m' = m-3$ and so, $5n'-m' = 5n-m-2 < 5n-m$.
  - Finally, in all other cases the recursive call happens at Step 3.2 (b) iii. Then, G' is obtained by adding an edge between two vertices $y, z \in N(b_v) \cap N(x)$ for some $x \in (N(a_v) \cap N(u_v)) \setminus b_v$. Therefore, $n' = n$, $m' = m + 1$ and so, $5n' - m' = 5n - m - 1 < 5n - m$.

■

6 Conclusion and Open questions

On the negative side, we proved the NP-hardness of computing five metric graph invariants (namely, tree-breadth, path-length, path-breadth, k-good tree and path decompositions) whose complexity has been left open in several works [24, 26, 27]. These results add up to the proof in [39] that it is NP-hard to compute the tree-length.

We leave as a future work further study on the border between tractable and intractable instances for the problem of computing the above metric graph invariants. Especially, what are the graph classes for which it can be decided in polynomial-time whether a graph admits a star-decomposition ? In this paper, we partially answer to this question by proving that it is the case for bipartite graphs and planar graphs. Based on these two positive results, we conjecture that the problem is Fixed-Parameter Tractable when it is parameterized by the *clique-number* of the graph (note that there is a large clique in all the graphs obtained from our polynomial-time reductions). Intermediate challenges could be to determine whether the problem is Fixed-Parameter Tractable when it is parameterized by the genus, the tree-width or the Hardwiger number.

Finally, we notice that all our NP-hardness results imply that the above metric graph invariants cannot be approximated below some constant-factor. There remains a gap between our inapproximability results and the constant-ratio of the approximation algorithms in [24, 27]. Therefore, we leave as an interesting open question whether we can fill in this gap.

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Appendix H

To approximate treewidth, use treelength!

TO APPROXIMATE TREEWIDTH, USE TREELENGTH![*]

DAVID COUDERT[†] [‡] AND GUILLAUME DUCOFFE[‡] [†] AND NICOLAS NISSE[†] [‡]

Abstract. Tree-likeness parameters have proven their utility in the design of efficient algorithms on graphs. In this paper, we relate the *structural* tree-likeness of graphs with their *metric* tree-likeness. To this end, we establish new upper-bounds on the diameter of *minimal separators* in graphs. We prove that in any graph G, the diameter of any minimal separator S in G is at most $\lfloor \ell(G)/2 \rfloor \cdot (|S|-1)$, with $\ell(G)$ the length of a longest isometric cycle in G. Our result relies on algebraic methods and on the cycle basis of graphs. We improve our bound for the graphs admitting a *distance preserving elimination ordering*, for which we prove that any minimal separator S has diameter at most $2 \cdot (|S|-1)$.

We use our results to prove that the *treelength* $tl(G)$ of any graph G is at most $\lfloor \ell(G)/2 \rfloor$ times its *treewidth* $tw(G)$. In addition, we prove that, for any graph G that excludes an *apex graph* H as a minor, $tw(G) \leq c_H \cdot tl(G)$ for some constant c_H only depending on H. We refine this constant when G has bounded genus. Altogether, we obtain a simple $\mathcal{O}(\ell(G))$-approximation algorithm for computing the treewidth of n-node apex-minor-free graphs in $\mathcal{O}(n^2)$-time.

Key words. Graph; Treewidth; Treelength; Cycle basis; Genus.

AMS subject classifications. 05C85, 68Q17, 68Q25, 68R10

1. Introduction.

It turns out that for a vast range of graph problems, the boundary between tractable and intractable cases depends on the *tree-like properties* of the graphs. This motivates us to study two tree-likeness invariants, that are called the *treewidth* [31] and the *treelength* [20]. Informally, the *width* of a tree-decomposition is the maximum size of its bags and its *length* is the maximum "diameter" of its bags. The treewidth and treelength of a graph are respectively the minimum width and length of its tree-decompositions (formal definitions can be found in Section 2). Note that bounded treelength graphs generalize the chordal graphs, split graphs, etc. which are well studied graph classes that have unbounded tree-width.

The treewidth aims to measure how close is the *structure* of a graph from the structure of a tree, whereas the treelength aims to measure the minimum distortion of the *distances* in a graph when it is embedded into a tree [1]. Since both invariants provide distinct, yet complementary, pieces of information on the closeness of a graph to a tree, we wish to relate treewidth and treelength through other graph properties so as to obtain a unifying view of tree-likeness in graphs.

Let us further motivate the need to compare treewidth with treelength, before presenting our main results.

One of the motivations is that we want to take the algorithmic advantages from both sides. Indeed, on the one hand there are many NP-hard problems that can be solved in polynomial-time on bounded-treewidth graphs [13]; on the other hand there exist compact routing schemes [7], approximation algorithms for packing, covering, and augmentation problems [10] up to an additive constant, as well as a PTAS for the well-known Traveling Salesman Problem on bounded-treelength graphs [26]. Therefore, finding relations between both invariants might lead to extend the use of some of the above-mentioned algorithms to a larger class of graphs. In particular,

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this might be beneficial to bounded-treelength graphs that are more common than bounded-treewidth graphs amongst the complex networks, but for which there seem to be less algorithmic applications. For instance, the graph of Autonomous Systems has large treewidth, while it is *hyperbolic* [1, 14], and so, it has bounded treelength [9].

Another advantage of relating treewidth and treelength is that such relations can improve the best-known complexities for their computation on certain graph classes. Indeed, despite the fact that treewidth and treelength are both NP-hard to compute [3, 28], treelength seems much easier to approximate than treewidth. Namely, there are 3-approximation algorithms for treelength that rely on a few breadth-first-searches [20], while the best known approximation algorithms for treewidth only achieve a ratio $\mathcal{O}(\sqrt{\log tw(G)})$ for general graphs —and a constant-ratio for minor-free graphs— through the use of semi-definite programming [22]. We thus highlight that by relating treelength with treewidth, one can obtain practical algorithms for approximating the treewidth on certain graph classes.

1.1. State of the art. To put our contributions in context, let it be said that treewidth and treelength are uncomparable in general. This fact prevents from expecting simple relations between both invariants.

On the one hand, it comes from the fact that the cycle C_n, with $n \geq 4$ vertices, satisfies that $tw(C_n) = 2$ while $tl(C_n) = \lceil n/3 \rfloor$. This suggests that having a large treelength relies on the existence of long cycles in the graph. The authors in [20] supported this intuition, proving that the treelength of a graph G is bounded from above by half of the maximum length of a chordless cycle in G. Yet it is a strong constraint, as seen with the case of the wheel W_n which contains an induced C_n while it has treelength ≤ 2. Therefore, it is natural to constrain ourselves to the subcase of *isometric* cycles in graphs. We remind that a subgraph H of G is isometric if for any two vertices of H, the distance between them is the same in H as in G. Note that it is known how to compute a longest isometric cycle in a graph in polynomial-time [27]. Unfortunately, there are graphs such as grids with bounded-length isometric cycles and arbitrarily large treelength. As we will show below, our results imply that in such a case, we always have that $tl(G) = \mathcal{O}(tw(G))$.

On the other hand, the complete graph with n vertices has treewidth $n-1$ and treelength 1. Another interesting example is the graph H obtained by adding a universal vertex to a square-grid with n^2 vertices, for which it holds $tw(H) = n+1$ and $tl(H) = 2$. Note that such graphs have a large *genus*, *i.e.*, they are in a sense arbitrarily far from planar graphs. In contrast, it holds that $tw(G) < 12 \cdot tl(G)$ for planar graphs [17]. Consequently, it is quite natural to ask whether a treewidth arbitrarily larger than the treelength requires a large genus. We will prove it is the case, *i.e.*, $tw(G) = \mathcal{O}(tl(G))$ for bounded-genus graphs.

Finally, and independently from this work, Belmonte et al. [5] proved that $tw(G) = \mathcal{O}(\Delta^{tl(G)})$ for any graph G with *maximum degree* Δ. They built upon this relation in order to design a fixed-parameter-tractable algorithm to compute the metric dimension on bounded treelength graphs. We will use different techniques in order to upper-bound the treewidth with linear dependency on the treelength.

1.2. Our contributions. We introduce a very generic method to upper-bound the *diameter*[1] of *minimal separators* in graphs, the latter denoting inclusion wise minimal subsets whose removal disconnects some fixed pair of vertices. Let us emphasize

[1]The *diameter* of a set S of vertices of a graph G is the maximum distance in G between two vertices in S.

that the minimal separators are at the cornerstone of various graph decompositions, such as the so-called k-connected decompositions [24]. Therefore, our method may find applications beyond the scope of tree-decompositions.

In a few more details, we prove that minimal separators in a graph G induce connected subsets in some of its powers G^j, where j only depends on the length of cycles in some arbitrary *cycle basis* of G (see Section 2 for a formal definition). We deduce from our method that, for any graph G with longest isometric cycle of size $\ell(G)$, and for any minimal separator S in G, the diameter of S is at most $\lfloor \ell(G)/2 \rfloor \cdot (|S|-1)$ and the upper-bound is sharp as shown by any cycle.

Then, we prove that for any graph G which is not a tree, $tl(G) \leq \lfloor \ell(G)/2 \rfloor \cdot (tw(G)-1)$. This upper-bound on treelength follows from our upper-bound on the diameter of minimal separators, and it is tight up to a small constant-factor [2]. We refine our bound in several particular graph classes (the formal definition of these classes are postponed to the technical sections of the paper).

- For any graph G in the class of null-homotopic graphs (including the class of dismantlable graphs), we prove that $tl(G) \leq tw(G)$. This is tight, as one can easily see on trees.
- In the class of graphs G that admit a distance preserving elimination ordering, we prove that $tl(G) < 2 \cdot tw(G)$.

We emphasize that the latter class contains the cobipartite graphs. Though the treelength of cobipartite graphs is trivially bounded by 3, computing their treewidth is an NP-hard problem. As a consequence, the treewidth of graphs that admit a distance preserving elimination ordering is also NP-hard to compute. Our results combined with the 3-approximation algorithm for treelength [20] provide a polynomial-time algorithm for computing a new non-trivial lower-bound for treewidth.

Finally, we consider lower-bounds for treelength. We prove that, for any graph excluding an *apex graph* H as a minor, there is a constant c_H such that $tw(G) \leq c_H \cdot tl(G)$. The constant c_H only depends on H. Our proofs in this part make use of the bidimensionality theory [15]. In the particular case of graphs with bounded genus $g > 0$, we use results from this theory so as to prove the more precise relation $tw(G) \leq 72\sqrt{2}(g+1)^{\frac{3}{2}} \cdot tl(G) + \mathcal{O}(g^2)$.

So, to sum up, we obtain that *any* approximation algorithm for treelength can be turned into an approximation algorithm for treewidth up to multiplying by an $\mathcal{O}(\ell(G) \cdot (g+1)^{\frac{3}{2}})$ the approximation ratio.

2. Preliminaries.

In this section, we recall some useful definitions and known results that will be used in the sequel. All graphs considered in this paper are simple (*i.e.*, without loops or multiple edges), connected and finite. Given a graph $G = (V, E)$, the number $|V|$ of vertices will be denoted by n and the number of edges $|E|$ by m. For any vertex $v \in V$, let $N_G(v) = \{u \in V \mid \{u, v\} \in E\}$ be the set of neighbors of v in G. Let $N_G[v]$ denote $N_G(v) \cup \{v\}$.

Minimal separators. A set $S \subseteq V$ is a *minimal separator* if there exist $a, b \in V \setminus S$ such that any path from a to b intersects S and, for any proper subset $S' \subset S$, there is a path from a to b which does not intersect S'. We name any such a set S an a-b

[2]Recently and independently of this work (see research report in [12]), Diestel and Muller [19] proved that $tl(G) \leq \ell(G) \cdot (tw(G)-1)$ (see also [2] for a slightly looser bound). Note that our upper-bound for treelength is sharper than theirs. Furthermore, unlike our results which apply to any minimal separator in a graph, theirs rely on minimal separators in a specific tree-decomposition called an atomic tree-decomposition.

minimal separator. A connected component $C \subseteq V \setminus S$ of $G[V \setminus S]$ is *full* with respect to S if every node in S has a neighbour in C. Any a-b minimal separator has at least two full components: the one containing a and the one containing b. Conversely, any separator having at least two full components is a minimal separator. A graph is said *well-connected* if each of its minimal separators induces a connected subgraph [21].

Cycle space. The set $\mathcal{C}(G)$ of Eulerian subgraphs of G is called the *cycle space* of G. It is well-known that every Eulerian subgraph can be obtained from the symmetric difference (on the edges) of cycles in G. In fact, the set $\mathcal{C}(G)$ with the symmetric difference is a vector space of dimension $m-n+1$ if G is connected[18, Theorem 1.9.6]. We will call the symmetric difference of two subgraphs H_1, H_2, denoted $H_1 \oplus H_2$, the *sum* of H_1 with H_2. A cycle basis is an inclusion wise minimal set of cycles generating the whole cycle space In particular, a graph is said *null-homotopic* if it has a cycle basis with only triangles.

THEOREM 2.1. *[21] Any connected null-homotopic graph is well-connected.*

In this paper, we will extend the class of null-homotopic graphs as follows.

DEFINITION 2.2. *Let $l \geq 3$. We define $\mathcal{G}_l$ as the class of graphs whose cycle space can be generated by cycles of length at most l.*

Note that $\mathcal{G}_3$ is exactly the class of null-homotopic graphs. Moreover, the isometric cycles in a graph can generate its cycle space [25] (see also Exercice 1.32 of the textbook [18]), so the class $\mathcal{G}_l$ contains all graphs with no isometric cycle longer than l. Therefore by varying the parameter l, classes $\mathcal{G}_l$ include all graphs and they form an inclusion wise increasing hierarchy. By [11], the smallest integer $l \geq 3$ such that a graph belongs to $\mathcal{G}_l$ can be computed in polynomial-time.

Diameter and Graph powers.. For any $X \subseteq V$, let $diam_G(X)$ denote the maximum distance in G between any pair of vertices in X, *a.k.a.* the *diameter* of X. Last, for any $j \geq 1$, the graph G^j is obtained from G by adding an edge between any two distinct nodes that are at distance at most j in G.

2.1. Tree-decompositions.

Minimal fill-in. A graph is *chordal* if all its induced cycles have length at most 3. For any graph $G = (V, E)$, we define a *fill-in* of G as any chordal supergraph $H = (V, E \cup F)$ of G [3]. A fill-in $H = (V, E \cup F)$ is *minimal* if, for any $f \in F$, the graph $H' = (V, E \cup F \setminus \{f\})$ is not chordal.
Let H be a fill-in of a graph G, and let V_C be the set of maximal cliques of H. A *clique-tree* of H is a tree $T_C = (V_C, F)$ such that for each vertex $x \in V$, the set of maximal cliques containing x induces a subtree of T_C. We define a (reduced) *tree-decomposition* of G as any clique-tree of an arbitrary fill-in of G. Equivalently, a tree-decomposition of G consists of a pair $(T, \mathcal{X})$ where T is a tree and $\mathcal{X} = (X_t)_{t \in V(T)}$ is a family of subsets of V, called *bags*, indexed by the nodes of T and that satisfies the following three properties.

1. $\bigcup_{t \in V(T)} X_t = V$;
2. for any $\{u, v\} \in E$, there is $t \in V(T)$ with $u, v \in X_t$;
3. for any $u \in V$, the set of bags containing u induces a subtree of T.

Tree-likeness invariants. Given a graph G, the *length* of a tree-decomposition $(T, \mathcal{X})$ equals the maximum diameter in G of its bags. The *treelength* of G, denoted by $tl(G)$, is the minimum length over all tree-decompositions of G. Equivalently, the treelength of G is the smallest integer j such that G^j contains a fill-in of G [28]. The *width* of $(T, \mathcal{X})$ equals the maximum size of its bags minus one. The *treewidth*

[3]Here we use the term fill-in to avoid confusion with planar triangulations.

of G, denoted by $tw(G)$, is the minimum width over all tree-decompositions of G. Equivalently, the treewidth of G is the minimum over all minimal fill-ins H of G of $\omega(H) - 1$, where $\omega(H)$ is the clique-number of H [6]. It can be checked that both invariants are *contraction-closed i.e.*, the contraction of an edge in the graph cannot increase its treewidth nor its treelength. We will often use the fact that treewidth and treelength are contraction-closed invariants in the following.

Parallel minimal separators. Finally, let S_1, S_2 be two minimal separators in a graph G. The separator S_1 *crosses* S_2 if there are two components of $G \setminus S_2$ that S_1 intersects. If S_1 does not cross S_2, then S_1 is said to be *parallel* to S_2.

THEOREM 2.3. *[30] H is a minimal fill-in of the graph G if and only if H is obtained by completing*[4] *all sets of a maximal set of pairwise parallel minimal separators in G.*

3. Diameter of Minimal Separators in Graphs.

In this section, we show the diameter of any minimal separator S in a graph G is $\mathcal{O}(\ell(G) \cdot |S|)$, where $\ell(G)$ is the length of a longest isometric cycle in G (Theorem 3.4). We then strengthen our results in particular graph classes that are defined by the existence of some *elimination ordering* of their vertices.

Before going into the details of the proof, let us describe the main intuition behind it and the difficulties we had to face on. Let us consider a minimal separator S. If it is connected, then the result easily follows. Hence, we may assume S consists of several connected components. The idea is to find a set of paths, each of length at most $\lfloor \ell(G)/2 \rfloor$, such that any of these paths connects two components and the subgraph induced by S and these paths is connected. If we do so, the result easily follows. Hence, the main difficulty is to find such paths. For this purpose, let us consider a minimum-length cycle crossing two components of S (such a cycle surely exists because there are at least two full components in $G \setminus S$). If this cycle is isometric, then the distance between the two components cannot exceed $\lfloor \ell(G)/2 \rfloor$. Otherwise, it means that there is a shortcut between two nodes of the cycle. However, this shortcut could intersect S more than once which does not help our purpose. The key point is that, using the shortcut, the initial cycle can be viewed as the combination (symmetric difference) of two cycles. This kind of local view can be generalized to a global one using our main tool, namely the cycle basis. Indeed, the initial cycle is actually the symmetric difference of a set of isometric cycles [25, 18]. Using this set, we can then prove our theorem.

3.1. Case of general graphs.

We start proving some properties of graphs in the class $\mathcal{G}_l$. This will lead us to the main result in this section (Theorem 3.4).

Let us first prove that the class $\mathcal{G}_l$ is stable under the following two operations.

LEMMA 3.1. *Let $l \geq 3$, the class $\mathcal{G}_l$ is stable under edge-contraction.*

Proof. Let $G \in \mathcal{G}_l$ with n vertices and m edges. W.l.o.g., G is connected. The dimension $dim(\mathcal{C}(G))$ of the cycle space $\mathcal{C}(G)$ is $s = m - n + 1$ ([18, Theorem 1.9.6]). Let $e \in E(G)$ such that e lies on $k \geq 0$ triangles in G. By contracting e, we loose one vertex and $k+1$ edges, the edge e and for each triangle which contains e we have to remove one of the resulting multi-edges. Hence, $dim(\mathcal{C}(G/e)) = dim(\mathcal{C}(G)) - k$. Let $\{C_1 \cdots, C_s\}$ be a basis of $\mathcal{C}(G)$ such that each C_i has length at most ℓ. Let $\{C'_1, \cdots, C'_t\}$ be the set of cycles in G/e which are obtained by contracting e on each C_i and by removing triangles that contain e from the list. Then $t \geq dim(\mathcal{C}(G/e)) = s - k$ (since at most k triangles have been removed) and each C'_i has length at most ℓ. We

[4]Completing a set of vertices is to make the set a clique.

show that $C'_1, \cdots, C'_t$ are linearly independent in $\mathcal{C}(G/e)$, which proves that they form a basis of $\mathcal{C}(G/e)$. For purpose of contradiction, let us assume that $C'_{i_1} \oplus \cdots \oplus C'_{i_r} = 0$ for $1 \leq i_1 < \cdots < i_r \leq s$, $r > 0$. Then $C_{i_1} \oplus \cdots \oplus C_{i_r}$ is either 0 or e. Therefore, the sum equals e since the C_{i_j}'s are linearly independent in $\mathcal{C}(G)$. This is a contradiction as $(V(G), \{e\})$ is not Eulerian.

Hence, since all cycles in the basis $\{C'_1, \cdots, C'_t\}$ have length at most ℓ, it implies that $G/e \in \mathcal{G}_l$. □

LEMMA 3.2. *Let G_1 and G_2 be two graphs such that $V(G_1) \cap V(G_2) = \{x, y\}$ and $E(G_1) \cap E(G_2) = \emptyset$, and let $G = G_1 \cup G_2 = (V(G_1) \cup V(G_2), E(G_1) \cup E(G_2))$. If $G_1, G_2 \in \mathcal{G}_l$ and $d_{G_1}(x, y) + d_{G_2}(x, y) \leq l$, then $G \in \mathcal{G}_l$.*

Proof. Let C be a cycle in G. We will prove that it is a sum of cycles of length at most l in G. If it is a cycle in G_1 (resp. in G_2), then we are done as it is the sum of cycles of length at most l by Definition 2.2. Else, it must contain the pair x, y and it can be decomposed into: a xy-path in G_1, and a xy-path in G_2. Let C_l be obtained from the union of a shortest xy-path in G_1 with a shortest xy-path in G_2. Note that C_l has length $d_{G_1}(x, y) + d_{G_2}(x, y) \leq l$ by the hypothesis. Furthermore, $H = C \oplus C_l$ is an Eulerian subgraph of G. Let H_1, H_2 be the respective subgraphs of H that are induced by the edges in G_1, G_2 (possibly empty). Note that $E(H_1) \cap E(H_2) = \emptyset$ by construction. We claim that both graphs H_1, H_2 are Eulerian subgraphs. Indeed, on the one hand the subsets $V(H_1) \setminus \{x, y\}, V(H_2) \setminus \{x, y\}$ are disjoint by the hypothesis and so, any vertex $\neq x, y$ in one of these graphs, say in H_1, has the same (even) degree in H_1 as in H. On the other hand, by construction each node amongst x, y is incident exactly to one edge in $E(C) \cap E(G_1)$ (resp. in $E(C) \cap E(G_2)$) and to one edge in $E(C_l) \cap E(G_1)$ (resp. in $E(C_l) \cap E(G_2)$). As a result, nodes x, y have degree either null or equal to 2 in H_1, and similarly they have degree either null or equal to 2 in H_2, which is even in both cases. Consequently, both H_1, H_2 are sums of cycles of length at most l by the hypothesis because they are respective Eulerian subgraphs of $G_1, G_2 \in \mathcal{G}_l$. Hence $H = H_1 \oplus H_2$ is also a sum of cycles of length at most l in G. This concludes the proof because $C = H \oplus C_l$. □

Then, we prove that for any graph $G \in \mathcal{G}_l$, every minimal separator in G must contain a pair of vertices that are at small distance to each other.

LEMMA 3.3. *Let $l \geq 3$, let $G \in \mathcal{G}_l$ and let S be a minimal separator in G. Either S is a cut-vertex, or there are two distinct nodes $x, y \in S$ such that $d_G(x, y) \leq \lfloor l/2 \rfloor$.*

Proof. Suppose that S does not consist of a single cut-vertex. If the subgraph induced by S contains at least one edge $\{x, y\}$, then we are done as in such case $d_G(x, y) = 1 \leq \lfloor \ell/2 \rfloor$. So, we assume that S is a stable set. Let A, B be two distinct full components of $G \setminus S$ and let $s, t \in S$ be two distinct vertices. By connectivity, there is an st-path P whose internal vertices are contained in A, and in the same way there is a st-path Q whose internal vertices are contained in B. Let C be a cycle composed of P and Q. Because $G \in \mathcal{G}_l$, there is some set $\mathcal{C}$ of cycles of length at most ℓ whose sum equals C. We claim that there is a cycle $C' \in \mathcal{C}$ which intersects both A and another component of $G \setminus S$. Otherwise, because S is a stable set, the sum of all cycles that intersect A must generate P. This is not possible, since it is not Eulerian. As S separates the components, there are $x, y \in S \cap V(C')$ and so, since the length of C' is at most ℓ, we deduce that $d_G(x, y) \leq \lfloor \ell/2 \rfloor$. □

Finally, we can prove Theorem 3.4 and Corollary 3.5 below. Intuitively, we consider a pair of nodes $x, y \in S$, where S is a minimal separator in some graph $G \in \mathcal{G}_l$. If x, y are connected in the induced subgraph $G[S]$, then it is clear that their distance in G is at most $|S| - 1$. Else, we prove that there is a xy-path that intersects the connected components $C_1, C_2, \ldots, C_k$ of $G[S]$ consecutively, and that satisfies: $x \in C_1, y \in C_k$, and $\forall 1 \leq i < k$, there exists a cycle of length at most l which intersects both C_i and C_{i+1}. Every two consecutive components C_i, C_{i+1} of $G[S]$ are thus at distance at most $\lfloor l/2 \rfloor$ in G, hence their union $C_i \cup C_{i+1}$ induces a connected subgraph of the power $G^{\lfloor l/2 \rfloor}$.

THEOREM 3.4. *Let $l \geq 3$. For any graph $G \in \mathcal{G}_l$, every minimal separator in G induces a connected subgraph in the power $G^{\lfloor l/2 \rfloor}$.*

Proof. By contradiction, let $G \in \mathcal{G}_l$, and let S be a minimal separator in G that does not satisfy the property. We first make adjacent every two vertices in S that are at distance at most $\lfloor l/2 \rfloor$ in G. We claim that the resulting graph is still in $\mathcal{G}_l$. Indeed, let $x, y \in S$ be non-adjacent and at distance at most $\lfloor l/2 \rfloor$ in G, let $G_1 = G$ and let G_2 be the complete graph on the two vertices x, y (i.e., G_2 is isomorphic to K_2). Since we have that $G_1 \in \mathcal{G}_l$ by the hypothesis, that $G_2 \in \mathcal{G}_3 \subseteq \mathcal{G}_l$ and that $d_{G_1}(x, y) + d_{G_2}(x, y) \leq \lfloor l/2 \rfloor + 1 \leq l$, then we deduce from Lemma 3.2 that $G_1 \cup G_2 \in \mathcal{G}_l$. The same argument can be applied iteratively because adding an edge in G cannot increase the distances between nodes in S. So, the claim is proved. Finally, we contract each connected component of the subgraph induced by S in a single node, thus contracting S to obtain a stable set S', and the resulting graph G' still belongs to $\mathcal{G}_l$ by Lemma 3.1. Furthermore, the stable set S' is a minimal separator in G' by construction. Since S does not satisfy the property of the theorem, we have that all nodes in S' are pairwise at distance at least $\lfloor l/2 \rfloor + 1$, but then it contradicts Lemma 3.3. □

Theorem 3.4 is tight, as it can be shown with any cycle C_l.

COROLLARY 3.5. *Let G be a graph that is not a tree. Any minimal separator S in G has diameter at most $\lfloor \ell(G)/2 \rfloor \cdot (|S| - 1)$, where $\ell(G)$ denotes the length of a longest isometric cycle in G.*

Proof. It follows from Theorem 3.4 combined with the fact that isometric cycles generate the cycle space [25, 18]. □

3.2. Graphs with distance-preserving elimination ordering. We strengthen the result of Corollary 3.5 in the case of graphs with a distance-preserving elimination ordering. Formally, we say that G admits a *distance-preserving elimination ordering* if there exists a total order of V, denoted by $v_1, v_2, \ldots, v_n$, such that, for any $1 \leq i \leq n$, the subgraph $G_i = G \setminus \{v_1, \ldots, v_i\}$ is isometric. Graphs with a distance-preserving elimination ordering arise from applications in graph searching (*e.g.*, dismantlable graphs [29]) and geometry [8]. Note that they contain the class of cobipartite graphs, for which computing the treewidth is NP-hard. Our main result in this section is that for every graph G with a distance-preserving elimination ordering, it holds that $G \in \mathcal{G}_4$.

PROPOSITION 3.6. *A graph G that admits a distance-preserving elimination ordering has its cycle space generated by all its triangles and quadrangles.*

Proof. We claim that it is enough to prove that the induced cycles of G can be generated by all its triangles and quadrangles. Indeed, the induced cycles of G generate its cycle space [18]. Let $v_1, v_2, \ldots, v_n$ be a distance-preserving elimination ordering of G. By contradiction, amongst all induced cycles that do not satisfy the property let C maximize the smallest index j such that $v_j \in C$. Note that C is a cycle of $G_{j-1} = G[\{v_j, \cdots, v_n\}]$ by the hypothesis. Moreover, all cycles contained in G_j are the sum of triangles and quadrangles of G because of the maximality of index j. Let $x, y \in V(C)$ be the two neighbours of v_j in cycle C. By the hypothesis, x, y are not adjacent because C is induced. So, because $x, y, v_j \in G_{j-1}$ which has a distance-preserving elimination ordering, there is $v_i, i > j$ such that x, y are adjacent to v_i. Moreover, $v_i \notin C$ because otherwise C would be the quadrangle (v_j, x, v_i, y, v_j), thus contradicting the fact that it does not satisfy the property. As a result, $C = Q \oplus C'$, with Q the quadrangle (v_j, x, v_i, y, v_j) and C' is the cycle of G_j obtained from C by replacing the path x, v_j, y with x, v_i, y. Furthermore, cycle C' is a sum of induced cycles of G_j that are themselves a sum of triangles and quadrangles by maximality of j. Hence so is cycle C, which contradicts the fact that it does not satisfy the property. □

Corollary 3.7. *Let G be a graph that admits a distance-preserving elimination ordering. Every minimal separator S in G has diameter at most $2 \cdot (|S| - 1)$.*

Given that the cycle of length four C_4 admits a distance-preserving elimination ordering, one can see that Corollary 3.7 is sharp.

Dismantlable graphs are an interesting subclass of graphs with a distance-preserving elimination ordering. Formally, a graph G is dismantlable if, for any $1 \leq i < n$, there exists $j > i$, such that $N_G[u_i] \setminus \{u_1, \cdots, u_{i-1}\} \subseteq N_G[u_j]$. It is immediate that if a graph is dismantlable, then it admits a distance-preserving elimination ordering. We obtain the following improvement over Proposition 3.6 for the subclass of dismantlable graphs.

Lemma 3.8. *A dismantlable graph is null-homotopic and so, well-connected.*

Proof. Let G be a dismantlable graph. We prove that cycles of G can be generated by its triangles, which proves that G is null-homotopic. The fact that G is well-connected follows from the fact that dismantlable graphs are connected and from Theorem 2.1.

It is enough to prove that all induced cycles can be generated by triangles. Let $(u_1, u_2, \ldots, u_n)$ be a dismantling ordering of G. By contradiction, amongst all induced cycles that do not satisfy the property, let C maximize the smallest index j such that $u_j \in C$. Let $x, y \in V(C)$ be the two neighbours of u_j in cycle C, and let u_i, with $i > j$, be a dominator of u_j in G_{j-1}. We have that $u_i \notin C$ because C is induced and it has length at least 4 by the hypothesis. As a result, $C = T_1 \oplus T_2 \oplus C'$, with T_1 the triangle induced by nodes u_i, x, u_j; with T_2 the triangle induced by nodes u_i, y, u_j; and with C' a cycle of G_j obtained from C by replacing the path x, u_j, y with x, u_i, y. Furthermore, cycle C' is a sum of induced cycles of G_j that are themselves a sum of triangles of G by maximality of j. Hence, so is cycle C, which contradicts the fact that it does not satisfy the property. □

We note that it was already noticed in [21] that dismantlable graphs are null-homotopic. However the proof was left to the reader. We give it in the paper for self-containment.

Corollary 3.9. *Let G be a dismantlable graph. Every minimal separator S in G has diameter at most $|S| - 1$.*

Last, we point out that by a result from [4], *every* graph is an isometric subgraph of some dismantlable graph. Therefore, there are graphs with arbitrarily long isometric cycles that admit a distance-preserving elimination ordering.

4. Relating treewidth with treelength.

4.1. Upper-bounds for treelength. Using the results recalled in Section 2.1, we are now able to upper-bound the treelength of a graph by a linear function depending on the size of its minimal separators. We then show that the treelength of a graph is upper-bounded by a function that is linear in its treewidth.

LEMMA 4.1. *Let G be a graph and $\mathcal{S}$ be a maximal set of pairwise parallel minimal separators in G. If there is a constant $c_{\mathcal{S}}$ such that $diam_G(S) \leq c_{\mathcal{S}}(|S|-1)$ for all $S \in \mathcal{S}$, then $tl(G) \leq \max \{1\} \cup \{c_{\mathcal{S}} \cdot (|S|-1) \mid S \in \mathcal{S}\}$.*

Proof. Let H be the supergraph of G obtained by completing all sets of $\mathcal{S}$. By Theorem 2.3, H is a minimal fill-in of G. Moreover, any clique-tree T_C of H corresponds to a reduced tree-decomposition of G where each clique of H induces a bag. Let Ω be any maximal clique in H, i.e., Ω is any bag of the tree-decomposition T_C. Let $x, y \in \Omega$. By definition of H, either $\{x, y\} \in E(G)$ or there is a minimal separator $S \in \mathcal{S}$ that contains both x and y. In the latter case, $d(x, y) \leq diam_G(S) \leq c_{\mathcal{S}} \cdot (|S|-1)$. ☐

THEOREM 4.2. *If every minimal separator in a graph G induces a connected subgraph in its power G^j, then $tl(G) \leq \max \{1, j \cdot (tw(G)-1)\}$.*

Proof. Let H be a minimal fill-in of G with maximum clique-size $tw(G)+1$. By Theorem 2.3, there is a maximal set $\mathcal{S}$ of pairwise parallel minimal separators of G such that H results from the completion of all elements in $\mathcal{S}$. Note that any $S \in \mathcal{S}$ induces a minimal separator in H that is a clique —*a.k.a.* a clique-minimal separator in H— and therefore S is strictly contained in a maximal clique in H. Hence, $\max_{S \in \mathcal{S}} |S| \leq tw(G)$. By Lemma 4.1, $tl(G) \leq \max \{1\} \cup \{j \cdot (|S|-1) \mid S \in \mathcal{S}\} \leq \max \{1, j \cdot (tw(G)-1)\}$. ☐

COROLLARY 4.3. *Let G be a connected graph which is not a tree, then $tl(G) \leq c_G \cdot (tw(G)-1)$, where:*

- *$c_G = 2$ if G admits a distance-preserving elimination ordering;*
- *$c_G = \lfloor \ell(G)/2 \rfloor$, with $\ell(G)$ the length of a longest isometric cycle in G.*

Proof. First item follows from Proposition 3.6 combined with Theorem 3.4 and Theorem 4.2. Second item follows from Theorem 3.4 combined with Theorem 4.2. ☐

We emphasize that it is NP-hard to compute the treelength of a graph [28], but there exist 3-approximation algorithms to compute it in polynomial-time [20]. Moreover, a longest isometric cycle in a graph can also be computed in polynomial-time [27]. Hence, the previous result gives a new way to compute lower-bounds for treewidth.

4.2. Lower-bound in case of bounded-genus graphs. In this section, we prove that the treewidth of a graph is upper-bounded by a function of its treelength and of its genus. Our result is mainly based on the result from [16] stating that any graph with large treewidth and genus contains a large "grid-like" graph as a contraction. We use their terminology.

Let us remind that a planar triangulation of a planar graph G is a planar supergraph of G whose faces are bounded by triangles. A *partially triangulated $(r \times r)$-grid* is any graph that contains an $(r \times r)$-grid as a subgraph and is a subgraph of some planar triangulation of the same $(r \times r)$-grid. A *(r, k)-gridoid* G is a partially triangulated $(r \times r)$-grid in which k extra edges have been added[5].

THEOREM 4.4. *[16] Let G be a graph with genus g and $tw(G) > 4k(g+1)$ with $k \geq 12g$, then G contains a $(k-12g, g)$-gridoid as a contraction.*

We prove that such a gridoid has large treelength and so, since the treelength is contraction-closed, such a graph has large treelength too.

LEMMA 4.5. *Let G be a partially triangulated $(r \times r)$-grid, then $tl(G) \geq \lfloor r/3 \rfloor - 1$.*

[5]Note that the notion of (r, k)-gridoid is more general in [16].

Proof. The result holds if $r \leq 3$ because in such a case $tl(G) \geq 1 \geq \lfloor r/3 \rfloor - 1$. Else, let G' be the $(r \times r)$-grid from which G is obtained by planar triangulation. Let V' be the set of vertices that are at distance at least $\left\lfloor \frac{r-1}{3} \right\rfloor$ from the external face of G'. The vertices of V' induce a partially triangulated $(r' \times r')$-grid F in G, $r = 2\left\lfloor \frac{r-1}{3} \right\rfloor + r'$, such that the external face has not been triangulated. Moreover, F is isometric in G. Hence, $tl(G) \geq tl(F)$. We show that $tl(F) \geq \lfloor r/3 \rfloor - 1$.

Our proof adapts from the lower-bound techniques in [20, Sec. 2.3]. Let $(T, \mathcal{X})$ be any tree-decomposition of F. Consider the two subsets of vertices A, B that contain the first and the last row of F respectively. Since A induces a connected subgraph of F, by the properties of tree-decompositions the bags in $\mathcal{X}$ that intersect A form a subtree T_A of T. Similarly, the bags in $\mathcal{X}$ that intersect B form a subtree T_B of T. Furthermore, either $T_A \cap T_B \neq \emptyset$ (in which case, the diameter of every bag in $T_A \cap T_B$ is at least $r' - 1$), or by [20, Lemma 5] there exists a bag which intersects all paths between A and B in F. In the latter case, such bag must intersect the first and last column of F, and so, it has diameter at least $r' - 1$. Therefore, $(T, \mathcal{X})$ has length at least $r' - 1$ in both cases, that proves that $tl(F) \geq r' - 1 \geq \lfloor r/3 \rfloor - 1$. □

LEMMA 4.6. *Let G be a (r,k)-gridoid, then $tl(G) > r/(18\sqrt{2k+1}) - 2$.*

Proof. The result holds if $r \leq 36\sqrt{2k+1}$ because in such case $tl(G) \geq 1 > r/(18\sqrt{2k+1}) - 2$. Hence, let us assume that $r > 36\sqrt{2k+1}$.

Let M be a set of at most k edges whose removal in G yields a partially triangulated $(r \times r)$-grid. Let $S = V(M)$ be the set of end-vertices of the edges of M. Note that $|S| \leq 2k$. Also, let G' be the $(r \times r)$-grid whose $G \setminus M$ is a partial planar triangulation. Let finally $4 \leq x \leq r$ be an integer. There are $(r - x + 1)^2$ distinct $(x \times x)$-grids as subgraphs in G', that give us as many distinct partially triangulated $(x \times x)$-grids as subgraphs in G. Furthermore, each node in S belongs to at most x^2 such subgraphs. Therefore assuming $(r - x + 1)^2 - 2k \cdot x^2 \geq 1$, there is one of these partially triangulated $(x \times x)$-grids, say H, that does not contain any node incident to one of the k extra edges. Consider the partially triangulated $(x' \times x')$-grid R which is in the center of H, with $x = 2 \cdot \left\lfloor \frac{x-1}{3} \right\rfloor + x'$. That is, R is a subgraph of H and any node of R is at distance at least $\left\lfloor \frac{x-1}{3} \right\rfloor$ from a node of $G \setminus H$ (it is possible because H does not contain an extremity of an extra edge). Therefore, R is isometric in G and $tl(R) \leq tl(G)$. By Lemma 4.5,

$$tl(R) \geq \lfloor x'/3 \rfloor - 1 \geq x/9 - 1.$$

It remains to maximize x satisfying the inequality $(r - x + 1)^2 - 2k \cdot x^2 \geq 1$ so that we maximize the above lower-bound for $tl(R)$. The polynomial

$$\begin{aligned}(r - X + 1)^2 - 2k \cdot X^2 - 1 &= r^2 + X^2 + 1 - 2r \cdot X + 2r - 2X - 2k \cdot X^2 - 1 \\ &= -\left[(2k-1) \cdot X^2 + 2(r+1) \cdot X - r(r+2)\right]\end{aligned}$$

has for reduced discriminant $(r+1)^2 + r(r+2)(2k-1) = 2k \cdot r(r+2) + 1$, hence its roots are equal to

$$\left\{ -\frac{\sqrt{2k \cdot r(r+2) + 1} + r + 1}{2k - 1}, \frac{\sqrt{2k \cdot r(r+2) + 1} - r - 1}{2k - 1} \right\}.$$

Since this polynomial is nonnegative only between its roots, the value maximizing x

is:

$$x_0 = \left\lfloor \frac{\sqrt{2k \cdot r(r+2)+1} - r - 1}{2k-1} \right\rfloor \geq \frac{\sqrt{2k \cdot r(r+2)+1} - r - 1}{2k-1} - 1 + \frac{1}{2k-1}$$
$$= \frac{r(r+2)}{\sqrt{2k \cdot r(r+2)+1} + r + 1} - 1 + \frac{1}{2k-1} > \frac{r(r+2)}{2\sqrt{2k \cdot r(r+2)+1}} - 1$$
$$> \frac{1}{2}\sqrt{\frac{r(r+2)}{2k+1}} - 1 > \frac{r}{2\sqrt{2k+1}} - 1.$$

Hence, $tl(G) \geq tl(R) \geq x_0/9 - 1 \geq r/(18\sqrt{2k+1}) - 2$. □

THEOREM 4.7. *Let G be a graph with genus g and $tw(G) > 4k(g+1)$ with $k \geq 12g$. Then*

$$tw(G) \leq 72\sqrt{2}(g+1)^{\frac{3}{2}} \cdot tl(G) + \mathcal{O}(g^2).$$

Proof. By Theorem 4.4, G contains a $(k-12g, g)$-gridoid R as a contraction. By Lemma 4.6,

$$tl(R) > \frac{k-12g}{18\sqrt{2g+1}} - 2.$$

Thus, by setting $k = (tw(G)-1)/(4(g+1))$, we obtain that:

$$tl(R) > \frac{tw(G) - 48g(g+1) - 1}{72(g+1)\sqrt{2g+1}} - 2 > \frac{tw(G)}{72\sqrt{2}(g+1)^{\frac{3}{2}}} - \frac{\sqrt{2}}{3} \cdot \sqrt{g+1} - 3.$$

The result then follows from the fact that treelength is contraction-closed. □

Extensions.. Theorem 4.7 can be extended to the broader class of apex-minor-free graphs. An *apex graph* is a graph such that the removal of one vertex creates a planar graph. Similar techniques from the bidimensionality theory allow us to deal with graphs that exclude a fixed apex graph as a minor. Namely, we will make use of the graph Γ_k as it is defined in [23]. The graph Γ_k is obtained from a $(k \times k)$-grid by triangulating its internal faces such that all internal vertices become of degree 6, all non-corner external vertices are of degree 4, and then one corner of degree two is joined by edges with all vertices of the external face.

THEOREM 4.8. *[23] For every apex graph H, there is a constant $c_H > 0$ such that every connected H-minor-free graph of treewidth at least $c_H \cdot k$ contains Γ_k as a contraction.*

THEOREM 4.9. *Let H be any apex graph and G be a connected H-minor-free graph of treewidth at least $c_H \cdot k$, where c_H is the constant of Theorem 4.8. Then $tl(G) \geq tw(G)/(3 \cdot c_H) - 1$.*

Proof. By Theorem 4.8, G contains Γ_k as a contraction. Moreover, Γ_k is a partially triangulated grid. The result follows from Lemma 4.5 and the fact that treelength is contraction-closed. □

5. Conclusion. We can deduce from Corollary 3.5 and Theorem 4.7 that for every n-node graph of genus g, the 3-approximation algorithms for treelength in [20] compute in $\mathcal{O}(g \cdot n^2)$-time an integer t^* satisfying:

$$\frac{tw(G)}{72\sqrt{2}(g+1)^{\frac{3}{2}}} - \frac{\sqrt{2}}{3} \cdot \sqrt{g+1} - 3 \leq t^* \leq 3\lfloor \ell(G)/2 \rfloor \cdot tw(G).$$

Observe that in case an upper-bound on the treewidth is given, we can also deduce from our relations a lower-bound on the graph genus.

The main drawback with our above approximation algorithm for treewidth is that it may output a tree-decomposition with unbounded width (the length is upper-bounded by t^*). We let open whether our method can be modified so that it outputs a tree-decomposition of width $\mathcal{O}(\ell(G) \cdot (g+1)^{3/2} \cdot t^*)$.

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Papers on coloring games

Appendix I

The Complexity of Hedonic coalitions under bounded cooperation

The Complexity of Hedonic Coalitions under Bounded Cooperation [*]

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Abstract

We consider additively separable symmetric hedonic games, that are a specific type of hedonic coalition formation in which players value joining a given group solely based on its members. In graph-theoretic terms, the game is defined by an edge-weighted complete graph, and a configuration of the game is a vertex-partition of this graph. The utility of a given vertex v w.r.t. the configuration is the sum of the weights of the edges that are incident to v and another vertex in the same group as v. Then, given an integer $k \geq 1$, a better-response dynamics for the hedonic game previously mentioned consists in iterating the following operation, until it is no more possible to do so. We move at most k vertices to a same group of the partition, provided they all increase their utility in the process.

We study the complexity of deciding whether a given such game admits an equilibrium that is robust to coalition of at most k players, where k is a fixed constant. In some cases where an equilibrium is known to exist, referred to as *colouring games* in the literature, we also study the time of convergence of the better-response dynamics toward an equilibrium.

Our main result proves how even a minimal amount of cooperation between players makes finding the final outcome of such games prohibitively difficult. This applies even in the simpler case of colouring games, for which it was previously conjectured that the better-response dynamics always converge in polynomial time, while our tight analysis proves the opposite. Precisely, our main result is that, already for $k = 4$, the better-response dynamics for colouring games converges in $\Omega(n^{\Theta(\ln(n))})$ steps. Furthermore, we show that minimum addition to the simplest game reinforces this view, making the mere existence of a stable outcome prohibitively hard to decide. That is, when all edge weights are in a fixed subset $\mathcal{W}$, either an equilibrium always exists or it is NP-complete to decide on its existence.

While our results may be interpreted as a criticism of solution concepts involving bounded cooperation in general, we also present conditions (based on the edge weights) under which the complexity of this form of cooperation remains tractable.

Coloring games; Hedonic Games; Equilibrium computation; Better-response dynamics; Graph theory; NP-hardness; Social networks.

1 Introduction

We consider process by which players of a game choose to belong to a group solely based on the members that it contains, as a way to model multiple situations pertaining to creation of

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coalitions. Below we introduce a model that generalizes previous games and dynamics related to information sharing [22], graph colouring [11, 26], creation of clubs and societies [4, 8] referred to as Hedonic [13]. Roughly in *Hedonic Games*, the following natural assumption is made: a player's appreciation of a coalition structure only depends on the members of the coalition she belongs to, and not on how players in other coalitions are arranged [13]. Our goal, like multiple works before [3, 4, 8, 16, 24, 25, 31], is to determine the merit of a solution concept for revealing stable and meaningful structures as final outcome of this game. However, unlike previous studies, we carefully control the level of cooperation among players to see how it impacts the complexity of computing an equilibrium and the convergence of multiple better response dynamics.

We consider the effect of two important features, only found in [22]: *Incompatibility* between some pairs of players, in the form of arbitrarily high penalty, is here to ensure that the dynamics of the game always avoid cases where any such two players set are in the same coalition. *Bounded cooperation of size* k stipulates that a new set of coalitions can be formed whenever a subset containing at most k players can move simultaneously so that each player in the subset benefits from this move. Computing stable outcomes of this game for any value of k allows one to gradually compare configurations that are individually stable ($k = 1$) — and hence attainable as Nash Equilibrium of a non-cooperative dynamics — with those that satisfy a stronger notion of stability ($k > 1$). This eventually culminates (when k is equal to the number of players) in finding exactly the configurations that remain stable even against any coalition of players. Such configurations are sometimes referred to as strong Nash Equilibrium, coalition proof equilibrium, or core stable coalition, as they relate to those in the core of an associated cooperative game.

On the one hand, it seems intuitive that, when it comes to understand the formation of clubs or groups, a purely individually rational solution concept (corresponding to $k = 1$) is rather limiting. On the other hand, allowing cooperation between players is expected to increase dynamics' complexity. Prohibitive complexity does not only come as computational cost for prediction, it also casts a doubt that the solution concept represents well the outcome of a process of decisions made by players. We hence aim at determining the conditions under which this complexity remains tractable (*i.e.,* a final outcome is reached by the dynamics in a number of steps that grows no more than a polynomial function of the number of players, where ideally this polynomial function grows not too large). It appears that a limited form of cooperation (*i.e.,* $k < \infty$) helps to reduce complexity as long as k is chosen small enough. As an example, the authors in [22] show that for the simplest version of the game above (that we call uniform), simple dynamics converge in polynomial time when $k = 1, 2$ and 3. They also conjecture that a similar property extends when $k > 3$. In this article, we disprove the above conjecture and shows that $k = 3$ is the maximum level of cooperation ensuring polynomial convergence for simple dynamics. Furthermore if $k \leq 2$ our novel analysis does not only provide the first non-trivial lower bounds but it determines the exact worst case convergence time in a closed form.

1.1 Related work

The role of coalitions – and under which conditions on player's incentive those can be sustained – has been a premier theme of Game Theory since its beginning. Ever since, it has played a key role in determining the theoretical and practical merits of solution concepts [1, 6, 7, 23, 28]. Most of the earliest works center on situations in which utility can be transferred among players. That leads to the possibility of bargaining and hence reach specific equilibria (Nash, Core, Strong Nash) depending on the axioms applying to players' expected behavior in similar situations. With a slight simplification, one can summarize the role of cooperation among players in this context as a major factor increasing complexity: indeed, determining that a Nash equilibrium exists is often trivial, while being assured that an equilibrium exists that is stable under cooperation (*i.e.,* the core is non-empty) remains prohibitively difficult. In other words, expecting solution concepts with cooperations to be normative implies that players or analyst in general have access to infinite or at least very large computational powers to behave accordingly. The only general case with utility transfers where cooperation does not contradict stability and leads to predictable outcome is when the game is convex and the only stable coalition is one that contains all players.

Here, we wish to determine the impact of cooperation among players in a different context where utility cannot be transferred between players. The systematic study of those games has been more recent, motivated primarily by the need to determine how individual choices governed by constraints set on player's interaction lead to the formation of different types of cartels, alliances, clubs, interest groups. The studies of such groups and how users are connected through them in a network paved the way to a novel economic analysis where a player's position in a structure governs its expected behaviors and eventual gains. Most of the work concentrates on studying the outcomes of so called *Hedonic Games*. In the general case, a stable outcome may not exist, even for a weak definition of stability that only allows certain individual strategies [8]. This holds even when preferences among coalitions are anonymous (*i.e.,* the utility of a player only depends on the size of her group). This also holds if the preferences are additively separable (*i.e.,* they derive from a simple utility function that sums up the effects of pairwise interaction between a player and members of her coalition), as long as they are not required to be symmetric. Perhaps unsurprisingly, for stronger stability notion when cooperation among players – and hence possibly more deviations from a given status quo – are allowed to take place, those negative results are only reinforced. Only when additional properties constraining preferences are assumed (see *e.g.,* [5, 10, 20]) can it be shown that such solutions (core stable or strong Nash equilibrium) exist, and/or are unique [27].

The results we mention above judge the merit of solution concepts merely by existence, and occasionally by unicity of a stable outcome. More recently, merit of solution concepts were discussed using an algorithmic approach [12], by analyzing how the cost of deciding on the existence of a stable outcome, or computing one when it exists, grows with the number of players n. Indeed, all the negative results aforementioned were strenghtened in recent works: for hedonic games in general, even anonymous ones, deciding if a coalition system that satisfies a stability condition exists is NP-hard [4]. Those results were shown to hold when preferences are additively separable (in the assymmetric case) [24]; and more recently even when the parameters definining the preferences among coalitions are bounded by a polynomial function of n [30]. It is noteworthy that those negative results are each different, but one can be found for *any* stability condition, whether or not cooperation between players is allowed[1]. Similar NP-hardness results apply in general to solution concepts defined by efficiency instead of stability such as maximizing sum of utility, or satisfying Pareto optimality under weak conditions (as shown in [2]).

For hedonic games, the effect of players' cooperation is chiefly of interest in the case where preferences are additively separable and symmetric. The interesting situation is when players' preferences among coalitions are defined using parameters which are constant or bounded by a polynomial function of the number of players [2]. Under those natural conditions, depending on which cooperation is assumed the properties of solution concepts are entirely at odds. First, if one assumes that only individual deviation is allowed, outcomes are Nash or individually stable equilibrium of this game (see definition below). Those always exist and they can be always attained

[1]Note that here and in the rest of the paper we ignore the case where in order to move a player is required to get approval from members of his current coalition [29]. This leads, in the separable case and many others, to have almost all coalition structures being stable, and hence provide little insight into the game.

[2]Otherwise, it is already known that finding stable outcome is hard even without cooperation, as computing Nash or Individually stable equilibria requires solving a PLS complete problem [16]

using some better response dynamics of the game within a pseudopolynomial number of steps [8] — following a potential function argument. In contrast, when unrestricted cooperation is allowed between players, sustainable outcomes are only those that are so called core stable; such an outcome may not exist in general. In fact, deciding if one exists in general is NP-hard, as previously shown independently in [3] for a specific set of weights, a result that we prove in this article in a more general case. This chasm motivates us to answer more precisely which forms of cooperation renders stability so much complex. Are pairwise cooperation involving two players, or triadic cooperation involving three, sufficient to cause a sudden increase in complexity? We gradually increase the size of possible subsets of players acting in concert to create a new deviation, from a subset of size 1 denoting absence of coordination to size n denoting unrestricted cooperation.

The above question was recently formulated in [22] when preferences are additively separable, symmetric, and formulated to either denote a complete incompatibility between two players, or a benefit to share the same coalition that is uniform among compatible players. In this case, solution concepts involving simultaneous cooperation of at most 2 or 3 players are shown to be tractable for those particular hedonic games. This result is remarkable: it offers the first example of a solution concept involving some cooperation and that has not been shown to be computationally prohibitive. Unfortunately, this paper brings no more light to extend any such results to other hedonic games. Indeed the tractability of any form of cooperation involving more than 3 players is left open. Here we explain and show why this is the case. Furthermore, although it has been proposed a partial analysis beyond the case $k = 3$, where it is proved that the outcome can be NP-Hard to find in general, this negative result relies on a unique form of deviations (called *gossip*) introduced by the authors and that has no equivalent in the theory of hedonic games.

1.2 Contribution of this paper

The main contribution of this paper is to completely solve the complexity analysis of hedonic games for any level of cooperation, in the general case where preferences are additively separable and symmetric. This includes in particular a specific study of the effect of cooperation when the values taken by weights defining players' preferences are fixed in advance.

- We first consider the binary incompatible/compatible case (uniform), where all compatible players benefit from each other uniformly as introduced in [22] (the latter corresponds to the above-mentioned uniform case). We prove that in such case better response dynamics always converge to an equilibrium, for any possible level of cooperation. Hence we focus on the time of convergence for the dynamics. We report on our results in Table 1. Previous work focuses on upper-bounds on the number of steps. We provide not only the first non-trivial lower-bound but even derive the exact worst case of convergence time when only individual and pairwise deviations are allowed. This requires an entire new analysis of this problem connecting its dynamic to sand piles, which is of independent interest.

- By leveraging more properties of our novel analysis, we are able to prove that the complexity suddenly increases when groups of more than 3 players are allowed to coordinate to act simultaneously. This result solves an open conjecture from [22]. It is also remarkable as it proves that cooperation affects computational complexity in multiple stages as more and more players are allowed to coordinate. To the best of our knowledge, no such progressive phase transitions were ever identified.

  All our results on the uniform case are listed in Table 1.

- We then consider general hedonic games, and for the first time analyze them when cooperation among players is gradually increased. We start with a case where preferences follow incompatible/indifferent/compatible interactions among players. We first show that solution concepts for pairwise cooperation in this case can be computed efficiently. On the other hand, this result is tight in multiple ways: any amount of further cooperation or slightly more complex preferences is sufficient to impose a prohibitive cost to decide if a stable outcome exists in the general case. We present new sufficient conditions on preferences under which an outcome is found in polynomial time, but those remain stringent.

Those results present a new level of details to assess solution concepts for hedonic games. Under different assumptions on cooperation, it allows one to see which coalition systems are likely to form among players or, on the contrary, are unlikely to exist or be found using reasonable time and resources.

2 Hedonic Games and Stability

Let us first define colouring games in a formal way.

Network We model the network with an edge-weighted graph $G = (V, E, w)$, where V denotes the set of players. There are $n = |V|$ players in the network. Moreover, it is supposed to be a *simple* graph, hence there is no loop and no multiple edges. The weight w_{uv} is defined for every edge $uv \in E$ as the utility both u and v receive if they interact. Note that $w_{uv} = w_{vu}$ by symmetry. In the general case, $w_{uv} \in \mathbb{Z} \cup \{-\infty\}$. In other words, for any two vertices $u, v \in V$, if $w_{uv} = -\infty$ then the players are *enemies* and they never interact. Given the natural dominance of weight $-\infty$ over all the other ones, we also say that $\{uv\}$ is a *conflict edge* when $w_{uv} = -\infty$.

Sometimes, the set of possible weights may be constrained, and we will denote it $\mathcal{W}$. Also, missing edges in the graph can be added with weight 0; so, without loss of generality, we assume that G is a complete graph, and we will simply write $G = (V, w)$ in the sequel. As an example, Figure 1(a) depicts a network with $\mathcal{W} = \{-\infty, 2, 3, 4\}$. Conflict edges are represented with dashed red lines, while edges with positive weight are represented with solid green lines.

Groups and Utilities We suppose in our model that the players are *partitioned* into n ordered sharing groups, some of them may be empty. Such a partition of the nodes is denoted $P = (X_1, X_2, \ldots, X_n)$. For every node $u \in V$, we denote by $c_u(P) \in [\![1, n]\!]$ the index of the group containing u. In other words, $u \in X_c$, where $c = c_u(P)$. The integer c is the *colour* of u in P.

Figure 1 presents three different partitions of the nodes for a graph with $\mathcal{W} = \{-\infty, 2, 3, 4\}$. Each of them has three non-empty groups (and so three empty groups).

For a given P, the *utility* for the player $u \in V$ is defined as $f_u(P) = \sum_{v \in X_c \setminus \{u\}} w_{uv}$, where $c = c_u(P)$ denotes the sharing group in P which u belongs to. The global utility, or social welfare, is $f(P) = \sum_{u \in V} f_u(P)$. For the partition of Figure 1(a), the respective utilities of $u_1, u_2, u_3, v_1, v_2, v_3$ are $7, 4, 0, 4, 5, 6$ and the global utility is equal to 26.

Deviations Let P be any partition of the nodes. Given a coalition S with at most k players, we say that S is a *k-deviation*, or k-set, when all the players in S have an incentive to join the same (possibly empty) group in P, so that they *all* increase their individual utility in the process. This way, we aim at modeling situations where players can join a given group without any approval of its current members, *e.g.,* , public communities in social networks, etc. The following definition formalizes the notion of k-deviation.

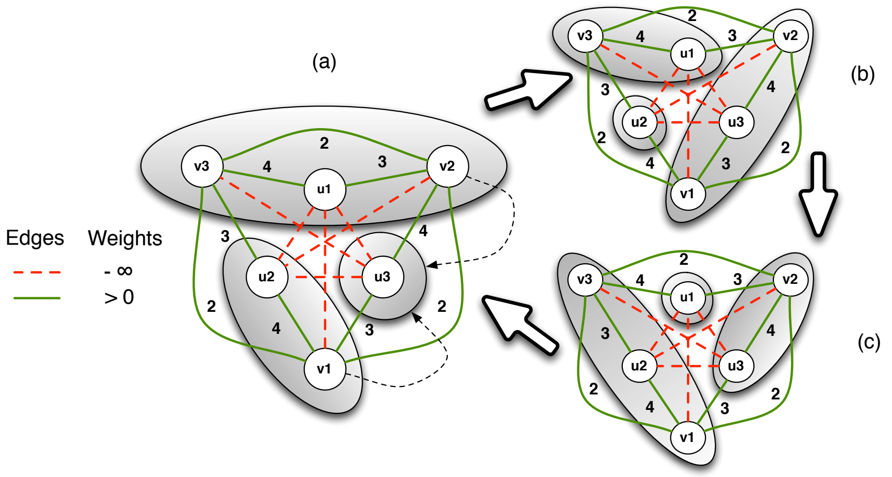

Figure 1: A network with set of weights $\mathcal{W} = \{-\infty, 2, 3, 4\}$ that does not admit a 2-stable partition. **(a)** 1-stable partition that is not 2-stable and that can be obtained after a 2-deviation in partition depicted in (c). **(b)** 1-stable partition that is not 2-stable and that can be obtained after a 2-deviation in partition depicted in (a). **(c)** 1-stable partition that is not 2-stable and that can be obtained after a 2-deviation in partition depicted in (b).

Definition 1 (k-deviation)**.** *Let $k \geq 1$ be any integer and let $P = (X_1, \ldots, X_n)$ be any partition of V. A k-deviation is defined as a pair (S, j), where $S \subseteq V$, $|S| \leq k$, $j \in [\![1, n]\!]$, such that the partition $P' = (X'_1, \ldots, X'_n)$, with $X'_i = X_i \setminus S$ if $i \neq j$ and $X'_j = X_j \cup S$ is such that $f_v(P') > f_v(P)$ for every $v \in S$.*

As an illustration, consider the partition $P = (\{v_3, u_1, v_2\}, \{u_3\}, \{u_2, v_1\}, \{\}, \{\}, \{\})$ of Figure 1(a). There exists a 2-deviation $(\{v_2, v_1\}, 2)$ because v_2 and v_1 have an incentive to join the singleton group $\{u_3\}$. We indicate it by dashed arrows. Let $P' = (\{v_3, u_1\}, \{v_2, u_3, v_1\}, \{u_2\}, \{\}, \{\}, \{\})$ be the partition obtained after the 2-deviation $(\{v_2, v_1\}, 2)$ *happens* (Figure 1(b)). Observe that $f_{v_1}(P') > f_{v_1}(P)$ and $f_{v_2}(P') > f_{v_2}(P)$. Note that there is no 1-deviation for the partition of Figure 1(a).

Stability Let $k \geq 1$ be any integer and let P be any partition of the nodes. We say that P is a k-stable partition if and only if there is no k-deviation.

As an illustration, the three different partitions depicted in Figure 1 are 1-stable. However, none of them is 2-stable. Indeed, there is 2-deviation for the partition of Figure 1(a) that permits to obtain the partition of Figure 1(b); there is 2-deviation for the partition of Figure 1(b) that permits to obtain the partition of Figure 1(c), and there is 2-deviation for the partition of Figure 1(c) that permits to obtain the partition of Figure 1(a). The arrows in Figure 1 describes this ”cycle” of partitions. It is possible to show for this graph, there is no 2-stable partition.

Dynamic of the game Players in the networks want to maximize their individual utility. Initially, none of them interact, and so, we only have singleton groups, that is $|X_j| = 1$ for every $j \in [\![1, n]\!]$. Then we fix a constant parameter $k \geq 1$, and the colouring game starts. At each round i, we consider the current partition P_i of the nodes. In particular, there are only singleton groups in P_0. When a k-deviation exists, we may allow any *one* of them to *happen* and, in so doing, we

Dynamic of the system (Algorithm 1)

Input: a positive integer $k \geq 1$, a set of weights $\mathcal{W}$, and a graph $G = (V, w)$.
Output: a partition k-stable for G.

```
1: Let $P_0$ be the partition composed of $n$ singletons groups.
2: Set $i = 0$.
3: while there exists a $k$-deviation for $P_i$ do
4:     Set $i = i + 1$.
5:     Compute the partition $P_i$ after any $k$-deviation.
6: return Partition $P_i$.
```

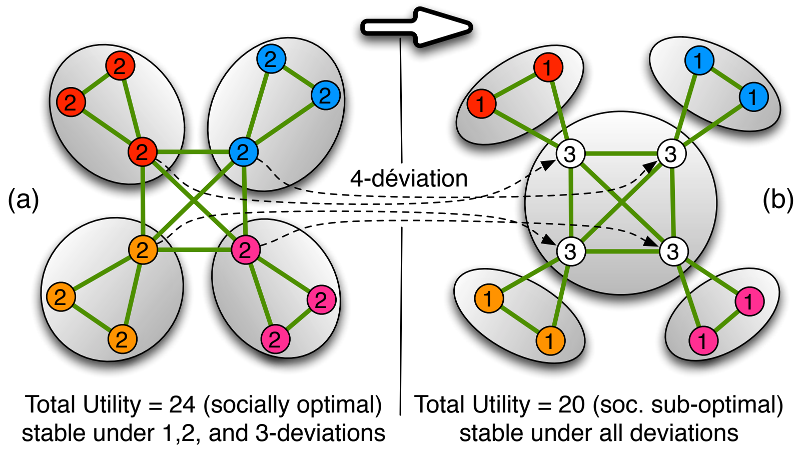
4-déviation
(a)
(b)
Total Utility = 24 (socially optimal)
stable under 1,2, and 3-deviations
Total Utility = 20 (soc. sub-optimal)
stable under all deviations

Figure 2: A network with set of weights $\mathcal{W} = \{-\infty, 1\}$. **(a)** 3-stable partition that is not 4-stable but it is optimal in terms of total utility. **(b)** k-stable partition for any $k \geq 1$ that is not optimal in terms of total utility.

break P_i, and we get a new partition P_{i+1}. If there is no k-deviation, the partition P_i is k-stable. An algorithmic presentation of the game is given in Algorithm 1.

For the graph of Figure 1, Algorithm 1 returns a k-stable partition if and only if $k = 1$ (otherwise the algorithm never ends because there is always a 2-deviation for this graph).

Example Consider the graph depicted in Figure 2 with $\mathcal{W} = \{-\infty, 1\}$. Figure 2(a) depicts a partition composed of 4 non-empty groups. The integers on the nodes represent their utilities. Observe that this partition is k-stable when $k \in \{1, 2, 3\}$. However, this partition is not 4-stable because there is a 4-deviation: the four central nodes can join an empty group (that corresponds to create a new group) and increase their utilities. The partition obtained after such a 4-deviation is depicted in Figure 2(b). This partition is k-stable for any $k \geq 1$. The utility of the four nodes that have joined the empty group is now 3 (instead of 2). However, the utility of the other nodes is now 1 (instead of 2). Thus, we deduce that this partition is not optimal in terms of total utility (the total utility has decreased from 24 to 20); but it is now stable under all deviations.

We will discuss in Section 5 several extensions of the model. We will show that most of our results still hold for these more general games.

3 The uniform case: are longest deviation sequences polynomial?

A colouring game is said *uniform* if, except for conflict edges, all edges have the same unit weight *i.e.,* $\mathcal{W} = \{-\infty, 1\}$. This game is entirely characterized by an unweighted and undirected *conflict graph* $G^- = (V, E)$ that contains all the conflict edges[3]. The complementary graph of G^- represents all the pairs of friends (with unit weight). Note also that given a partition P, for any player u, the individual utility $f_u(P)$ equals $|X_c| - 1$ with $c = c_u(P)$, which is how many players have the same colour as u. Recall that we only consider partition such that any two enemies do not belong to a same group. As shown in [15, 22] k-stable partitions always exist for any value of k. Their proof is algorithmic, but it does not compute a k-stable partition in polynomial-time *even if k is fixed.* As a first step toward a polynomial-time computation, we now prove that the better-response dynamic always terminates. Hence, the problem of computing a k-stable partition —in the uniform case— is in the complexity class PLS, for any fixed k (*e.g.,* see [19]).

In the following, given a partition P we define $\lambda_i(P)$ to be the number of groups of size i, and we denote by $\overrightarrow{\Lambda}(P) = (\lambda_n(P), \ldots, \lambda_1(P))$ the *partition vector.*

Lemma 2. *For any $k \geq 1$, for any conflict graph G^-, Algorithm 1 converges to a k-stable partition.*

Proof. Let P_i, P_{i+1} be two partitions for G^- such that P_{i+1} is obtained from P_i after a k-deviation. We prove that $\overrightarrow{\Lambda}(P_i) <_L \overrightarrow{\Lambda}(P_{i+1})$ where $<_L$ is the lexicographical ordering. To do so, let (S, j) be the k-deviation which breaks P_i. By definition, for any $u \in S$, we have $f_u(P_i) < f_u(P_{i+1})$. Furthermore the size of the group X_j has increased by $|S|$. Therefore, no vertex of S was in a group of size at least $|X_j| + |S|$ in P_i. Thus, we get $\overrightarrow{\Delta} = \overrightarrow{\Lambda}(P_{i+1}) - \overrightarrow{\Lambda}(P_i) = (0, \ldots, 0, \Delta_{|X_j|+|S|} = 1, \ldots)$, and so $\overrightarrow{\Lambda}(P_i) <_L \overrightarrow{\Lambda}(P_{i+1})$. Finally, as the number of possible vectors is finite, we obtain the convergence of Algorithm 1. $\square$

We can then define $L(k, n)$ as the size of a longest sequence of k-deviations among all the colouring games defined on a conflict graph with (at most) n nodes.

Let $G^\emptyset$ be the empty conflict graph. An instrumental observation for our next proofs is that:

Observation 1. *$L(k, n)$ is always attained in the colouring game defined on the empty conflict graph $G^\emptyset$ of order n, containing no conflict edges.*

Prior to this work, no lower bound on $L(k, n)$ was known, and the analysis was limited to potential function that only applies when $k = 1, 2,$ and 3 [15, 22]. The analysis of the game becomes much more difficult as soon as 4-deviations are allowed. Table 1 summarizes our contributions:

Table 1: Previous Bounds and results we obtained on $L(k, n)$.

k	Prior to our work	**Our results**	
1	$O(n^2)$ [22]	exact analysis, which implies $L(k,n) \sim \frac{(2n)^{3/2}}{3}$	Theorem 8
2	$O(n^2)$ [22]	exact analysis, which implies $L(k,n) \sim \frac{(2n)^{3/2}}{3}$	Theorem 9
3	$O(n^3)$ [15, 22]	$\Omega(n^2)$	Theorem 12
≥ 4	$O(2^n)$ [22]	$\Omega(n^{\Theta(\ln(n))})$, $O(\exp(\pi\sqrt{2n/3})/n)$	Theorem 13

[3]The reader may wonder why we consider the conflict graph rather than the *friendship graph*: which is induced by the edges with unit weight. Our choice is motivated by the usual terminology for colouring games [22, 26], and because the conflict graph is the best suited to show the link between equilibria and vertex colouring.

3.1 Exact analysis for $\mathbf{k \leq 2}$

In [22], the authors proved that the global utility increases for each k-deviation when $k \leq 2$. As that potential function is also upper bounded by $O(n^2)$, Algorithm 1 converges to a 2-stable partition in at most a quadratic time. We improve this result as we completely solve this case and give the exact (non-asymptotic) value of $L(k,n)$ when $k \leq 2$. The gist of the proof is to re-interpret sequences of deviations in the Dominance Lattice. This object has been widely used in theoretical physics and combinatorics to study systems in which the addition of one element (*e.g.,* a grain of sand) creates consequences in cascade (*e.g.,* the reconfiguration of a sand pile) [17]. Let us define an integer partition:

Definition 3 ([9])**.** *An integer partition of $n \geq 1$, is a non-increasing sequence of integers $Q = q_1 \geq q_2 \geq \ldots \geq q_n \geq 0$ such that $\sum_{i=1}^{n} q_i = n$.*

Given any game with n players, there are as many partition vectors as there are integer partitions of n. Thus in the following, we will make no difference between a partition vector and the integer partition it represents. If we denote the number of integer partitions by p_n, then we know that Algorithm 1 reaches a stable partition in at most $p_n = \Theta((e^{\pi\sqrt{\frac{2n}{3}}})/n)$ steps (the upper-bound directly follows from Lemma 2 *i.e.,* , the lexicographical ordering argument). This is already far less than 2^n, which was shown to be the best upper bound that one can obtain for $k \geq 4$ when using an additive potential function [22].

For $n \geq 6$ it can be seen that some partitions P of the players may never be in the same sequence of 1-deviations. It is hence important to deal with a partial ordering instead of a total one. Brylawski proved in [9] that dominance ordering creates a lattice on integer partitions, where successors and predecessors can be defined using a covering relation:

Definition 4. *(dominance ordering) Given two integer partitions of $n \geq 1$, denoted by $Q = q_1 \geq \ldots \geq q_n$ and $Q' = q'_1 \geq \ldots \geq q'_n$, we say that Q' dominates Q if $\sum_{j=1}^{i} q'_j \geq \sum_{j=1}^{i} q_j$, for all $1 \leq i \leq n$.*

Definition 5. *(covering) Given two integer partitions Q, Q' of $n \geq 1$, Q'* covers *Q if and only if Q' dominates Q and no other integer partition Q'' satisfies that Q' dominates Q'' and Q'' dominates Q.*

The following lemma characterizes when an integer partition covers another one.

Lemma 6 ([9])**.** *Given Q, Q', Q' covers Q if and only if there are j, k such that: (i) $q'_j = q_j + 1$; (ii) $q'_k = q_k - 1$; (iii) for all $i \notin \{j,k\}$, we have $q'_i = q_i$; (iv) either $k = j+1$ or $q_j = q_k$.*

The main ingredient of our analysis is to exploit a strong relationship between covering and 1-deviations in a game, that holds as long as no conflict edges exist.

Lemma 7. *Assuming no conflict edges exist* i.e., *$G^- = G^\emptyset$, let Q, Q' be two integer partitions of $n = |V|$. Then, Q' dominates Q if and only if there exist two partitions P, P' of the players such that: $\overrightarrow{\Lambda}(P') = Q'$, $\overrightarrow{\Lambda}(P) = Q$, and there is a valid sequence of 1-deviations from P to P'.*

Proof. ($\Rightarrow$) To prove the first direction (*a.k.a.*, the 'only if part'), it suffices to prove the result whenever Q' covers Q. In such case, we have by Lemma 6 that there exist j, k satisfying: $q'_j = q_j + 1$, $q'_k = q_k - 1$, and for all i such that $i \notin \{j,k\}$, $q'_i = q_i$. Moreover, since $k = j+1$ or $q_j = q_k$, we get $q_j \geq q_k$.

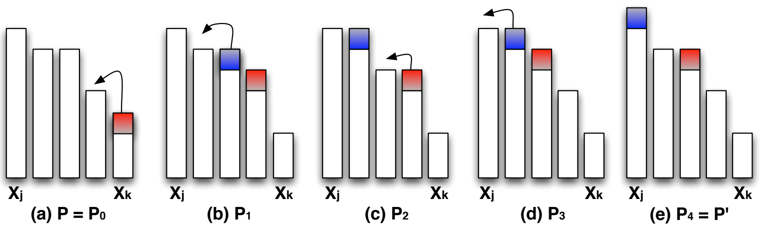

Figure 3: An example of decomposition for a 1-deviation from group X_k to group X_j.

Let P be any partition of the players such that $\overrightarrow{\Lambda}(P) = Q$. We can write w.l.o.g. $P = (X_1, \ldots, X_n)$ with $|X_i| = q_i$ for all $1 \leq i \leq n$. We take a vertex $v \in X_k$, which exists because $|X_k| = q_k > 0$, and we claim that $(\{v\}, j)$ is a 1-deviation that breaks P. Indeed, we have that $|X_j| = q_j \geq q_k$, and no conflict edges exist by the hypothesis. So, we can break P by making $(\{v\}, j)$ happen and in so doing, we get a new partition $P' = (X'_1, \ldots, X'_n)$ for the players such that: $|X'_j| = |X_j| + 1$, $|X'_k| = |X_k| - 1$, and for all i such that $i \notin \{j, k\}$, $|X'_i| = |X_i|$. In other words, $\overrightarrow{\Lambda}(P') = Q'$.

$(\Leftarrow)$ To prove the converse direction, assume the existence of two partitions P, P' such that $\overrightarrow{\Lambda(P)} = Q$, $\overrightarrow{\Lambda(P')} = Q'$ and P' can be obtained from P after the 1-deviation $(\{v\}, j)$ happens. Then, v picks j as her new colour instead of her former colour k, with $|X_j| \geq |X_k|$ by the hypothesis. Furthermore, we can suppose w.l.o.g. that the n groups in P are ordered by decreasing size, up to a recolouring. So, we get either $|X_j| = |X_k|$, or $|X_j| > |X_k|$, hence $j \leq k - 1$. By a reordering of groups with equal size, we can also assume that X_j is the first group with size $|X_j|$, whereas X_k is the last group with size $|X_k|$ in P. Then:

- if $i \in \{1, \ldots, j-1\}$, then $\sum_{l=1}^{i} |X'_l| = \sum_{l=1}^{i} |X_l|$;
- if $i \in \{j, \ldots, k-1\}$, then $\sum_{l=1}^{i} |X'_l| = [\sum_{l=1}^{i} |X_l|] + 1$;
- if $i \in \{k, \ldots, n\}$, then $\sum_{l=1}^{i} |X'_l| = \sum_{l=1}^{i} |X_l|$.

As a consequence, we have that Q' dominates Q by the hypothesis. □

In other words, any sequence of 1-deviations, from a partition P to another partition P', can be decomposed into more elementary 1-deviations, with the property that if there is such an elementary deviation from the partition P_i to the partition P_{i+1}, then the integer partition $\overrightarrow{\Lambda}(P_{i+1})$ covers $\overrightarrow{\Lambda}(P_i)$. Note that, by doing so, we may get another final partition $P'' \neq P'$ but it will have the same partition *vector*, as seen on an example in Figure 3. Since it has been proven in [18] that for $n = \frac{m(m+1)}{2} + r$, the longest chain in the Dominance Lattice has length $2\binom{m+1}{3} + mr$, we finally obtain the *exact* value for $L(1, n)$.

Theorem 8. *Let m and r be the unique non negative integers such that $n = \frac{m(m+1)}{2} + r$, and $0 \leq r \leq m$. We have $L(1, n) = 2\binom{m+1}{3} + mr$. This implies that $L(1, n) \sim \frac{2\sqrt{2}}{3} n\sqrt{n}$ as n gets large.*

Interestingly, we prove that 2-deviations have a similar action on partition vectors, which implies:

Theorem 9. *$L(2, n) = L(1, n) = \Theta(n\sqrt{n})$.*

Proof. Clearly, $L(2,n) \geq L(1,n)$.
For the other direction, let $G^{\emptyset} = (V,E)$ be the conflict graph such that $|V| = n$ and $|E| = 0$. Let P be any partition of the players for $G^{\emptyset}$ such that there exists some 2-deviation $(\{u,v\},j)$ that breaks P. In the following, let $c = c_u(P)$ and let $c' = c_v(P)$. If $|X_j| \geq |X_c|$ or $|X_j| \geq |X_{c'}|$, then the 2-deviation can be decomposed into 1-deviations. So, we suppose that $|X_j| = |X_c| - 1 = |X_{c'}| - 1$. There are two cases:

- Suppose $c = c'$. Then after the 2-deviation happens, the groups X_c, X_j are replaced with $X_c \setminus \{u,v\}, X_j \cup \{u,v\}$; equivalently, we obtain two groups of respective size $|X_c| - 2$, $|X_c| + 1$ instead of two groups of respective size $|X_c| - 1$, $|X_c|$. It thus follows that for any vertex $u_j \in X_j$, one can obtain the same partition vector by making the 1-deviation $(\{u_j\}, c)$ happen.
- Else, after the 2-deviation happens the groups $X_c, X_{c'}, X_j$ of respective size $|X_c|, |X_c|, |X_c| - 1$ are replaced with the groups $X_c \setminus \{u\}, X_{c'} \setminus \{v\}, X_j \cup \{u,v\}$ of respective size $|X_c| - 1, |X_c| - 1, |X_c| + 1$. Again, one can obtain the same partition vector, this time by making the 1-deviation $(\{v\}, c)$ happen.

Finally, any partition vector that is obtained from a 2-deviation may also be obtained from a sequence of 1-deviations. Thus, $L(2,n) \leq L(1,n)$.
Consequently, $L(2,n) = L(1,n) = \Theta(n\sqrt{n})$. □

3.2 Lower bounds for k > 2

On the one hand, the classical dominance ordering does not suffice to describe all k-deviations as soon as $k \geq 3$. It can be seen with the two following integer partitions of 10: $Q = (3,3,3,1)$ and $Q' = (4,2,2,2)$, that are uncomparable, yet one can break Q to obtain Q' using a 3-deviation. On the other hand, we can reuse some techniques inspired from [18] so that we can obtain lower-bounds on $L(k,n)$. The method heavily relies on specific sequences of deviations that we will call *cascades*.

Overview To give a flavor of the method, we first observe there is only *one* k-stable partition in the empty conflict graph $G^{\emptyset}$ namely, the one with partition vector (n) composed of only one summand. Then given two partitions P, P' of the players, we notice that if P' is obtained from P using a k-deviation, then we may have that $h(P') \geq h(P)$ as soon as $k \geq 3$, with $h(P)$ the length of a longest sequence in the Dominance Lattice from the integer partition $\overrightarrow{\Lambda}(P)$ to the integer partition (n). Moreover, we also noticed that the larger k the larger $h(P') - h(P)$ may be. Thus it motivates the following strategy to lower-bound $L(k,n)$: at each step of Algorithm 1, one should break the current partition using a set S of maximum size[4].
To ensure that many k-deviations can happen *consecutively*, we will seek for partitions containing a group of *each* size: from one to some value p. For instance, consider a partition with three groups of size p, and one group of size i for $1 \leq i \leq p-2$. A first 3-deviation can happen so that a vertex in each of the three groups of size p changes her colour to join the group of size $p-2$. In such case, we are left with a partition containing: one group of size $p+1$, three groups of size $p-1$, and one group of size i, for $0 \leq i \leq p-3$. Hence, another 3-deviation can happen, so that a vertex in each of the three groups of size $p-1$ changes her colour to join the group of size $p-3$, and so on.

[4]We only consider *elementary* k-deviations *e.g.,* deviations such that the partition vector one obtains after they happen cannot be gotten using a sequence of smaller deviations.

Vectorial notations In order to define our cascades, we will rely on a *vectorial representation* of partitions and deviations. This novel representation allows us to describe, in simpler terms, the "patterns" that are applied recursively until we obtain a long sequence of k-deviations. Formally, given two partitions P, P' of the players, if P' is obtained from P using a k-deviation, then we represent the deviation by the vector $\overrightarrow{\Lambda}(P') - \overrightarrow{\Lambda}(P)$.

- In case of a 1-deviation, there are four possibilities. If some player leaves a group of size $q+1$ for a group of size $p-1$, hence $p \geq q+2$, then the deviation is represented by a vector $\overrightarrow{\alpha}[p,q]$[5] whose entries all equal zero, except:
  - if $p = 2, q = 0$ then $\alpha_1 = -2, \alpha_2 = 1$;
  - if $p > 2, q = 0$ then $\alpha_1 = \alpha_{p-1} = -1, \alpha_p = 1$;
  - if $p = q+2, q > 0$ then $\alpha_p = \alpha_q = 1$, and $\alpha_{p-1} = -2$;
  - if $p > q+2, q > 0$ then $\alpha_{p-1} = \alpha_{q+1} = -1$, and $\alpha_p = \alpha_q = 1$.
- The case of 2-deviations can be ignored by Theorem 9.
- In case of a 3-deviation, we consider there are three groups of size $p-1$ and a player leaves each group to join some group of (possibly null) size $p-3$. Hence it is represented by a vector $\overrightarrow{\gamma}[p]$[5] whose entries all equal zero except: $\gamma_p = 1$, $\gamma_{p-1} = -3$, $\gamma_{p-2} = 3$, and if $p \neq 3$ $\gamma_{p-3} = -1$.
- Finally, in case of a 4-deviation, we consider there are four groups of size $p-1$, one group of size $p-4$, and a player in each group of size $p-1$ changes her colour so that she joins the group of size $p-4$. Therefore it is represented by a vector $\overrightarrow{\delta}[p]$[5] whose entries all equal zero, except: $\delta_p = 1, \delta_{p-1} = -4, \delta_{p-2} = 4$, and if $p \neq 4$ $\delta_{p-4} = -1$.

Throughout the remaining of the section, we will ignore all other k-deviations.

Properties To go further with our vectorial approach, one needs to check whether a given deviation $\overrightarrow{\varphi} = \overrightarrow{\Lambda}(P') - \overrightarrow{\Lambda}(P)$ is *valid i.e.,* the vector $\overrightarrow{\Lambda}(P) + \overrightarrow{\varphi}$ has no negative entries. Let us now introduce the notion of *balanced sequence.*

Definition 10. *Given any integer $h > 0$, let $\overrightarrow{\varphi}^1, \overrightarrow{\varphi}^2, \ldots, \overrightarrow{\varphi}^t$ be vectors. We call this sequence h-balanced if, for any $1 \leq i \leq t$, the sum of the i first vectors, namely $\sum_{j=1}^{i} \overrightarrow{\varphi}^j$, has all its entries greater than or equal to $-h$.*

Given a h-balanced sequence $(\overrightarrow{\varphi}^1, \overrightarrow{\varphi}^2, \ldots, \overrightarrow{\varphi}^t)$ of k-deviations, let $\overrightarrow{\Phi} = \sum_{i=1}^{t} \overrightarrow{\varphi}^i$ be the sum of all deviations, and let $p_{\max}$ be the largest index j that satisfies $\overrightarrow{\Phi}_j \neq 0$. Equivalently, $p_{\max}$ is the largest size of a group modified (hence created) after some deviation in the sequence happens (*i.e.,* $\forall l, \forall p > p_{\max}, \varphi_p^l = 0$). One can observe that a sufficient condition so that the sequence is valid is that it starts from a partition with at least h groups of each size j, for $1 \leq j \leq p_{\max}$.
In the following, we will often make use of a *symmetric* property to find a balanced sequence:

Definition 11. *The minimum-size sub-vector that contains all non-zero entries of a vector is called the* support *of the vector. We say a vector has the* symmetric property *if, and only if, the support of the vector is symmetric. Equivalently, a vector has the symmetric property if, and only if, the coordinates of its support are invariant under the reverse permutation.*

[5]The index p represents the largest group created *after* the k-deviation happens.

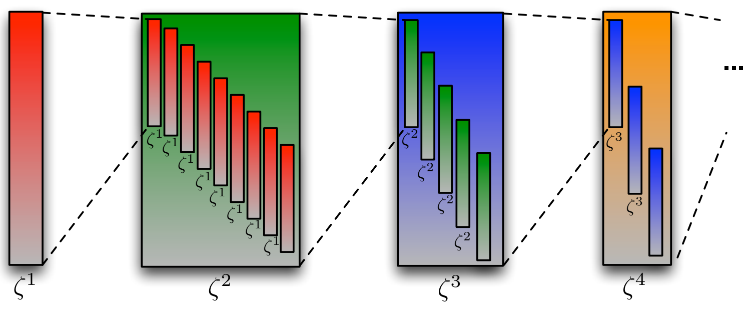

Figure 4: Long sequence using recursive cascades.

Given a vector, it might be useful in the following to notice that the size of the support is exactly $p_{\max} - p_{\min} + 1$, where $p_{\max}, p_{\min}$ denote the largest non-zero index and the least non-zero index.
One can also notice every 1-deviation yields an elementary vector of the form $\overrightarrow{\alpha}[p,q]$ that has the symmetric property provided $p \geq q \geq 1$. But the property does not hold in general for k-deviations whenever $k \geq 3$.

Results Prior to our work, it was known $L(3,n) = O(n^3)$, which follows from another application of the potential function method [22]. But nothing proved that $L(3,n) > L(2,n)$, and in fact it was conjectured in [15] that both values are equal. Theorem 12 proves for the first time that deviations of multiple players can delay convergence and that the gap between $k = 2$ and $k = 3$ obtained from potential function is indeed justified. Using a considerable refinement of the cascade technique, we are able to prove in Theorem 13 a much more significant result: that 4-deviations are responsible for a sudden complexity increase, as we now prove that no polynomial bounds exist for $L(4,n)$.

Theorem 12. $L(3,n) = \Omega(n^2)$.

Theorem 13. $L(4,n) = \Omega(n^{\Theta(\ln(n))})$.

The rest of this section is mainly devoted to prove Theorem 13. At the end of this section, we also give a proof of Theorem 12 using the same techniques.

Theorem 13. As before, we assume no conflict edge exists. W.l.o.g. we also assume that the number of players is $n = cL(L+1)/2$. The values c and L will be defined later, and we only assume for the moment that c is sufficiently large.
Starting from the partition with n singleton groups, let P^0 be such that $\overrightarrow{\Lambda}(P^0) = (0,\ldots,0,\lambda_L = c,\ldots,\lambda_1 = c)$. Using our notations, one can obtain a group of size j with the sequence of 1-deviations defined by $\sum_{i=2}^{j} \overrightarrow{\alpha}[i,0]$ and so, one can obtain P^0 using the sequence of 1-deviations defined by $c \cdot \left(\sum_{j=2}^{L} \sum_{i=2}^{j} \overrightarrow{\alpha}[i,0]\right)$.

Our proof relies on a "shift" operator: given a vector $\overrightarrow{\varphi}$ whose support ranges between indices $p_{\min}, p_{\max}$, the vector $^{\mathtt{tr}(i)}\overrightarrow{\varphi}$, $i < p_{\min}$, is a vector of the same size *and the same support* as $\overrightarrow{\varphi}$, but whose support ranges between indices $p_{\max} - i, p_{\min} - i$. For instance, we have $^{\mathtt{tr}(1)}(0,1,-2,1,0,0,0) = (0,0,1,-2,1,0,0)$. In particular, if $\overrightarrow{\varphi}$ represents a k-deviation, then $^{\mathtt{tr}(i)}\overrightarrow{\varphi}$ represents the same k-deviation, up to a decrease by i of all groups involved; that is, we have $^{\mathtt{tr}(i)}\overrightarrow{\alpha}[p,q] = \overrightarrow{\alpha}[p-i,q-i]$, $^{\mathtt{tr}(i)}\overrightarrow{\gamma}[p] = \overrightarrow{\gamma}[p-i]$, $^{\mathtt{tr}(i)}\overrightarrow{\delta}[p] = \overrightarrow{\delta}[p-i]$.

One can extend the operator and its meaning to sequences of k-deviations as well. Formally, let $\overrightarrow{\varphi}^1, \ldots, \overrightarrow{\varphi}^t$ be a sequence of k-deviations, and let $\overrightarrow{\Phi} = \sum_{l=1}^{t} \overrightarrow{\varphi}^l$. Then, if no group of size less than $i+1$ is modified nor created by the sequence (*i.e.,* $\forall l, \forall p \leq i, \varphi_p^l = 0$), we obtain by linearity of the operator that ${}^{\texttt{tr}(i)}\overrightarrow{\Phi} = \sum_{l=1}^{t} {}^{\texttt{tr}(i)}\overrightarrow{\varphi}^l$.

Interestingly, the so-called "shift" operator keeps the symmetric properties of a vector:

Claim 14. *Let $\overrightarrow{\phi}$ be any vector that has a support of size $s = p_{\max} - p_{\min} + 1$, and with the symmetric property. For any positive integers r and d such that $1 + (r-1)d \leq p_{\min}$, the vector $\overrightarrow{\phi}' = \sum_{h=0}^{r-1} {}^{tr(hd)}\overrightarrow{\phi}$ also has the symmetric property.*

Proof. The support of vector $\overrightarrow{\phi}'$ has size $s' = (r-1)d + s$. In the following, we will assume up to padding the vector $\overrightarrow{\phi}$ with additional null entries that it is unbounded *i.e.,* it is indexed by $\mathbb{Z}$. By the hypothesis the vector $\overrightarrow{\phi}$ has the symmetric property and so, $\forall 1 \leq j \leq p_{\max} + p_{\min} - 1, \phi_j = \phi_{p_{\min}+p_{\max}-j}$. Let $0 \leq j \leq s'/2 - 1$. We have that:

$$\phi'_{p_{\max}-j} = \sum_{h=0}^{r-1} \phi_{p_{\max}-j+hd} = \sum_{h=0}^{r-1} \phi_{p_{\max}+p_{\min}-(p_{\max}-j+hd)}$$

$$= \sum_{h=0}^{r-1} \phi_{p_{\min}+j-(r-1-h)d} = \sum_{h=0}^{r-1} \phi_{p_{\min}-(r-1)d+j+hd} = \phi'_{p_{\min}-(r-1)d+j}.$$

Thus, $\overrightarrow{\phi}'$ also has the symmetric property. ◇

Let $t > 0$ and $T > 0$ be such that $2^{T-1}(2t^2 + 2) \leq L$. In order to prove Theorem 13, we construct sequences of deviations that we denote by $\overrightarrow{\zeta}^i$ for all $i = 1, \ldots T$. The construction is recursive. To construct the vector $\overrightarrow{\zeta}^{i+1}$ from $\overrightarrow{\zeta}^i$, we follow a particular construction that we will show valid and that is illustrated in Figure 4. The construction is composed of a repetition of the sequence defined by $\overrightarrow{\zeta}^i$ a certain number of times (linear in t) shifting the "starting point" of each sequence by the same value. The construction then adds 1-deviations in order to get a technical property, called *Good property* (*e.g.,* see Definition 15 below).

Definition 15. *Let i be a positive integer. We will say the sequence $\overrightarrow{\zeta}^i$ has the* Good Property *if it has the symmetric property, its support has even size s_i, and there exist t_1^i, t_2^i satisfying:*

- $1 < t_1^i < t_2^i < 2t_1^i$*;* $t_2^i \leq 2^{i+1}$*;*
- *and all entries of $\overrightarrow{\zeta}^i$ are null except for: $\zeta_L^i = \zeta_{L+1-s_i/2}^i = 1$, $\zeta_{L-t_1^i}^i = \zeta_{L-t_2^i}^i = -1$, and symmetrically: $\zeta_{L-s_i+1}^i = \zeta_{L-s_i/2}^i = 1$, $\zeta_{L-s_i+t_1^i+1}^i = \zeta_{L-s_i+t_2^i+1}^i = -1$.*

Note that in terms of k-deviations, Definition 15 implies that L is the largest size of a group created after the sequence $\overrightarrow{\zeta}^i$ happens.

Let us construct the base-case $\overrightarrow{\zeta}^1$. It starts with a cascade of t^2 consecutive 4-deviations, namely $\sum_{i=0}^{t^2-1} \overrightarrow{\delta}[L-i]$. Then, a player in some group of size $L-2$ picks a new colour so that she joins another group of size $L-2$; another player leaves her group of size $L - t^2 - 1$ to join another one of the same size; a third player in a group of size $L - t^2 - 5$ picks a new colour so that she joins a group of size $L - t^2 - 4$; last, a fourth player leaves her group of size $L-4$ for a group of size $L-2$, followed by a player leaving her group of size $L-3$ for another one of the same size. Altogether, we obtain the sequence

$$\overrightarrow{\Phi}^1 = \sum_{i=0}^{t^2-1} \overrightarrow{\delta}[L-i] + \overrightarrow{\alpha}[L-1, L-3] + \overrightarrow{\alpha}[L-t^2, L-t^2-2] + \overrightarrow{\alpha}[L-t^2-3, L-t^2-6] + \overrightarrow{\alpha}[L-1, L-5] + \overrightarrow{\alpha}[L-2, L-4].$$

The sum-vector $\overrightarrow{\Phi}^1$ has all its entries equal to zero, except for: $\Phi^1_L = \Phi^1_{L-5} = \Phi^1_{L-t^2-1} = \Phi^1_{L-t^2-6} = 1$, and $\Phi^1_{L-1} = \Phi^1_{L-2} = \Phi^1_{L-t^2-4} = \Phi^1_{L-t^2-5} = -1$.
We finally construct $\overrightarrow{\zeta}^1$ by repeating the sequence[6] $\overrightarrow{\Phi}^1$ many times, up to various shiftings, followed by a sequence of 1-deviations that yields:

$$\overrightarrow{\zeta}^1 = \sum_{i=0}^{t^2-5} {}^{\mathtt{tr}(i)}\overrightarrow{\Phi}^1 + \sum_{i=0}^{t^2-4} \overrightarrow{\alpha}[L-4-i, L-2t^2+3+i] + \overrightarrow{\alpha}[L-t^2+4, L-t^2-5] + \overrightarrow{\alpha}[L-t^2+3, L-t^2-4].$$

Claim 16. *There is a constant h_1 such that the sequence defined by $\overrightarrow{\zeta}^1$ is h_1-balanced.*

Proof. First, note that any k-deviation modifies a *constant* number of groups in the partition (at most $k+1$). Thus, for any i, $0 \le i \le t^2-5$, the sequence defined by ${}^{\mathtt{tr}(i)}\overrightarrow{\Phi}^1$ is balanced for some constant because, for any j, $1 \le j \le n$, the number of deviations that modifies some group of size j is constant as well. In addition, the vector ${}^{\mathtt{tr}(i)}\overrightarrow{\Phi}^1$ contains a constant number of non-zero values and so, for any j, $1 \le j \le n$, the sequence defined by $\sum_{i=0}^{t^2-5} {}^{\mathtt{tr}(i)}\overrightarrow{\Phi}^1$ also modifies a constant number of groups of size j. Since this sequence $\sum_{i=0}^{t^2-5} {}^{\mathtt{tr}(i)}\overrightarrow{\Phi}^1$ is only completed with a subsequence of 1-deviations so that we obtain $\overrightarrow{\zeta}^1$, and that $\forall j$ there is also a constant number of such 1-deviations that modify or create some group of size j, we can safely conclude there exists a constant h_1 such that the sequence induced by $\overrightarrow{\zeta}^1$ is h_1-balanced. $\diamond$

By the calculation, we obtain that all values in $\overrightarrow{\zeta}^1$ equal to zero, except for: $\zeta^1_L = \zeta^1_{L-t^2} = \zeta^1_{L-t^2-1} = \zeta^1_{L-2t^2-1} = 1$, and $\zeta^1_{L-2} = \zeta^1_{L-3} = \zeta^1_{L-2t^2+2} = \zeta^1_{L-2t^2+1} = -1$. This proves that $\overrightarrow{\zeta}^1$ satisfies the so-called Good Property of Definition 15 (with $t^1_1 = 2, t^1_2 = 3$, $s_1 = 2(t^2+1)$). Then, one can apply the following inductive step.

Claim 17. *Suppose that $\overrightarrow{\zeta}^i$ is defined, it has a support of size s_i and it has the Good Property. Then there exist two positive integers denoted by a_i, t^i_1, and there exists a sequence of 1-deviations denoted by $\overrightarrow{\xi}^{i+1}$ so that:*

$$\overrightarrow{\zeta}^{i+1} = \sum_{j=0}^{a_i} {}^{tr(jt^i_1)}\overrightarrow{\zeta}^i + \overrightarrow{\xi}^{i+1}$$

also has the Good Property.
In addition we have that if $\overrightarrow{\zeta}^i$ is h_i-balanced then $\overrightarrow{\zeta}^{i+1}$ is (h_i+1)-balanced, and it holds that $s_i \le s_{i+1} < \frac{3}{2}s_i$ where s_{i+1} denotes the size of the support of $\overrightarrow{\zeta}^{i+1}$.

Proof. We first note that s_i is even by Definition 15. Let t^i_1, t^i_2 be as defined in Definition 15. Also, let a_i be the largest even integer j such that $L - jt^i_1 - t^i_2 > L - s_i/2 + 1$.
We set $\overrightarrow{\Phi}^{i+1} = \sum_{j=0}^{a_i} {}^{\mathtt{tr}(jt^i_1)}\overrightarrow{\zeta}^i$, that has the symmetric property by Claim 14.

[6]Note that we will often abuse of our "vector-sum" notation $\overrightarrow{\Phi} = \sum_{i=1}^{t} \overrightarrow{\varphi}^i$ to represent the whole sequence $\overrightarrow{\varphi}^1, \ldots, \overrightarrow{\varphi}^t$.

In addition, let $t_1^{i+1} = t_2^i$ and $t_2^{i+1} = t_1^i + t_2^i$[7]. Since we have $1 < t_1^i < t_2^i < 2t_1^i$, $t_2^i \leq 2^{i+1}$ by the hypothesis, one obtains $1 < t_1^{i+1} < t_2^{i+1} < 2t_1^{i+1}$, $t_2^{i+1} < 2t_2^i \leq 2 \cdot 2^{i+1} = 2^{i+2}$.
We finally introduce $s_{i+1} = s_i + a_i t_1^i < \frac{3}{2}s_i$ the size of the support of $\overrightarrow{\Phi}^{i+1}$, and we observe that it is an even number because a_i, s_i are both even.

We aim to construct from $\overrightarrow{\Phi}^{i+1}$ a sequence $\overrightarrow{\zeta}^{i+1}$ that satisfies the Good Property w.r.t. $t_1^{i+1}, t_2^{i+1}, s_{i+1}$. To do so, we first introduce for any $0 \leq l \leq a_i$ the truncated sum-vector $\overrightarrow{\Psi}^l = \sum_{j=0}^{l} {}^{\mathtt{tr}(jt_1^i)}\overrightarrow{\zeta}^i$. In particular, we have $\overrightarrow{\Psi}^0 = \overrightarrow{\zeta}^i$ while $\overrightarrow{\Psi}^{a_i} = \overrightarrow{\Phi}^{i+1}$. Note that each $\overrightarrow{\Psi}^l$ has the symmetric property by Claim 14. Furthermore we have that all entries of $\overrightarrow{\Psi}^l$ are equal to zero, except for:

- $\Psi^l_L = \Psi^l_{L-s_i-lt_1^i+1} = 1$; $\forall 0 \leq j \leq l, \Psi^l_{L-s_i/2-jt_1^i+1} = \Psi^l_{L-s_i/2-(l-j)t_1^i} = 1$;
- $\Psi^l_{L-lt_1^i} = \Psi^l_{L-s_i+1} = -1$; $\forall 0 \leq j \leq l, \Psi^l_{L-jt_1^i-t_2^i} = \Psi^l_{L-s_i-(l-j)t_1^i+t_2^i} = -1$.

In particular, we have that: $\Phi^{i+1}_L = \Psi^{a_i}_L = 1$; $\Phi^{i+1}_{L-s_{i+1}/2+1} = \Psi^{a_i}_{L-s_i/2-\frac{a_i}{2}t_1^i+1} = 1$; $\Phi^{i+1}_{L-t_1^{i+1}} = \Psi^{a_i}_{L-t_2^i} = -1$, and $\Phi^{i+1}_{L-t_2^{i+1}} = \Psi^{a_i}_{L-t_1^i-t_2^i} = -1$. So, in order to obtain the so-called Good property of Definition 15, we are left to set to zero all other entries of the -sum-vector $\overrightarrow{\Phi}^{i+1}$, using 1-deviations. To achieve the result, let us partition the $4a_i$ indices we want to set to zero in 4-tuples $(L-j_1, L-j_2, L-s_{i+1}+1+j_2, L-s_{i+1}+1+j_1)$ such that: $j_1 < j_2$, and $\Phi^{i+1}_{L-j_1} = -1, \Phi^{i+1}_{L-j_2} = 1$. For each such 4-tuple, we add to the vector-sum $\overrightarrow{\Phi}^{i+1}$ the sequence of 1-deviations $\sum_{j=0}^{j_2-j_1-1} \overrightarrow{\alpha}[L-j_1-j, L-s_{i+1}+1+j_1+j]$ whose all entries are equal to zero, except for those indexed by the 4-tuple that are respectively equal to $1, -1, -1, 1$.

Finally, let us assume $\overrightarrow{\zeta}^i$ is h_i-balanced. It remains to prove that $\overrightarrow{\zeta}^{i+1}$ is (h_i+1)-balanced. By the hypothesis, we have that $\forall j, {}^{\mathtt{tr}(j)}\overrightarrow{\zeta}^i$ is h_i-balanced, and $\forall l, p, \Psi^l_p \geq -1$, hence $\overrightarrow{\Phi}^{i+1}$ is (h_i+1)-balanced. Furthermore, we have by construction each subsequence of 1-deviations in the sequence $\overrightarrow{\xi}^{i+1}$ is 1-balanced. As a result, $\overrightarrow{\Phi}^{i+1}$ is (h_i+1)-balanced implies that $\overrightarrow{\zeta}^{i+1}$ is (h_i+1)-balanced. $\diamond$

Recall that $t, T > 0$ are such that $2^{T-1}(2t^2+2) \leq L$, and $n = cL(L+1)/2$. Set $T = \lceil \log_2(t)+1 \rceil$ and, without loss of generality, assume $2(t^3+t) = L$. By the proof of Claim 17, one obtains a maximum shift of:

$$\sum_{i=1}^{T-1} a_i \cdot t_1^i < \sum_{i=1}^{T-1} \frac{s_i}{2} < \sum_{i=1}^{T-1} \left(\frac{3}{2}\right)^{i-1} \frac{s_1}{2} = \frac{2s_1}{3}\left(\left(\frac{3}{2}\right)^{T-1} - 1\right) = O(t^{\log_2(3)+1}) = o(t^3)$$

for the range of the support of vector $\overrightarrow{\zeta}^T$ w.r.t. the range of the support of $\overrightarrow{\zeta}^1$. By comparison, we remind that the sequence $\overrightarrow{\zeta}^1$ solely modifies groups of size $\Omega(L) = \Omega(t^3)$. As a result, the vector $\overrightarrow{\zeta}^L$ indeed represents a sequence of k-deviations, and by Claim 17 it is (h_1+T-1)-balanced. So, $n = (h_1+T-1)(2t^3+2t)(2t^3+2t+1)/2 = (h_1+\lceil \log_2(t) \rceil)(2t^3+2t)(2t^3+2t+1)/2$ is sufficient to make this sequence valid. One can note that since h_1 is a universal constant, $n = O(t^6 \log_2(t))$.

Claim 18. *The sum-vector $\overrightarrow{\zeta}^{i+1}$, as it is defined in Claim 17, represents a sequence of at least $(\frac{s_i}{2^{i+2}} - 5)$-times more deviations than in the sequence $\overrightarrow{\zeta}^i$, where s_i denotes the size of the support of $\overrightarrow{\zeta}^i$.*

[7] By induction, we get $t_i^1 = F_{i+3}$ and $t_i^2 = F_{i+4}$, where $F_i = \frac{1}{\sqrt{5}}\left(\left(\frac{1+\sqrt{5}}{2}\right)^i - \left(\frac{1-\sqrt{5}}{2}\right)^i\right)$ is the i^{th} Fibonacci number.

Proof. The sequence $\overrightarrow{\zeta}^i$ is repeated a_i times using the "shift" operator, with a_i the largest even integer j such that $L - jt_1^i - t_2^i > L - s_i/2 + 1$. Furthermore if $L - jt_1^i - t_2^i > L - s_i/2 + 1$ then $j \leq \frac{s_i - 4 - 2t_2^i}{2t_1^i}$. Since we have by Definition 15 that $t_1^i < t_2^i \leq 2^{i+1}$, then $\frac{s_i-4-2t_2^i}{2t_1^i} > \frac{s_i}{2^{i+2}} - \frac{1}{2^i} - 1$ and so, $a_i \geq \lfloor \frac{s_i}{2^{i+2}} - \frac{1}{2^i} - 1 \rfloor - 2 \geq \frac{s_i}{2^{i+2}} - 5$. ◇

Since the support of $\overrightarrow{\zeta}^1$ has size $2t^2 + 2$ by construction, it follows that $\overrightarrow{\zeta}^T$ represents a sequence of at least $\prod_{i=1}^{T-1}(\frac{2t^2+2}{2^{i+2}} - 5) \geq (\frac{2t^2+2}{2^{T+1}} - 5)^{T-1} \geq (\frac{2t^2+2}{4t} - 5)^{\log_2(t)} = \Omega(t^{\log_2(t)})$ deviations. As $n = O(t^6 \log_2(t))$, it proves Theorem 13. □

We finally prove that $L(3, n) = \Omega(n^2)$.

Proof. [Theorem 12] As usual let $G^{\emptyset} = (V, E)$ be the empty conflict graph with $|V| = n$ and $|E| = 0$. The number of players is here assumed to be $n = O(cL^2)$, where c denotes a large constant integer. We start our sequence from any partition P^0 which satisfies $\overrightarrow{\Lambda}(P^0) = (0, \ldots, 0, \lambda_L = c, \ldots, \lambda_1 = c)$. Note that one can reach such a partition using a sequence of 1-deviations, namely $c \cdot \left(\sum_{j=2}^{L}\sum_{i=2}^{j} \overrightarrow{\alpha}[i, 0]\right)$.

Let then $t = \frac{L-1}{4}$. We construct a sequence $\overrightarrow{\zeta}^1 = \sum_{i=0}^{t} \overrightarrow{\gamma}[L - i]$ of $t + 1$ consecutive 3-deviations *a.k.a.*, a cascade. The sum-vector $\overrightarrow{\zeta}^1$ has all its entries equal to zero, except for: $\zeta_L^1 = \zeta_{L-2}^1 = 1$, $\zeta_{L-t-1}^1 = \zeta_{L-t-3}^1 = -1$, $\zeta_{L-1}^1 = -2$ and $\zeta_{L-t-2}^1 = 2$.
Using the so-called "shift" operator of Section 3.2, one can repeat the above sequence that yields $\overrightarrow{\zeta}^2 = \sum_{i=0}^{t-2} {}^{\mathtt{tr}(i)}\overrightarrow{\zeta}^1$. The sum-vector $\overrightarrow{\zeta}^2$ has all its entries equal to zero, except for: $\zeta_L^2 = \zeta_{L-t}^2 = \zeta_{L-t-2}^2 = \zeta_{L-2t}^2 = 1$, and $\zeta_{L-1}^2 = \zeta_{L-t+1}^2 = \zeta_{L-t-1}^2 = \zeta_{L-2t-1}^2 = -1$.
Again, we repeat the sequence $\overrightarrow{\zeta}^2$ using the so-called "shift" operator, and one obtains $\overrightarrow{\zeta}^3 = \sum_{i=0}^{t-4} {}^{\mathtt{tr}(i)}\overrightarrow{\zeta}^2$. The sum-vector $\overrightarrow{\zeta}^3$ has all its entries equal to zero, except for: $\zeta_L^3 = \zeta_{L-3t+3}^3 = \zeta_{L-3t+1}^3 = 1$, and $\zeta_{L-t+3}^3 = \zeta_{L-t+2}^3 = \zeta_{L-t}^3 = \zeta_{L-4t}^3 = -1$.
We finally repeat the sequence $\overrightarrow{\zeta}^3$ until we obtain $\overrightarrow{\zeta}^4 = \sum_{i=0}^{t-1} {}^{\mathtt{tr}(i)}\overrightarrow{\zeta}^3$. Note that since the sequence $\overrightarrow{\zeta}^1$ is a cascade, then it is h_1-balanced for some constant h_1 (*e.g.,* see the proof of Claim 16) and so, since in addition each sequence $\overrightarrow{\zeta}^i$ has a constant number of non-zero entries, then it follows that the whole sequence $\overrightarrow{\zeta}^4$ is also h-balanced, for some larger constant $h \geq h_1$. Hence, it is a valid sequence whenever we start from P^0 and the constant c is large enough, and it represents a sequence of $\theta(t^4) = \theta(L^2) = \theta(n^2)$ deviations. As a result, we have $L(3, n) = \Omega(n^2)$. □

4 The general case: Are games stable under deviations?

More generally, a colouring game may be defined with weights taking values in a larger set $\mathcal{W}$. Players then choose to interact with each others according to more complex preferences and the individual utility is not always related to the size of the sharing group. For the remaining of the section, let w_p be the largest positive weight in a graph, if any, and 0 otherwise.

Nash equilibria On the positive side, we first show the following result.

Theorem 19. *For any weighted graph, Algorithm 1 converges in $O(w_p n^2)$ steps to a 1-stable partition.*

The proof follows from a more general potential-function technique:

Lemma 20. *Given a graph $G = (V, w)$, let P, P' be partitions of the nodes. Let (S, j) be a k-deviation which breaks P, $S = \{u_1, u_2, \ldots, u_k\}$. If one can obtain P' from P after this deviation happens then we have: $f(P') - f(P) \geq 2[k - \sum_{1 \leq i,l \leq k} w_{u_i u_l} + \sum_{\{u_i, u_l | c_{u_i}(P) = c_{u_l}(P)\}} w_{u_i u_l}]$.*

The proof of the lemma is deferred to the appendix. Theorem 19 follows from an application of Lemma 20 to the case of a 1-deviation.

Proof. [Theorem 19] Let P_i, P_{i+1} be two consecutive partitions of the players in Algorithm 1, and let $(\{u_1\}, j)$ be the 1-deviation that breaks P_i. By Lemma 20, we get that $f(P_{i+1}) - f(P_i) \geq 2[1 - 0 + 0] = 2$. Hence the global utility increases at each step of the dynamic, and it is upper bounded by an $O(w_p n^2)$. $\square$

Theorem 19 proves that *all* colouring games admit a 1-stable partition, or equivalently a Nash-equilibrium, and that one can be reached in pseudo-polynomial time. Note on the other hand that our dependency on the weights can be exponential. It is unlikely one can improve this analysis, as the problem of computing a 1-stable partition is PLS-complete[8].

We now fix a set of weights $\mathcal{W}$ for the analysis, and we look at the greatest value of k for which a k-stable partition *always* exists. In the following, we will denote this maximum value by $k(\mathcal{W})$, and we will establish it for various sets of weights. Finally, we will strengthen the aforementioned results by proving that deciding if a graph with weights in $\mathcal{W}$ admits a k-stable partition is either trivial (*i.e.,* it is true for all such graphs) or NP-complete.

4.1 Games with a unique positive weight

We first focus on the subsets of $\{-\infty, 0, 1\} \cup -\mathbb{N}$. A good representative amongst these is the subset $\{-\infty, 0, 1\}$, which is the simplest set of weights extending the uniform case ($\mathcal{W} = \{-\infty, 1\}$) to accommodate *indifferent* edges. Surprisingly, we will show that introducing the null weight radically alters the stability properties of colouring games. Indeed, whereas $k(\{-\infty, 1\}) = \infty$, we will prove $k(\{-\infty, 0, 1\}) = 2$ after exhibiting a surprising counterexample for $k = 3$.

Let us first show that $k(\mathcal{W}) \geq 2$. In fact, Theorem 21 is a global stability result, which is more precise and uses structural properties of the graphs. Given a graph $G = (V, w)$, let us define the "friendship graph" $G^+ = (V, E^+)$ of G, where $E^+ = \{uv \in E : w_{uv} > 0\}$. We remind that the *girth* of a graph is the length of its shortest cycle. By definition, an acyclic graph has infinite girth.

Theorem 21. *Let k be a positive integer, and $G = (V, w)$ be constrained to $\mathcal{W} \subseteq \{-\infty, 0, 1\} \cup -\mathbb{N}$. If the girth of the friendship graph G^+ is at least $k + 1$, then Algorithm 1 always reaches a k-stable partition in $O(n^2)$ steps in that case.*

Proof. As in the case $k = 1$, let P_i, P_{i+1} be two consecutive partitions of the players in Algorithm 1, and let $(S = \{u_1, u_2, \ldots, u_l\}, j)$ be the l-deviation that breaks P_i, with $l \leq k$. By Lemma 20, we get that $f(P_{i+1}) - f(P_i) \geq 2[l - \sum_{\{u_t, u_s | c_{u_t}(P_i) \neq c_{u_s}(P_i)\}} w_{u_t u_s}] \geq 2[l - |E^+ \cap S \times S|]$ because by the hypothesis the largest positive weight is 1. Furthermore, since the girth is at least $k + 1$ by the hypothesis, S induces a forest in G^+, and so, $|E^+ \cap S \times S| \leq l - 1$. Hence, $f(P_{i+1}) - f(P_i) \geq 2$, and as the result the global utility increases at each step of the dynamic. The latter concludes the proof as the global utility is upper bounded by an $O(n^2)$. $\square$

Particularly, if G^+ is cycle-free, then we get there is a k-stable partition for G, for any $k \geq 1$; if G^+ is triangle-free, then there always exists a 3-stable partition for G. Furthermore, as the girth of any graph is at least 3, then there always exists a 2-stable partition.

[8]A simple reduction from cut games can be found *e.g.,* see [19].

Unlike the uniform case, one can show the quadratic bound on the number of steps is indeed tight. To show it, assume the set V can be partitioned in three distinct subsets V_1, V_2, V_3. We assume the induced (friendship) subgraph $G^+[V_3]$ is the clique K_{p+1}, the induced subgraph $G^+[V_1 \cup V_2]$ is the complete bipartite graph $K_{p,p}$, and each node in V_2 is adjacent in G^+ to every node in V_3. Note that $n = 3p + 1$. We obtain the graph $G = (V, w)$ by completing G^+ with all missing edges and setting their weight to zero. Here is a sequence one can obtain for the colouring game defined on G: in p consecutive 1-deviations, all nodes in V_3 pick the same colour, say 1; then, in p consecutive 1-deviations all nodes in V_1 pick the same colour as some node in V_2, say 2, before the unique node in V_2 of colour 2 picks colour 1. By repeating the same process with all other $p - 1$ nodes in V_2, one finally obtains a sequence of $(p + 1)^2 = \theta(n^2)$ 1-deviations.

Proposition 22. *There is a graph $G = (V, w)$ constrained to $\mathcal{W} = \{-\infty, 0, 1\}$ such that there does not exist a 3-stable partition for the colouring game defined on G.*

Figure 5 presents a graph with 18 vertices that does not admit any stable partition for $k = 3$. Note in particular the presence of 4 indifferent edges shown in dashed lines: without these edges a k-stable partition would exist for all values of k. The proof illustrates the complexity of sequences of 3-deviations, which are able to create infinite sequences of deviations at *constant* global utility! To keep the graph readable, we use conventions. (1) Some sets of nodes are grouped within a circle; an edge from another node to that circle denotes an edge to *all* elements of this set. (2) All nodes that are not connected by an edge on the Figure are enemies with weights $-\infty$. (3) Green solid edges represent edges with weight 1, whereas blue dashed edges represent edges with weight 0.

The proof of Proposition 22 relies on another structural result which we state as follows.

Definition 23. *Let $G = (V, w)$, and let $u, u' \in V$. We say that u and u' are* quasi-twins *if $w_{uu'} > 0$ and for all nodes $v \in V \setminus \{u, u'\}$ $w_{uv} = w_{u'v}$ except maybe for one v_0 for which $|w_{uv_0} - w_{u'v_0}| = 1$.*

Lemma 24. *Given a graph $G = (V, w)$, let P be a 1-stable partition for the colouring game defined on it. Then, $c_u(P) = c_{u'}(P)$ for all quasi-twin vertices u, u'.*

Proof. Without loss of generality we have that for all vertices $v \in V \setminus \{u, u'\}$, $w_{uv} \geq w_{u'v}$. Equivalently, either $w_{uv} = w_{u'v}$ for all $v \in V \setminus \{u, u'\}$, or there is a unique v_0 such that $w_{uv_0} = w_{u'v_0} + 1$ and $w_{uv} = w_{u'v}$ for all $v \in V \setminus \{u, u', v_0\}$. Suppose by contradiction $c_u(P) \neq c_{u'}(P)$. There are two cases to be considered.

- **Case $f_u(P) > f_{u'}(P)$.** Then $(u', c_u(P))$ breaks the partition because, after it happens we get a new partition P' so that $f_{u'}(P') \geq (f_u(P) - 1) + w_{uu'} \geq f_u(P) > f_{u'}(P)$.
- **Case $f_u(P) \leq f_{u'}(P)$.** Then $(u, c_{u'}(P))$ breaks the partition because, after it happens we get a new partition P' so that $f_u(P') \geq f_{u'}(P) + w_{uu'} > f_{u'}(P) \geq f_u(P)$.

There is a contradiction in both cases, hence $c_u(P) = c_{u'}(P)$. □

Proof. [Proposition 22] The set of vertices consists of four sets A_i, $0 \leq i \leq 3$, each of equal size $h \geq 2$ and with a special vertex a_i, plus four vertices b_i, $0 \leq i \leq 3$, and two vertices c_0 and c_1. In what follows, indices are taken modulo 2 for c_j, $j \in \{0, 1\}$, and they are taken modulo 4 everywhere else. Figure 5 represents the example with $h = 3$. The friendship graph G^+ here consists of all the edges with weight 1; it contains:

1. all the edges between nodes in A_i ($0 \leq i \leq 3$);
2. edges between b_i and A_i ($0 \leq i \leq 3$);

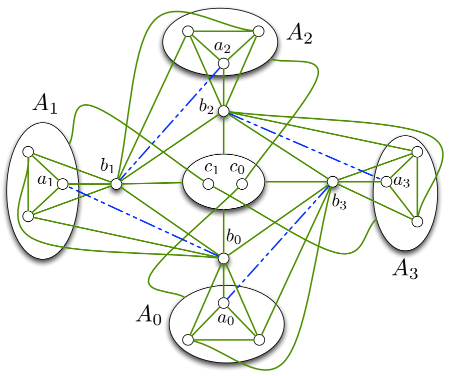

Figure 5: Graph that does not admit a 3-stable partition.

3. edges between b_i and $A_{i+1} \setminus \{a_{i+1}\}$ $(0 \leq i \leq 3)$;
4. edges between b_i and b_{i-1} and b_{i+1} $(0 \leq i \leq 3)$;
5. edges between c_0 and all the b_i, and edges between c_1 and all the b_i;
6. edges between c_0 and $A_0 \cup A_2$, and edges between c_1 and $A_1 \cup A_3$.

Moreover, there are four edges with weight 0, namely the edges $b_i a_{i+1}$. All the remaining edges have weight $-\infty$. That is two nodes in different $A_i, A_{i'}$ are enemies; a user b_i is enemy of b_{i+2} and of the nodes in A_{i+2} and A_{i+3}; c_0 and c_1 are enemies; c_0 is enemy of the nodes in A_1 and A_3, and c_1 is enemy of the nodes in A_0 and A_2. We now assume there exists a 3-stable partition P for the colouring game defined on $G = (V, w)$.

Claim 25. *Every node in A_i picks the same colour.*

Proof. It directly follows from Lemma 24 because all vertices in A_i are pairwise quasi-twins. ◇

Claim 26. *b_i picks the same colour as nodes in A_i or nodes in A_{i+1}.*

Proof. Suppose it is not the case. Then $X_{c_{b_i}(P)}$ contains at most two other nodes: one of b_{i-1} and b_{i+1} (together enemies), and one of c_0 and c_1 (enemies). If $|X_{c_{b_i}(P)}| \leq 2$ or the group X_j containing A_i has size at least 3, then $(\{b_i\}, j)$ is a 1-deviation. So, we assume $|X_{c_{b_i}(P)}| = 3$, $h = 2$ and $A_i = X_j$. There are two cases. If $c_{b_i}(P) = c_{c_i}(P)$ then $(\{b_i, c_i\}, j)$ is a 2-deviation. Else, $c_{c_{i-1}}(P) = c_{b_i}(P)$, and $X_{c_{b_i}(P)} \cap \{b_{i-1}, b_{i+1}\} \neq \emptyset$; hence we can break P using $(X_{c_{b_i}(P)} \cap \{c_{i-1}, b_{i-1}, b_{i+1}\}, j')$, with $A_{i-1} \subseteq X_{j'}$ or $A_{i+1} \subseteq X_{j'}$. ◇

Claim 27. *There is an i such that nodes A_i, b_i and b_{i-1} pick the same colour.*

Proof. Again, we show the claim by contradiction. We distinguish two cases:

Case 1: b_{i-1} is with A_i, but not b_i. So, as the claim is supposed to be false, b_i is with A_{i+1}, b_{i+1} is with A_{i+2}, and b_{i+2} is with A_{i+3}. Either $c_{b_{i-1}}(P) = c_{c_i}(P)$, hence $(\{b_i\}, c_{b_{i-1}}(P))$ breaks P, or $c_{b_{i-1}}(P) \neq c_{c_i}(P)$, hence $(\{b_i, c_i\}, c_{b_{i-1}}(P))$ breaks the partition.

Case 2: b_i is with A_i, but not b_{i-1}. So, as the claim is supposed to be false, b_{i-1} is with A_{i-1}, b_{i+1} is with A_{i+1}, and b_{i+2} is with A_{i+2}. Note either $c_{c_i}(P) = c_{b_i}(P)$ or $c_{c_i}(P) = c_{b_{i+2}}(P)$.

W.l.o.g., suppose $c_{c_i}(P) = c_{b_{i+2}}(P)$. Either $c_{b_{i-1}}(P) = c_{c_{i-1}}(P)$, hence $(\{b_i\}, c_{b_{i-1}}(P))$ breaks P, or $c_{b_{i-1}}(P) \neq c_{c_{i-1}}(P)$, hence it is $(\{b_i, c_{i-1}\}, c_{b_{i-1}}(P))$. $\diamond$

By Claim 27, it follows there is an i such that nodes in A_i, b_i, b_{i-1}, c_i all pick the same colour. Moreover, such a group is unique in P due to the conflict graph in (G, w) (induced by the conflict edges). By symmetry, we will assume $X_{c_{a_0}(P)} = \{b_0, b_3, c_0\} \cup A_0$.

Case 1: $c_{a_2}(P) = c_{b_1}(P) = c_{b_2}(P)$.
Either $c_{c_1}(P) = c_{a_1}(P)$ and $(\{b_1\}, c_{a_1}(P))$ breaks P, or $c_{c_1}(P) \neq c_{a_1}(P)$ and it is $(\{b_1, c_1\}, c_{a_1}(P))$.

Case 2: $c_{a_2}(P) = c_{b_2}(P) \neq c_{b_1}(P)$.
Either $c_{c_1}(P) = c_{a_3}(P)$ and $(\{b_2, b_3\}, c_{a_3}(P))$ breaks P, or $c_{c_1}(P) \neq c_{a_3}(P)$ and it is $(\{b_2, b_3, c_1\}, c_{a_3}(P))$.

Case 3: $c_{a_2}(P) = c_{b_1}(P) \neq c_{b_2}(P)$.
In that case, $(\{b_1\}, c(a_1))$ breaks P.

Case 4: $c_{a_2}(P) \neq c_{b_1}(P), c_{a_2}(P) \neq c_{b_2}(P)$, that implies $c_{b_2}(P) = c_{a_3}(P)$.
Either $c_{c_1}(P) = c_{a_3}(P)$ and $(\{b_3\}, c_{a_3}(P))$ breaks P, or $c_{c_1}(P) \neq c_{a_3}(P)$ and it is $(\{b_3, c_1\}, c_{a_3}(P))$.

Finally, there does not exist a 3-stable partition P for the colouring game defined on (G, w). $\square$

We emphasize the following consequence of Proposition 22.

Observation 2. *For $k > 1$, Algorithm 1 may not terminate even if a k-stable partition exists.*

Proof. Let $G = (V, w)$ be the counter-example of Proposition 22 that does not admit a 3-stable partition. We construct the instance $G' = (V, w')$ from G by replacing every conflict edge by an edge with weight zero. On the one hand there exists a 3-stable partition for the colouring game defined on G'. On the other hand, one can construct an infinite sequence of steps by taking G as input for Algorithm 1, and it is a valid sequence of 3-deviations for G' as well. $\square$

4.2 Game with general weights

While the two results we obtained ($k(\mathcal{W}) \geq 1$ in general, $k(\mathcal{W}) = 2$ when $\mathcal{W}$ contains a single positive weight) seem constrained, we now prove that these are the best results that one can hope for. Furthermore, we also want to consider in this section the case of "*best friends*" *i.e.*, two friends who want to interact unless there is an enemy of one of them to interfere. For this purpose, we put $w_{uv} = N$ where N denotes an arbitrarily large positive weight that is at least n times greater than any other (finite) weight in absolute value. Table 2 summarizes the most important values for $k(\mathcal{W})$, and it refers to the lemmas and proposition in the appendix where they are proved.

$\mathcal{W}$	$k(\mathcal{W})$	
$\{-\infty, a\}, a > 0$	∞	[22]
$\{-\infty, 0, a\}, a > 0$	2	Theorem 21, Proposition 22
$\{-\infty, a, b\}, b > a > 0$	1	Lemma 32
$\{-a, b\}, a > 0, b > 0$	$\leq 2 \cdot \lceil \frac{a+1}{b} \rceil + 1$	Lemma 35
$\{-\infty, N, -a\}, a > 0$	≤ 2	Corollary 34
$\mathbb{N} \cup \{N\}$ or $-\mathbb{N} \cup \{-\infty\}$	∞	*(trivial)*
$-\mathbb{N} \cup \{N\}$	∞	Proposition 36

Table 2: Values of $k(\mathcal{W})$ for different $\mathcal{W}$.

Finally we completely characterize the sets of weights $\mathcal{W}$ which satisfy $k(\mathcal{W}) = \infty$.

Theorem 28. *$k(\mathcal{W}) = \infty$ if, and only if: $\mathcal{W} \subseteq \mathbb{N} \cup \{N\}$; or $\mathcal{W} \subseteq -\mathbb{N} \cup \{-\infty\}$; or $\mathcal{W} = \{-\infty, a\}, a > 0$ (possibly $a = N$); or $\mathcal{W} \subseteq -\mathbb{N} \cup \{N\}$ (and so, $-\infty \notin \mathcal{W}$).*

4.3 Intractability with conflict graphs

Under general weights, we have proved that not all games in general have a k-stable partition, even for relatively simple sets of weights and small values of k. On the other hand, one could argue that these results come from pathological cases which could be ruled out after checking a property of the graph. We prove it is unlikely to be the case: not only is the stability not guaranteed for a given game when $k > k(\mathcal{W})$, but it is computationally prohibitive to decide it. We first define:

Definition 29 (k-Stable decision problem). *Let $k \geq 1$ and let $\mathcal{W}$ be a (fixed) set of weights. Given a graph $G = (V, w)$ constrained to these weights, does there exist a k-stable partition for the colouring game defined on it ?*

Theorem 30. *For $k \geq 1$ and $\mathcal{W}$ containing $-\infty$, either a k-stable partition always exists (*i.e.*, $k \leq k(\mathcal{W})$); or the* k-Stable decision problem *is NP-complete.*

The previous result of NP-hardness in [22] requires another kind of deviations in addition to the classical k-deviations we consider in our paper (see *gossip deviations* in Section 5). Moreover, the large positive weight N is essential in their proof, whereas ours overrules these strong constraints.

The rest of the section is devoted to prove Theorem 30. The k-Stable decision problem is clearly in NP because one can decide whether a k-deviation exists in polynomial-time $n^{O(k)}$, for any fixed k. Informally, to prove the NP-hardness we will assume a counter-example to the k-Stable decision problem exists, and we will build a supergraph of it that is arbitrarily large. We will characterize k-stable partitions for the colouring game defined on the supergraph. In particular, we will prove a necessary and sufficient condition so that a partition is k-stable is that one player from the counter-example picks the same colour as a large independent set from the supergraph. By doing so, we will be able to reduce the well-known Maximum Independent Set problem to the k-Stable decision problem. The latter NP-complete problems seems to well encapsulate the difficulty of colouring games, as already observed in the uniform case [22].

For technical reasons, we will require one can lower-bound the utility of a player, in *any* 1-stable partition, by some positive constant. Intuitively, we make use of this lower-bound to ensure that in case a k-stable partition exists for the colouring game, then it means that some player from the counter-example picks the same colour as an independent set from the supergraph which is even larger. We now introduce two reductions so that one can obtain the lower-bound.

Reduction 1. *Let t be a positive integer, let $\mathcal{W}$ be finite and such that $\mathcal{W} \cap (\mathbb{N} \cup \{N\}) \neq \emptyset$. We set $w_p = \max \mathcal{W}$, which is positive and may equal N.*

Given $G = (V, w)$ constrained to $\mathcal{W}$, and $n' \geq n = |V|$, we construct $\tilde{G_{t,n'}}$ as follows. We add to the graph n' distinct copies of the complete graph K_t whose edges are all weighted w_p. Then we add a conflict edge between any two nodes in two distinct copies of K_t, and an edge weighted w_p between any node in V and any node belonging to some copy of K_t.

Intuitively, Reduction 1 increases the minimum utility of the nodes to $w_p t$.

Reduction 2. *Let α be a positive integer, let $\mathcal{W}$ be finite and such that $\mathcal{W} \cap (\mathbb{N} \cup \{N\}) \neq \emptyset$. We set $w_p = \max \mathcal{W}$, which is positive and may equal N.*

Given $G = (V, w)$ constrained to $\mathcal{W}$, we construct KG_α as follows. We replace every node $u \in V$ with a clique of α nodes $K_\alpha(u) \subseteq V(KG_\alpha)$. For all $u, v \in V$, every two nodes in $K_\alpha(u)$ are linked by an edge weighted w_p, and all nodes in $K_\alpha(u)$ are linked to all nodes in $K_\alpha(v)$ by edges weighted w_{uv}.

Said differently, we substitute every node in the graph by a clique.
Our reduction will make use of the following lemma that we will prove in the appendix.

Lemma 31. *Let $\mathcal{W}$ be finite and such that $\mathcal{W} \cap (\mathbb{N} \cup \{N\}) \neq \emptyset$. Given $G = (V, w)$, $n' \geq n = |V|$ and $t > n$, there exists a k-stable partition for the colouring game defined on G if, and only if, there exists a k-stable partition for the colouring game defined on $\tilde{G_{t,n'}}$.*

We are now able to prove Theorem 30:

Proof. [Theorem 30] Suppose there is $G_0 = (V_0, w^0)$ constrained to $\mathcal{W}$ and such that it does not admit a k-stable partition. W.l.o.g. we constrain $\mathcal{W}$ to the set of weights on the edges of G_0 so that it is finite. We notice that $\mathcal{W} \cap (\mathbb{N} \cup N) \neq \emptyset$ because otherwise, the partition with only singleton groups is k-stable for G_0. One can also assume there exists some $x_0 \in V_0$ whose removal makes the existence of a k-stable partition for the gotten subgraph. Indeed, otherwise, we remove nodes sequentially until obtaining this property.
Let P^0 be a k-stable partition for the colouring game defined on $G_0 \setminus x_0$. The partition $P^0 \cup \{x_0\}$ is not k-stable by the hypothesis and so, let $f_0^{P^0}$ be the *maximum* utility node x_0 can obtain after any k-deviation happens which breaks $P^0 \cup \{x_0\}$. We define f_0 as the maximum value $f_0^{P^0}$, taken amongst all such k-stable partitions; if $f_0 \leq 0$, then we replace G_0 with $\tilde{G}_{0t',n_0'}$ for t', n_0' large enough (in such case, all above properties of the counter-example still hold by Lemma 31). By setting $w_p = \max \mathcal{W}$, one can define two other constants, namely $\alpha = \lceil \frac{f_0}{w_p} \rceil$ and $c_0 = 2n_0 + 1$, with $n_0 = |V_0|$.

We can now prove the NP-hardness by using a polynomial reduction for the Maximum Independent Set problem. Let $G = (V, E)$ be a graph, and let $c \geq c_0$ be an integer. We define $D_G = (V, w_G)$ such that $\forall uv \in E, w_{uv} = -\infty$ and $\forall uv \notin E, w_{uv} = w_p$. Let $t = \lfloor \alpha c - \frac{f_0}{w_p} \rfloor$, and let $G_1 = \tilde{G}_{0t,n_0}$, let $G_2 = KD_{G\alpha}$. Observe that $t > \alpha c - \frac{f_0}{w_p} - 1 \geq \alpha c - n_0 - 1 \geq c - n_0 - 1 \geq n_0$, because $f_0 \leq n_0 w_p$.
We finally build the graph H_G from G_1 and G_2 as follows. We add a conflict edge between any node of $G_1 \setminus x_0$ and any node of G_2. All nodes of G_2 are linked to x_0 with an edge weighted w_p.

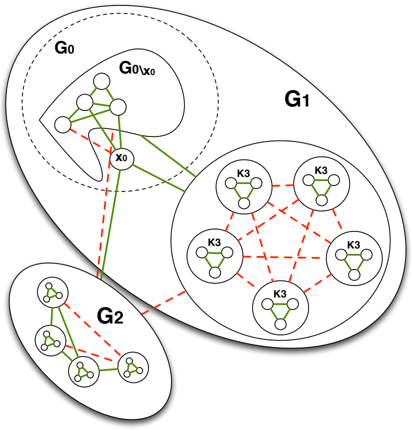

Figure 6: The transformation of an input.

The transformation above is illustrated in Figure 6. First assume that every independent set of G has a size lower than c. By contradiction, suppose there exists a k-stable partition for the colouring game defined on H_G. In such case, there can be no group with more than $\alpha(c-1)$ vertices of $V(G_2)$. Furthermore, nodes coloured as x_0 are either all in $V(G_1)$ or all in $V(G_2)$. Since $\alpha(c-1) = \alpha c - \lceil \frac{f_0}{w_p} \rceil \leq \alpha c - \frac{f_0}{w_p} - 1 < t$, it follows all such nodes belong to $V(G_1)$. Consequently, any k-stable partition for the colouring game defined on H_G, can be decomposed as follows: a k-stable partition for the colouring game defined on G_1, and a k-stable partition for the colouring game defined on G_2. Since G_0 does not admit a k-stable partition, hence G_1 does not admit one either by Lemma 31, it follows that H_G does not admit a k-stable partition.

Conversely, assume that there exists an independent set of G with size at least c. By [22], there exists a k-stable partition P^α for $G_2 \cup \{x_0\}$ which contains as a group X_j a maximum independent set of $G \cup \{x_0\}$. Moreover, $x_0 \in X_j$ because x_0 is an isolated vertex in the graph $G \cup \{x_0\}$. We also have that there exists a k-stable partition P^0 for $G_0 \setminus x_0$ and so, there exists a k-stable partition P^1 for $G_1 \setminus x_0 = \widetilde{(G_0 \setminus x_0)}_{t,n_0}$ by Lemma 31. Last, we claim that $P^H = P^\alpha \cup P^1$ is a k-stable partition for H_G. Indeed, on the one hand we have that the utility of x_0 in P^α is at least $w_p \alpha c$. On the other hand, the maximum utility x_0 can get after a k-deviation that breaks P^1 is $f_0^{P^0} + w_p t \leq f_0 + w_p t = w_p(t + \frac{f_0}{w_p}) \leq w_p \alpha c$. We can conclude the NP-hardness, as our transformation is polynomial, and the Maximum Independent Set problem is NP-complete [21]. □

5 Extensions of colouring games

All theoretical models of social dynamics should consider whether the overall behavior of the model is not too limited by some simplifying assumptions. We now discuss the way our results extend to account for various situations in the formation of social groups, including variants previously discussed and new ones. Full proofs of our results are provided in our technical report [14].

5.1 Gossiping

In this model, all k-deviations as previously defined are allowed. In addition two players in two distinct groups may "gossip" *i.e.,* both groups they are part of are merged. Obviously, and as before, this deviation will only take place if the two players benefit from the merge, but what is unique here is that the deviation does not require that other players in these groups benefit from the merge. They may even see a decrease in utility, but they are not given a choice to block the deviation — although they are in some sense seeing a modification of their group. This actually turns out to be equivalent to our model *in the uniform case*: one can check that there is a 1-deviation whenever there exists a gossip-deviation. Consequently all our results apply in that case, closing previously open problem with this model. In the general case, we prove that gossip creates instability even when a unique and fixed positive weight exists. We remind that without gossip, in such case a 2-stable partition always exists (see Theorem 21).

5.2 Asymmetry

Studying directed graphs rather than undirected graphs is a natural generalization. In this case, we may not have that $w_{uv} = w_{vu}$ for all players u, v. However, even if modest generalization of the model, asymmetrical weights lead to intractability. This can be seen with a simple digraph $D = (\{u, v\}, w)$ such that $w_{uv} > 0$ whereas $w_{vu} < 0$. Furthermore, the problem of deciding whether there exists a 1-stable partition is NP-hard. This result holds even when there can be no more than two groups in the partition.

5.3 Multichannel model and overlapping groups

One assumption of our model is that players form a partition, hence they are limited to a single channel to interact with their peers. In reality participants in social networks may engage in *multiple* groups. This motivates us to extend partitions into multisets, that we call 'configurations'. A configuration C is said to use q channels if each player participates (at most) to q groups. The utility of u depends on the number of groups that u shares with each peer:

$$f_u(C) = \sum_{v \in V} h\left(|X(u) \cap X(v)|\ ,\ w_{uv}\right)\ , \tag{1}$$

where $X(u)$ denotes the list of colours of u, and $h(g, w)$ is a function measuring the utility of sharing g groups with a player with weight w. Note that we assume, without loss of generality, that

$$\begin{array}{l} h(0,.) = 0\,,\, h(.,0) = 0 \ \text{ and } \ \forall w \in \mathbb{Z}\,,\, h(1,w) = w\,, \\ \forall g \in \mathbb{N}\,,\, w \mapsto h(g,w) \ \text{ is a non-decreasing function,} \\ \forall w \in \mathbb{Z}\,,\, g \mapsto w \cdot h(g,w) \ \text{ is a non-decreasing function.} \end{array}$$

The last property simply ensures that $h(g, w)$ increases with g when w is positive, and decreases with g when w is negative. Using the same potential function as before *e.g.,* global utility, it follows that there always exists a 1-stable configuration with q channels. It is now natural to wonder what is the behavior of $k_q(\mathcal{W})$ when the number of channels q is higher than 1. While it may have none or positive effects, we show that it is not always the case. Indeed, even for uniform games, we prove $k_2(\{-\infty, 1\}) \leq 2$ with 2 channels, while $k_1(\{-\infty, 1\}) = k(\{-\infty, 1\}) = \infty$.

5.4 Multi-modal relationship

Our model so far is heavily biased towards pairwise relationships, as the utility of a player depends on the sum of her interactions with all other members of the groups. In reality, more subtle interactions occur: one may be interested to interact with either friend u or v, but would not like to join a group where both of them are present. Our analysis also generalizes to this case. We use a hypergraph based model and we prove that, for instance, there always exists a 1-stable partition.

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.1 Proofs of Section 4

Proof. [Lemma 20] By the hypothesis, the utility of each vertex in S increases by at least 1. So, we get as the variation of the utility for the whole k-set: $\sum_{i=1}^{k}[f_{u_i}(P') - f_{u_i}(P)] \geq k$.
For every $1 \leq i \leq k$, we then define $\delta_i = \sum_{v \in X_{c_{u_i}(P)} \setminus S} w_{u_i v}$ and $\sigma_i = \sum_{u_l \in X_{c_{u_i}(P)}} w_{u_l u_i}$.
We define $\delta'_i = \sum_{v \in X_j} w_{u_i v}$ and $\sigma'_i = \sum_{l=1}^{k} w_{u_i u_l}$ in a similar way.
Then, $f_{u_i}(P) = \delta_i + \sigma_i$ and $f_{u_i}(P') = \delta'_i + \sigma'_i$. So, we get by summation that:
$\sum_{i=1}^{k} f_{u_i}(P) = \sum_{i=1}^{k} \delta_i + 2\sum_{\{u_i,u_l | c_{u_i}(P) = c_{u_l}(P)\}} w_{u_i u_l}$,
while $\sum_{i=1}^{k} f_{u_i}(P') = \sum_{i=1}^{k} \delta'_i + 2\sum_{1 \leq i,l \leq k} w_{u_i u_l}$. Note that we have a factor 2 for any occurence of $w_{u_i u_l}$, as it is counted once for u_i and once for u_l.

Furthermore, the variation of the global utility includes that of the nodes in S, that of the nodes in X_j, plus that of the nodes in $X_{c_{u_i}(P)} \setminus S$ for every $1 \leq i \leq k$. In other words, we get by symmetry that:
$f(P') - f(P) = \sum_{i=1}^{k}[f_{u_i}(P') - f_{u_i}(P)] + \sum_{i=1}^{k}[\delta'_i - \delta_i]$
$= 2\sum_{i=1}^{k}[f_{u_i}(P') - f_{u_i}(P)] - 2\sum_{1 \leq i,l \leq k} w_{u_i u_l} + 2\sum_{\{u_i,u_l | c_{u_i}(P) = c_{u_l}(P)\}} w_{u_i u_l}$
$\geq 2k - 2\sum_{1 \leq i,l \leq k} w_{u_i u_l} + 2\sum_{\{u_i,u_l | c_{u_i}(P) = c_{u_l}(P)\}} w_{u_i u_l}$. □

Proof. [Lemma 31] We first remind that one obtains $\tilde{G_{t,n'}}$ from G using n' distinct copies of the complete graph K_t, that we will denote by $K_t^1, \ldots, K_t^{n'}$ in the following.
First, let $P = (X_1, X_2, \ldots, X_n)$ be a k-stable partition for the colouring game defined on G. We claim $P' = (X_1 \cup V(K_t^1), X_2 \cup V(K_t^2), \ldots, X_n \cup V(K_t^n), V(K_t^{n+1}), \ldots, V(K_t^{n'}))$ is a k-stable partition for $\tilde{G_{t,n'}}$. By contradiction, let (S, j) be a k-deviation that breaks P', with $1 \leq j \leq n + tn'$. Note that w.l.o.g., one can assume no node in S is coloured j in P, as $(S \setminus X_j, j)$ is still a k-deviation that breaks P'. In addition, we must have $S' = S \cap V(G) \neq \emptyset$. Let $1 \leq j' \leq n$ be such that $X_{j'} \cap (V(G) \setminus S') = \emptyset$. Either nodes in S pick a colour j no node in $V(G) \setminus S'$ was using and so, (S', j') is a k-deviation that breaks P; or $S = S'$, and (S, j) also breaks P. A contradiction in both cases, because P is assumed to be k-stable.

Conversely, assume by contradiction that there is no k-stable partition for G, whereas there exists a k-stable partition $P' = (X'_1, \ldots, X'_{n+tn'})$ for $\tilde{G_{t,n'}}$. By Lemma 24, for any i all nodes in K_t^i are coloured accordingly. Furthermore, we note by construction of $\tilde{G_{t,n'}}$ that for all nodes $u \in V(G)$, she has to be pick the same colour as some clique K_t^i (else, the partition P' would not even be 1-stable). Let P be the partition of $V(G)$ whose non-empty groups are those amongst $X'_1 \cap V(G), X'_2 \cap V(G), \ldots, X'_{n+tn'} \cap V(G)$. By construction, P is not k-stable but then, every k-deviation (S, j) that breaks P also breaks P'. Consequently, there does not exist any k-stable partition for $\tilde{G_{t,n'}}$. □

Counter-examples for stability Counter-examples with different sets of weights are presented in the following. We first make an observation which is the starting point of most of our counter-examples for stability: namely, the weights $2, 3, 4$ in the counter-example of Figure 1 can be replaced by any weights w_1, w_2, w_3 such that $w_1 < w_2 < w_3$, and $w_1 + w_2 > w_3$. Especially, they can be replaced by $b, b+1, b+2$, for any $b \geq 2$. We now show through a counter-example no 2-stable partition exists in general when $\mathcal{W}$ contains two positive elements, even when the zero is not present.

Lemma 32. *Let a, b be two positive integers such that $a < b$. There is a graph $G = (V, w)$ constrained to $\mathcal{W} = \{-\infty, a, b\}$ that does not admit a 2-stable partition.*

Proof. Users are partitioned into four sets $U_1 = \{x_1, x_2, x_3\}$, $U_2 = \{y_1, y_2, y_3\}$, $U_3 = \{z_1, z_2, z_3\}$ and $\{v_1, v_2, v_3\}$. Each of these sets is a clique with edges weighted b. In addition, each edge between a node in U_i and another node in $U_{i'}, i \neq i'$ is a conflict edge. Node v_1 is linked to nodes in U_2 with edges weighted b, to nodes in U_1 with conflict edges. In the same way, node v_2 is linked to nodes in U_3 with edges weighted b, to nodes in U_2 with conflict edges; node v_3 is linked to nodes in U_1 with edges weighted b, to nodes in U_3 with conflict edges. We finally set: $w_{v_1 z_1} = w_{v_1 z_2} = b$, $w_{v_1 z_3} = a$; $w_{v_2 x_1} = w_{v_2 x_2} = b$, $w_{v_2 x_3} = a$; $w_{v_3 y_1} = w_{v_3 y_2} = b$, $w_{v_3 y_3} = a$.
Let us assume by contradiction there exists a 2-stable partition P.

Claim 33. *For any $1 \leq i \leq 3$, nodes in U_i are coloured accordingly.*

Proof. By symmetry, it suffices to show the claim for U_1. First, nodes x_1, x_2 pick the same colour by Lemma 24. Furthermore, by construction there can be no node coloured $c_{x_1}(P)$ that is an enemy of x_3. Since $\sum_{s \in V \setminus V_1} \max\{0, w_{x_3 s}\} = b + a < 2b$, it follows $c_{x_3}(P) = c_{x_1}(P) = c_{x_2}(P)$ (otherwise, the partition would not even be 1-stable). $\diamond$

We can then substitute subsets U_i with nodes u_i through contractions, and by doing so, one obtains the variation of Figure 1 with weights $w_1 = b$, $w_2 = 2b + a$, $w_3 = 3b$. Let P' be the partition of the nodes one obtains from P in this new graph. Since one can always find a 2-deviation using nodes v_1, v_2, v_3 that breaks P', one can deduce from such deviation a 2-deviation in G that breaks P. $\square$

Corollary 34. *If $\{-\infty, N\}$ is a strict subset of $\mathcal{W}$, then $k(\mathcal{W}) \leq 2$.*

Proof. First assume there exists a positive weight $a \in \mathcal{W} \setminus \{N\}$. Then we can apply Lemma 32 to the subset $\{-\infty, a, N\}$, and then one obtains $k(\mathcal{W}) = 1$. Else, let G_0 be the counter-example from Proposition 22, constrained to $\{-\infty, 0, 1\}$ and that does not admit a 3-stable partition. Let a non-negative be such that $-a \in \mathcal{W} \setminus \{N\}$. We construct G_1 from G_0 by replacing edges weighted 1 with edges weighted N, and null-weight edges with edges weighted $-a$. As there does not exist any 3-stable partition for G_0, there does not exist any 3-stable partition for G_1 either. Thus, $k(\mathcal{W}) \leq 1$. $\square$

Lemma 35. *Let a, b be positive integers (not necessarily distinct). There is $G = (V, w)$ constrained to $\mathcal{W} = \{-a, b\}$ that does not admit a $2 \cdot \left(1 + \lceil \frac{a+1}{b} \rceil\right)$-stable partition.*

Proof. Let x, y non-negative be such that $bx - ay = \gcd\{a, b\} = d$. The vertex-set is partitioned in $V_1, V_2, V_3, U_1^+, U_2^+, U_3^+, U_1^-, U_2^-, U_3^-$ plus three vertices $u_1^=, u_2^=, u_3^=$.
Any subset V_i has size $1 + \lceil \frac{a+1}{b} \rceil$, and there are constants k_1, k_2, k_3 that we assume sufficiently large so that subsets U_i^+, U_i^- have respective size $\left\lceil \frac{1+b\left(1+\lceil \frac{a+1}{b} \rceil\right)}{d} \right\rceil \cdot x + k_i \cdot a$, $\left\lceil \frac{1+b\left(1+\lceil \frac{a+1}{b} \rceil\right)}{d} \right\rceil \cdot y + k_i \cdot b - 1$.
As for the weights, subsets $V_1 \cup V_2 \cup V_3$ and $U_i = U_i^+ \cup U_i^- \cup \{u_i^=\}$ all induce complete subgraphs of the friendship graph G^+ (here induced by edges weighted b). Any node of U_i^+ is also linked to all nodes in $(V_1 \cup V_2 \cup V_3) \setminus V_i$ with edges weighted positively. Last, node u_1 is adjacent in G^+ to all nodes in V_3, and similarly node u_2 is adjacent in G^+ to all nodes in V_1, node u_3 is adjacent in G^+ to all nodes in V_2. Every remaining edge has weight $-a$.

Suppose by contradiction there is a $2\left(1 + \lceil \frac{a+1}{b} \rceil\right)$-stable partition P for the colouring game defined on G. By Lemma 24, all nodes in subsets $V_1, V_2, V_3, U_1^+, U_2^+, U_3^+, U_1^-, U_2^-, U_3^-$ are coloured accordingly. Furthermore for any $i > j$, assuming $k_i >> k_j >> 1 + \lceil \frac{a+1}{b} \rceil$ we have that no node of $U_j \cup V_i$ picks the same colour as nodes in U_i^+, nor the same colour as nodes in U_i^- (else, the partition would not even be 1-stable). Under similar assumptions, one obtains that all nodes in U_i are coloured accordingly. By contracting subsets V_i and U_i in the obvious way, one thus obtains

the variation of Figure 1 with weights $w_1 = \left(1 + \lceil\frac{a+1}{b}\rceil\right) \cdot b \geq b + a + 1; w_2 = \left\lceil \frac{1+b\left(1+\lceil\frac{a+1}{b}\rceil\right)}{d} \right\rceil \cdot d > w_1; w_3 = b + a + w_2 < w_1 + w_2$.
Let P' be the partition of the nodes one obtains from P in this new graph. Since one can always find a 2-deviation using nodes v_1, v_2, v_3 that breaks P', one can deduce from such deviation a $2 \cdot \left(1 + \lceil\frac{a+1}{b}\rceil\right)$-deviation in G that breaks P. □

Positive result

Proposition 36. *If $\mathcal{W} \subseteq -\mathbb{N} \cup \{N\}$, then $k(\mathcal{W}) = \infty$.*

Proof. Let $G = (V, w)$ constrained to $\mathcal{W}$, and let G^+ be the friendship graph that is here induced by edges weighted N. We define P as the partition of the nodes whose non-empty groups are exactly the connected components of G^+. Suppose (S, j) is a deviation that breaks P. On the one hand, no node has an incentive to decrease the number of best friends in her group, which means S is a collection of groups in P whose all vertices change their colour. On the other hand we have by the definition of P that no node in S can increase her number of best-friends by changing her colour. As a result, no such deviation can exist and so, P is a k-stable partition for any $k \geq 1$. □

Appendix J

The parallel complexity of coloring games

The parallel complexity of coloring games [⋆]

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Abstract. We wish to motivate the problem of finding *decentralized lower-bounds* on the complexity of computing a Nash equilibrium in graph games. While the centralized computation of an equilibrium in polynomial time is generally perceived as a positive result, this does not reflect well the reality of some applications where the game serves to implement distributed resource allocation algorithms, or to model the social choices of users with limited memory and computing power. As a case study, we investigate on the parallel complexity of a game-theoretic variation of graph coloring. These "coloring games" were shown to capture key properties of the more general welfare games and Hedonic games. On the positive side, it can be computed a Nash equilibrium in polynomial-time for any such game with a local search algorithm. However, the algorithm is time-consuming and it requires polynomial space. The latter questions the use of coloring games in the modeling of information-propagation in social networks. We prove that the problem of computing a Nash equilibrium in a given coloring game is PTIME-hard, and so, it is unlikely that one can be computed with an efficient distributed algorithm. The latter brings more insights on the complexity of these games.

1 Introduction

In algorithmic game theory, it is often the case that a problem is considered "tractable" when it can be solved in polynomial time, and "difficult" only when it is NP-hard or it is PLS-hard to find a solution. On the other hand, with the growing size of real networks, it has become a boiling topic in (non game-theoretic) algorithmic to study on the finer-grained complexity of polynomial problems [16]. In our opinion, the same should apply to graph games when they serve as a basis for new distributed algorithms. We propose to do so in some cases when it can be easily computed a Nash equilibrium in polynomial time. The following case study will make use of well-established parallel and space complexity classes to better understand the hardness of a given graph game.

Precisely, we investigate on a "coloring game", first introduced in [14] in order to unify classical upper-bounds on the chromatic number. Since then it has been rediscovered many times, attracting attention on the way in the study of information propagation in wireless sensor networks [4] and in social networks [12]. We choose to consider this game since it is a good representative of the *separable welfare games* – proposed in [13] as a game-theoretic toolkit for distributed

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resource allocation algorithms – and the *additively separable symmetric Hedonic games* [3]. A coloring game is played on an undirected graph with each vertex being an agent (formal definitions will be given in the technical sections of the paper). Agents must choose a colour in order to construct a proper coloring of the graph. The individual goal of each agent is to maximize the number of agents with the same colour as hers. Furthermore, it can always be computed a Nash equilibrium in polynomial time with a simple local-search algorithm [6, 12, 14].

However, for n-vertex m-edge graphs, the above-mentioned algorithm has $\mathcal{O}(m + n\sqrt{n})$-time complexity and $\mathcal{O}(n + m)$-space complexity. Therefore, when the graph gets larger, potential applications of coloring games as a *computational mechanism design* (*e.g.*, in order to assign frequencies in sensor networks in a distributed fashion, or to model the behaviour of social network users with limited power and storage) can be questioned. In particular, the authors in [11] report on the limited abilities of human subject networks to solve a coloring problem. In this note, we will investigate on the belonging of our problem – the computation of a Nash equilibrium in coloring games – to some complexity classes that are related to parallel and space complexity. Our goal in doing so is to bring more insights on the complexity of the problem.

Related work. Apart from lower-bounds in communication complexity [7], we are not aware of any analysis of decentralized complexity in game theory. Closest to our work are the studies on the sequential complexity of Hedonic games. Deciding whether a given Hedonic game admits a Nash equilibrium is NP-complete [1]. Every additively separable symmetric Hedonic games has a Nash equilibrium but it is PLS-complete to compute one [8]. Coloring games are a strict subclass where the local-search algorithm terminates on a Nash equilibrium within a polynomial number of steps. We will go one step further by considering their parallel complexity, something we think we are the first to study.

In [4], they introduced a distributed algorithm in order to compute the Nash equilibrium of a given coloring game. Their algorithm is a natural variation of the classical local-search algorithm for the problem, however, it does not speed up the computation of equilibria (at least theoretically). In addition, each agent needs to store locally the colouring of the graph at any given step, that implies *quadratic* space and communication complexity. Additional related work is [6, 12], where it is studied the number of steps of more elaborate local-search algorithms when up to k players are allowed to *collude* at each step. Informally, collusion means that the players can simultaneously change their colours for the same new colour provided they all benefit from the process (note that the classical local-search algorithm corresponds to the case $k = 1$).

Contributions. We prove that the problem of computing a Nash equilibrium in a given coloring game is PTIME-hard (Theorem 2). This is hint that the problem is inherently *sequential*, *i.e.*, it is unlikely the computation of an equilibrium can be sped up significantly on a parallel machine with polynomially many processors. In particular, our negative result applies to the *distributed* setting since any distributed algorithm on graphs can be simulated on a parallel machine with one processor per edge and per vertex. By a well-known relationship between space and parallel complexity [15], Theorem 2 also extends to show that no *space efficient* algorithm for the problem (say, within logarithmic workspace) can exist. Altogether, this may be hint that coloring games are a too powerful computational mechanism design for "lightweight" distributed applications.

Our reduction is from the standard MONOTONE CIRCUIT VALUE problem. However, the gadgets needed are technically challenging, and we will need to leverage nontrivial properties of coloring games in order to prove its correctness. Definitions and useful background will be given in Section 2. We will detail our reduction in Section 3 before concluding this paper in Section 4.

2 Definitions and notations

We use the graph terminology from [2]. Graphs in this study are finite, simple, and unweighted.

Coloring games. Let $G = (V, E)$ be a graph. A *coloring* of G assigns a positive integer, taken in the range $\{1, \ldots, n\}$, to each of the n vertices in V. For every i, let L_i be the subset of vertices coloured i. We name L_i a *colour class* in what follows. Nonempty colour classes partition the vertex set V. The partition is a *proper coloring* when no two adjacent vertices are assigned the same colour, *i.e.*, for every $1 \leq i \leq n$ and for every $u, v \in L_i$, $\{u, v\} \notin E$.

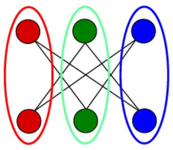

Fig. 1. Proper coloring of a graph G. Each colour class is represented by an ellipse. Every agent receives unit payoff.

Every graph G defines a *coloring game* whose n agents are the vertices in V. The strategy of an agent is her colour. Furthermore, every $v \in L_i$ receives payoff: -1 if there is $u \in L_i$ s.t. $\{u, v\} \in E$ (in which case, the coloring is not proper), and $|L_i| - 1$ otherwise. We refer to Figure 1 for an illustration. Finally, a *Nash equilibrium* of the coloring game is any coloring of G where no agent can increase her payoff by changing her strategy. In particular, the proper coloring in Figure 1 is a Nash equilibrium. More generally, observe that a Nash equilibrium in this game is always a proper coloring of G. In what follows, we will focus on the computation of Nash equilibria in coloring games.

Theorem 1 ([6, 12]). *For any coloring game that is specified by an n-vertex m-edge graph $G = (V, E)$, a Nash equilibrium can be computed in $\mathcal{O}(m + n\sqrt{n})$-time and $\mathcal{O}(n + m)$-space.*

Parallel complexity. Computations are performed on a parallel random-access machine (PRAM, see [9]) with an unlimited amount of processors. However, as stated in the conclusion, our results also apply to more realistic parallel complexity classes. In what follows, we will use the fact that processors are numbered. We will handle with read/write conflicts between processors with the strategy CREW-PRAM (concurrent read, exclusive write). Let PTIME contain the decision problems that can be solved in *sequential* polynomial-time (that is, with a single processor). Problem A reduces to problem B if given an oracle to solve B, A can be solved in polylogarithmic-time with a polynomial number of processors. In particular, a problem B is PTIME-hard if every problem in PTIME reduces to B (this is formally defined as quasi-PTIME-hardness in [9]). Such reductions are finer-grained than the more standard logspace reductions.

3 Main Result

Theorem 2. *Computing a Nash equilibrium for coloring games is PTIME-hard.*

In order to prove Theorem 2, we will reduce from a variation of the well-known Monotone Circuit Value problem, defined as follows.

*Problem 1 (*Monotone Circuit Value*).*

Input: A boolean circuit $\mathcal{C}$ with m gates and n entries, a word $w \in \{0,1\}^n$ such that:
- the gates are either AND-gates or OR-gates;
- every gate has exactly two entries (in-degree two);
- a *topological ordering* of the gates is given, with the m^{th} gate being the output gate.

Question: Does $\mathcal{C}$ output 1 when it takes w as input ?

Monotone Circuit Value is proved to be PTIME-complete in [9].

3.1 The reduction

Let $\langle \mathcal{C}, w \rangle$ be any instance of Monotone Circuit Value. We will reduce it to a coloring game as follows. Let $\mathcal{G} := (g_1, g_2, \ldots, g_m)$ be the gates of the circuit, that are topologically ordered.

Construction of the gate-gadgets. For every $1 \leq j \leq m$, the j^{th} gate will be simulated by a subgraph $G_j = (V_j, E_j)$ with $12(n+j) - 9$ vertices. We refer to Figure 2 for an illustration. Let us give some intuition for the following construction of G_j. We aim at simulating the computation of the (binary) output of all the gates in $\mathcal{C}$ when it takes w as input. To do that, given a supergraph G of G_j (to be defined later), and a fixed Nash equilibrium for the coloring game that is defined on G, we aim at guessing the output of the j^{th} gate from the subcoloring of G_j. More precisely, the subcoloring will encode a "local certificate" that indicates which values on the two entries of g_j cause the output.

Observe that to certify that an OR-gate outputs 1, it suffices to show that it receives 1 on any one of its two entries, whereas for an AND-gate it requires to show that it outputs 1 on its two entries. Since by de Morgan's laws, the negation of an AND-gate can be transformed into an OR-gate and vice-versa, therefore, we need to distinguish between three cases in order to certify the output of the gate. So, the vertices in V_j are partitioned in three subsets of equal size $4(n+j)-3$, denoted by $V_j^1,\ V_j^2,\ V_j^3$. Furthermore, for every $1 \leq t \leq 3$, every vertex in V_j^t is adjacent to every vertex in $V_j \setminus V_j^t$.

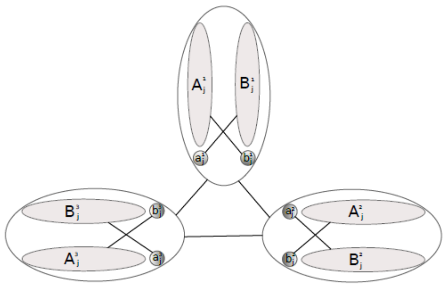

Fig. 2. Gadget subgraph G_j representing the j^{th} gate. An edge between two subsets of vertices (delimited by an ellipse) denotes the existence of a complete bipartite subgraph.

Let us now describe the structure of the three (isomorphic) subgraphs $G_j[V_j^t] = (V_j^t, E_j^t)$ with $1 \leq t \leq 3$. Informally, we will need this internal structure in order to ensure that every of the three subsets V_j^t will behave as a "truthful" certificate to decide on the output of the gate; *i.e.*, only a few vertices of V_j will be used to certify the output of the j^{th} gate, while all others will be divided into artificial aggregates that we name "private groups" whose role is to ensure "truthfulness" of the certificate (this will be made clearer in the following). There are two nonadjacent vertices $a_j^t, b_j^t \in V_j^t$ playing a special role. The other vertices in $V_j^t \setminus \{a_j^t, b_j^t\}$ are partitioned in two subsets A_j^t, B_j^t of respective size $2(n+j)-3$ and $2(n+j)-2$. The sets A_j^t, B_j^t are called the *private groups* of a_j^t, b_j^t. Furthermore, every vertex in A_j^t is adjacent to every vertex in $V_j^t \setminus (A_j^t \cup \{a_j^t\})$, similarly every vertex in B_j^t is adjacent to every vertex in $V_j^t \setminus (B_j^t \cup \{b_j^t\})$.

Since all edges are defined above independently the one from the other, the graph $G_j[V_j^1] = (V_j^1, E_j^1)$ (encoded by its adjacency lists) can be constructed with $|V_j^1| + |E_j^1| = 4(n+j)^2 - 2(n+j) - 2$ processors simply by assigning the construction of each vertex and each edge to a different processor. Note that each processor can decide on the vertex, resp. the edge, it needs to compute from its number. Overall, it takes $\mathcal{O}(\log(n+j))$-time in order to construct $G_j[V_j^1]$ in parallel. The latter can be easily generalized in order to construct G_j in $\mathcal{O}(\log(n+j))$-time with $|V_j|+|E_j|$ processors. Therefore, the graphs $G_1, G_2, \ldots, G_m$ can be constructed in parallel in $\mathcal{O}(\log(n+m))$-time with $\sum_{j=1}^{m}(|V_j|+|E_j|)$ processors, that is polynomial in $n+m$.

Construction of the graph. Let $X = \{x_1, x_1', \ldots, x_i, x_i', \ldots, x_n, x_n'\}$ contain $2n$ nonadjacent vertices, that are two vertices per letter in the binary word w. The graph $G = (V, E)$ for the reduction has vertex-set $V = X \cup \left(\bigcup_{j=1}^{m} V_j\right)$. In particular, it has $2n - 9m + 6m(m+2n+1)$ vertices. Furthermore, $G[V_j]$ is isomorphic to G_j for every $1 \le j \le m$. In order to complete our reduction, let us now describe how our gadgets are connected the one with the other.

For technical reasons, we will need to make adjacent every vertex in the private group A_j^t (resp. B_j^t), with $1 \le j \le m$ and $1 \le t \le 3$, to every vertex in $V \setminus V_j$. By doing so, note that every vertex in $V \setminus (A_j^t \cup \{a_j^t\})$ is adjacent to every vertex in A_j^t (resp., every vertex in $V \setminus (B_j^t \cup \{b_j^t\})$ is adjacent to every vertex in B_j^t). Furthermore, each edge is defined independently the one from the other. Hence, similarly as above, $\sum_{j=1}^m \sum_{t=1}^3 (|A_j^t| + |B_j^t|)|V \setminus V_j|$ processors are sufficient in order to construct these edges in $\mathcal{O}(\log(n+m))$-time, that is polynomial in $n+m$.

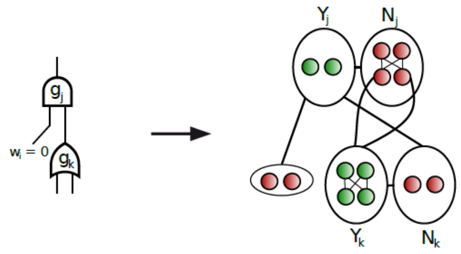

Fig. 3. Edges in G to simulate the two connections of an AND-gate in the circuit.

Finally, we recall that for every j, there are three cases to distinguish in order to decide on the output of the j^{th} gate, with each case being represented with some subset V_j^t. The union of subsets representing a *positive* certificate (output 1) is named Y_j, while the union of those representing a *negative* certificate (output 0) is named N_j. In particular, if the j^{th} gate is an OR-gate, let $Y_j := \{a_j^1, b_j^1, a_j^2, b_j^2\}$ and $N_j := \{a_j^3, b_j^3\}$ (it suffices to receive 1 on one input). Else, the j^{th} gate is an AND-gate, so, let $Y_j := \{a_j^1, b_j^1\}$ and $N_j := \{a_j^2, b_j^2, a_j^3, b_j^3\}$.

Suppose the j^{th} gate is an OR-gate (the case when it is an AND-gate follows by symmetry, up to interverting Y_j with N_j, see also Figure 3). Let us consider the first entry of the gate. There are two cases. Suppose that it is the i^{th} entry of the circuit, for some $1 \le i \le n$. If $w_i = 0$ then we make both x_i, x_i' adjacent to both a_j^1, b_j^1; else, $w_i = 1$, we make both x_i, x_i' adjacent to both a_j^3, b_j^3. Else, the entry is some other gate of the circuit, and so, since gates are topologically ordered, it is the k^{th} gate for some $k < j$. We make every vertex in N_k adjacent to both a_j^1, b_j^1, and we make every vertex in Y_k adjacent to both a_j^3, b_j^3.

The second entry of the gate is similarly considered, up to replacing above the two vertices a_j^1, b_j^1 with a_j^2, b_j^2. We refer to Figure 3 for an illustration. In particular, observe that there is only a constant number of edges that are added at this step for each gate. Furthermore, the construction of these new edges only requires to read the two in-neighbours of the gate in the circuit $\mathcal{C}$. As a result, the last step can be done in parallel in $\mathcal{O}(\log(n+m))$-time with m processors.

3.2 Structure of a Nash equilibrium

The graph $G = (V, E)$ of our reduction (constructed in Section 3.1) defines a coloring game. Let us fix any Nash equilibrium for this game (that exists by

Theorem 1). We will show that it is sufficient to know the colour of every vertex in $Y_m \cup N_m$ in order to decide on the output of the circuit $\mathcal{C}$ (recall that the m^{th} gate is the output gate). To prove it, we will need the following technical claims in order to gain more insights on the structure of the equilibrium.

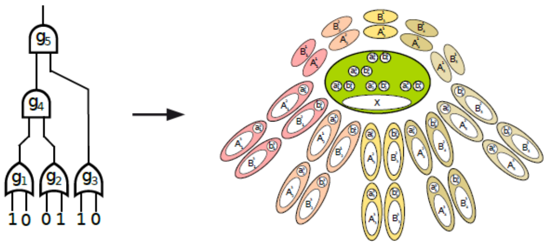

Fig. 4. A boolean circuit (left) with a Nash equilibrium of the coloring game from our reduction (right). Each colour class is represented with an ellipse. Intuitively, vertices in the central colour class simulate the computation of the output. Other colour classes contain a private group and they are "inactive".

More precisely, we will prove that there are exactly $6m + 1$ colour classes, that are one colour class per private group A_j^t or B_j^t and an additional colour for the vertices in X. The intuition is that there are $2(n + m)$ vertices in one special colour class (including X) that simulates the computation of the output of $\mathcal{C}$, whereas all other vertices are "trapped" with the vertices in their respective private group. We refer to Figure 4 for an illustration.

Claim 1. *For every j, any colour class does not contain more than two vertices in every $Y_j \cup N_j$. Furthermore, if it contains exactly two vertices in $Y_j \cup N_j$ then these are a_j^t, b_j^t for some $1 \leq t \leq 3$.*

Proof. A Nash equilibrium is a proper coloring of G. Therefore, since any two vertices in different subsets among V_j^1, V_j^2, V_j^3 are adjacent by construction, they cannot have the same colour. Since $Y_j \cup N_j = \{a_j^1, b_j^1, a_j^2, b_j^2, a_j^3, b_j^3\}$ and $a_j^t, b_j^t \in V_j^t$ for every $1 \leq t \leq 3$, the claim follows directly. $\diamond$

Claim 2. *Any two vertices that are in a same private group have the same colour. Similarly, x_i and x_i' have the same colour for every $1 \leq i \leq n$.*

Proof. Let S be either a private group ($S = A_j^t$ or $S = B_j^t$ for some $1 \leq j \leq m$ and $1 \leq t \leq 3$), or a pair representing the same letter of word w (*i.e.*, $S = \{x_i, x_i'\}$ for some $1 \leq i \leq n$). Let $v \in S$ maximize her payoff and let c be her colour. Note that v receives payoff $|L_c| - 1$ with L_c being the colour class composed of all the vertices with colour c. Furthermore, every $u \in S$ receives payoff lower than or equal to $|L_c| - 1$ by the choice of v. In such case, every $u \in S$ must be coloured c, or else, since the adjacency and the nonadjacency relations are the same for u and v (they are twins), furthermore u, v are nonadjacent, the agent u would increase her payoff to $|L_c|$ by choosing c as her new colour, thus contradicting the hypothesis that we are in a Nash equilibrium. $\diamond$

The argument we use in Claim 2 is that twin vertices must have the same colour. In what follows, we will use the same argument under different disguises.

Claim 3. *Let $1 \leq j \leq m$ and $1 \leq t \leq 3$. Either A_j^t or $A_j^t \cup \{a_j^t\}$ is a colour class, and in the same way either B_j^t or $B_j^t \cup \{b_j^t\}$ is a colour class. Furthermore, either $B_j^t \cup \{b_j^t\}$ is a colour class, or a_j^t and b_j^t have the same colour.*

Proof. Recall that a Nash equilibrium is a proper coloring of G. Since a_j^t is the only vertex in $V \setminus A_j^t$ that is nonadjacent to A_j^t, furthermore every two vertices in A_j^t have the same colour by Claim 2, therefore, either A_j^t or $A_j^t \cup \{a_j^t\}$ is a colour class. Similarly, either B_j^t or $B_j^t \cup \{b_j^t\}$ is a colour class. In particular, suppose that b_j^t does not have the same colour as her private group. Then, she must receive payoff at least $|B_j^t| = 2(n+j) - 2$ (else, she would increase her payoff by choosing the same colour as her private group, thus contradicting the hypothesis that we are in a Nash equilibrium). Furthermore, there can be only vertices in $V \setminus (A_j^t \cup B_j^t)$ with the same colour c as b_j^t. Suppose for the sake of contradiction that a_j^t does not have colour c. There are two cases to be considered.

Suppose that $A_j^t \cup \{a_j^t\}$ is a colour class. Then, a_j^t receives payoff $|A_j^t| = 2(n+j) - 3$. In such case, since a_j^t and b_j^t are twin vertices in $G \setminus (A_j^t \cup B_j^t)$, vertex a_j^t could increase her payoff to at least $2(n+j) - 1$ by choosing c as her new colour, thus contradicting the hypothesis that we are in a Nash equilibrium.

Else, a_j^t and b_j^t do not have the same colours as their respective private groups. In such case, A_j^t and B_j^t are colour classes, hence we can constrain ourselves to the subgraph $G \setminus (A_j^t \cup B_j^t)$. In particular, the constriction of the Nash equilibrium to the subgraph must be a Nash equilibrium of the coloring game defined on $G \setminus (A_j^t \cup B_j^t)$. Since a_j^t and b_j^t are twin vertices in $G \setminus (A_j^t \cup B_j^t)$, they must have the same colour by a similar argument as for Claim 2.

As a result, a_j^t must have colour c in both cases, that proves the claim. $\diamond$

We recall that we aim at simulating the computation of the output of all the gates in $\mathcal{C}$. To do that, we will prove the existence of a special colour class containing X and some pair in $Y_j \cup N_j$ for every j. Intuitively, the two vertices of $Y_j \cup N_j$ are used to certify the output of the j^{th} gate. However, this certificate is "local" in the sense that it assumes the output of the $j-1$ smaller gates to be already certified. Therefore, we need to prove that there can be no "missing gate", *i.e.*, every gate is represented in the special colour class.

Claim 4. *Let c be a colour such that $L_c \not\subseteq X$ and L_c does not intersect any private group (A_j^t or B_j^t for any $1 \leq j \leq m$ and $1 \leq t \leq 3$).*

Then, $X \subseteq L_c$ and there exists an index j_0 such that the following holds true: $|L_c \cap (Y_j \cup N_j)| = 2$ for every $1 \leq j \leq j_0$, and $L_c \cap (Y_j \cup N_j) = \emptyset$ for every $j_0 + 1 \leq j \leq m$.

Proof. By the hypothesis $L_c \not\subseteq X$ and L_c does not intersect any private group, so, there is at least one vertex of $\bigcup_{j=1}^m (Y_j \cup N_j)$ with colour c. Let j_0 be the largest index j such that there is a vertex in $Y_j \cup N_j$ with colour c. Since by Claim 1, there can be no more than two vertices of $Y_j \cup N_j$ that are in L_c for every j, therefore, by maximality of j_0 we get $|L_c| \leq |X| + 2j_0 = 2(n + j_0)$. In particular, observe that if $|L_c| = 2(n + j_0)$ then $X \subseteq L_c$ and for every $1 \leq j \leq j_0$ there are exactly two vertices in $Y_j \cup N_j$ with colour c. So, let us prove that $|L_c| = 2(n + j_0)$, that will prove the claim. By the choice of j_0, there is some $1 \leq t \leq 3$ such that $a^t_{j_0} \in L_c$ or $b^t_{j_0} \in L_c$. In particular, $|L_c| \geq \min\{|A^t_{j_0}|, |B^t_{j_0}|\} + 1 = 2(n + j_0) - 2$ or else, every vertex $v^t_{j_0} \in L_c \cap \{a^t_{j_0}, b^t_{j_0}\}$ would increase her payoff by choosing the colour of the vertices in her private group (that is a colour class by Claim 3), thus contradicting the hypothesis that we are in a Nash equilibrium.

We prove as an intermediate subclaim that for any $1 \leq j \leq j_0 - 1$ such that $L_c \cap (Y_j \cup N_j) \neq \emptyset$, there is some $1 \leq t' \leq 3$ such that $a^{t'}_j, b^{t'}_j \in L_c$. Indeed, in this situation, there is some t' such that $a^{t'}_j \in L_c$ or $b^{t'}_j \in L_c$. If $b^{t'}_j \in L_c$ then we are done as by Claim 3, $a^{t'}_j \in L_c$. Otherwise, $b^{t'}_j \notin L_c$ and we prove this case cannot happen. First observe that $a^{t'}_j \in L_c$ in this case. Furthermore, since $a^{t'}_j$ and $b^{t'}_j$ do not have the same colour we have by Claim 3 that $B^{t'}_j \cup \{b^{t'}_j\}$ is a colour class. In this situation, $b^{t'}_j$ receives payoff $2(n+j) - 2 \leq 2(n+j_0-1) - 2 < |L_c|$. Since in addition $a^{t'}_j$ and $b^{t'}_j$ are twins in $G \setminus (A^{t'}_j \cup B^{t'}_j)$, vertex $b^{t'}_j$ could increase her payoff by choosing colour c, thus contradicting that we are in a Nash equilibrium. This proves $a^{t'}_j, b^{t'}_j \in L_c$, and so, the subclaim.

By the subclaim, there is an even number $2k$ of vertices in $\bigcup_{j=1}^{j_0-1}(Y_j \cup N_j)$ with colour c, for some $k \leq j_0 - 1$. Similarly, since by Claim 2 the vertices x_i, x'_i have the same colour for every $1 \leq i \leq n$, $|X \cap L_c| = 2n'$ for some $n' \leq n$. Now there are two cases to be considered.

Suppose that $b^t_{j_0} \in L_c$. Then, by Claim 3 $a^t_{j_0} \in L_c$. Furthermore $|L_c| \geq 2(n + j_0) - 1$ or else, vertex $b^t_{j_0}$ would increase her payoff by choosing the colour of the vertices in $B^t_{j_0}$ (that is a colour class by Claim 3), thus contradicting the hypothesis that we are in a Nash equilibrium. As a result, $|L_c| = 2(n'+k+1) \geq 2(n+j_0) - 1$, that implies $n'+k \geq n+j_0-1$, and so, $|L_c| \geq 2(n+j_0)$, as desired.

Else, $b^t_{j_0} \notin L_c$ and we prove this case cannot happen. First observe that $a^t_{j_0} \in L_c$. Furthermore, $|L_c| = 2(n' + k) + 1 \geq 2(n + j_0) - 2$, that implies $n' + k \geq n + j_0 - 1$, and so, $|L_c| \geq 2(n + j_0) - 1$. However, since $a^t_{j_0}$ and $b^t_{j_0}$ do not have the same colour, $B^t_{j_0} \cup \{b^t_{j_0}\}$ is a colour class by Claim 3. In particular, $b^t_{j_0}$ receives payoff $2(n+j_0) - 2 < |L_c|$. Since $a^t_{j_0}, b^t_{j_0}$ are twins in $G \setminus (A^t_{j_0} \cup B^t_{j_0})$, vertex $b^t_{j_0}$ could increase her payoff by choosing colour c, thus contradicting that we are in a Nash equilibrium.

Altogether, $|L_c| \geq 2(n + j_0)$, that proves the claim. ◇

We point out that by combining Claim 1 with Claim 4, one obtains that for every $1 \leq j \leq m$, there are either zero or two vertices in $Y_j \cup N_j$ in each colour class not containing a private group, and in case there are two vertices then these are a^t_j, b^t_j for some $1 \leq t \leq 3$.

Claim 5. *Any two vertices in X have the same colour. Furthermore, for every $1 \leq j \leq m$, every vertex in $Y_j \cup N_j$ either has the same colour as vertices in X or as vertices in her private group.*

Proof. Let L_c be any colour class with at least one vertex in $\bigcup_{j=1}^{m}(Y_j \cup N_j)$. Let j_0 be the largest index j such that there is a vertex in $Y_j \cup N_j$ with colour c. In order to prove the claim, there are two cases to be considered. Suppose that

$L_c \neq A^t_{j_0} \cup \{a^t_{j_0}\}$ and $L_c \neq B^t_{j_0} \cup \{b^t_{j_0}\}$ for any $1 \leq t \leq 3$. We will prove that $X \subseteq L_c$, that will imply that L_c is unique in such a case, and so, will prove the claim. By the choice of colour c, $L_c \nsubseteq X$. Further, observe that there can be no private group with a vertex in L_c. As a result, this case follows directly from Claim 4.

Else, either $L_c = A^t_{j_0} \cup \{a^t_{j_0}\}$ or $L_c = B^t_{j_0} \cup \{b^t_{j_0}\}$ for some $1 \leq t \leq 3$, and we may assume that it is the case for any colour class L_c that contains at least one vertex in $\bigcup_{j=1}^m (Y_j \cup N_j)$ (or else, we are back to the previous case). So, let us constrain ourselves to the subgraph $G[X]$. In particular, the constriction of the Nash equilibrium to the subgraph must be a Nash equilibrium of the coloring game defined on $G[X]$. Since the vertices in X are pairwise nonadjacent, they must form a unique colour class in such case, that proves the claim. $\diamond$

We will need a "truthfulness" property to prove correctness of our reduction. Namely, the value of the output of any gate in the circuit must be correctly guessed from the agents with the same colour as vertices in X.

Claim 6. *Let $1 \leq j_0 \leq m$ such that for every $1 \leq j \leq j_0$, there is at least one vertex in $Y_j \cup N_j$ with the same colour c_0 as all vertices in X. Then for every $1 \leq j \leq j_0$, $L_{c_0} \cap Y_j \neq \emptyset$ if and only if the output of the j^{th} gate is 1.*

Proof. In order to prove the claim by contradiction, let $1 \leq j_1 \leq j_0$ be the smallest index j such that either $Y_j \cap L_{c_0} = \emptyset$ and the output of the j^{th} gate is 1 (false negative) or $Y_j \cap L_{c_0} \neq \emptyset$ and the output of the j^{th} gate is 0 (false positive). We will show that in such case, there is an edge with two endpoints of colour c_0, hence the coloring is not proper, thus contradicting the hypothesis that we are in a Nash equilibrium. Note that since by de Morgan's laws, the negation of an AND-gate can be transformed into an OR-gate and vice-versa, both cases are symmetrical, and so, we can assume w.l.o.g. that the j_1^{th} gate is an OR-gate. There are two subcases to be considered.

Suppose that the output of the j_1^{th} gate is 0 (false positive). In such case, $Y_{j_1} \cap L_{c_0} \neq \emptyset$. Let us consider the first entry of the gate. If it is the i^{th} entry of the circuit for some $1 \leq i \leq n$ then $w_i = 0$ (because the output of the j_1^{th} gate is 0) and so, by construction, $x_i, x'_i \in L_{c_0}$ are adjacent to $a^1_{j_1}, b^1_{j_1}$. Else, it is the k^{th} gate of the circuit for some $k < j_1$. By minimality of j_1, since the output of the k^{th} gate must be 0 (because the output of the j_1^{th} gate is 0), $Y_k \cap L_{c_0} = \emptyset$, and so, $N_k \cap L_{c_0} \neq \emptyset$. By construction, every vertex in N_k is adjacent to $a^1_{j_1}, b^1_{j_1}$. As a result, $a^1_{j_1}, b^1_{j_1}$ have a neighbour in L_{c_0} in this subcase. We can prove similarly (by considering the second entry of the gate) that $a^2_{j_1}, b^2_{j_1}$ have a neighbour in L_{c_0} in this subcase. The latter implies the existence of an edge with both endpoints in L_{c_0} since $Y_{j_1} = \{a^1_{j_1}, b^1_{j_1}, a^2_{j_1}, b^2_{j_1}\}$.

Else, the output of the j_1^{th} gate is 1 (false negative). In such case, $Y_{j_1} \cap L_{c_0} = \emptyset$, hence $N_{j_1} \cap L_{c_0} \neq \emptyset$. Since the output of the gate is 1, there must be an entry of the gate such that: either it is the i^{th} entry of the circuit for some $1 \leq i \leq n$, and $w_i = 1$ (in which case, the two vertices $x_i, x'_i \in Lc_0$ are adjacent to both $a^3_{j_1}, b^3_{j_1}$ by construction); or it is the k^{th} gate of the circuit for some $k < j_1$ and this gate outputs 1. In the latter case, by minimality of j_1, $Y_k \cap L_{c_0} \neq \emptyset$. By construction, every vertex in Y_k is adjacent to $a^3_{j_1}, b^3_{j_1}$. As a result, $a^3_{j_1}, b^3_{j_1}$ have a neighbour in L_{c_0} in this subcase. The latter implies the existence of an edge with both endpoints in L_{c_0} since $N_{j_1} = \{a^3_{j_1}, b^3_{j_1}\}$. $\diamond$

3.3 Proof of Theorem 2

Proof of Theorem 2. Let $\langle \mathcal{C}, w\rangle$ be any instance of Monotone Circuit Value. Let $G = (V, E)$ be the graph obtained with our reduction from Section 3.1, which can be constructed in polylogarithmic-time with a polynomial number of processors. The graph G defines a coloring game. We fix any Nash equilibrium for this game, that exists by Theorem 1. By Claim 5, any two vertices in X have the same colour c_0. We will prove that there is at least one vertex in Y_m with colour c_0 if and only if the circuit $\mathcal{C}$ outputs 1 when it takes w as input. Since Monotone Circuit Value is PTIME-complete [9], the latter will prove that computing a Nash equilibrium for coloring games is PTIME-hard.

By Claim 6, we only need to prove that for every $1 \leq j \leq m$, there is at least one vertex in $Y_j \cup N_j$ with colour c_0. To prove it by contradiction, let j_0 be the smallest index j such that no vertex in $Y_j \cup N_j$ has colour c_0. By Claim 5, every vertex in $Y_{j_0} \cup N_{j_0}$ has the same colour as her private group. In particular, the three of $a^1_{j_0}, a^2_{j_0}, a^3_{j_0}$ receive payoff $2(n + j_0) - 3$. We will prove that one of these three agents could increase her payoff by choosing c_0 as her new colour, thus contradicting that we are in a Nash equilibrium. Indeed, by the minimality of j_0, it follows by Claim 4 that for any $1 \leq j \leq j_0 - 1$, there are exactly two vertices of $Y_j \cup N_j$ with colour c_0, while for every $j_0 \leq j \leq m$ there is no vertex in $Y_j \cup N_j$ with colour c_0. As a result, $|L_{c_0}| = 2(n + j_0) - 2$. In particular, any agent among $a^1_{j_0}, a^2_{j_0}, a^3_{j_0}$ could increase her payoff by choosing c_0 as her new colour — provided she is nonadjacent to every vertex in L_{c_0}. We will show it is the case for at least one of the three vertices, that will conclude the proof of the theorem. Assume w.l.o.g. that the j_0^{th} gate is an OR-gate (indeed, since by de Morgan's laws, the negation of an AND-gate can be transformed into an OR-gate and vice-versa, both cases are symmetrical). There are two cases.

Suppose that the output of the j_0^{th} gate is 1. In such case, there must be an entry of the gate such that: it is the i^{th} entry of the circuit, for some $1 \leq i \leq n$, and $w_i = 1$; or it is the k^{th} gate of the circuit for some $k < j_0$ and the output of that gate is 1. In the latter case, we have by Claim 6 that the two vertices of $Y_k \cup N_k$ with colour c_0 are in the set Y_k. Assume w.l.o.g. that the above-mentioned entry is the first entry of the gate. By construction, the two vertices $a^1_{j_0}, b^1_{j_0}$ are nonadjacent to every vertex in L_{c_0}. Else, the output of the j_0^{th} gate is 0. Therefore, for every entry of the gate: either it is the i^{th} entry of the circuit, for some $1 \leq i \leq n$, and $w_i = 0$; or it is the k^{th} gate of the circuit for some $k < j_0$ and the output of that gate is 0. In the latter case, we have by Claim 6 that the two vertices of $Y_k \cup N_k$ with colour c_0 are in the set N_k. By construction, the two vertices $a^3_{j_0}, b^3_{j_0}$ are nonadjacent to every vertex in L_{c_0}. In both cases, it contradicts that we are in a Nash equilibrium. $\square$

4 Conclusion and open perspectives

We suggest through this case study a more in-depth analysis of the complexity of computational mechanism designs. We would find it interesting to pursue similar investigations for other games. Experiments in the spirit of [11] could be helpful for our purposes. Further, we note that PRAM is seen by some as a too unrealistic model for parallel computation. Thus, one may argue that proving our reduction in this model casts a doubt on its reach. However, we can leverage on the stronger statement that MONOTONE CIRCUIT VALUE is *strictly* PTIME-hard [5]. It implies roughly that the sequential time and the parallel time to solve this problem cannot differ by more than a moderate polynomial-factor (unless the solving of *all* problems in PTIME can be sped up on a parallel machine by at least a polynomial-factor). Our reduction directly shows the same holds true for the problem of computing a Nash equilibrium in a given coloring game, that generalizes our hardness result to more recent parallel complexity classes (*e.g.*, [10]).

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Papers on Web's transparency

Appendix K

Xray: enhancing the Web's transparency with differential correlation

XRay: Enhancing the Web's Transparency with Differential Correlation

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Abstract

Today's Web services – such as Google, Amazon, and Facebook – leverage user data for varied purposes, including personalizing recommendations, targeting advertisements, and adjusting prices. At present, users have little insight into how their data is being used. Hence, they cannot make informed choices about the services they choose.

To increase transparency, we developed *XRay*, the first fine-grained, robust, and scalable personal data tracking system for the Web. XRay predicts which data in an arbitrary Web account (such as emails, searches, or viewed products) is being used to target which outputs (such as ads, recommended products, or prices). XRay's core functions are service agnostic and easy to instantiate for new services, and they can track data within and across services. To make predictions independent of the audited service, XRay relies on the following insight: by comparing outputs from different accounts with similar, but not identical, subsets of data, one can pinpoint targeting through correlation. We show both theoretically, and through experiments on Gmail, Amazon, and YouTube, that XRay achieves high precision and recall by correlating data from a surprisingly small number of extra accounts.

1 Introduction

We live in a "big data" world. Staggering amounts of personal data – our as locations, search histories, emails, posts, and photos – are constantly collected and analyzed by Google, Amazon, Facebook, and a myriad of other Web services. This presents rich opportunities for marshaling big data to improve daily life and social well-being. For example, personal data improves the usability of applications by letting them predict and seamlessly adapt to future user needs and preferences. It improves business revenues by enabling effective product placement and targeted advertisements. Twitter data has been successfully applied to public health problems [36], crime prevention [44], and emergency response [22]. These beneficial uses have generated a big data frenzy, with Web services aggressively pursuing new ways to acquire and commercialize it.

Despite its innovative potential, the personal data frenzy has transformed the Web into an opaque and privacy-insensitive environment. Web services accumulate data, exploit it for varied and undisclosed purposes, retain it for extended periods of time, and possibly share it with others – *all without the data owner's knowledge or consent*. Who has what data, and for what purposes is it used? Are the uses in the data owners' best interests? Does the service adhere to its own privacy policy? How long is data used after its owner deletes it? Who shares data with whom?

At present, users lack answers to these questions, and investigators (such as FTC agents, journalists, or researchers) lack robust tools to track data in the ever-changing Web to provide the answers. Left unchecked, the exciting potential of big data threatens to become a breeding ground for data abuses, privacy vulnerabilities, and unfair or deceptive business practices. Examples of such practices have begun to surface. In a recent incident, Google was found to have used institutional emails from ad-free Google Apps for Education to target ads in users' personal accounts [18, 37]. MySpace was found to have violated its privacy policy by leaking personally identifiable information to advertisers [25]. Several consumer sites, such as Orbitz and Staples, were found to have adjusted their product pricing based on user location [29, 43]. And Facebook's 2010 ad targeting was shown to be vulnerable to micro-targeted ads specially crafted to reveal a user's private profile data [23].

To increase transparency and provide checks and balances on data abuse, we argue that new, robust, and versatile tools are needed to effectively track the use of personal data on the Web. Tracking data in a *controlled environment*, such as a modified operating system, language, or runtime, is an old problem with a well-known solution: taint tracking systems [12, 16, 7, 48]. However, is it possible to track data in an *uncontrolled environment*, such as the Web? Can robust, generic mechanisms assist in doing so? What kinds of data uses are trackable and what are not? How would the mechanisms scale with the amount of data being tracked?

As a first step toward answering these questions, we built *XRay*, a personal data tracking system for the Web.

XRay correlates designated data *inputs* (be they emails, searches, or visited products) with data *outputs* results (such as ads, recommended products, or prices). Its correlation mechanism is service agnostic and easy to instantiate, and it can track data use within and across services. For example, it lets a data owners track how their emails, Google+, and YouTube activities are used to target ads in Gmail.

At its core, XRay relies on a *differential correlation* mechanism that pinpoints targeting by comparing outputs in different accounts with similar, but not identical, subsets of data inputs. To do so, it associates with every personal account a number of *shadow accounts*, each of which contains different data subsets. The correlation mechanism uses a simple Bayesian model to compute and rank scores for every data input that may have triggered a specific output. Intuitively, if an ad were seen in many accounts that share a certain email, and never in accounts that lack that email, then the email is likely to be responsible for a characteristic that triggers the ad. The email's score for that ad would therefore be high. Conversely, if the ad were seen rarely in accounts with or lacking that email, that email's score for this ad would be low.

Constructing a practical auditing system around differential correlation raises significant challenges. Chief among them is scalability with the number of data items. Theoretically, XRay requires a shadow account for each combination of data inputs to accurately pinpoint correlation. That would suggest an *exponential number of accounts*! Upon closer examination, however, we find that a few realistic assumptions and novel mechanisms let XRay reach high precision and recall with only a *logarithmic number of accounts in number of data inputs*. We deem this a major new result for the science of tracking data-targeting on the Web.

We built an XRay prototype and used it to correlate Gmail ads, Amazon product recommendations, and YouTube video suggestions to user emails, wish lists, and previously watched videos, respectively. While Amazon and YouTube provide detailed explanations of their targeting, Gmail does not, so we manually validated associations. For all cases, XRay achieved 80-90% precision and recall. Moreover, we integrated our Gmail and YouTube prototypes so we could track cross-service ad targeting. Although several prior measurement studies [10, 47, 21, 20, 31] used methodologies akin to differential correlation, we believe we are the first to build a generic, service agnostic, and scalable tool based on it. Overall, we make the following contributions:

1. The first general, versatile, and open system to track arbitrary personal Web data use by uncontrolled services. The code is available from our Web page `https://xray.cs.columbia.edu/`.
2. The first in-depth exploration into the scalability challenges of tracking personal data on the Web.
3. The design and implementation of robust mechanisms to address scaling, including data matching.
4. System instantiation to track data on three services (Gmail, Amazon, YouTube) and across services (YouTube to Gmail).
5. An evaluation of our system's precision and recall on Gmail, Amazon, and YouTube. We show that XRay is accurate and scalable. Further, it reveals intriguing practices now in use by Web services and advertisers.

2 Motivation

This paper lays the algorithmic foundations for a new generation of scalable, robust, and versatile tools to lift the curtain on how personal data is being targeted. We underscore the need for such tools by describing potential usage scenarios inspired by real-life examples (§2.1). We do this not to point fingers at specific service providers; rather, we aim to show the many situations where transparency tools would be valuable for end-users and auditors alike. We conclude this section by briefly analyzing how current approaches fail to address these usage scenarios (§2.2).

2.1 Usage Scenarios

Scenario 1: Why This Ad? Ann often uses her Gmail ads to discover new retail offerings. Recently, she discussed her ad-clicking practices with her friend Tom, a computer security expert. Tom warned her about potential privacy implications of clicking on ads without knowing what data they target. For example, if she clicks on an ad targeting the keyword "gay" and then authenticates to purchase something from that vendor, she is unwittingly volunteering potentially sensitive information to the vendor. Tom tells Ann about two options to protect her privacy. She can either disable the ads altogether (using a system like AdBlock [1]), or install the XRay Gmail plugin to uncover targeting against her data. Unwilling to give up the convenience of ads, Ann chooses the latter. XRay clearly annotates the ads in the Gmail UI with their target email or combination, if any. Ann now inspects this targeting before clicking on an ad and avoids clicking if highly sensitive emails are being targeted.

Scenario 2: They're Targeting *What*? Bob, an FTC investigator, uses the XRay Gmail plugin for a different purpose: to study sensitive-data targeting practices by advertisers. He suspects a potentially unfair practice whereby companies use Google's ad network to collect sensitive information about their customers. Therefore, Bob creates a number of emails containing keywords such as "cancer," "AIDS," "bankruptcy," and "unemployment." He refreshes the Gmail page many times, each time recording the targeted ads and XRay's explanations for them. The experiment reveals an interesting result: an online insurance company, TrustInUs.com, has targeted multiple ads against his illness-related emails. Bob hypothesizes that the company might use the data to set higher premiums for users reaching their site through a disease-targeted ad. He uses XRay results as initial evidence to open an investigation of TrustInUs.com.

Scenario 3: What's With The New Policy?[1] Carla, an investigative journalist, has set up a watcher on privacy policies for major Web services. When a change occurs, the watcher notifies her of the difference. Recently, an important sentence in Google's privacy policy has been scrapped:

> *If you are using Google Apps (free edition), email is scanned so we can display conceptually relevant advertising in some circumstances.* ~~*Note that there is no ad-related scanning or processing in Google Apps for Education or Business with ads disabled.*~~

To investigate scientifically whether this omission represents a shift in implemented policy, she obtains institutional accounts, connects them to personal accounts, and uses XRay to detect the correlation between emails in institutional accounts and ads in corresponding personal accounts. Finding a strong correlation, Carla writes an article to expose the policy change and its implications.

Scenario 4: Does Delete Mean Delete? Dan, a CS researcher, has seen the latest news that Snapchat, an ephemeral-image sharing Website, does not destroy users' images after the requested timeout but instead just unlinks them [41]. He wonders whether the reasons for this are purely technical as the company has declared (e.g., flash wearing levels, undelete support, spam filtering) [39, 38] or whether these photos, or metadata drawn from them, are mined to target ads or other products on the Website. The answer will influence his decision about whether to continue using the service. Dan instantiates XRay to track the correlation between his expired Snapchat photos and ads.

2.2 Alternative Approaches

The preceding scenarios illustrate the importance of transparency in protecting privacy across a range of use cases. *We need robust, generic auditing tools to track the use of personal data at fine granularity (e.g., individual emails, photos) within and across arbitrary Web services.* At present, no such tools exist, and the science of tracking the use of personal Web data at a fine grain is largely non-existent.

[1]In Feb. 2014, it was revealed based on court documents that Google could have used institutional emails to target ads in personal accounts [18]. In May 2014, Google committed to disable that feature [30]. Scenario 3 presents an XRay-based approach to investigate the original allegation.

Existing approaches can be broadly classified in two categories: *protection tools*, which prevent Web services' acquisition or use of personal data, and (2) *auditing tools*, which uncover Web services' acquisition or use of personal data. We discuss these approaches next; further related work is in §9.

Protection Tools. A variety of protection tools exist [11, 35, 1, 49]. For example, Ann could disable ads using an ad blocker [1]. Alternatively, she could encrypt her emails, particularly the sensitive ones, to prevent Google from using them to target ads. Dan could use a self-destructing data system, such as Vanish [14], to ensure the ephemerality of his Snapchat photos.

While we encourage the use of protection tools, they impose difficult tradeoffs that make them inapplicable in many cases. If Ann blocks all her ads, she cannot benefit from those she might find useful; if she encrypts all of her emails, she cannot search them; if she encrypts only her sensitive emails, she cannot protect any sensitive emails she neglected to encrypt in advance. Similarly, if Dan encrypts his Snapchat photos, sharing them becomes more difficult. While more sophisticated protection systems address certain limitations (e.g., searchable [5], homomorphic [15, 33], and attribute-based encryption [19], or privacy-preserving advertising [42, 13]), they are generally heavyweight [15], difficult to use [45], or require major service-side changes [15, 42, 13].

Auditing Tools. Given the limitations of protection tools, transparency is gaining increased attention [47, 12, 21]. If protecting data proves too cumbersome, limiting, or unsupportive of business needs, then users should at least be able to know: (1) *who is handling their data?*, and (2) *what is it being used for?*

Several tools developed in recent years partially address the first question by revealing where personal data flows from a local device [34, 12, 8]. TaintDroid [12] uses taint tracking to detect leakage of personal data from a mobile application to a service or third-party backend. ShareMeNot [34] and Mozilla's Lightbeam Firefox add-on [27] identify third parties that are observing user activities across the Web. These systems track personal data – such as location, sensor data, Web searches, or visited sites – *until it leaves the user's device*. Once the data is uploaded to Web services, it can be used or sold without a trace. In contrast, XRay's tracking just begins: we aim to tell users how services use their data *once they have it*.

Several new tools and personalization measurement studies partially address the second question: what data is being used for [10, 47, 21, 20, 31]. In general, all existing tools are highly specialized, focusing on specific input types, outputs, or services. No general, principled foundation for data use auditing exists, that can be applied effectively to many services, a primary motivation for this our work. For example, Bobble [47] reveals search result personalization based on user location (e.g., IP) and search history. Moreover, existing tools aim to discover only *whether* certain types of user inputs – such as search history, browsing history, IP, etc. – influence the output. None pinpoints at fine grain *which* specific input – which search query, which visited site, or which viewed product – or combination of inputs explain which output. XRay, whose goals we describe next, aims to do just that.

3 Goals and Models

Our overarching goal is to develop the core abstractions and mechanisms for tracking data within and across arbitrary Web sites. After describing specific goals (§3.1), we narrow our scope with a set of simplifying assumptions regarding the data uses that XRay is designed to audit (§3.2) and the threats it addresses (§3.3).

3.1 Goals

Three specific goals have guided XRay's design:

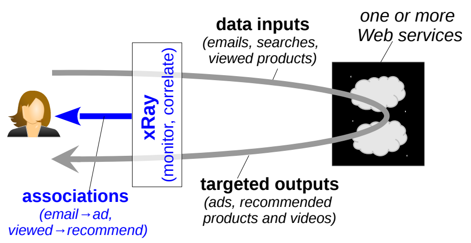
Goal 1: *Fine-Grained and Accurate Data Tracking.* Detect which specific data inputs (e.g., emails) have likely triggered a particular output (e.g., an ad). While coarse-grained data use information (such as Gmail's typical statement, "This ad is based on emails from your mailbox.") may suffice at times, knowing the specifics can be revelatory, particularly when the input is highly sensitive and aggressively targeted.

Goal 2: *Scalability.* Make it practical to track significant amounts of data (e.g., past month's emails). We aim to support the tracking of hundreds of inputs with reasonable costs in terms of shadow accounts. These accounts are generally scarce resource since their creation is being constrained by Web services. While we assume that users and auditors can obtain *some* accounts on the Web services they audit (e.g., a couple dozen), we strive to minimize the number required for accurate and fine-grained data tracking.

Goal 3: *Extensibility, Generality, and Self-Tuning.* Make XRay generic and easy to instantiate for many services and input/output types. Instantiating XRay to track data on new sites should be simple, although it may require some service-specific implementation of input/output monitoring. However, XRay's correlation machinery – the conceptually challenging part of a scalable auditing tool – should be turn key and require no manual tuning.

3.2 Web Service Model

These goals may appear unsurmountable. An extremely heterogeneous environment, the Web has perhaps as many data uses as services. Moreover, data mining algorithms can be complex and proprietary. How can we abstract away this diversity and complexity to design robust and generic building blocks for scalable data tracking? Fortunately, we find that certain popular classes of Web data uses lend themselves to principled abstractions that facilitate scalable tracking.



data inputs
(emails, searches, viewed products)
one or more Web services
xRay
(monitor, correlate)
associations
(email→ad, viewed→recommend)
targeted outputs
(ads, recommended products and videos)

Figure 1: **XRay Conceptual View.** XRay views Web services as black boxes, monitors user *inputs* and *outputs* to/from them, and detects data use through correlation. It returns to the user or auditor *associations* of specific inputs and outputs.

Figure 1 shows XRay's simplified view of Web services. Services, and networks of services that exchange user data, are *black boxes* that receive personal data *inputs* from users – such as emails, pictures, search queries, locations, or purchases – and use them for varied purposes. Some uses materialize into *outputs* visible to users, such as ads, product or video recommendations, or prices. Others invisible to the users. XRay correlates some visible data inputs with some visible outputs by monitoring them, correlating them, and reporting strong *associations* to users. An example association is which email(s) contributed to the selection of a particular ad.

XRay relates only *strongly correlated* inputs with outputs. If an output is strongly correlated to an input (i.e., the input's presence or absence changes the output), then XRay will likely be able to detect its use. If not (i.e., the monitored input plays but a small role in the output), then it may go undetected. XRay also relates small combinations of inputs with strongly correlated outputs.

Although simple, this model efficiently addresses several types of personal data functions, including product recommendations, price discriminations, and various personalization functions (e.g., search, news). We refer to such functions generically as *targeting functions* and focus XRay's design on them.

Three popular forms of targeting are:

1. *Profile Targeting*, which leverages static or slowly evolving explicit information – such as age, gender, race, or location – that the user often supplies by filling a form. This type of targeting has been studied profusely [10, 47, 21, 20, 31]; we thus ignore it here.
2. *Contextual Targeting*, which leverages the content currently being displayed. In Gmail, this is the currently open email next to which the ad is shown. In Amazon or Youtube, the target is the product or video next to which the recommendation is shown.
3. *Behavioral Targeting*, which leverages a user's past actions. An email sent or received today can trigger an ad tomorrow; a video watched now can trig-

ger a recommendation later. Use of histories makes it harder for users to track which data is being used, a key motivation for our development of XRay.

Theoretically, our differential correlation algorithms could be applied to all three forms of targeting. From a systems perspective, XRay's design is geared towards *contextual targeting* and *a specific form of behavioral targeting*. The latter requires further attention. We observe that this broad targeting class subsumes multiple types of targeting that operate at different granularities. For example, a service could use as inputs a user's most recent few emails to decide targeting. This would be similar to an extended context. Alternatively, a service could use historical input to learn a user's coarse interests or characteristics and base its targeting on that.

XRay currently aims to disclose any targeting applied at the level of individual user data, or small combinations thereof. Our differential correlation algorithms could be applied to detect targeting that operates on a coarser granularity. However, the XRay system itself would require significant changes. Unless otherwise noted, we use *behavioral targeting* to denote the restricted form of behavioral targeting that XRay is designed to address. We formalize these restrictions in §4.2.

3.3 Threat Model

To further narrow our problem's scope, we introduce threat assumptions. We assume that data owners (users and auditors) are trusted and do not attempt to leverage XRay to harm Web services or the Web ecosystem. While they trust Web services with their data, they wish to better understand how that data is being used. Data owners are thus assumed to upload the data in clear text to the Web services.

The threat models relevant for Web services depend on the use case. For example, Scenarios 1 and 2 in §2.1 assume Google is trusted, but its users wish to understand more about how advertisers target them through its ad platform. In contrast, in Scenarios 3 and 4, investigators may have reason to believe that Web services might intentionally frustrate auditing.

This paper assumes an *honest-but-curious* model for Web services: they try to use private data for financial or functional gains, but they do not try to frustrate our auditing mechanism, e.g., by identifying and disabling shadow accounts. The service might attempt to defend itself against more general types of attacks, such as spammers or DDoS attacks. For example, many Web services constrain the creation of accounts so as to limit spamming and false clicks. Similarly, Web services may rate limit or block the IPs of aggressive data collectors. XRay must be robust to such inherent defenses. We discuss challenges and potential approaches for stronger adversarial models in §7.

4 The XRay Architecture

XRay's design addresses the preceding goals and assumptions. For concreteness, we draw examples from our three XRay instantiations: tracking email-to-ad targeting association within Gmail, attributing recommended videos to those already seen on YouTube, and identifying products in a wish list that generate a recommendation on Amazon.

4.1 Architectural Overview

XRay's high-level architecture (Figure 2) consists of three components: (1) a *Browser Plugin*, which intercepts tracked inputs and outputs to/from an audited Web service and gives users visual feedback about any input/output associations, (2) a *Shadow Account Manager*, which populates shadow accounts with inputs from the plugin and collects outputs (e.g., ads) for each shadow account, and (3) the *Correlation Engine*, XRay's core, which infers associations and provides them to the plugin for visualization. While the Browser Plugin and Shadow Account Manager are *service specific*, the Correlation Engine, which encapsulates the science of Web-data tracking, is *service agnostic*. After we describe each component, we focus on the design of the Correlation Engine.

Browser Plugin. The Browser Plugin intercepts designated inputs and outputs (i.e., *tracked inputs/outputs*) by recognizing specific DOM elements in an audited service's Web pages. Other inputs and outputs may not be tracked by XRay (i.e., *untracked inputs/outputs*). The decision of what to track belongs to an investigator or developer who instantiates XRay to work on a specific service. For example, we configure the XRay Gmail Plugin to monitor a user's emails as inputs and ads as outputs. When the Plugin gets a new tracked input (e.g., a new email), it forwards it both to the service and to the Shadow Account Manager. When the Plugin gets a new tracked output (e.g., an ad), it queries the Correlation Engine for associations with the user's tracked inputs (message `get_assoc`).

Shadow Account Manager. This component: (1) populates the shadow accounts with subsets of a user account's tracked inputs (denoted D_i), and (2) periodically retrieves outputs (denoted O_k) from the audited service for each shadow account. Both functions are service specific. For Gmail, they send emails with SMTP and call the ad API. For YouTube, they stream a video and scrape recommendations, and for Amazon, they place products in wish lists and scrape recommendations. The complexity of these tasks depends on the availability of APIs or the stability of a service's page formats. Outputs collected from the Web service are placed into a *Correlation Database* (DB), which maps shadow accounts to their input sets and output observations. Figure 2 shows a par-

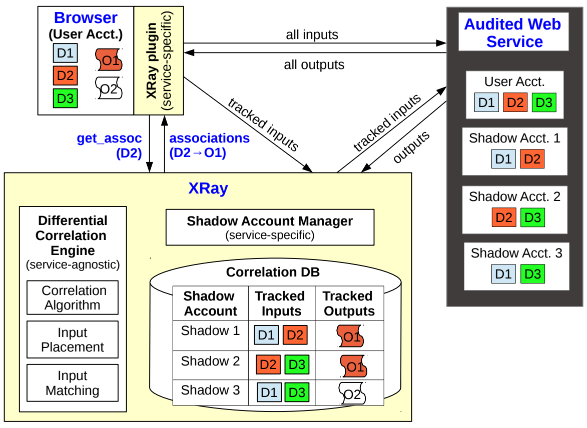


Figure 2: **The XRay Architecture.**

ticular assignment of tracked inputs across three shadow accounts. For example, Shadow 1 has inputs D_1 and D_2. The figure also shows the outputs collected for each shadow account. Output O_1 appears in Shadows 1 and 2 but not in 3; output O_2 appears in Shadow 3 only.

Differential Correlation Engine. This engine, XRay's service-agnostic "brain," leverages the data collected in the Correlation DB to infer input/output associations. When new outputs from shadow accounts are added into the Correlation DB, the engine attempts to diagnose them using a *Correlation Algorithm*. We developed several such algorithms and describe them in §4.3. This process, potentially time-consuming process, is done as a background job, asynchronously from any user request. In Figure 2, differential correlation might conclude that D_2 triggers O_1 because O_1 appears consistently in accounts with that D_2. It might also conclude that O_2 is *untargeted* given inconsistent observations. The engine saves these associations in the Correlation DB.

When the plugin makes a `get_assoc` request, the Correlation Engine looks up the specified output in its DB and returns any pre-computed association. If no output is found, then the engine replies *unknown* (e.g., if an ad never appeared in any shadow account or there is insufficient information). Periodic data collection, coupled with an online update of correlation model parameters, minimizes the number of unknown associations. Our experience shows that collecting shadow account outputs in Gmail every ten hours or so yielded few unknown ads.

While the preceding example is simple, XRay can handle complex challenges occurring in practice. First, outputs are never consistently seen across all shadow accounts containing the input they target. We call this the *limited-coverage* problem; XRay handles it by placing each data input in more shadow accounts. Second, an output may have been triggered by one of several targeted inputs (e.g., multiple emails on the same topic may cause related ads to appear), a problem we refer to as *overlapping-inputs*. This exacerbates the number of accounts needed, since it diminishes the differential signal we receive from them. XRay uses robust, service-agnostic mechanisms and algorithms to match overlapping inputs, place them in the same accounts, and detects their use as a group.

Organization. The remainder of this section describes the Differential Correlation Engine. After constructing it for Gmail, we applied it as-is for Amazon and YouTube, where it achieved equally high accuracy and scalability despite observable differences in how targeting works on these three services. After establishing notations and formalizing our assumptions (§4.2), we describe multiple correlation algorithms, which build up to our self-tuning correlation algorithm that made this adaptation convenient (§4.3). §4.4 describes our input matching.

4.2 Notation and Assumptions

We use f to denote the black-box function that represents the service (e.g., Gmail) associating inputs D_is (e.g., the emails received and sent) to targeted outputs O_ks (e.g., ads). Other inputs are either ignored by XRay, known only to the targeting system, or under no known control. We assume they are independent or fixed, captured in the randomness of f.

We assume that f decides targeting using: (1) a single input (e.g., show O_k if D_4 is in the account), (2) a conjunctive combination of inputs (e.g., show O_k if D_5 *and* D_8 are in the account), or (3) a disjunctive combination of the previous (e.g., show O_k if (D_5 *and* D_8) are in the account *or* if D_4 is in the account). We refer to conjunctive and disjunctive combinations as AND and OR combinations, respectively, and assume that their is bounded by a maximum *input size*, r. This corresponds to the preceding definition of behavioral targeting from §3.2. Contextual targeting will always be a single-input (size-one) combination.

Our goal is to decide whether f produced each output O_k as a reaction to a bounded-size combination of the D_is. We define as *untargeted* any ad that is not targeted against any combination of D_is, though in reality the ad could be targeted against untracked inputs. We denote untargeting as $D_\emptyset$, meaning that the ad is targeted against the "void" email. Our algorithms compute the most likely combination from the N inputs that explains a particular set of observations, $\vec{x}$, obtained by XRay.

We define three probabilities upon which our algorithms and analyses depend. First, the *coverage*, p_{in}, is the probability that an account j containing the input D_i targeted by a particular ad, will see that ad at least once. Second, an account j' lacking input D_i will see the ad with a smaller probability, p_{out}. Third, if the ad is not behaviorally targeted, it will appear in each account with the same probability, $p_\emptyset$. We assume that $p_{\text{in}}, p_\emptyset, p_{\text{out}}$ are constant across all emails, ads, and time, and that p_{out} is strictly smaller than p_{in} (bounded noise hypothesis).

Finally, we consider all outputs to be independent of each other across time. §8 discusses the implications.

4.3 Correlation Algorithms

A core contribution of this paper is our service-agnostic, self-tuning differential correlation algorithm, which requires only a logarithmic number of shadow accounts to achieve high accuracy. We wished not only to validate this result experimentally, but also to prove it theoretically in the context of our assumptions. This section constructs the algorithm in steps, starting with a naïve polynomial algorithm that illustrates the scaling challenges. We then define a base algorithm using set intersections and prove that it has the desired logarithmic scaling properties; it has parameters which, if not carefully chosen, can lead to poor results. We therefore extend this base algorithm into a self-tuning Bayesian model that automatically adjusts its parameters to maximize correctness.

4.3.1 Naïve Non-Logarithmic Algorithm

An intuitive approach to differential correlation is to create accounts for every combination of inputs, gathering maximum information about their behaviors. With a sufficient number of observations, one could expect to detect which accounts, and hence which subsets of inputs, target a particular ad. Unfortunately, this method requires a number of accounts that grows *exponentially* as the number of items N to track grows. When restricting the size of combinations to r, as we do in XRay, the number of accounts needed is *polynomial* (in $O(N^r)$), or *linear* if we study unique inputs only. Even a linear number of accounts in the number N of inputs remains impractical to scale to large input sizes (e.g., a mailbox).

4.3.2 Threshold Set Intersection

We now show that it is possible to infer behavioral targeting using no more than a *logarithmic* number of accounts as a function of the number of inputs. Specifically, we prove the following theorem:

Theorem 1 *Under §4.2 assumptions, for any $\varepsilon > 0$ there exists an algorithm that requires $C \times \ln(N)$ accounts to correctly identify the inputs of a targeted ad with probability $(1-\varepsilon)$. The constant C depends on ε and the maximum size of combinations r ($O(r2^r \log(\frac{1}{\varepsilon}))$).*

To demonstrate the theorem, we define the *Set Intersection Algorithm* and prove that it has the correctness and scaling properties specified in the theorem. Given that outputs will appear more often in accounts containing the targeting inputs, the core of the algorithm is to determine the set of inputs appearing in the highest number of accounts that also see a given ad. This paper describes a basic version of the algorithm that makes

```
// Set Intersection Algo:
// Runs with each collected ad.
In: Output $O_k$ (e.g. an ad).
Params: MIN_ACTIVE_ACCTS, THRESHOLD.
Out: Targeted input combination.
// Step 1: Compute active accounts.
$A_k$ = the accounts that see ad $O_k$.
if $|A_k| <$ MIN_ACTIVE_ACCTS
    return $\emptyset$
end
// Step 2: Create input combination hypothesis.
targeted_set = $\emptyset$
foreach input $D_i$ do
    if $\frac{\textit{number of } A_k \textit{ containing } D_i}{|A_k|}$ >THRESHOLD
        targeted_set += $D_i$
    end
end
// Step 3: Verify it is a real combination.
if $\frac{\textit{number of } A_k \textit{ containing entire targeted\_set}}{|A_k|}$ <THRESHOLD
    return $\emptyset$
end
// targeted_set triggered the output.
return targeted_set
```

Figure 3: **The Set Intersection Algorithm.** Can be proven to predict targeting correctly under certain assumptions with a logarithmic number of accounts.

some simplifying assumptions and provides a brief proof sketch. The detailed proof and complete algorithm are described in our technical report [26].

Algorithm. The algorithm relies on a randomized placement of inputs into shadow accounts, with some redundancy to cope with imperfect coverage. We thus pick a probability, $0 < \alpha < 1$, create $C\ln(N)$ shadow accounts, and place each input D_i randomly into each account with probability α. Figure 3 shows the Set Intersection algorithm for a set of observations, $\vec{x}$. Given an output O_k collected from the user account, we compute the set of *active accounts*, A_k, as those shadow accounts that have seen the output (Step 1). We then compute the set of inputs that appear in at least a threshold fraction of active accounts; this set is our candidate for the combination being targeted by the ad (Step 2). Finally, we check that the entire combination is in a threshold fraction of the active accounts (Step 3). Theoretically, we prove that there exists a threshold for which the algorithm is arbitrarily correct with the available $C\ln(N)$ accounts. Practically, this threshold must be tuned experimentally to achieve good accuracy on every service – a key reason for our Bayesian enhancement in §4.3.3.

Correctness Proof Sketch. The proof shows that if there were targeting, every non-targeting input would have a vanishingly small probability to be in a significant fraction of the active accounts. Let us call S the set of inputs

```
// Bayesian Prediction Alg:
// Runs with each collected ad.
In: Output $O_k$ (e.g. an ad).
Out: Targeted input.
// Compute probabilities.
foreach input $D_i$ do
    $\mathbb{P}[D_i | \vec{x}]$ = bayes($\mathbb{P}[\vec{x} | D_i]$)
end
// Compute untargeted prob.
$\mathbb{P}[D_\emptyset | \vec{x}]$ = bayes($\mathbb{P}[\vec{x} | D_\emptyset]$)
// Return event with max prob.
return $D_i$ with max $\mathbb{P}[D_i | \vec{x}]$
```

```
// Parameter Learning Alg:
// Runs periodically.
// Initialize params (arbitrary).
$p_{in} = .7, p_{out} = .01, p_\emptyset = .1$
do
    foreach output $O_k$ do
        Run Bayesian Prediction.
    end
    Update $p_{in}$, $p_{out}$, $p_\emptyset$
        from predictions.
until $p_{in}$, $p_{out}$, $p_\emptyset$ converge
end
```

Figure 4: **Bayesian Correlation.** Left: Bayesian prediction algorithm for behavioral targeting. Right: typical iterative inference process to learn parameters.

contained in a significant fraction of the active accounts. Without targeting, these inputs would be present in the accounts by mere chance. Since inputs are independently distributed into the accounts, we show that the probability of S not being empty decreases exponentially with the number of active accounts (through Chernoff bounds). With targeting, we show that with high probability no other input than the explaining combination is in S, because of the bounded noise hypothesis. Appendix A.2 provides further proof details.

The proofs and algorithm included in this paper work only for conjunctive combinations (e.g., D_1 and D_2, see §4.2). The theory, however, can be extended to disjunctive combinations (e.g., (D_1 and D_2) or D_5), but the algorithm for detecting such combinations is more complex and relies on a recursive argument: if we find one combination from the disjunction, then the active accounts that include this combination define a context where the combination appears non-targeting because it is everywhere. If we recursively apply our algorithm in this context, we can detect the second combination in the disjunction, then the third, etc (see technical report [26]).

4.3.3 Self-Tuning Bayesian Algorithm

The Set Intersection algorithm provides a good theoretical foundation; however, it requires parameters be tuned and applies only to behavioral targeting, not contextual targeting. Thus, we include in XRay a more robust, self-tuning version that leverages a Bayesian algorithm to adjust parameters automatically through iterated inference. Our algorithm relies on three models: one that predicts behavioral targeting, one that predicts contextual targeting, and one that combines the two.

Behavioral Targeting. The Bayesian behavioral targeting model uses the same random assignment as the Set Intersection algorithm, and it leverages the same information from the shadow account observations, $\vec{x}$. It counts the observations x_j of ad O_k in an account j as a binary signal: if the ad has appeared at least once in account j, we count it once; otherwise we do not count it. Briefly, the Bayesian model is a simple generative model that simulates the audited service given some targeting associations (e.g., D_i triggers O_k). It computes the probability for this model to generate the outputs we do observe for every targeting association. The most likely association will be the one XRay returns.

In more detail if the ad were targeted towards D_i, then an account j containing D_i would see this ad at least once with a *coverage* probability p_{in}; otherwise, it would miss it with probability $(1 - p_{\text{in}})$. An account j' without input D_i would see the ad with a smaller probability, p_{out}, missing it with probability $(1 - p_{\text{out}})$. If the ad were not behaviorally targeted, it would appear in each account with the same probability, $p_\emptyset$. If we define A_k as the set of active accounts that have seen the ad, and A_i as the set of accounts that contain email D_i, then we have the following definitions for the probabilities:

$$\begin{aligned}\mathbb{P}[\vec{x} | D_i] = \;& (p_{\text{in}})^{|A_i \cap A_k|} (1 - p_{\text{in}})^{|A_i \cap \bar{A_k}|} \\ & \times (p_{\text{out}})^{|\bar{A_i} \cap A_k|} (1 - p_{\text{out}})^{|\bar{A_i} \cap \bar{A_k}|}, \\ \mathbb{P}[\vec{x} | D_\emptyset] = \;& (p_\emptyset)^{|A_k|} (1 - p_\emptyset)^{|\bar{A_k}|},\end{aligned}$$

where $D_\emptyset$ designates the untargeted prediction.

The preceding formula has an interesting interpretation that is visible if placed in the equivalent form:

$$\begin{aligned}\mathbb{P}[\vec{x} | D_i] = \;& (p_{\text{in}})^{|A_k|} (1 - p_{\text{out}})^{|\bar{A_k}|} \\ & \times \left(\frac{1 - p_{\text{in}}}{1 - p_{\text{out}}}\right)^{|A_i \cap \bar{A_k}|} \left(\frac{p_{\text{out}}}{p_{\text{in}}}\right)^{|\bar{A_i} \cap A_k|}\end{aligned}$$

From the point of view of the event D_i, an account found in $A_i \cap \bar{A_k}$ is a false positive (an ad was expected but was not shown). This should lower the probability, especially when the *coverage* p_{in} is close to 1. Inversely, an account found in $\bar{A_i} \cap A_k$ acts as a false negative (we observed an ad where we did not expect it), which should decrease the probability, especially when p_{out} is close to 0.

These formulas let us infer the likelihood of event D_i according to Bayes' rule: $\mathbb{P}[A | B] = \frac{\mathbb{P}[B|A] \times \mathbb{P}[A]}{\mathbb{P}[B]}$. Figure 4 shows two algorithms. First, the prediction algorithm (left) predicts the targeting of O_k by computing the probabilities defined above, applying Bayes' rule, and returning the input with the maximum probability. Second, the parameter learning algorithm (right) computes the variables that those probabilities depend upon (p_{in}, p_{out}, and $p_\emptyset$) using an iterative process. It repeatedly runs the prediction algorithm for all outputs and re-computes p_{in}, p_{out}, and $p_\emptyset$ based on the predictions. It stops when the variables converge (i.e., their variation from one iteration to another is small).

Contextual Targeting. Contextual targeting is more straightforward since it uses content shown next to the ad. XRay also uses Bayesian inference and defines the observations as how many times ad O_k is seen next to email D_i. Our causal model assumes imperfect coverage: if this ad were contextually targeted towards D_i, it would occur next to that email with probability $p_{\text{in}} < 1$ and next to any other email with probability p_{out}. Alternatively, if the ad were untargeted, our model predicts it would be shown next to any email with probability $p_{\emptyset}$. Hence, $\mathbb{P}[\vec{x}|D_i] = (p_{\text{in}})^{x_i} (p_{\text{out}})^{\sum_{i' \neq i} x'_i}, \mathbb{P}[\vec{x}|D_{\emptyset}] = (p_{\emptyset})^{\sum_i x_i}$. For this model, parameters are also automatically computed by iterated inference.

Composite Model (XRay). The contextual and behavioral mechanisms were designed to detect different types of targeting. To detect both types, XRay must combine the two scores. We experimented with multiple combination functions, including a decision tree and the arithmetic average, and concluded that the arithmetic average yields sufficiently good results. XRay thus defines the *composite model* that averages scores from individual models, and we demonstrate in §6.3 that doing so yields higher recall for no loss in precision.

4.4 Input Matching and Placement

Our design of differential correlation, along with our logarithmic results for random input placement, relies on the fundamental assumption that the probability of getting an ad O_1 targeted at an input D_1 in a shadow account that lacks D_1 is vanishingly small. However, when inputs attract the same ads (a.k.a., overlapping inputs), a naive input placement can contradict this assumption. Imagine a Gmail account with multiple emails related to a Caribbean trip. If placement includes Caribbean emails in every available shadow account, related ads will appear in groups of accounts with no email object in common. XRay will thus classify them as untargeted. Our Amazon experiments showed XRay's recall dropping from 97% to 30% with overlapping inputs (§6.5).

To address this problem, XRay's Input Matching module identifies similar inputs and directs the Placement Module to co-locate them in the same shadow accounts. The key challenge is to identify similar inputs. One method is to use content analysis (e.g., keywords matching), but this has limitations. First, it is not service agnostic; one needs to reverse engineer complex and ever-changing matching schemes. Second, it is hard to apply to non-textual media, such as YouTube videos.

In XRay, we opt for a more robust, systems technique rooted in the key insight that we can deduce similar inputs from contextual targeting. Intuitively, inputs that trigger similar targeting from the Web service should attract similar outputs in their context. The Input Matching module builds and compare inputs' *contextual signatures*. Contextual signature similarity is the distance between inputs (e.g., email) in a Euclidean space, where each output (e.g., ad) is a dimension. The coordinate of an email in this dimension is the number of times the ad was seen in the context of the email. XRay then forwards close inputs to the same shadow accounts. Once the placement is done, behavioral targeting against that email's group can be inferred effectively.

This input matching mechanism differs fundamentally from any content analysis technique, such as keyword matching, because it groups inputs *the same way the Web service does*.[2] It is robust and very general: we used it on both Gmail and Amazon without changing a single line of code to change.

5 XRay-based Tools

To evaluate XRay's extensibility, we instantiated it on Gmail, YouTube, and Amazon. The engine, about 3,000 lines of Ruby, was first developed for Gmail. We then extended it to YouTube and Amazon, without any changes to its correlation algorithms. We did need to do minor code re-structuring, but the experience felt turn key when integrating a new service into the correlation machinery.

Building the full toolset required non-trivial coding effort, however. Instantiating XRay for a specific Web service is a three-step process. First, the developer instantiates appropriate data models (less than 20 code lines for our prototypes). Second, she implements a service-specific shadow account manager and plugin; care must be taken not be too aggressive to avoid adversarial service reactions. While these implementations are conceptually simple, they require some coding; our Amazon and YouTube account managers were built by two graduate students new to the project, and have around 500 lines of code. Third, the developer creates a few shadow accounts for the audited service and runs a small exploratory experiment to determine the service's coverage. XRay uses the coverage to estimate the number of shadow accounts needed for a given input size. All other parameters are self-tuned at runtime.

6 Evaluation

We evaluated XRay with experiments on Gmail, Amazon, and YouTube. While Amazon and YouTube provide ground truth for their targeting, Gmail does not. We therefore manually labeled ads on Gmail and measured XRay's accuracy, as described in §6.1 and validated in §6.2. We sought answers to four questions:

Q1 How accurate are XRay's inference models? (§6.3)
Q2 How does XRay scale with input size? (§6.4)
Q3 Can input matching manage overlap? (§6.5)
Q4 How useful is XRay in practice? (§6.6)

[2]We call this method "monkey see, monkey do" because we watch how the service groups inputs and group them similarly.

Ad Keyword	Targeted Email	Detected by XRay?	XRay Scores	# Accounts & Displays
Chaldean Poetry	Like Chaldean Poetry?	Yes	0.99, 1.0	13/13, 1588/1622
Steampunk	Fan of Steampunk?	Yes	0.99, 1.0	13/13, 888/912
Cosplay	Discover Cosplay.	Yes	0.99, 1.0	13/13, 440/442
Falconry	Learn about Falconry.	Yes	0.99, 1.0	13/13, 1569/1608

Figure 5: **Self-Targeted Ads.** Fourth column shows XRay's correlation scores X, Y, (Bayesian) Behavioral and Contextual scores, respectively. Fifth column shows raw behavioral and contextual data for interpretation: X/Y, Z/T means that the ad was seen in X active accounts that contain the targeted email out of a total of Y active accounts; the ad was shown Z times in the context of the targeted email out of a total of T times.

6.1 Methodology

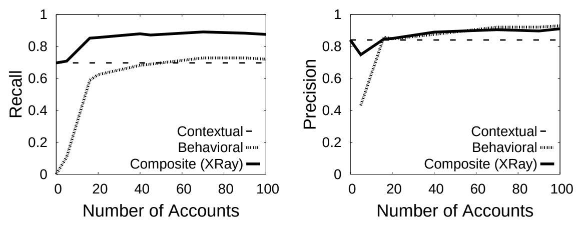
We evaluated XRay with experiments on Gmail, Amazon, and YouTube. For inputs, we created a workload for each service by selecting topics from well-defined categories relevant for that service. For Gmail and YouTube, we crafted emails and selected videos based on AdSense categories [17]; for Amazon, we selected products from its own product categories [2]. We used these categories for most of our experiments (§6.3–§6.5). We used these categories to create two types of workloads: (1) a non-overlapping workload, in which each data item belonged to a distinct category, and (2) an overlapping workload, with multiple data items per category (described in §6.5).

To assess XRay's accuracy, we needed the ground truth for associations. Amazon and YouTube provide it for their recommendations. For instance, Amazon provides a link "Why recommended?" which explicitly explains the recommendation. For Gmail, we manually labeled ads based on our personal assessment. The ads for different experiments were labeled by different people, generally project members. A non-computer scientist labeled the largest experiment (51 emails).

We evaluate two metrics: (1) *recall*, the fraction of positive associations labeled as such, and (2) *precision*, the fraction of correct associations. We define *high accuracy* as having both high recall and high precision.

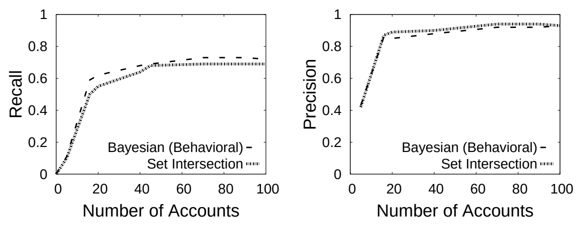
6.2 Sanity-Check Experiment

To build intuition into XRay's functioning, we ran a simple sanity-check experiment on Gmail. Recall that, unlike Amazon and YouTube, Gmail does not provide any ground truth, requiring us to manually label associations, a process that can be itself faulty. Before measuring XRay's accuracy against labeled associations, we checked that XRay can detect associations for our own ads, whose targeting we control. For this, we strayed away from the aforementioned methodology to create a highly controlled experiment. We posted four Google AdWords campaigns targeted on very specific keywords (Chaldean Poetry, Steampunk, Cosplay, and



(a) **Recall** (b) **Precision**

Figure 6: **Bayesian Model Accuracy.** Recall and precision for each of the three Bayesian models vs. shadow account number, using the Bayesian algorithm. XRay needed 16 accounts to reach the "knee" with high recall and precision.



(a) **Recall** (b) **Precision**

Figure 7: **Bayesian vs. Set Intersection Comparison.** Recall and precision for detecting *behavioral* targeting with each algo.

Falconry), crafted an inbox that included one email per keyword, and used XRay to recover the associations between our ads and those emails. In total, we saw our ads 1622, 912, 442, and 1608 times, respectively, across all accounts (shadows and master). Figure 5 shows our results. After one round of ad collection (which involved 50 refreshes per email), XRay correctly associated all four ads with the targeted email. It did so with very high confidence: composite model scores were 0.99 in all cases, with very high scores for both contextual and behavioral models. The figure also shows some of the raw contextual/behavioral data, which provides intuition into XRay's perfect precision and recall in this controlled experiment. We next turn to evaluating XRay in less controlled environments, for which we use the workloads and labeling methodology described in §6.1.

6.3 Accuracy of XRay's Inference Models (Q1)

To assess the accuracy of XRay's key correlation mechanisms (Bayesian behavioral, contextual, and composite), we measured their recall and precision under non-overlapping workloads. Figures 6(a) and 6(b) show how these two metrics varied with the number of shadow accounts for a 20-email experiment on Gmail. The results indicate two effects. First, both contextual and behavioral models were required for high recall. Of the 193 distinct ads seen in the user account, 121 (62%) were targeted, and XRay found 109 (90%) of them, a recall we deem high. Of the associations XRay found, 37% were found by only one of the models: 15

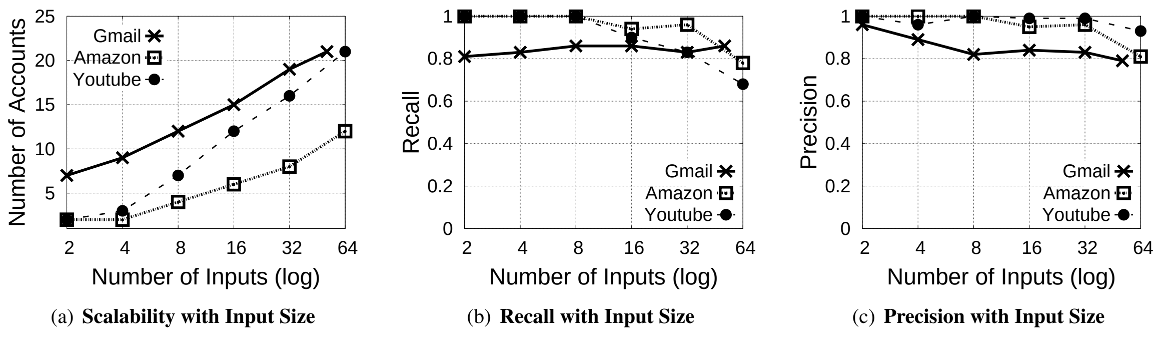


Figure 8: **Scalability.** (a) Number of accounts required to achieve the knee accuracy for varied numbers of inputs. (b), (c) Recall/precision achievable with the number of accounts in (a). Behavioral uses the Bayesian algorithm.

by the contextual model only, and 24 by the behavioral model only. Thus, both models were necessary, and composing them yielded high recall. Our Amazon and YouTube experiments (which provide ground truth) yielded very similar results: on a 20-input experiment, we reached over 90% recall and precision with only 8 and 12 accounts, respectively.

Second, the composite model's recall exhibited a knee-shaped curve for increasing shadow account numbers, with a rapid improvement at the beginning and slow growth thereafter. With 16 accounts, XRay exceeded 85% recall; increasing the number of accounts to 100 yielded a 1.9% improvement. Precision also remained high (over 84%) past 16 accounts. We define the *knee* as the minimum number of accounts needed to reap most of the achievable recall and precision.

We also wished to compare the accuracy of the Bayesian algorithm, which conveniently self-tunes its parameters, to the parameterized Set Intersection algorithm. We manually tuned the latter as best as we could. Figures 7(a) and 7(b) show the recall and precision for detecting behavioral targeting with the two methods for a non-overlapping workload. The two algorithms performed similarly, with the Bayesian staying within 5% of the manually tuned algorithm. We also tested the algorithms on an Amazon dataset, and using a version of the Set Intersection algorithm with empirical optimizations. The conclusion holds: the Bayesian algorithm, with self-tuned parameters, performs as well as the Set Intersection technique with manually tuned parameters. We focus the remainder of this evaluation on the Bayesian algorithm.

6.4 Scalability of XRay with Input Size (Q2)

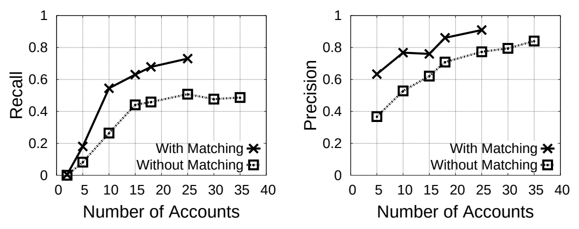
A main contribution of this paper is the realization that, under certain assumptions, the number of accounts needed to achieve high accuracy for XRay scales logarithmically with the number of tracked inputs. We have proven that under certain assumptions, the Set Intersection algorithm scales logarithmically. This theoretical result is hard to extend to the Bayesian algorithm, so we evaluated it experimentally by studying three metrics with growing input size: the number of accounts required to reach the recall knee and the value of recall/precision at this knee. Figures 8(a), 8(b) and 8(c) show the corresponding results for Gmail, YouTube and Amazon. For Gmail, the number of accounts necessary to reach the knee increased less than 3-fold (from 8 to 21) as input size increased more than 25-fold (from 2 to 51). For Amazon and YouTube, the increases in accounts were 6- and 8-fold respectively, for a 32-fold increase in input size. In general, the roughly linear shapes of the log-x-scale graphs in Figure 8(a) confirm the logarithmic increase in the number of accounts required to handle different inputs. Figure 8(b) and 8(c) confirm that the "knee number" of accounts achieved high recall and precision (over 80%).

What accounts for the large gap between the number of accounts needed for high accuracy in Gmail versus Amazon? For example, tracking a mere two emails in Gmail required 8 accounts, while tracking two viewed products in Amazon needed 2 accounts. The distinction corresponds to the difference in coverage exhibited by the two services. In Gmail, a targeted ad was typically seen in a smaller fraction of the relevant accounts compared to a recommended product in Amazon. XRay adapted its parameters to lower coverage automatically, but it needed more accounts to do so.

Overall, these results confirm that our theoretical scalability results hold for real-world systems given carefully crafted, non-overlapping input workloads. We next investigate how more realistic overlapping input workloads challenge the accuracy of our theoretical models and how input matching – a purely systems technique – helps address this challenge.

6.5 Input Matching Effectiveness (Q3)

To evaluate XRay's accuracy with overlapping inputs, we infused our workloads with multiple items from the same category. (e.g., multiple emails targeting the



(a) **Recall** (b) **Precision**

Figure 9: **Input Matching effectiveness.** Behavioral (Bayesian) recall and precision in Gmail with overlapping inputs, with and without Matching.

same topic on Gmail and multiple products in the same category in Amazon). For the Gmail experiments, we (as users) could not tell when Gmail targeted a specific email from a group of similar emails. We therefore ran two different types of experiments. First, a controlled, albeit unrealistic, one for Gmail. We replicated various emails *identically* in a user's inbox: 1 email was replicated 4 times, 2 emails 3 times, 4 emails 2 times, and 12 were single, for a total of 30 emails. This end-of-a-spectrum workload demonstrates how matching works ideally. XRay matched *all* redundant emails correctly. More importantly, Figures 9(a) and 9(b) show XRay's precision/recall with and without matching-aware placement for XRay's behavioral model, the only model improved by matching. Without input matching, XRay struggled to find differential signals: even with 35 shadow accounts for a 30-email experiment, recall was only 48%. With input matching, XRay's correlation model drew a stronger signal from each account and attained close to 70% recall for 16 accounts.

Second, for Amazon, we created a more realistic overlapping workload by selecting three *distinct* products in each of six product categories (e.g., from the Outdoor & Cycling category, we selected a helmet, pedals, and shoes). With a total workload of 18 products, XRay's input matching matched all but one item (shoes) into its correct group. With the new grouping, XRay's recall improved by a factor of 3 (from 30% to 93%) compared to the no-matching case for 18 products with 10 accounts; precision was 2.6 times higher (from 34% to 88%).

These results demonstrate that XRay's matching scheme is both portable across Web services and essential for high accuracy with overlapping workloads.

6.6 Anecdotal Use Experience (Q4)

To gain intuition into XRay's practical value, we ran a small-scale, anecdotal experiment that fished for Gmail ads targeted against a few specific topics. We created emails focused on topics such as cancer, Alzheimer, depression, HIV, race, homosexuality, pregnancy, divorce, and debt. Each email consisted of keywords closely related to one topic (e.g., the depression-related email included *depression*, *depressed*, and *sad*; the homosexuality email included *gay*, *homosexual*, and *lesbian*). We then launched XRay's Gmail ad collection and examined the targeting associations. We acknowledge that a much larger-scale experiment is needed to reach statistically-meaningful conclusions. Hence, we relate our experience by example.

Topic	**Targeted Ads**	**XRay Scores**	**# Accounts & Displays**
Alzheimer	Black Mold Allergy Symptoms? Expert to remove Black Mold.	0.99, 0.05	9/9, 61/198
	Adult Assisted Living. Affordable Assisted Living.	0.99, 0.99	8/8, 12/14
Cancer	Ford Warriors in Pink. Join The Fight.	0.96, 0.98	9/9, 1022/1106
	Rosen Method Bodywork for physical or emotional pain.	0.98, 0.05	7/7, 24/598
Depression	Shamanic healing over the phone.	0.99, 0.99	16/16, 117/117
	Text Coach - Get the girl you want and Desire.	0.93, 0.04	7/7, 31/276
African American	Racial Harassment? Learn your rights now.	0.99, 0.2	10/10, 851/5808
	Racial Harassment, Hearing racial slurs?	0.99, 0.2	10/10, 627/7172
Homosexuality	SF Gay Pride Hotel. Luxury Waterfront.	0.99, 0.1	9/9, 50/99
	Cedars Hotel Loughborough, 36 Bedrooms, Restaurant, Bar.	0.96, 1.0	8/8, 36/43
Pregnancy	Find Baby Shower Invitations. Get Up To (60% Off) Here!	0.99, 1.0	9/9, 22/22
	Ralph Lauren Apparel. Official Online Store.	0.99, 0.6	10/10, 85/181
	Clothing Label-USA. Best Custom Woven Labels.	0.99, 1.0	9/9, 14/14
	Bonobos Official Site, Your Closet Will Thank You.	0.99 0.99	9/9 64/71
Divorce	Law Attorneys specializing in special needs kids education.	0.99, 0.99	9/9, 635/666
	Cerbone Law Firm, Helping Good People Thru Bad Times	0.99, 1.0	10/10, 94/94
Debt	Take a New Toyota Test Drive, Get a $50 Gift Card On The Spot.	0.99, 0.9	7/7, 58/65
	Great Credit Cards Search. Apply for VISA, MasterCard...	0.99, 0.0	9/9, 151/2358
	Stop Creditor Harassment, End the Harassing Calls.	0.99, 0.96	8/8, 256/373

Figure 10: **Example of Targeted Ads.** Columns three and four show the same data as columns four and five in Figure 5.

Figure 10 shows ads that XRay associated with each topic, with its confidence scores. Conservatively, we only consider ads with high scores. We make two observations. First, our small-scale experiment confirms that it is possible to target sensitive topics in users' inboxes. All disease-related emails, except for the HIV one, are strongly correlated with a number of ads. A "Shamanic healing" ad appears exclusively in accounts containing the depression-related email, and many times in its context; ads for assisted living services target the Alzheimer email; and a Ford campaign to fight breast cancer targets the cancer email. Race, homosexuality, pregnancy, divorce, and debt also attract plenty of ads. For example, the pregnancy email is strongly targeted by an ad for baby-shower invitations (shown in the figure), maternity- and lactation-related ads (not shown), and, interestingly, a number of ads for general-purpose clothing (shown). As another example, the debt email is strongly targeted by a car dealership ad that entices the targeted users to take a Toyota test drive using a $50 gift offering. Discussing the morality of targeting such sensitive topics is beyond our statute, however we believe that the lack of transparency, coupled with sensitive-topic targeting, opens users to subtle dangers, a topic we discuss next.

Second, for many ads, the association with the targeted email is not obvious at all. Nothing in the "Shamanic healing" ad suggests targeting against depression; nothing in the general-purpose clothing ads suggest targeting against pregnancy; and nothing in the "Cedars hotel" ad suggests an orientation toward the homosexuality email. If no keyword in the ad suggests relation with sensitive topics, a user clicking on the ad may not realize that they could be disclosing private information to advertisers. Imagine an insurance company wanted to gain insight into pre-existing conditions of its customers before signing them up. It could create two ad campaigns – one that targets cancer and another youth – and assign different URLs to each campaign. It could then offer higher premium quotes to visitors who come through the cancer-related ads to discourage them from signing up while offering lower premium quotes to those who come through youth-related ads. We believe that the potential for this attack illustrates the urgent need for increased transparency in ad targeting.

6.7 Summary

Our evaluation results show that XRay supports fine-grained, accurate data tracking in popular Web services, scales well with the size of data being tracked, is general and flexible enough to work efficiently for three Web services, and robustly uses systems techniques to discover associations when ad contents provide no indication of them. We next discuss how XRay meets its last goal: robustness against honest-but-curious attackers.

7 Security Analysis

As stated in §3.3, two threat models are relevant for XRay and applicable to different use cases. First, an *honest-but-curious* Web service does not attempt to frustrate XRay, but it could incorporate defenses against typical Web attacks, such as DDoS or spam, that might interfere with XRay's functioning. Second, a *malicious service* takes an adversarial stand toward XRay, seeking to prevent or otherwise disrupt its correlations. Our current XRay prototype is robust against the former threat and can be extended to be so against the latter. In either case, third-party advertisers can attempt to frustrate XRay's auditing. We discuss each threat in turn.

Non-Malicious Web Services. Many services incorporate protections against specific automated behaviors. For example, Google makes it hard to create new accounts, although doing so remains within reach. Moreover, many services actively try to identify spammers and click fraud. Gmail includes sophisticated spam filtering mechanisms, while YouTube rate limits video viewing to prevent spam video promotion. Finally, many services rate limit access from the same IP address.

XRay-based tools must be aware of these mechanisms and scale back their activities to avoid raising red flags. For example, our prototype for Gmail, YouTube, and Amazon rate limit their output collection in the shadow accounts. Moreover, XRay's very design is sensitive to these challenges: by requiring as few accounts as possible, we minimize: (1) the load on the service imposed by auditing, and (2) the amount of input replication across shadow accounts. Moreover, XRay's workloads are often atypical of spam workloads. Our XRay Gmail plugin sends emails from one to a few other accounts, while spam is sent from one account to many other accounts.

Malicious Third-Party Advertisers. Third-party advertisers have many ways to obfuscate their targeting from XRay, particularly if it may arouse a public outcry. First, an advertiser could purposefully weaken its targeting by, for example, targeting the same ad 50% on one topic and 50% on another topic. This weakens input/output correlation and may cause XRay to infer untargeting. However, it also makes the advertisers' targeting less effective and potentially more ambiguous if their goal is to learn specific sensitive information about users. Second, an advertiser might target complex combinations of inputs that XRay's basic design cannot discover. Our accompanying technical report shows an example of how advertisers might achieve this [26]. It also extends our theoretical models so they can detect targeting on linear combinations with only a constant factor increase in the number of accounts. We plan to incorporate and evaluate these extensions in a future prototype.

Malicious Web Services. A malicious service could identify and disable shadow accounts. Identification could be based on abnormal traffic (successive reloads of email pages), data distribution within accounts (several accounts with subsets of one account), and perhaps more. XRay could be extended to add randomness and deception (e.g., fake emails, varying copies). More importantly, a collaborative approach to auditing, in which users contribute their ads and input topics in an privacy-preserving way is a promising direction for strengthening robustness against attacks. Web services cannot, after all, disable legitimate user accounts to frustrate auditing. We plan to pursue this direction in future work.

8 Discussion

XRay takes a significant step toward providing data management transparency in Web services. As an initial effort, it has a number of limitations. First, both the Set

Intersection and Bayesian algorithms assume independent targeting across accounts and over time. In reality, ad targeting is not always independent across either. For example, advertisers set daily ad budgets. When the budget runs out, an ad can stop appearing in accounts mid-experiment even though it has the targeted attributes. The system might incorrectly assume that no targeting is taking place, when it could resume the next day. XRay takes reduced coverage into account, but differences between ads can let some targeting pass unnoticed. XRay does not currently account for these dependencies, but estimating their impact is an important goal for future work.

Second, we assume that targeting noise is bounded and smaller than the targeting signal. While this condition seems to hold on the evaluated services, other services making more local decisions may be harder to audit. For example, Facebook might target ads based on friends' information, potentially creating noise that is as high as the targeting signal. A future solution might imitate the social network in shadow accounts.

Third, XRay uses Web services atypically. To the best of our knowledge, it does not violate any terms of service. It does, however, collect ads paid for by advertisers to detect correlation. Ad payment is per impression and pay per click. The former is vastly less expensive than the latter [32]. XRay creates false impressions only but never clicks on ads. A back-of-the-envelope calculation using impression pricing from [32] of $0.6/thousand impressions reveals that XRay's cost should be minimal: at most 50 cents per ad for our largest experiments.

Despite these limitations, XRay has proven itself useful for many needs, particularly in an auditing context. An auditor can craft inputs that avoid many of these limitations. For example, emails can be written to avoid as much overlap as possible and keep the size of inputs used for targeting within reasonable bounds. We hope that XRay's solid correlation components will streamline much-needed investigations – by researchers, journalists, or the FTC – into how personal data is being used.

9 Related Work

While §2.2 covered Web data protection and auditing related works, we next cover other related topics. Our work relates to recent efforts to measure various forms of personalization, such as search [21, 47], pricing [31], and ad discrimination [40]. They generally employ a methodology similar in spirit to differential correlation, but their goals differ from ours. They aim to quantify *how much* output is personalized and what *type* of information is used overall. In contrast, XRay seeks to provide fine-grained diagnosis of which *input data* generates which personalized results. Through its scaling mechanisms – unique in the personalization and data tracking literature – XRay scales well even when the relevant inputs are many and unknown in advance.

Our work also relates to a growing body of research measuring advertising networks. These networks, notably complex and difficult to crawl [3], are rendered opaque by the need to combat click fraud [9], and have been shown to be susceptible to leakage [24] and profile reconstruction attacks [6]. As for other personalization, prior studies focused mostly on macroscopic trends (e.g., What fraction of ads are targeted?) [3] or qualitative trends (e.g., Which ads are targeted toward gay males?) [20]. Various studies showed traces – but not a prevalence – of potential abuse through concealed targeting [20] and data exchange between services [46]. These works primarily focus on display advertising, and each distinguishes contextual advertising using a specific classifier with semantic categories obtained from Google's Ad Preferences Managers or another public API [28].

XRay departs significantly from these works. First, since it entirely ignores the content and even the domain of targeting, it is readily applied as-is to ads in Gmail, product recommendations, and videos. Second, while previous methods label ads as "behavioral" in bulk once other explanations fail [28], XRay remains grounded on positive evidence, and determines to *which* inputs an output should be attributed. Third, XRay's mechanisms to avoid exponential input placement and deal with overlapping inputs are unprecedented in the Web-data-tracking context. While they resemble *black box* software testing [4], the specific targeting assumption we leverage have, to our knowledge, no prior equivalent.

10 Conclusions

The tracking of personal data usage poses unique challenges. XRay shows for the first time that accurate, *fine-grained* tracking need not compromise portability and scalability. For users who care about *which* piece of their data has been targeted, it offers a unique level of precision and protection. Our work calls for and promotes the best practice of voluntary transparency, while at the same time empowering investigators and watchdogs with a significant new tool for increased vigilance.

11 Acknowledgements

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A Proof of Theorem 1

A.1 Targeting functions, Axioms and Core Family

A *combination* $\mathscr{C}$ of order r, also called r_combination, is a subset of r elements among the N inputs.

Each given ad is associated with a *targeting function* defined as a mapping f from any subset $\mathscr{C}$ of the N inputs into $\{0,1\}$, where $f(\mathscr{C}) = 1$ denotes that an account containing $\mathscr{C}$ as inputs should be targeted. By convention, untargeted ads are associated with the null function $f(.) = 0$. Any targeting function f satisfies two axioms:

- **monotonicity**: $\mathscr{C} \subseteq \mathscr{C}' \implies f(\mathscr{C}) \leq f(\mathscr{C}')$.
- **input-sensitivity**: $\exists \mathscr{C}, \mathscr{C}'$ s.t. $f(\mathscr{C}) = 0, f(\mathscr{C}') = 1$.

Monotonicity simply reflects that an account with strictly more interest or hobbies should in theory be relevant to more ads, and never to less. Input sensitivity prevents the degenerate case where a targeting function is constant.

A *family* S of size l is any collection of l distinct combination. The *order* of this family is defined as the largest order of a combination it contains. For any family S, one can define a targeting function that takes value 1 whenever the subset contains at least one combination in S. Indeed, as shown in [26], the converse is true:

Lemma 1 *For each monotone, input-sensitive targeting function there exists a unique family S satisfying:*

(i) S has size l and order r and it explains *f, which means $f(\mathscr{C}) = 1$ holds if and only if $\exists \mathscr{C}' \in S, \mathscr{C}' \subseteq \mathscr{C}$.*

(ii) No family of size $l' < l$ explains f.

(iii) No family of order $r' < r$ explains f.

Hence, associated with each ad and therefore each targeting function is a unique family of input combination that are targeted, called the ad's *core family*, and we now sketch why it is correctly identified by our algorithm.

A.2 Algorithm and Correctness

For any family of subsets S and fraction $0 \leq x \leq 1$, we say a subset of inputs $\mathscr{C}$ is an x_intersecting subset of S if x subsets in S have at least one input in $\mathscr{C}$. Our proof exploits an original connection between small intersecting subsets (that can be found efficiently) to show how they can reveal a core family. One way to understand why is the following: say, for instance, that the targeting function f takes value 1 exactly when one of the inputs within $\mathscr{C}$ is found in the account. Then $\mathscr{C}$ is exactly the union of inputs found in the core family and intersects all accounts within scope, i.e., forms a large fraction of those receiving the ad.

The key property to explain our algorithm is random subsets. We can show under the conditions of the theorem that there exists $0 < x < 1$ that satisfies two properties related to the inputs of accounts receiving the ads: (1) if targeting does not occur, then with a large probability we cannot find a subset of l inputs that meets at least a fraction x of the accounts seeing the ad, and (2) if targeting does occur, we have accounts receiving the ads for various reasons, within and outside the targeting scope. But we can show with high probability that at least a fraction x of them are within scope and hence must include one combination in the core family. Since with each core family of size l one can associate an intersecting subset that contains at most l elements, checking the existence of such a subset reveals the presence of targeting.

This explains why an algorithm can qualitatively conclude whether targeting occurs or not, but it does not explain how the core family can be computed. However, leveraging stronger results of random subsets allows to apply the same rule recursively, offering multiple ways to determine exactly the core family even with a polynomial number of operations.

More formally, we define: A random *Bernoulli subset*, denoted by $B(n,p)$, is a subset such that any of n elements is contained with probability p independently of all others. A random *Bernoulli family* of size m is a collection of m independent Bernouilli subsets. We first show property (1) above more formally:

Lemma 2 *Let $x > 0$, $s \in \mathbb{N}$, $p < 1-(1-x)^{\frac{1}{s}}$, and a Bernouilli family $B_1(n,p), B_2(n,p), \ldots, B_m(n,p)$. For any $\varepsilon > 0$ and polynomial P of degree $\leq r$, there exists $A > 0$ such that with probability $\left(1 - \frac{\varepsilon}{P(n)}\right)$ no x_intersection subset exists of size s whenever we have:*

$$m \geq A \cdot ((s+r)\ln(n) + \ln(1/\varepsilon)) .$$

To prove property (2), we need to bound, among accounts receiving an ad, the fraction that is outside the scope of targeting but still receives the ads because $p_{\text{out}} > 0$. Formally, we have:

Lemma 3 *Let $x > 0$, $\alpha > 0$, and a core family of size l and order r p_{in}, p_{out} where we have $p_{out}/p_{in} < \frac{1-x}{x}\frac{\alpha^r}{1-\alpha^r}$. Let $\mathscr{C}$ be a combination of order r.*

For any $\varepsilon > 0$ and polynomial P of degree $\leq r$, there exists $A > 0$ such that with probability $(1-\varepsilon/P(n))$ the following holds: Among accounts containing $\mathscr{C}$ and receiving the ad, at least x fraction of them is within the targeting scope whenever we have:

$$m \geq A \cdot (r\ln(n) + \ln(1/\varepsilon)) .$$

The two lemmas above (proved in [26]) can be combined whenever α satisfies the inequality for p in the first lemma, which shows that an algorithm can detect the presence of targeting whenever $p_{\text{out}}/p_{\text{in}} < \frac{1-x}{x}\frac{(1-(1-x)^{\frac{1}{l}})^r}{1-(1-(1-x)^{\frac{1}{l}})^r}$.

A naive exponential algorithm could be used to exhaustively search for a core family using this brick. We also show that a polynomial algorithm can refine this analysis to compute the core family at the expense of a more complex recursion in [26].

Appendix L

Web Transparency for Complex Targeting: Algorithms, Limits and Tradeoffs

Web Transparency for Complex Targeting: Algorithms, Limits, and Tradeoffs

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Big Data promises important societal progress but exacerbates the need for due process and accountability. Companies and institutions can now discriminate between users at an individual level using collected data or past behavior. Worse, today they can do so in near perfect opacity. The nascent field of *web transparency* aims to develop the tools and methods necessary to reveal how information is used, however today it lacks robust tools that let users and investigators identify targeting using multiple inputs.

Here, we formalize for the first time the problem of detecting and identifying targeting on *combinations of inputs* and provide the first algorithm that is asymptotically exact. This algorithm is designed to serve as a theoretical foundational block to build future scalable and robust web transparency tools. It offers three key properties. First, our algorithm is *service agnostic* and applies to a variety of settings under a broad set of assumptions. Second, our algorithm's analysis delineates a *theoretical detection limit* that characterizes which forms of targeting can be distinguished from noise and which cannot. Third, our algorithm establishes *fundamental tradeoffs* that lead the way to new metrics for the science of web transparency. Understanding the tradeoff between effective targeting and targeting concealment lets us determine under which conditions predatory targeting can be made unprofitable by transparency tools.

1. QUICK OVERVIEW

A primer on web transparency tools.

To address the big-data web's untenable opacity, a new set of transparency tools have been proposed recently [7, 4, 5, 6, 3, 9]. Generally speaking, they assume no insider information about how the data-driven web service operates and instead rely on a specific form of *black box testing* [2] to detect data use. Briefly, a transparency tool works as follows. First, it collects the results of a series of tests in which *inputs* vary, *e.g.*, browsing history [7], search history [4], emails [6], locations [9], or explicit profile information [3]. Second, by examining the observed *outputs* – *e.g.*, search results [4, 9], ads seen [3, 6], recommendations [6, 5], or prices [7, 5] – the tool deduces how the system personalizes its behavior based on this input. Finally, the tool's deductions are used as *hypotheses* that are further analyzed for implications by the tool's users, such as end users, journalists, privacy watchdogs, or federal investigators.

To be valuable to their users, transparency tools strive to meet three requirements:

1. **Scalability:** Each test may involve multiple preliminary steps to open a new web account and populating its inputs. These steps cannot always be automated and may be expensive (e.g., creating a Google account requires buying a new phone number). It is also important to keep resources to a minimum as the size of outputs/inputs grows.

2. **Accuracy:** The deduction that the tool provides should be *sound*, which means that it can be trusted not to originate from noise or other limitations of the experiments. The tool should also be *complete* which specifies that it rarely misses an important deduction.

3. **Broad Applicability:** Ideally, the same tool should apply not only to many different services but also various forms of data usage within those services, with only minor and intellectually simple changes.

Perhaps unsurprisingly, the first two requirements are often in conflict. The third makes the problem extremely challenging, and has barely been considered to date. With few exceptions [6, 3], previous transparency tools were designed for a specific service or usage in order to detect a particularly sensitive topic: price discrimination [7], search results personalization [4], censorship [9]. Only recently has development of widely-applicable, generic tools begun to be considered to allow generic data collections [5] and service-agnostic detection methods [6, 3]. Despite appearences, however, we find that even the latest transparency tools are limited in the kind of data uses they can support accurately and scalably. We believe that the biggest roadblock is the lack of support for detecting complex, multi-input targeting, which we find mandatory for building scalable, accurate, and broadly applicable tools.

Our new findings.

We prove that targeting that uses one or several combinations of N inputs can be detected and identified with asymptotically perfect accuracy, and that this only requires

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a logarithmic order $O(\ln(N))$ of experimental observations. To place our contribution in respect to prior work, this shows that a web transparency tool can remain scalable and accurate, without being strictly restricted to single input targeting. However, and this is where our contribution contrasts the most with previous results, it comes at a cost: the intensity of targeting (defined below) needs to be sufficiently large. In other words, web transparency need not always be blind to combined targeting, however as the inherent complexity of targeting increases, targeting becomes easier to conceal. Our results open a new chapter in the understanding of Big Data: to determine sufficient and necessary conditions under which one can prevent its opacity.

2. PROBLEM FORMULATION & RESULTS

We formalize the following intuitive problem: given a set of N inputs representing possible information items present in a user's account (such as emails or searches), we wish to determine how they affect occurence of one particular output of interest (such as an ad or a recommendation).

Our main assumption is that the output is affected through an unknown targeting function f of the inputs, to be determined. The function f is defined separately for each output. The targeting function f is a mapping from the set of all combinations to $\{0;1\}$. By convention, $f(\mathcal{C})=1$ indicates that an account containing $\mathcal{C}$ is targeted, and we denote $f(.)=0$ if the ad is untargeted.

Experiments and outcome properties.

Because in practice we have no access to the targeting function, we rely on experiments to observe its reaction to various inputs. Intuitively, these experiments collect outputs from a set of accounts that contain subsets of the inputs and produce a set of observations of f. For example, experiments could collect ads for accounts with different subsets of emails. More formally, the experimental infrastructure we assume is similar to an *oracle* from function learning theory [8, 1]. We assume that our experimental oracle satisfies the following axiom. There exist two probabilities p_{in}, p_{out} such that:

$$\mathbb{P}\left[\mathcal{O}(\mathcal{C}_i)=1|f(\mathcal{C}_i)=1\right] \geq p_{\text{in}} > p_{\text{out}} \geq \mathbb{P}\left[\mathcal{O}(\mathcal{C}_j)=1|f(\mathcal{C}_j)=0\right].$$

where p_{in} is a minimal bound on the probability that an account receives an output that is relevant for it and p_{out} is a maximal bound on the probability that an account receives an output that is not relevant for it. This axiom properly states that f is related to the outcome we study. It allows the variables to also depend on other factors: hidden inputs that are not in the set of N we study, external sources of randomness such as availability of ad-slot, competition. One experimental design used in practice [6, 3] and that fits this axiom is to populate each account randomly so that an input independently appears with probability α.

Under the assumptions above, we say that an algorithm using m observations solves the targeting detection problem if it can correctly decide whether $f(.) \neq 0$ and hence that the output is targeted using at most m queries to $\mathcal{O}$. Going further, an algorithm solves the targeting identification problem if it correctly returns the function f. Naturally, both problems rely on random observations and hence our goal is to design algorithms whose detection/identification error is arbitrarily small for large N.

Since one should distinguish (at least) between N inputs, it seems that a minimum of $\Omega(\ln(N))$ binary observations are absolutely necessary at least for the identification. This is hence what we assume and we aim at keeping it at this absolute minimum.

THEOREM 1. *Assuming that f is a monotone DNF with size at most s and width at most w, and that ratio p_{out}/p_{in} is below a predetermined bound, we provide a targeting detection algorithm that for any $\varepsilon > 0$ requires $O(\ln(N/\varepsilon))$ observations, $O(N^s \ln(N/\varepsilon))$ operations and is correct with probability $(1-\varepsilon/N)$.*

THEOREM 2. *Under the same assumption, we provide a targeting identification algorithm that for any $\varepsilon > 0$ requires $O(\ln(N/\varepsilon))$ observations, $O(N^{s+w} \ln(N/\varepsilon))$ operations and is correct with probability $(1-\varepsilon/N)$.*

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Appendix M

Can Web Transparency Tools Cope with Complex Targeting?

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Abstract: Big Data promises important societal progress but exacerbates the need for algorithmic accountability as more and more decisions affecting millions of users are being automated using personal and private information. The recent area of *web transparency* has developed generic methods to reveal *which* information item or input generates personalization and differentiated treatments. We surveyed 13 transparency tools and found that they all make stringent assumptions on personalization; unless an algorithm exploits a *single input*, it can be *undetected* – or to be more precise, ensuring its detection incurs a *prohibitive exhaustive search.* The ever increasing set of relevant inputs to monitor exacerbates the difficulty of this task. As personalization becomes ever more complex, we see the familiar conditions of an arms race, where transparency and evasion techniques grow more sophisticated. Until now, we understand little of it, let alone how to best address it to make the web more transparent.

In this paper, we present the first algorithms for transparency enhancing tools that are efficient and correct even with general complex targeting. To take a simple example, ad-targeting can usually depend on multiple inputs in a way that may not satisfy previous properties like linearity. Here we formalize it for the first time, and show how to combine simple heuristics into transparency algorithms that are provably correct while keeping the cost of queries and computations minimum (actually matching computational lower bounds). We introduce a key metric, the *targeting lift*, and show it dictates the conditions for algorithms with different computation cost to succeed. Small scale experiments with 20 or 50 inputs, and large scale simulations with up to 100,000 inputs complement our theoretical analysis: they prove that our algorithms expand the scope of targeting found beyond the state of the art, that they exhibit excellent scaling properties as the set of inputs grows, and that they resist even challenging targeting lift values.

Keywords: transparency enhancing tools, behavioural targeting, blackbox analysis, computational learning, analysis of random algorithms

1 Introduction

"Just as neighborhoods can serve as a proxy for racial or ethnic identity, there are new worries that big data technologies could be used to digitally redline unwanted groups, either as customers, employees, tenants, or recipients of credit."
– Executive Office of the President, *Big Data: Seizing Opportunities, Preserving Values*, [16].

Big Data – a set of measurement and decision tools leveraging large sets of records such as emails, web visits, voice calls, credit card transactions, tweets, and geotagged content – is becoming central to any business today. Tomorrow it promises to unlock opportunities in myriad public services, promoting healthy behaviors [18], environmental sustainability [17], preventing crime [21], mitigating congestion and pollution in transportation [14], improving disaster recovery [13], and economic development [9]. However, the availability and use of this information can also challenge our society's values, as illustrated by recent cases of online discrimination found in advertising [20], pricing [8, 15], and hiring [1]. Our society must be able to celebrate Big Data's potential for progress *and* perpetuate our commitment to equal opportunities for all: We should be ready to guard all from the intended or unintended consequences that differentiation enables.

Today, most systems handling personal data, such as web services and mobile applications, behave as *blackboxes*, which no one outside the service provider – neither the end-users nor privacy watchdogs or federal investigators like the Federal Trade Commission – can understand and monitor. *Web transparency* is a nascent area that takes an engineering approach to promote better accountability. Its goal is to enable everyone to answer critical questions about *how* personal data is being used. However, this is a complex question to answer and

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current tools quickly show their limits. For example, we found that state of the art tools [6, 11] have been designed and evaluated primarily to detect when a single input is responsible for an action. But personal data is growing in size and complexity. For example, as we present later in three potential scenarios of data use, it could be a *combination* of inputs (*i.e.*, multiple inputs together) that explain personalized outputs. One may then ask "Can transparency enhancing tools extend beyond single-input personalization? or would they meet a computational barrier or restriction which impedes their practicality? If the success of these tools depends on the environment, which metrics matter?"

This paper answers the aforementioned questions as it provides a formal definition of the detection and the identification problem posed by web transparency under complex targeting. We introduce multiple new algorithms, and a new metric that is shown through rigourous proof and experimental/simulated evidence to control the accuracy (or lack thereof) for those tools. Most importantly we show that web transparency continues to scale even with complex targeting, but that it poses new combinatorial challenges and computational tradeoffs. Several of our results suggest future research avenues to design future robust transparency enhancing tools.

We now present the following contributions.

– After reviewing 13 transparency tools, we identify multi-input targeting as a key missing feature, motivated by multiple scenarios in which it may be relevant. We introduce a formal model of online targeting that allows us to pose detection and identification in rigorous terms. This model encompasses arbitrarily more complex targeting and introduces a key metric: the targeting lift. (§2)
– We then introduce an heuristic algorithm which leverages intuitive facts about random subsets to detect when multi-input targeting is taking place. In a small experiment comparing this heuristic to the state of the art, we find that it significantly increases the coverage of transparency tools. This observation even holds when an approximation is used in lieu of the exact suggested heuristic and it motivates a more thorough analysis to prove it rigorously. (§3)
– By a mathematical analysis of properties of random subsets, we show that those detection algorithms (exact and approximate) are provably correct under a specific condition that relates to the targeting lift we introduced above. Moreover, we prove these algorithms can be used iteratively or recursively not only to detect but to exactly identify the function that is being applied to the inputs. All the algorithms we present scale remarkably well as the number of inputs grows, *i.e.*, they require only $O(\ln N)$ observations. While the first algorithm we introduce is polynomial in computation cost, we prove a (much more involved) approximation exists that correctly identifies the function with linear computation cost, matching a trivial lower bound. (§4)
– Finally, we come back to analyze more thoroughly the impact of the targeting lift, they key metric enabling web transparency. First, our analysis shows that transparency enhancing tools exhibit a tradeoff where lighter forms of targeting can - at least in theory - only be found by more expensive algorithms. Second, we run large numerical simulations proving that even moderate numbers of accounts (around 300) allow us to decipher complex multi-input targeting among 100,000 of inputs, while remaining robust to noise in the targeting lift. These reports demonstrate the possibility of running transparency with 1000 times more inputs than any experiment to date. We show that the greedy heuristic we introduced is robust and efficient, and typically succeeds for much higher levels of noise than what our theoretical bounds would suggest. Finally, we discuss the practical consequences of our results: we define the price of opacity which measures the added cost incurred by an advertiser that aims at running illegal targeting under the radar of current transparency-enhancing tools. (§5)

Our results greatly enhance the complexity that can be handled by transparency tools, and also delineate where they may fail. This is the first formal definition of algorithms that can provably exactly identify targeting in the general case we present here. Before this analysis, the only previous mention of input combination appears as an unvalidated extensions in the XRay paper [11], which centers on a different Bayesian algorithm restricted to single input targeting (used for comparison in our small experiment). The authors present no formal proof beyond some initial steps (resembling (Lemma 1, 2 and 3 here) reproduced her to keep this paper self-contained. All other results, proofs and algorithms involved are new, and only partly appeared as part of an unpublished appendix in a technical report [REMOVED FOR ANONYMITY].

2 Problem formulation

2.1 Requirements of transparency tools

To address the big-data web's untenable opacity, a new set of transparency tools have been proposed recently [6–8, 11, 15, 22]. Generally speaking, they assume no insider information about how the data-driven web service operates and instead rely on a specific form of *black box testing* [4] to detect data use. Briefly, a transparency tool works as follows. First, it collects the results of a series of tests in which *inputs* vary, *e.g.*, browsing history [15], search history [7], emails [11], locations [22], or explicit profile information [6]. Second, by examining the observed *outputs* – *e.g.*, search results [7, 22], ads seen [6, 11], recommendations [8, 11], or prices [8, 15] – the tool deduces how the system personalizes its behavior based on this input. Finally, the tool's deductions are used as *hypotheses* that are further analyzed for implications by the tool's users, such as end users, journalists, privacy watchdogs, or federal investigators. The deductions are generally not considered as definite proof, but as quantified hypotheses that require further investigation and reasoning. For example, an FTC investigator might use a transparency tool's deductions to glean at potential predatory targeting against some vulnerable population, but will open his/her own detailed investigation to validate whether the targeting was intentional or automatic, which of many potential parties applied this targeting, etc.

To be valuable to their users, transparency tools strive to meet three requirements:

1. **Scalability:** Each test may involve multiple preliminary steps to open a new web account and populate its inputs. These steps cannot always be automated and may be expensive (e.g., creating a Google account requires buying a new phone number). It is also important to keep resources to a minimum as the size of outputs/inputs grows.
2. **Accuracy:** The deduction that the tool provides should be *sound*, which means that it can be trusted not to originate from noise or other limitations of the experiments. The tool should also be *complete* which specifies that it rarely misses an important deduction.
3. **Broad Applicability:** Ideally, the same tool should apply not only to many different services but also various forms of data usage within those services, with only minor and intellectually simple changes.

Perhaps unsurprisingly, the first two requirements are often in conflict. The third makes the problem extremely challenging, and has barely been considered to date. With few exceptions [6, 11, 12], previous transparency tools were designed for a specific service or usage in order to detect a particularly sensitive topic, such as price discrimination [15], search personalization [7] or censorship [22]. Only recently has development of widely-applicable, generic tools begun to be considered to allow generic data collections [8] and service-agnostic detection methods [6, 11, 12]. However, we find that even the latest transparency tools are limited in the kind of data usage they can detect or identify in large scale examples. We believe that the biggest roadblock is the lack of support for detecting complex, multi-input targeting, which we argue must be addressed for building scalable, accurate, and broadly applicable tools. We motivate this need next.

2.2 Why does multi-input targeting matter?

Without exception, all existing transparency tools are designed to detect situations in which a *single input* is responsible for an algorithmic decision. AdFisher [6] builds for a given individual input (*i.e.*, gender, or race) a classifier that *retroactively* predicts the presence of an input based on the outputs observed for this account. This allows sound predictions of whether individual inputs are treated differently by the audited system. The XRay tool [11] relies on a Bayesian inference procedure that determines the likelihood that a given input explains the distribution of ads seen across accounts. Sunlight [12] introduces a machine learning technique that approximates targeting functions in a linear model, with no proven guarantee, especially when input combinations are found to affect the targeting function (see below).

We first argue that targeting function that depends on multiple inputs are *far from unusual.* We provide three scenarios where those can be found:

- For years, search engines have combined previous and current queries for input *disambiguation* (*e.g.*, deciding whether a user querying the word "apple" is looking for fruits or electronics). Similarly, advertisers today can define their targets by combining multiple keywords together, and even jointly with given demographics or location [10].
- Even if the target is specified by a unique term or topic, it is common for inputs to *overlap* (*e.g.*, two

emails may trigger the same output because they both contain the same important keyword). In fact, ad-targeting platforms like adwords often leverage relation between inputs, such as different keywords, as suggestions for how to expand the target of a given campaign. Some overlap is common even among a small number of inputs, as evidence of our experiments prove.

– Third, using multiple terms could be a way to *conceal* targeting. There are situations in which sensitive information such as race, gender or sexual orientation are forbidden to be used explicitly for targeting. But the nature of big data makes it possible to exploit other inputs that correlate with the intended target to obtain a similar effect. A collection of first names, for instance, was shown to be used as a proxy for race [20].

We now would like to highlight how those scenarios illustrate the limitations of current transparency tools. For example, if multiple inputs overlap and they all cause a personalized ads, XRay's tests [11] conclude that no targeting takes place since all hypotheses associated with a single input yield poor likelihood. AdFisher [6] is more robust as it can detect that an input plays a partial role and causes increased likelihood of an ad. But that knowledge applies only if the experimenter knows a priori which input to test and conduct an experiment about. For instance, in the concealed targeting case, monitoring the use of N inputs as potential proxy requires an exhaustive search with queries growing linearly with N. Sunlight [12] approximates targeting functions through linear combinations of inputs. In the disambiguation case, when different subsets of inputs cause targeting only when they are found together, Sunlight can only return a linear approximation of the targeting function. While extensions may be considered with an exhaustive list of subsets as new dimensions of an input space, this appears costly and has not been considered or validated.

In contrast to the above, our approach presents transparency algorithms directly designed for the complex case where the targeting function depends on multiple inputs. We would like, also in contrast to the above, for our algorithm to provide a formal theoretical guarantee under a small set of conditions. To do so, we first need to formally define the problem.

2.3 A formal model of complex targeting

We formalize the following intuitive problem: given a set of N inputs representing possible information items present in a user's account (such as emails, searches, or other examples above), we wish to determine how they affect a web service's choice of one particular output of interest (such as an ad or a recommendation).

Our main assumption is that the output is affected through an unknown targeting function f of the inputs, to be determined. The function f is defined separately for each output (i.e., it should be called f_{output} but we elide the subscript for simplicity). Formally, we define a combination $\mathcal{C}$ of width r as a subset of r elements chosen among the N inputs. The targeting function f is a mapping from the set of all combinations to $\{0;1\}$. We distinguish between two types of functions. Those that are untargeted will randomly assign their output with a probability that is independent of the tracked inputs. Those that are targeted will assign their output based on the presence of certain inputs in the account. For these targeted functions, we say an account $\mathcal{C}$ is inside the target if $f(\mathcal{C}) = 1$, and outside the target otherwise.

Any targeting function $f \neq 0$ should satisfy two assumptions (a.k.a., axioms):
A1 **monotonicity**: $\mathcal{C} \subseteq \mathcal{C}' \implies f(\mathcal{C}) \leq f(\mathcal{C}')$.
A2 **input-sensitivity**: $\exists\, \mathcal{C},\ \mathcal{C}'$ s.t. $f(\mathcal{C}) \neq f(\mathcal{C}')$.

Monotonicity simply reflects that an account with strictly more inputs that may indicate interest or hobbies should in theory be relevant to more ads, and never to less. Input sensitivity prevents the degenerate case where a targeting function is constant.

In practice we have no access to the targeting function directly. Instead we rely on experiments to observe how various inputs are treated. Intuitively, these experiments collect outputs from a set of accounts that contain subsets of the inputs and produce a set of noisy observations of f. For example, experiments could collect ads for accounts with different subsets of emails. More formally, the experimental infrastructure we assume is similar to a *noisy oracle* $\mathcal{O}$ as defined in computational learning theory [2, 3, 19]. It can be interpreted as a collection of random variables $\mathcal{O}(\mathcal{C})$ associated with each combination of input $\mathcal{C}$.

We assume that this oracle $\mathcal{O}$ (*i.e.*, the family of random variables it defines) satisfies the following third axiom:
A3 **targeting lift**: There exist $p_{\text{in}}, p_{\text{out}}$ such that

$$P\left[\mathcal{O}(\mathcal{C})=1 \middle| f(\mathcal{C})=1\right] = p_{\text{in}} > p_{\text{out}} = P\left[\mathcal{O}(\mathcal{C}')=1 \middle| f(\mathcal{C}')=0\right].$$

The targeting lift axiom properly states that f is related to the outcome we observe. It allows the variables to also depend on other factors: hidden inputs that are not in the set of N we study, external sources of randomness such as availability of ad-slot, competition. This axiom is also here to avoid the degenerate case where the values taken by $\mathcal{O}(\mathcal{C})$ for each $\mathcal{C}$ are simply not affected by $f(\mathcal{C})$. We note that $p_{\text{in}}/p_{\text{out}} > 1$ and we call this ratio the targeting lift which denotes how much more likely are the ads to be shown for an account in-target. A function is more likely to be easy to detect or identify when the targeting lift is high, while for moderate or small targeting lift, the presence of ads in many accounts outside the target makes this more difficult.

2.3.1 Core family

A family S of *size* l is any collection of l distinct combinations. The width of the family is defined as the largest width of a combination it contains. Interestingly, there is a duality between families and targeting functions. On the one hand, one can define for any family S a targeting function $f : \mathcal{C} \to \max_{\mathcal{S}\in S} I_{\{\mathcal{S}\subseteq\mathcal{C}\}}$ that takes value $f(\mathcal{C}) = 1$ whenever the subset $\mathcal{C}$ contains at least one combination in S. On the other hand, we show (proof omitted due to space constraints) that the converse holds: for a targeting function f, there is a *unique* family with the property that it is of both minimum width and minimum size:

Lemma 1. *For each monotone, input-sensitive targeting function, f, there exists a unique family S satisfying:*
(i) S has size l and width r and it explains f, i.e.,

$$f(\mathcal{C}) = 1 \textit{ holds if and only if } \exists\, \mathcal{C}' \in S, \mathcal{C}' \subseteq \mathcal{C}\,.$$

(ii) No family of size $l' < l$ explains f.
(iii) No family of width $r' < r$ explains f.

For each targeting function, this family is the core family. Similarly, the size and the width of f is defined by its core family. Lemma 1 follows from the monotonicity axiom and does *not* hold for non-monotonic functions.

For example, with $N = 4$, let $S = \{\{1,3\}, \{4\}\}$, and $S' = \{\ \{1,2,3\}, \{4\}, \{2,4\}, \{1,3\}\ \}$ and consider the function $f : \mathcal{C} \mapsto \max_{\mathcal{S}\in S'} I_{\{\mathcal{S}\subseteq\mathcal{C}\}}$. We see that S' explains f by definition, and S also explains f. Intuitively, if S explains f, then if we were to observe that all combinations in S' receive an ad, this could in theory be explained by the hypothesis that the ad is targeted at accounts which contain any of the combinations of inputs in S. Alternatively, if S does not explain S', then it shows that S is not sufficient on its own to interpret this observation.

2.3.2 Targeting Detection, Targeting Identification

Under the assumptions above, an algorithm using m observations solves the targeting detection problem if it can correctly decide whether the output is the product of a targeted or untargeted function. Going further, an algorithm solves the targeting identification problem if it correctly returns the core family defining f. Naturally, both problems rely on random observations and hence our goal is to design algorithms whose detection/identification error is arbitrarily small for large N.

Let us quickly discuss the computational cost that we can hope to achieve. Since one should distinguish (at least) between N inputs, it seems that a minimum of $\Omega(\ln(N))$ binary observations are absolutely necessary at least for the identification. Similarly each input needs to be considered so a minimum of $\Omega(N)$ elementary computations are to be performed. This is hence what we assume and we aim at keeping it at this absolute minimum. Note that those condition imply that we cannot detect function of any arbitrary size and width (*e.g.*, the function $f : \mathcal{C} \mapsto I_{\{|\mathcal{C}|\geq N/2\}}$ has a core family with a size growing *exponentially* in N). So our goal is to solve detection/identification given bounded size and width, a priori known[1], while carefully analyzing how those bounds affect the complexity and correctness of the algorithm. In fact, at the end of the next section we show that an algorithm solving identification exists that matches the computational lower bounds above, provided that the targeting lift is sufficiently strong.

3 Transparency Algorithms

In this section, we present our new transparency algorithm that we justify informally through an intuitive heuristic argument. We then present immediate empirical evidence, from a small scale experiment, that algorithms based on this heuristic are promising to ex-

1 If the bounds are unknown, one could run algorithms with increasing values of maximum size and width and stop when targeting is correctly detected and/or identified.

pand the scope of transparency enhancing tools. All the claims we made here are formally proved in the next section, but can be found here without superfluous technicalities.

3.1 Heuristic for targeting detection

We assume that a collection of m accounts are created. For each of those accounts, every one of the N inputs we study is independently and randomly included with probability α. For a given advertisment we wish to study, we observe multiple accounts that receive it in our experiment, which we generally call the active accounts.

Let us first discuss how one could design a test to distinguish untargeted ads from ads with infinite targeting lift ($pin > 0$ and $p_{\text{out}} = 0$). The essential argument follows from a simple yet powerful intuition: First, if on the one hand the ad is targeted with an infinite targeting lift, then any combinations of inputs $\mathcal{C}$ for an active account must verify $f(\mathcal{C}) = 1$ and hence it must contain one combination from the core-family of f. In the later case, let us denote by l the size of the core family of f. Then there exists a subset $\mathcal{C}'$ of l inputs among N such that each active account contains at least one element of $\mathcal{C}'$. Basically $\mathcal{C}'$ is a small subset that intersects all set of inputs found in all active account. On the other hand, if we assume that none of the inputs that we included play any role in the appearance of this particular ad - *i.e.*, if the ad is not targeted - then the inputs of the active accounts are the sole results of our random choices. In that case, having a small subset that intersects all of those random choices is a very unlikely event.

This informally suggests that looking for a small subset intersecting the inputs of all (or most) active accounts in which the ads appear may potentially serve as a good test that the ad is targeted. Note that when it is the case, the inputs found in this small intersecting subset are primary candidates to be the ones defining the target. With this in mind, we introduce a simple heuristic algorithm for detection:

```
Heuristic Detection-x Algorithm
Known parameters: $m$, maximum size $l$, probability $\alpha$.
Entries: a threshold parameter $x > \alpha$.
Result: 1 if the ad is targeted, 0 otherwise.
1: Create $m$ accounts, include each input independently with
   probability $\alpha$.
2: Construct the family $S^{(\text{ad})}$ containing all combinations of
   inputs in accounts seeing the ad.
3: for $\mathcal{C}'$ of $l$ inputs do
4:     if $|\{\mathcal{C} \in S^{(\text{ad})} | \mathcal{C} \cap \mathcal{C}' \neq \emptyset|\} > x \cdot |S^{(\text{ad})}|$ then
5:         return 1.
6:     end if
7: end for
8: return 0.
```

Note that, while this simple heuristic appears natural, it requires in the worst case to test all subsets of size up to l to find one intersecting a large number of the active accounts. This can be overly expensive, so one may decide to simplify this procedure by simply testing the subset returned by a simple greedy dynamic, which may often be a good approximation.

```
Heuristic Greedy Detection-x Algorithm
Known parameters: $m$, maximum size $l$, probability $\alpha$.
Entries: a threshold parameter $x > \alpha$.
Result: 1 if the ad is targeted, 0 otherwise.
1: Create $m$ accounts, include each input independently with
   probability $\alpha$.
2: Construct the family $S^{(\text{ad})}$ containing all combinations of
   inputs in accounts seeing the ad.
3: $\mathcal{C}' = \emptyset$,
4: while $|\mathcal{C}'| < l$ do
5:     $\mathcal{C}' \leftarrow \mathcal{C}' \cup \text{argmax}_i \left|\{\mathcal{C} \in S^{(\text{ad})} | \mathcal{C} \cap (\mathcal{C}' \cup \{i\})\}\right|$
6:     if $|\{\mathcal{C} \in S^{(\text{ad})} | \mathcal{C} \cap \mathcal{C}' \neq \emptyset|\} > x \cdot |S^{(\text{ad})}|$ then
7:         return 1.
8:     end if
9: end while
10: return 0.
```

Finally, one may decide to build a simple identification algorithm which, instead of returning a simple binary value, actually returns the set $\mathcal{C}'$ that was found in this procedure. One can hope under some conditions (for instance, if the width of the targeting is known to be 1) that this procedure returns the correct core family of f.

However naive these procedures may seem, we prove later that under some conditions they are essentially correct. Moreover they can be used effectively as building blocks for exact identification in the general case. But before proving that formally, we first test them in a practical setting.

3.2 Report from a small scale experiment

We run two small scale experiments to gain experience and inform our model of online advertising and the presence of ad targeting leveraging multiple inputs. The full content of those preliminary experiments will be made available. For each experiment, we first manually created one *master* Gmail account a well as 100 other *shadow* Gmail accounts. Inputs in these experiments are emails, which are all included in the master account, and independently assigned to each shadow account with probability 1/2. In the first experiment, we used 20 emails on unrelated topics (*e.g.*, the purchase of a new car, TV, college applications). In the second experiment, after creating different accounts we used 50 emails, including 15 groups with 2,3 or 4 emails on the same topic (*e.g.*, two emails that are distinct but both relate to biking), and 12 separate unrelated emails. The outputs are ads shown to each account, collected by opening and refreshing multiple times each email.

To study targeting, we reproduced the state of the art Bayesian algorithm from [11] as well as a simple greedy algorithm. The former was previously designed and evaluated to accurately identify single input targeting. The latter is new and picks sequentially, among emails included in accounts seeing the ads, the email that is found in the most remaining number of accounts (this design is defined formally and analyzed later, see Section 4). In the latter, we conclude that targeting takes place when the fraction of accounts containing one email in the subset is sufficiently large. For simplicity we used here fixed thresholds: an ad is classified as targeted if either an email is found in at least 70% of the accounts with ads, or two emails are found so that either of them is included in at least 90% of those accounts. This last case in particular indicates that subset of two inputs are simultaneously targeted.

Our first experiment was a simple sanity check. Using the same ground truth as in [11], we consider 108 ads seen in at least 30 accounts including the master account, and found that for single input targeting, Bayesian has 95% precision and 86% recall, whereas the greedy algorithm finds 95% precision and 88% recall. As expected, emails are on unrelated topics, so considering subset of size 2 yields no specific improvement. In the second experiment, with more inputs and some overlap, results are quite different: Among 230 ads seen in at least 30 accounts including the master, we find that 81 (35%) are classified as targeted on a single input by Bayes, and are all found by the Greedy algorithm (by manually checking the content of the ads, as in previous ground truth, we found the vast majority of those, 85%, are correct classified). More interestingly, 79 ad (34%) are found *in addition* by the Greedy algorithm: another manual check based on the ad content proved that this classification is correct 70% of the time. We present some representative examples in Figure 1. Note that some multi-input targeting are direct consequences of the experiment design (*e.g.*, the left example with two emails with almost identical topic). This proves

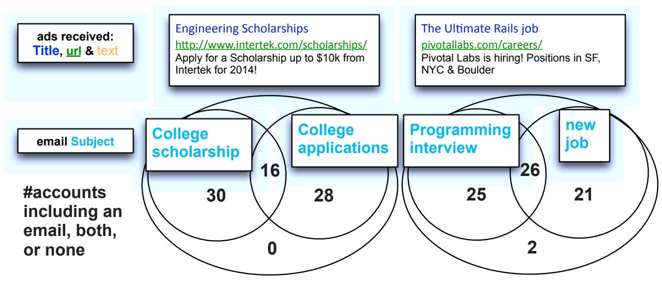

Fig. 1. Multi-input targeting in Exper. 2.

the limit of previous methods, since each email alone appears insufficient to explain targeting. Interestingly, some examples are less obvious (*e.g.*, the right example with subject "programming interview" and "new job" were not initially considered to be on the same topic, but happened to target similar ads). We believe this situation would be common in experiments with many emails. Note finally that, although we found quite a lot of multi-input targeting (at least 25% of the ads we analyzed), we cannot a priori conclude that this occurs with such frequency as it typically depends on many factors including the input sets. At best we can expect that it is not infrequent, and that our experience of exploiting simple heuristics can be made more systematic.

In this paper, motivated by this preliminary evidence, we wish to study the problem of multi-input targeting more formally. In particular, are heuristics like those we used above sound and complete to find this form of targeting when it takes place? Since multi-input targeting raises a combinatorial difficulty, how likely are the properties that make simple detection easy or hard? To answer those questions, we turn to a systematic mathematical analysis of a model reproducing the essential ingredients that we observed.

4 Proof of Correctness

Now that we found algorithms based on intersecting subsets to be intuitively justified, at least for detection, and practically useful, it remains to determine under which conditions those are rigourously correct. Moreover, beyond mere detection it remains to be shown that those test could be effectively used for exact identification. In this section, we do not only prove that, but also that this can be done while matching the computational lower bound of a linear number of operation.

4.1 Polynomial Targeting Detection

The first detection test we introduced runs naively using a polynomial number of operations to test for small subsets intersecting many active accounts. We first determine conditions under which it is provably correct.

Theorem 1. *Assuming $S^{(core)}$ has size at most l and width at most r, and $\frac{p_{out}}{p_{in}} < \varphi_{l,r}(\alpha) = \frac{\alpha^r}{1-\alpha^r}\frac{(1-\alpha)^l}{1-(1-\alpha)^l}$, then there exists $x > \alpha$ and $C > 0$ satisfying:*

For any $\varepsilon > 0$, if $m \geq C \cdot (\ln(N) + \ln(1/\varepsilon))$, Heuristic detection-x is correct with probability $(1 - \frac{\varepsilon}{N})$.

Proof. A subset of inputs $\mathcal{C}$ is an x_intersecting subset of a family S (for $0 \leq x \leq 1$) if at least a fraction x of the subsets in S intersect $\mathcal{C}$ (*i.e.*, each contains an input chosen in $\mathcal{C}$):

$$|\{\ \mathcal{S} \in S\ \mid \exists\, D_i \in \mathcal{C}, D_i \in \mathcal{S}\ \}| \geq x \cdot |S|\,.$$

Similarly, we say that S' is an x_intersecting family of a family S if at least a fraction x of the subsets contained in S contain a combination chosen in S':

$$\left|\left\{\ \mathcal{S} \in S\ \middle|\ \exists\, \mathcal{C} \in S', \mathcal{C} \subseteq \mathcal{S}\ \right\}\right| \geq x \cdot |S|\,.$$

If S' satisfies this property, one can chose for each combination of S' one given input in this combination. Those inputs together form an x_intersecting subset, proving:

Fact 1. *Let S' be an x_intersecting family of S, there exists $\mathcal{C}$ an x_intersecting subset of S with $|\mathcal{C}| \leq |S'|$.*

Given a particular advertisement an account is said active if it has received the advertisement during the experiment. We denote by $S^{(\mathrm{ad})}$ the active family that is built after considering all active accounts and adding for each of them the combination of its inputs to $S^{(\mathrm{ad})}$. Finally, as seen in the previous section, if an advertisement is targeted it admits a unique core family. We then denote it by $S^{(\mathrm{core})}$ and observe that it is never empty. By convention the case where the advertisement is non-targeted is denoted by $S^{(\mathrm{core})} = \emptyset$.

Our first preliminary result a property of random subsets and ensures that our test is *sound*, *i.e.*, it almost never returns targeting when it's not the case.

- A random Bernoulli subset, denoted by $B(N, \alpha)$, is a subset such that any of N elements is contained with probability α independently of all others.
- A random Bernoulli family of size m is a collection of m independent Bernouilli subsets.

Since Bernouilli subsets and families derive from many independent decisions to include or not a single element, we can use concentration inequalities on the distribution of sum of binary variables. Indeed such variable remains close to its expectation (*i.e.*, up to a constant multiplicative factor) except on an event of polynomially small probability. This holds as soon as its expectation is at least logarithmic and it implies:

Lemma 2. *Let $1 > x > 0$, $l \in \mathbb{N}$, $\alpha < 1-(1-x)^{\frac{1}{l}}$, and a Bernouilli family $B_1(N,\alpha), B_2(N,\alpha), \ldots, B_m(N,\alpha)$. There exists $C > 0$ such that for any $\varepsilon > 0$ and polynomial P, if $m \geq C \cdot (l\ln(N) + \ln P(N) + \ln(1/\varepsilon))$, then with probability $(1 - \varepsilon/P(N))$ no x_intersecting subset exists of size l for this Bernouilli family.*

Lemma 3. *Assume $x, \alpha > 0$, and $\frac{p_{out}}{p_{in}} < \frac{1-x}{x}\frac{\alpha^r}{1-\alpha^r}$, where no combination in the core family has width larger than r.*

There exists $C > 0$ such that for any $\varepsilon > 0$ and polynomial P, for any combination $\mathcal{C}$, whenever we have

$$m \geq \alpha^{-|\mathcal{C}|} \cdot C \cdot (\ln P(N) + \ln(1/\varepsilon))\,.$$

then with probability $(1 - \varepsilon/P(N))$ the following holds: among accounts containing $\mathcal{C}$ and seeing the ad, at least a fraction x of them is within the targeting scope $S^{(in)}$,

$$\text{i.e., } \frac{\left|\left\{\ \mathcal{S} \in S^{(ad,in)}\ \mid \mathcal{C} \subseteq \mathcal{S}\ \right\}\right|}{\left|\left\{\ \mathcal{S} \in S^{(ad)}\ \mid \mathcal{C} \subseteq \mathcal{S}\ \right\}\right|} \geq x\,,$$

where $S^{(in)}$ denotes the family of combinations $\mathcal{C}$ such that $f(\mathcal{C}) = 1$ and $S^{(ad,in)} = S^{(ad)} \cap S^{(in)}$.

As a consequence, we see that the targeting lift does affect the inputs found in $S^{(\mathrm{ad})}$ as it is responsible for a fraction of them. Under the condition of this lemma, since we saw that a 1_intersecting set exists for $S^{(\mathrm{ad,in})} = S^{(\mathrm{ad})} \cap S^{(\mathrm{in})}$ that is constructed using $S^{(\mathrm{core})}$, it is also an x_intersecting subset of $S^{(\mathrm{ad})}$.

Based on the above results, we can expect that with high probability two claims hold when m has order $O(\ln(N))$:

- **Soundness:** If targeting does not occur, *i.e.*, if we have $S^{(\mathrm{core})} = \emptyset$, then $S^{(\mathrm{ad})}$ has no x_intersecting subset of size l.
- **Completeness:** If targeting occurs, *i.e.*, if we have $S^{(\mathrm{core})} \neq \emptyset$, an x_intersecting subset for $S^{(\mathrm{ad})}$ of size $|S^{(\mathrm{core})}|$ exists.

However, it is important that we prove that the same value of x is used simultaneously for both claims, which is why a careful analysis is required.

In order to apply both claims for the same x, we need that $\alpha < 1 - (1-x)^{1/l}$ and $p_{\mathrm{out}}/p_{\mathrm{in}} < \frac{1-x}{x}\frac{\alpha^r}{1-\alpha^r}$

are verified. Fortunately it is easy to show that such x exists as soon as $\frac{p_{\text{out}}}{p_{\text{in}}} < \varphi_{l,r}(\alpha) = \frac{\alpha^r}{1-\alpha^r}\frac{(1-\alpha)^l}{1-(1-\alpha)^l}$ which completes the proof. □

4.2 Detection with Linear Cost

In this section, we prove that, under stricter condition on the ratio $p_{\text{out}}/p_{\text{in}}$, it is possible to prove the correctness of the approximate detection test that uses a greedy heuristic. This shows that targeting detection is feasible in linear cost. We first introduce

$$\hat{\varphi}^{(\text{gr})}_{l,r}(\alpha) = \frac{(1-\alpha)^l - \left(1-\frac{1}{l}\right)^l}{1-(1-\alpha)^l}\frac{\alpha^r}{1-\alpha^r}\,. \tag{1}$$

Theorem 2. *Assuming $S^{(core)}$ has size at most l and width at most r, and $\frac{p_{out}}{p_{in}} < \hat{\varphi}^{(gr)}_{l,r}(\alpha)$, then there exists $x > \alpha$ and $C > 0$ satisfying:*

For any $\varepsilon > 0$, if $m \geq C\cdot(\ln(N) + \ln(1/\varepsilon))$, Heuristic Greedy detection-x is correct with probability $(1-\frac{\varepsilon}{N})$.

Proof. Let us first formalize our greedy building block. For any family S, we introduce the function that counts for any combination $\mathcal{S}$ how many elements of S it intersects: $g^S : \mathcal{S} \mapsto \left|\left\{\ \mathcal{S}' \in S\ \middle|\ \mathcal{S}\cap\mathcal{S}' \neq \emptyset\ \right\}\right|$. Note that $\mathcal{S}$ is an x_intersecting subset if and only if $g^S(\mathcal{S}) \geq x\cdot|S|$. Our tests relate to maxima of g^S under constraints.

This function is submodular, non-decreasing, non-negative. Hence one way to find $\mathcal{S}$ maximizing its value is to follow an iterative greedy algorithm, starting with $\mathcal{S}_0 = \emptyset$ that constructs $\mathcal{S}_1,\ldots,\mathcal{S}_l$ as follows:

$$\mathcal{S}_{i+1} := \operatorname{argmax}\left\{\ g^S(\mathcal{S}')\ \middle|\ \mathcal{S}_i \subseteq \mathcal{S}', |\mathcal{S}'| = |\mathcal{S}_i| + 1\ \right\}.$$

Using standard argument on maximum of such submodular functions, one can show that for *any* subset $\mathcal{S}$ of size l, we have $g^S(\mathcal{S}_l) \geq (1-(1-\frac{1}{l})^{1/l})g^S(\mathcal{S})$. This immediately implies that if an x_intersecting subset is to exist (which we can show when targeting occurs with high probability), then the greedy heuristic necessarily returns an $(1-(1-\frac{1}{l})^{1/l})\cdot x$ intersecting subset.

Following the same argument as the proof of the detection test in the previous section, this implies that the greedy algorithm offers a detection test that asymptotically correct under a more restricted conditions on the value of $p_{\text{out}}/p_{\text{in}}$. □

Note that the condition in the theorem is stronger than $p_{\text{out}}/p_{\text{in}} < \varphi_{l,r}(\alpha)$ as we have for all $l > 1$:

$$\forall\alpha > 0\,,\ \frac{(1-\alpha)^l - \frac{1}{e}}{(1-\alpha)^l}\cdot\varphi_{l,r}(\alpha) < \hat{\varphi}^{(\text{gr})}_{l,r}(\alpha) < \varphi_{l,r}(\alpha)\,. \tag{2}$$

This implies (see §5) that some targeting found by the exact exhaustive algorithm is missed by the greedy version.

4.3 From Detection to Identification

Here we show rigorously that the previous heuristic of intersecting subsets can be leveraged to provide exact identification of the targeting function.

Theorem 3. *Assuming $S^{(core)}$ has size at most l and width at most r, and $\frac{p_{out}}{p_{in}} < \varphi_{l,r}(\alpha)$, then there exists $x > \alpha$ and $C > 0$ satisfying:*

For any $\varepsilon > 0$, if $m \geq C\cdot(\ln(N) + \ln(1/\varepsilon))$, an identification algorithm using no more than $O(N^{l+r}\ln(N))$ operations is correct with probability $(1-\frac{\varepsilon}{N})$.

We prove this result in the rest of this section. Relating back to the requirements formulated for web transparency tools in, our results show that targeting on bounded-size combinations can be detected and identified *accurately* with very few resources (*scalably*). Our entire formalism is kept on purpose generic and its treatment of noisy combined targeting makes it more *broadly applicable* than prior systems.

Previously in this section, we designed a provably approximately correct *targeting detection* test that produces a provable certificate: an x_intersecting subset obtained under specific conditions. To go beyond mere detection, one would like to identify exactly *which* inputs are being targeted, a much more difficult task. Those are *a priori* related to inputs found in the intersecting subset. However, this intersecting subset is not unique, it may contain only a subset on relevant inputs of the core family.

Key observation: How targeting behaves "beyond" some combination We first answer to the following key question: For a combination $\mathcal{C}$, what can be said about the set of accounts that contain it and those among them that are active, $\{\mathcal{S} \in S^{(\text{ad})} \mid \mathcal{C} \subseteq \mathcal{S}\}$? By definition, all of those subsets contain all inputs in $\mathcal{C}$ so we are interested in understanding how other inputs affect them. This is where exactly two cases emerge: Firstly, if we assume that $\mathcal{C}$ does contain a combination of the core, it automatically implies that independently of any other inputs, they all receive the ad with the same probability. Secondly, if we assume on the other hand the opposite, then among all accounts including $\mathcal{C}$, there will be specific sets of inputs that may complete a combination from the core family and hence be targeted more heavily than others. This latter case resembles the situation of a targeting lift which can be detected. The former case resembles a situation where ads appear randomly. We can therefore design a new test as follows, that is sound and complete to determine in which case we are.

Definitions and main building block We remind that we denote $S^{(\text{in})}$ the set of combinations $\mathcal{C}$ that satisfy $f(\mathcal{C}) = 1$. One can observe these are all supersets of combinations in the core family $S^{(\text{core})}$. Our test will determine whether a given combination $\mathcal{C}$ belongs to this family. Indeed, we now show how to leverage the above observations to determine whether $\mathcal{C} \in S^{(\text{in})}$ using intersecting subsets. As it will be useful later to generalize this test to apply to intersecting subsets of smaller size $k \leq l$, we directly write the most general case. Note that this requires a new condition:

$$\hat{\varphi}^{(k)}_{l,r}(\alpha) = \frac{1 - \frac{l}{k}(1-(1-\alpha)^l)}{\frac{l}{k}(1-(1-\alpha)^l)} \frac{(1-(1-\alpha)^{l/k})^r}{1-(1-(1-\alpha)^{l/k})^r} \,. \tag{3}$$

When k is chosen equal to l, this condition is equivalent to previous one as the one above. The case where $k < l$, also proved here, will be of importance to design a linear identification algorithms in the next section.

We introduce the following key proposition

Proposition 1. *Assuming $S^{(core)}$ has size at most l and width at most r, $\frac{p_{out}}{p_{in}} < \hat{\varphi}^{(k)}_{l,r}(\alpha)$, for $k \leq l$, then there are $x, C > 0$ satisfying:*

For any $\varepsilon > 0$, polynomial P, and combination $\mathcal{C}$, when $m \geq \alpha^{-|\mathcal{C}|} \cdot C \cdot (\ln(N) + \ln P(N) + \ln(1/\varepsilon))$, then with probability $(1-\varepsilon/P(N))$ exactly <u>one</u> of the following claims holds:

(i) $\mathcal{C}$ contains a core combination, i.e., *it is in $S^{(in)}$.*

(ii) an x_intersecting subset of size k exists for

$$\Delta^{(ad)}(\mathcal{C}) = \left\{ \mathcal{S} \cap \overline{\mathcal{C}} \;\middle|\; \mathcal{S} \in S^{(ad)}, \mathcal{C} \subseteq \mathcal{S} \right\}.$$

Identification using exhaustive local search Assume we are equipped with the test of Prop 1 and that the targeting function to detect has width at most r. A first (costly) algorithm to compute the core family searchs for the results of all tests and in the worst case it examines all the $O(N^r)$ possible combinations.

This algorithm maintains a current core $S^{(\text{core})}$ that is initially empty. At each step $i \geq 1$ it considers all combinations of size i that are not strict supersets of a combination already found in $S^{(\text{core})}$. In particular, note that it considers all the possible N singletons for $i = 1$. For each combination $\mathcal{C}$ considered at step i (*i.e.*, $|\mathcal{C}| = i$), we apply to $\mathcal{C}$ the recognition test from Prop 1 (using $k = l$). If $\mathcal{C} \in S^{(\text{in})}$, then $\mathcal{C}$ is indeed in the core of the function by inclusion wise minimality and so, we put the combination in $S^{(\text{core})}$. Otherwise we drop it. When the algorithm stops after r steps, all core combinations have been necessarily identified.

Some final remarks are required to prove the correctness of the above algorithm: First, to perform the recognition test of Prop 1 (using $k = l$), we need a bound on the size of $S^{(\text{core})}$ and that the bound on the targeting lift is satisfied. We also need to observe that, since all tested combinations have width at most r, the value of $\alpha^{-|\mathcal{C}|}$ that appears in the bound for m indeed remains bounded. Finally, since we conduct $O(N^r)$ tests, we need to ensure that *none* of them fail. Using the fact that by choosing C large enough, Prop 1 holds for any polynomial P, we can choose $P(N) = N^r$ and applies the union bound to all tests. As a final remark, since each test boils down to identifying an intersecting subset of size l among m accounts, it uses at most $O(N^l m) = O(N^l \ln(N))$ operations so, the total number of operations in the algorithm is $O(N^{l+r} \ln(N))$.

4.4 Identification with linear cost

Getting rid of the exhaustive local search step in the identification of the targeting function is much more difficult. This requires each test to be computationally cheaper and more importantly to conduct a much smaller number of them. However, surprisingly, it can be done using more properties of intersecting subsets and a significantly more elaborate algorithm.

The gist: getting more from each test Given $\mathcal{C}$, §3 presents a test to determine if it belongs to the target $S^{(\text{in})}$, but more importantly if this answer is negative it produces a certificate which is an x_intersecting subset, or even the family of all such subsets. We first extract more information from this output.

Lemma 4. *Assuming $S^{(core)}$ has size at most l and width at most r, that $k \leq l$ and $\frac{p_{out}}{p_{in}} < \sup_{\alpha \in]0;\frac{k}{l}[} \hat{\varphi}^{(k)}_{l,r}(\alpha)$, then there are $x, \alpha, C > 0$ satisfying:*

For any $\varepsilon > 0$, polynomial P, and combination $\mathcal{C}$, when $m \geq \alpha^{-|\mathcal{C}|} \cdot C \cdot (\ln(N) + \ln P(N) + \ln(1/\varepsilon))$, then with probability $(1 - \varepsilon/P(N))$ the following two claims hold:

(i) All combinations in $S_{x,k}$ intersect $\bigcup_{\mathcal{S} \in S^{(core)}} \mathcal{S}$.

(ii) $\mathcal{C} \cup \bigcup_{\mathcal{S} \in S_{x,k}} \mathcal{S}$ is empty or contains a core comb.

$$S_{x,k} = \left\{ \mathcal{S} \;\middle|\; \mathcal{S}\ \ x\_\text{intersecting for}\ \ \Delta^{(ad)}\left(\mathcal{C}\right), |\mathcal{S}| \le k \right\}.$$

For the rest of this section, we will apply this lemma with $k = 1$; it then has a quasi-linear cost. Under this condition there is targeting if, and only if, there is an x_intersecting subset of size 1. Fact (i) above implies that all such x_intersecting subsets are included in $\bigcup_{\mathcal{S}\in S^{(\text{core})}} \mathcal{S}$, hence we have at most lr of them.

A recursive identification test using eliminations. It seems *a priori* promising to operate by elimination for the following reason: assuming $\mathcal{C}$ contains a core combination, we can remove elements from $\mathcal{C}$ one by one and only keep those whose removal changes the outcome of the test from Prop. 1. By inclusion wise minimality, the resulting combination belongs to the core family. Applying Lemma 4 to the empty combination provides a first detection test of targeting (*i.e.*, if this one fails, the algorithm returns $S^{(\text{core})} = \emptyset$) and a superset of a core combination (Line 1). By the elimination process aforementioned, we obtain a core combination (Line 3-7). We then recursively apply the same algorithm to multiple scenarios where we carefully remove exactly one input from the first combination (Line 9-12). This ensures that future combinations obtained by the same methods are different.

`Generalized-Set-Intersection(GSI)` Algorithm

Entries: a family $S^{(\text{ad})}$; and a threshold parameter x.
Result: The core-explaining family $S^{(\text{core})}$.

```
 1: $S^{(\text{core})} \leftarrow \{\}$; $\mathcal{S} \leftarrow \{D_i \mid \frac{|\{A_j \in S^{(\text{ad})} | D_i \in A_j\}|}{|S^{(\text{ad})}|} \ge x\}$;
 2: if $\mathcal{S} \neq \emptyset$ then
 3:     for all $D_i \in \mathcal{S}$, $\hat{S} = S \setminus D_i$ do
 4:         if $\{D_i' \notin \hat{S} \mid \frac{|\{A_j \in S^{(\text{ad})} | \hat{S} \cup \{D_i'\} \subseteq A_j\}|}{|\{A_j \in S^{(\text{ad})} | \hat{S} \subseteq A_j\}|} \ge x\} = \emptyset$ then
 5:             $\mathcal{S} \leftarrow \mathcal{S} \setminus D_i$.
 6:         end if
 7:     end for
 8:     $S^{(\text{core})} \leftarrow S^{(\text{core})} \cup \{\mathcal{S}\}$.
 9:     for all $D_i \in \mathcal{S}$ do
10:         $S_i \leftarrow \texttt{GSI}(S^{(\text{ad})} \setminus \{A_j \mid D_i \in A_j\}, x)$.
11:         $S^{(\text{core})} \leftarrow S^{(\text{core})} \cup S_i$.
12:     end for
13: end if
```

Proposition 2. *Assume $S^{(core)}$ has size at most l and width at most r, and $\frac{p_{out}}{p_{in}} < \frac{1-lx}{l}\frac{x^{r-1}}{1-x^r}$, for some $0 < x < 1/l$.*

There exist α, C satisfying $\forall \varepsilon > 0$, for all polynomial P, whenever $m \ge C \cdot (\ln P(N) + \ln \frac{1}{\varepsilon})$, the GSI algorithm identifies the core family with probability $1 - \varepsilon/P(N)$

Analysis of complexity It is straightforward to prove that `GSI` terminates, because the number of data inputs decreases at each recursive call to the algorithm. To upper-bound its time complexity in the worst-case, we introduce the so-called "relevant set" $\mathcal{I}$. Its definition is inductive, following the trace of some execution of the algorithm. Namely, let $\mathcal{S}$ be the union of all x_intersecting subsets of size 1. If $\mathcal{S} = \emptyset$, then we set $\mathcal{I} = \emptyset$. Else, for each recursive call $\texttt{GSI}(\mathcal{A} \setminus \{A_j \mid D_i \in A_j\}, x)$ of the algorithm, we name $\mathcal{I}_i$ its relevant set and we set $\mathcal{I} = \mathcal{C} \cup \left(\bigcup_i \mathcal{I}_i\right)$. Note that we have by construction $\forall i, |\mathcal{I}_i| \le |\mathcal{I}| - 1$.

We state below (proof omitted) that `GSI` is Fixed-Parameter Tractable (FPT) when the size $|\mathcal{I}|$ of the relevant set is fixed.

Lemma 5. *GSI can be implemented to run in a time bounded by $O\left(|\mathcal{I}|! \cdot N \cdot |S^{(ad)}|\right)$.*

Proposition 3. *Under the assumptions of Prop. 2 GSI terminates in $O((lr)! \cdot Nm)$-time with probability $1 - \varepsilon/P(N)$.*

5 Impact of Targeting Lift

5.1 Targeting lift defines in theory a limit to web transparency

As seen above, the tests we design can dramatically expand the scope of web transparency tools. We proved that observations from inputs and outputs can reveal how a targeting function affects what is shown to a population based on combination of multiple inputs. Since the ability to discriminate using such functions is fundamental to Big Data, and since our tests made minimal assumptions, our results can be readily used in many more applications to come beyond ad-targeting, our primary motivation.

This poses an important question: Is there a fundamental limit to web transparency? That would be a situation in which all tests so far fail no matter how parameters such as x, α and C are chosen. We show it is the case, and we compute the exact conditions under which all known tests fail. We also measure the detection power of other simpler tests to understand how they affect those limitations.

We showed tests always exists to successfully detect and identify a targeting of size l and order r such that

$$\frac{p_{\text{out}}}{p_{\text{in}}} \le \sup_{\alpha\in]0;1[} \varphi_{l,r}(\alpha) = \sup_{\alpha\in]0;1[} \frac{\alpha^r}{1-\alpha^r}\frac{(1-\alpha)^l}{1-(1-\alpha)^l}\,.$$

This condition leads to a closed form.

Lemma 6. *Let $M_{l,r} = \sup_{\alpha\in]0;1[}\varphi_{l,r}(\alpha)$, we have*

$$\begin{cases} \text{if } \ l=1, & M_{1,r} = 1/r\,, \\ \text{if } \ r=1, & M_{l,1} = 1/l\,, \\ \text{for all } \ r,l, & \frac{1}{(2^{\max(l,r)}-1)^2} \le M_{l,r} \le \frac{1}{(2^{\min(l,r)}-1)^2}\,, \\ \text{for all } \ r,l, & M_{l,r} = M_{r,l}\,, \\ \text{if } \ r=l=n, & M_{n,n} = 1/(2^n-1)^2\,. \end{cases}$$

If $r>1, l>1$, $M_{l,r} = \dfrac{(\alpha^*)^r}{1-(\alpha^*)^r}\dfrac{(1-\alpha^*)^l}{1-(1-\alpha^*)^l}$ where α^* is the only solution in $]0;1[$ of

$$r\alpha^{r+1} - l(1-\alpha)^{l+1} - (r+l)\alpha + r = 0\,.$$

Consequence on the concealment of targeting From our analysis important observations arise: First, when a single input is used for targeting *i.e.*, $l=1, r=1$, we have $M_{l,r}=1$ and the condition above is always verified except for the trivial case where $p_{\text{out}} = p_{\text{in}}$, impossible by definition. This confirms that *single input targeting never can stay hidden from all transparency tests*. However, all other forms of targeting that leverage multiple inputs stand sharply in contrast. Indeed any function whose core family is not a single input exhibits a non-trivial *undetected targeting lift*: it can in practice discriminate users to some extent without being detected by any of the tests known. Note that, in practice, a web transparency tool can restrict itself to test a few assumptions on carefully selected inputs, and it may in some cases detect their use, but it becomes a very different task as no method is shown to work *in general.*

It is particularly informative to see how this *undetected targeting lift* grows with the complexity of the formula used. Figure 2 presents the value of the function $\varphi_{l,r}$ that defines it (it is drawn up to a change of variable to make it easier to read). As proved in the lemma and shown in the Figure, if the targeting solely uses disjunction (resp. conjunction) of inputs, *i.e.*, $r=1$ (resp. $l=1$) as shown in Figure 2 (left), the targeting lift behaves as $1/l$ and hence it is polynomial. This polynomial expansion remains if l grows while r remains small. The proof is omitted but Figure 2 (middle) presents an example. In contrast, when l and r grow simultaneously, *e.g.*, if they are equal as shown in Figure 2 (right) one can show that targeting lift can be *exponential* and *undetected.* While this demonstrate the hardness of web-transparency, we note that such forms of complex targeting combining so many inputs to decide may be relatively rare in practice.

Limits of web transparency for simpler tests We present in Figure 3 along with other conditions the condition that allows our linear identification algorithm to be correct, *i.e.*, $\hat{\varphi}^{(k)}_{l,r}$ with $k=1$,for the case $l=r=2$. It illustrates some important observations: First, the conditions to apply the linear identification algorithm are more restricted (In this case, the targeting lift must be approximately 10 times larger). This points to another qualitative interesting insight: There exist instances of targeting for which a linear algorithm may be able to detect them without necessarily being able to completely identify them.

5.2 Simulations Targeting lift in large scale systems

Synthetic Experiments Both the Bayesian algorithm from [11] and the greedy algorithms here have several parameters upon which the accuracy of their predictions depends. While the XRay paper presents sufficient conditions for the success of the bayesian algorithm, the performance of the algorithm outside these conditions is not well understood. For the greedy algorithm, no such conditions are known. While there are known optimization methods for computing the ideal parameters for these algorithms, these methods rely critically on the availability of ground-truth data. For many important systems, this data is unlikely to ever be made available to anybody outside the proprietor. Thus, in the interest of measuring the boundaries and limiting conditions for these algorithms, as well as determining their efficacy beyond the theoretical guarantees provided in their definitions, we have measured their accuracy through a series of experiments that simulate our model of online interactions. These findings are intended to provide guidelines for what can and cannot be done, and to inform on the cost associated to particular endeavors.

Experimental Setup We will analyze four algorithms. The *Exhaustive Detection Algorithm*, the *Exhaustive Identification Algorithm*, and a pair of *Greedy Detection/Identifcation Algorithms.* The core components of the exhaustive algorithms are Proposition 1 and Proposition 2 from [11] respectively. All of these algorithms can roughly be divided into a *collection phase* and a *computation phase.*

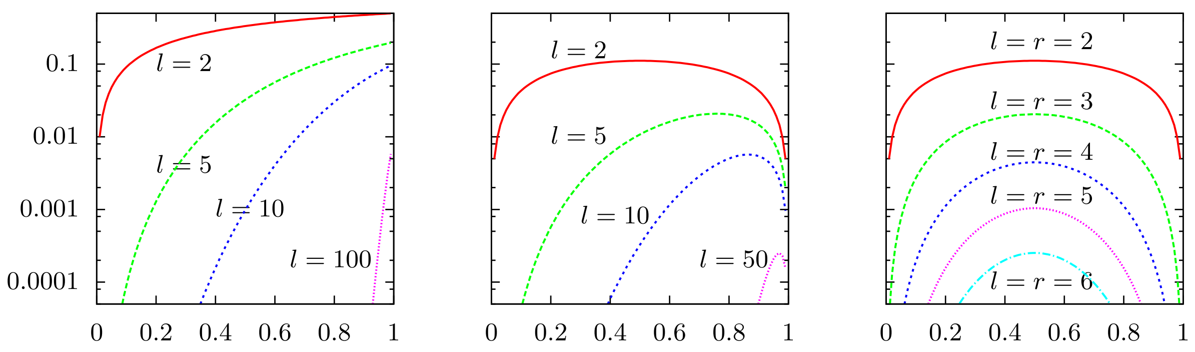

Fig. 2. Value of $\varphi_{l,r}$ as a function of $1 - \alpha$ for $r = 1$ (left), $r = 2$ (middle) and $r = l$ (right).

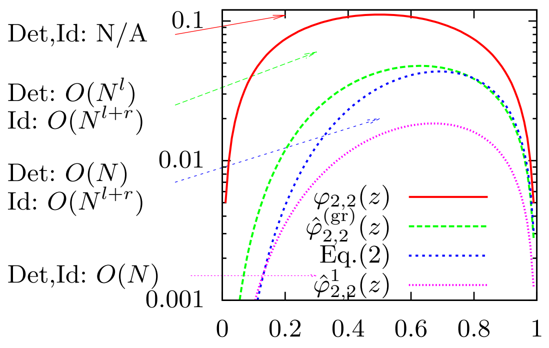

Fig. 3. Comparing the detection/identification region of various algorithms for $l = r = 2$.

During the collection phase, we take a pool of N emails and create m accounts. Each account contains each email with independent probability α. These accounts are then exposed to the targeting system and allowed to collect ads. In lieu of an actual targeting system, our synthetic experiments simulate the ad-targeting algorithm with a boolean stochastic targeting function T_C. This function has an underlying core family C. In the noiseless case, $T_C(A)$ is true if and only if A matches C. In order to simulate untargeted ads, we have a special function $T_\emptyset$ which randomly targets an account with fixed probability β. For our synthetic experiments, we have used $\beta = 0.5$.

During the computation phase, our algorithm no longer has access to T_C, and only sees body of ads which have been targeted by T_C. This mirrors the state of available information that is available to the researcher when attempting to test the targeting properties of a particular system. In this phase, an identification algorithm is required to produce a core family C' that matches C with high probability. For detection, we are merely required to produce a bit which matches, with high probability, the truth value of "$C \neq \emptyset$".

Our model admits two noise rates, each affecting the negative and positive instances of T_C, respectively. If A matches C, then $T_C(A)$ will be positive with probability p_{in}, otherwise, $T_C(A)$ will be positive with probability p_{out}. We will generally be interested in *symmetric noise*, where there is a certain noise value η, such that $p_{out} = \eta$ and $p_{in} = 1 - \eta$. For this type of noise, the *targeting lift* τ is given by $\tau = p_{out}/p_{in} = \eta/(1 - \eta)$.

To measure the success of an algorithm, we independently evaluate its performance in both targeted and untargeted scenarios, producing measures for targeted accuracy a_t and untargeted accuracy a_u. In any application, the actual accuracy of the algorithm will be given by $a_{real} = pa_t + (1 - p)a_u$, where p is the prevalence of targeted ads. However, since this parameter p is unknown to us a priori, and indeed may differ for each ad, we will assume it is chosen by an adversary who wishes to minimize our total accuracy. This provides us with a unified accuracy measure which we call min-accuracy a_m, which provides a lower bound for a_{real} and is equivalent to $a_m = \min\{a_t, a_u\}$.

For each algorithm under consideration, our primary interest is to find the maximum value of τ that can be tolerated, such that with a proper setting of the other parameters, we can still achieve a min-accuracy of 99%. We know that the optimal value for α is the one that guarantees $P[T_C(A)] = 0.5$ over a random choice of A. With sufficient information about the targeting function, this value can be determined algebraically. The proper value for x can then be found through a simple optimization procedure. First note that for all algorithms under consideration, a_t is monotonically decreasing in x, while a_u is monotonically increasing with x. Further note that a_u is totally independent of τ, while a_t is monotonically decreasing in τ Thus, it suffices to find the smallest value of x such that $a_u > 99\%$ when $\tau = 0$, which can be achieved via binary search. We may then use this value of x and find the maximum value of τ that will still guarantee $a_t > 99\%$, also via binary search. Per our prior observations, we know that this combination of α, x and τ will achieve $a_m > 99\%$.

Experimental Results

In Fig. 4(left) we may observe that the greedy algorithm is noise-tolerant, even for relatively high levels of τ. Noise-tolerance decays almost linearly, even as N increases exponentially, indicating a logarithmic dependence on N. Furthermore, we may note that while for $L = 1$ the difficulty of identification and detection are comparable, as L increases the cost of precise identification of the targeting function becomes steeper, and the decrease in noise-tolerance for increasing values of N is more pronounced. This suggests for very complex targeting, only detection is possible when noise levels are expected to be high and accounts are limited or the inputs under consideration are abundant.

Given the high cost associated with obtaining new accounts, and the deliberate barriers placed by content providers on automation of this task, the number of available accounts is often the limiting reagent in targeting inversion problems. Observing Fig. 4(middle), we note that accuracy can be boosted significantly by allowing ourselves access to a greater number of accounts. This allows the greedy algorithm to attain a noise-tolerance level much greater than the theoretical bound. Moreover, as we can see in Fig. 4(right), the greedy algorithm can very nearly approximate the noise tolerance of the optimal exhaustive search procedure.

These results highlight the importance of the greedy algorithm, which can be seen as applying the well-known greedy heuristic to solve a version of the optimal set cover problem. In particular, the algorithm achieves high noise-tolerance, approximates the exhaustive algorithm when l and r are small, and reduces the computations from an polynomial function using l and r to a linear one. For extremely large values of N, such as those often encountered in practice, the greedy algorithm is the only computationally tractable option.

5.3 An application: The price of opacity

We specified the theoretical limits to targeting detection. However, to complete the picture one must wonder whether it is economically feasible for an advertiser to conceal her targeting. To answer this question, we introduce a simplistic ad purchase model, in which the advertiser has to pay a fixed cost $C > 0$ for every account receiving the ad and she gains on average a fixed positive revenue $R > C$ for each active account *within her scope* which encompasses a fraction q of the users. We assume that through various bids, this advertiser controls the values of $p_{\text{in}}, p_{\text{out}}$ that users experience.

In case the advertiser is fully transparent, she can minimize the cost of her targeting campaign simply by setting p_{out} to 0. She would then potentially earn $p_{\text{in}} q(R - C)$ during that campaign. However, if she wishes to keep her advertising method concealed from transparency tools, she needs to increase p_{out} at least to $p_{\text{in}} \cdot M_{l,r}$. We immediately deduce that her cost increases by $p_{\text{out}}(1 - q)C = p_{\text{in}} \cdot M_{l,r}(1 - q)C$. It is hence multiplied by a factor $(1 + M_{l,r}\frac{1-q}{q})$, which denotes the *Price of Opacity*. As an example, for $l = 2, r = 2$ and $q = 0.05$, an advertiser already spent *three times* more on advertising just to avoid detection, and this price is particularly damaging when the target is small. To remain opaque she loses at least a fraction $\frac{1-q}{q}\frac{C}{R-C} \cdot M_{l,r}$ of her revenue. A necessary condition for the advertiser to remain profitable is that $\frac{1-q}{q}\frac{C}{R-C} \cdot M_{l,r} < 1$. Note that, with the exception of l and r, these parameters are not set by the advertisers.

In face of the above result, an advertiser might be tempted to decrease her targeting scope artifically so that a small value of p_{out} is enough to avoid detection. Formally, such an attack consists in replacing the core family of her targeting function by another one with larger dimensions $l' > l, r' > r$. Our preliminary analysis (omitted due to lack of space) shows that the decrease in p_{out} is offset by the opportunity loss of being too restricted in the definition of the target. It can quickly become economically unviable, especially when fixed costs are present. The analysis of this attack and how to best cope with it remains beyond the scope of our work.

6 Related Work

Our formulation resembles identification of monotone DNF formulae from an oracle (*e.g.*, see [2, 3, 19]) and more generally the theory of formal learning. However, it is quite distinct for three main reasons: First, and most importantly, we only care about *proper exact learning*, by which an algorithm is required not to produce an function closely approximating the monotone formula (as in [5, 19]), but to compute an exact representation of the formula itself. Second, previous proper exact learning techniques make adaptive queries [2, 3], which is impractical as typically web transparency in-

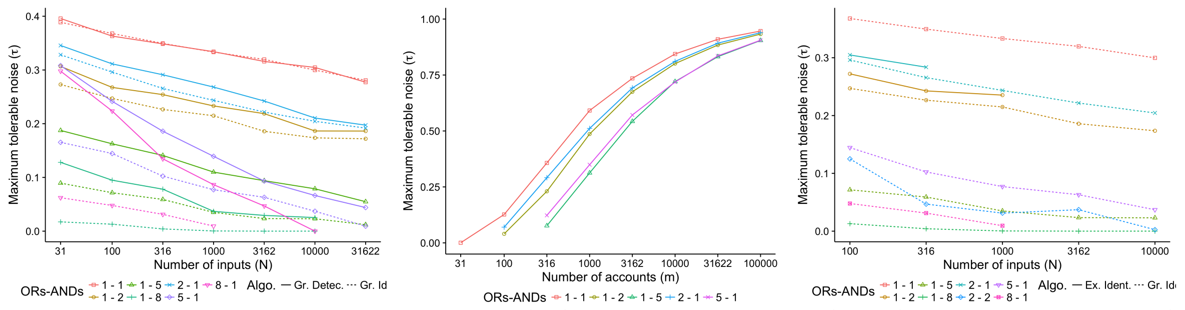

Fig. 4. Greedy Algorithms: Identification vs. Detection (left) using increasing accounts (middle) compares with exhaustive (right).

volves a large data collection that take significant time. Our algorithm in contrast makes non-adaptive queries: the set of combination to test is fixed and data are collected prior to any steps of the algorithm. Finally, since each query is resource intensive, we require the number of queries to grows as a logarithm of the number of variables. We are not aware of any previous algorithm – or extension of previously known techniques – that can fit all of these stringent conditions.

Another parameter of learning model often introduced is the VC dimension. However, in the case we study, it grows linearly[2] with N. This makes such algorithms impractical in this case.

Our work relates to recent efforts to measure various forms of personalization [7, 15, 20, 22]. They aim to quantify *how much* output is personalized and what *type* of information is used overall. In contrast, we seek to analyze fine-grained diagnosis of which combinations of *data inputs* generate which personalized results. Our analyses of scaling properties and tradeoffs are unique in the personalization literature.

Closest to our work are XRay [11] and AdFisher [6] – to our knowledge the very first two systems that fit in the emerging vision of data use transparency (described in Section 2). XRay aims to meet all the scalability, accuracy, and broad applicability requirements of web transparency, however the tool it currently provides lacks support for combinations – uniquely addressed in this paper through three new algorithms. We hope this can remove a critical roadblock to achieving any or all of these properties in practice. AdFisher aims to meet the accuracy and in some respect the broad applicability requirements, but does not consider scaling as a core requirement. This paper uniquely considers the theoretical underpinnings of tools that aim to support all three requirements at once. We believe that support for linear combinations of inputs is a crucial step toward achieving those requirements.

7 Conclusion

Web transparency – a nascent and critical field to deploy big data while protecting us against its abuse – poses brand new challenge to the analysis of personalization algorithms. By providing the first theoretical analysis of web transparency for general targeting functions, and the promise of simple random algorithms, we show that web transparency can indeed be successful at scale. However, our research clearly indicates that transparency will also be governed by theoretical limits of detection and inherent tradeoffs.

We believe that our results create many opportunities for further research at the frontier of stochastic models, distributed systems, and algorithms handling personal data. Beyond understanding how to design efficient personalization algorithms, one hopes in addition to decipher their operations from the outside using the minimum number of information and operations available. Our works suggest many open problems that this field will grow to encompass, such as new methods to improve detection when other conditions are satisfied by the targeting functions, a careful analysis of computational lower-bounds that could leverage information theory, or new algorithms achieving better tradeoffs.

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2 Indeed, if the targeting only depends on at most k inputs, then it is easy to prove that the $N - k$ inputs of which the function f does not depend on form a set that is shattered by the function. Hence the VC dimension of f is at least $N - k$ in such case

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8 Proofs

8.1 Proof of Lemma 1

Lemma 1. We define $S^{(\text{in})}$ the set of all combinations for which f takes value 1. Let $\overrightarrow{D}_f$ be the digraph with vertex-set $S^{(\text{in})}$ and with arc-set $\left\{ (\mathcal{C}, \mathcal{C}') \;\middle|\; \mathcal{C} \subsetneq \mathcal{C}' \right\}$. We have that $\overrightarrow{D}_f$ is a DAG because the subset-containment relation defines a partial order. So, let S be the non-empty set of combinations with null in-degree in $\overrightarrow{D}_f$. By construction, each combination in $S^{(\text{in})}$ contains some combination of S and $S \subseteq S^{(\text{in})}$, hence S explains f. Furthermore, we claim that S is contained in *any* family S' explaining f: indeed, since S' is required to contain a subset of any combination $\mathcal{C} \in S$, and no combination of $S^{(\text{in})}$ is strictly contained in $\mathcal{C}$, then it must contain $\mathcal{C}$. This shows that S satisfies all conditions of Lemma 1. Finally, since another family explaining f needs to include S, then it will necessarily have a higher size l, hence S is the unique with both minimum size and order. □

8.2 Chernoff bound

Lemma 7. *If Y is a sum of independent binary variables, let $\mu = E\left[Y\right]$, we have for any $0 < \delta \leq 1$:*

$$P\left[Y \geq (1+\delta)\mu\right] \leq \exp\left(-\frac{\delta^2\mu}{3}\right) \quad \text{, and}$$
$$P\left[Y \leq (1-\delta)\mu\right] \leq \exp\left(-\frac{\delta^2\mu}{2}\right)$$

Thus, for any polynomial P, integer N and value $\varepsilon > 0$,

$$\mu \geq \frac{3}{\delta^2} \ln\left(\frac{2P(N)}{\varepsilon}\right) \implies P\left[|Y-\mu| \leq \delta\mu\right] \geq 1 - \frac{\varepsilon}{P(N)}.$$

8.3 Proof of Lemma 2

Lemma 2. Let us consider an arbitrary combination $\mathcal{C}$ of size l. We introduce Y the variable counting how many Bernouilli subsets $\mathcal{C}$ intersects, and we note that $\mathcal{C}$ is an x_intersecting subset exactly if $Y \geq xm$. We also observe that Y is a sum of binary independent variables and so, since the probability that $\mathcal{C}$ intersects an arbitrary Bernouilli subset is $1-(1-\alpha)^l$, it has expectation $\mu = \left(1-(1-\alpha)^l\right)m$. Assuming $\alpha < 1-(1-x)^{\frac{1}{l}}$ as we do, μ is multiplicatively smaller than xm. Hence we can apply Chernoff Bound to conclude that $P\left[Y \geq xm\right] \leq \frac{\varepsilon}{P(N)N^l}$ when

$$m \geq C \cdot \ln\left(N^l P(N)/\varepsilon\right) \text{ with } C = \frac{3\left(1-(1-\alpha)^l\right)}{\left(x - \left(1-(1-\alpha)^l\right)\right)^2}.$$

Since there are $\binom{N}{l} \leq N^l$ choices of $\mathcal{C}$, by the union bound the probability that at least one of them is an x_intersecting subset is at most $\frac{\varepsilon}{P(N)}$. □

8.4 Proof of Lemma 3

Lemma 3. We introduce the set of inputs associated with each account $\mathcal{S}_1 = B_1(N,\alpha), \ldots, \mathcal{S}_m = B_m(N,\alpha)$, and for each of them we define Y_j a variable with the following value:

$$\begin{cases} 1 & \text{if } \mathcal{S}_j \text{ is in target, sees the ad, and } \mathcal{C} \subseteq \mathcal{S}_j, \\ -\frac{x}{1-x} & \text{if } \mathcal{S}_j \text{ not in target, sees the ad, and } \mathcal{C} \subseteq \mathcal{S}_j, \\ 0 & \text{otherwise} \end{cases}$$

We introduce $Y = \sum_{j=1}^{m} Y_j$, it is a sum of binary independent variables. We also note that the property of the theorem holds exactly if $Y \geq 0$. It is then sufficient to prove that this occurs with high probability.

First by the linearity of expectation we have that:

$$\begin{aligned} \mathbb{E}[Y] &= \sum_{j=1}^{m} \left(\alpha^{|\mathcal{C}|} q_{\mathcal{C}} p_{in} - \frac{x}{1-x}\alpha^{|\mathcal{C}|}\left(1-q_{\mathcal{C}}\right)p_{out}\right) \\ &= \left(q_{\mathcal{C}} p_{in} - \frac{x}{1-x}\left(1-q_{\mathcal{C}}\right)p_{out}\right)\alpha^{|\mathcal{C}|} m, \end{aligned}$$

where $q_{\mathcal{C}}$ denotes the probability for an account to be within scope knowing that it contains $\mathcal{C}$. This expectation is positive as long as it holds that $p_{\text{out}}/p_{\text{in}} < \frac{1-x}{x}\frac{q_{\mathcal{C}}}{1-q_{\mathcal{C}}}$. Moreover, the above upper-bound is monotonically increasing with $q_{\mathcal{C}}$, which is at least α^r because it suffices to complete $\mathcal{C}$ with any combination of the core to be within scope. As a result, it always holds that $E[Y] > 0$ (with respect to our assumption about the ratio $p_{\text{out}}/p_{\text{in}}$ for the lemma).

Hence $P\left[Y \geq 0\right] \geq 1 - \frac{\varepsilon}{P(N)}$ whenever $m \geq \alpha^{-|\mathcal{C}|} \cdot C \cdot \ln\left(P(N)/\varepsilon\right)$ with $C \leq \frac{2}{\alpha^r p_{\text{in}}}\left(1 - \frac{x}{1-x}\frac{1-\alpha^r}{\alpha^r}\frac{p_{\text{out}}}{p_{\text{in}}}\right)^{-1}$. □

8.5 Proof of Proposition 1

Proposition 1. Pick α so that $\frac{p_{\text{out}}}{p_{\text{in}}} < \hat{\varphi}_{l,r}^{(k)}(\alpha)$, x arbitrarily close to $1-(1-\alpha)^k$. First we prove (i) implies (ii) cannot hold which is the easy part of the result. Indeed, if a combination of the core is contained in $\mathcal{C}$, then any account that contains $\mathcal{C}$ as part of its input is in the target $S^{(\text{in})}$, hence it sees the ad with probability p_{in}, and this holds irrespective of all other inputs. One deduces that $\Delta^{(\text{ad})}(\mathcal{C})$ in that case is a Bernouilli family of expected size $\alpha^{|\mathcal{C}|}p_{\text{in}}m$, thus we can apply Lemma 2 if $\alpha < 1-(1-x)^{1/k}$, and conclude that (ii) may only occur with small probability $\varepsilon/P(N)$.

To show that if (i) does not hold, then (ii) does, we define the two following subsets.

$$\text{Let } \Delta^{(\text{ad,in})}(\mathcal{C}) = \left\{ \mathcal{S} \cap \overline{\mathcal{C}} \;\middle|\; \mathcal{S} \in S^{(\text{ad,in})}, \mathcal{C} \subseteq \mathcal{S} \right\},$$

$$\text{and } \Delta^{(\text{core})}(\mathcal{C}) = \left\{ \mathcal{S} \cap \overline{\mathcal{C}} \;\middle|\; \mathcal{S} \in S^{(\text{core})} \right\}.$$

Note that since no combination of the core family is included in $\mathcal{C}$, no element of $\Delta^{(\text{core})}(\mathcal{C})$ is empty. Furthermore, observe that by definition a combination in $S^{(\text{ad,in})} = S^{(\text{ad})} \cap S^{(\text{in})}$ should contain a combination of the core. This directly implies that a combination in $\Delta^{(\text{ad,in})}(\mathcal{C})$ necessarily contains a combination from $\Delta^{(\text{core})}(\mathcal{C})$, which is by consequence a 1_intersecting family of $\Delta^{(\text{ad,in})}(\mathcal{C})$.

We can apply Lemma 3 not using x but $(l/k) \cdot x$, as Eq.(3) ensures the condition of the lemma is satisfied for this value and α. This shows that with probability at least $(1-\varepsilon/P(N))$, $|\Delta^{(\text{ad,in})}(\mathcal{C})|/|\Delta^{(\text{ad})}(\mathcal{C})| \geq (l/k) \cdot x$.

The family $\Delta^{(\text{core})}(\mathcal{C})$ contains at most l elements, and it intersects all combinations in $\Delta^{(\text{ad,in})}(\mathcal{C})$. Moreover:

$$\forall (X_i)_{i=1}^{I}, \max_{i_1,\ldots,i_a} |X_{i_1} \cup \ldots \cup X_{i_a}| \geq \frac{a}{I}\left|\bigcup_{i=1}^{I} X_i\right|.$$

Hence there exists a subset of $k \leq l$ combinations chosen in $\Delta^{(\text{core})}(\mathcal{C})$ that collectively intersect at least $(k/l) \cdot$

$|\Delta^{(\text{ad,in})}(\mathcal{C})|$ elements. It is hence an x_intersecting family of $\Delta^{(\text{ad})}(\mathcal{C})$ with probability $(1-\varepsilon/P(N))$, proving (ii). □

8.6 Proof of Lemma 4

Lemma 4. The expected size of $\Delta^{(\text{ad})}(\mathcal{C})$ is $\alpha^{|\mathcal{C}|}q_{\mathcal{C}}m$ with

$$q_{\mathcal{C}} = P\left[B_j(N,\alpha) \in S^{(\text{in})} \middle| \mathcal{C} \in B_j(N,\alpha)\right] \geq \alpha^r .$$

Hence by Chernoff bound there exists C_0 such that whenever $m \geq \alpha^{-|\mathcal{C}|} \cdot C_0 \cdot \log \frac{P(N)}{\varepsilon}$, with high probability we have $|\Delta^{(\text{ad})}(\mathcal{C})| \geq \alpha^{|\mathcal{C}|}q_{\mathcal{C}}m/2$. If we constrain all combinations of $\Delta^{(\text{ad})}(\mathcal{C})$ to the $N' < N$ data inputs that are not part of $\bigcup_{\mathcal{S}\in S^{(\text{core})}} \mathcal{S}$, we thus obtain a random Bernouilli family of large size $\geq \alpha^{|\mathcal{C}|}q_{\mathcal{C}}m/2$ with parameters N', α. Assuming $\alpha < 1-(1-x)^{1/k}$, this family does not admit an x_intersecting subset of size $\leq k$ w.h.p. by Lemma 2, hence no combination in $S_{x,k}$ can be fully contained into it.

Moreover if it holds that $\frac{p_{\text{out}}}{p_{\text{in}}} < \sup_\alpha \hat{\varphi}^{(k)}_{l,r}(\alpha)$, then by the proof of Proposition 1 there is an x_intersecting family composed of $\leq k$ combinations from $\Delta^{(\text{core})}(\mathcal{C})$, hence w.h.p. there are $\leq k$ combinations from $S^{(\text{core})}$ fully contained in $\mathcal{C} \cup (\bigcup_{\mathcal{S}\in S_{x,k}} \mathcal{S})$. □

8.7 Proof of Proposition 2

Proposition 2. We will prove the proposition by induction on the size $s \leq l$ of the core family. If $s = 0$, then we are done as by Proposition 1 we have w.h.p. that $\{D_i \mid \frac{|\{A_j\in S^{(\text{ad})} | D_i \in A_j\}|}{|S^{(\text{ad})}|} \geq x\} = \emptyset$ whenever $m \geq C_0 \cdot \log \frac{P(N)}{\varepsilon}$, for some constant C_0.

Suppose by the induction hypothesis that for all $0 \leq s' \leq s-1$, there exists a constant $C_{s'}$ such that GSI is correct w.h.p. whenever $m \geq C_{s'} \cdot \log \frac{P(N)}{\varepsilon}$ and the core family has size s'. Let $S^{(\text{core})}$ be of size s. By the dichotomy result from Proposition 1, there is C' such that $\mathcal{S} = \{D_i \mid \frac{|\{A_j\in S^{(\text{ad})} | D_i \in A_j\}|}{|S^{(\text{ad})}|} \geq x\} \neq \emptyset$ w.h.p. whenever $m \geq C' \cdot \log \frac{P(N)}{\varepsilon}$. Furthermore by Lemma 4, this set contains a combination from the core family. GSI iterates over the data inputs $D_i \in \mathcal{S}$, it removes each temporarily and it applies the recognition test from Prop.1 to decide whether $\mathcal{S} \setminus D_i$ is within target. If so, then it still contains a combination of the core family and we can delete D_i from $\mathcal{S}$ permanently. Else, the data input D_i is *critical i.e.*, , it intersects all combinations of $S^{(\text{core})}$ contained into $\mathcal{S}$, and we put is back in $\mathcal{S}$. As a result, the remaining data inputs in $\mathcal{S}$ at the end of the iteration are a combination from $S^{(\text{core})}$ that we will denote by $\mathcal{C}$ in the following.

Let $D_i \in \mathcal{C}$ be fixed, and let $\mathcal{A}_i$ be the active accounts amongst those in the random Bernouilli subfamily $\mathcal{B}_i$, defined as all the $B_j(N,\alpha)$ not containing this data input. Note that $\mathcal{B}_i$ has size $(1-\alpha)m$ on expectation, and that f constrained to $\mathcal{B}_i$ is equivalent to the targeting function f_i whose core family is $S_i = S^{(\text{core})} \setminus \{\mathcal{S} \mid D_i \in \mathcal{S}\}$. Thus by the induction hypothesis, there is C_{s_i}, with $s_i = |S_i|$, such that w.h.p. the output of the recursive call $\text{GSI}(S^{(\text{ad})} \setminus \{A_j \mid D_i \in A_j\}, x)$ is exactly the core subfamily S_i if $|\mathcal{B}_i| \geq C_{s_i} \cdot \log \frac{P(N)}{\varepsilon}$. Furthermore, there is C^i such that $|\mathcal{B}_i| \geq (1-\alpha)m/2$ w.h.p. if $m \geq C^i \cdot \log \frac{P(N)}{\varepsilon}$.

Consequently, the output of the algorithm is with high probability $\{\mathcal{C}\} \cup (\bigcup_{D_i\in\mathcal{C}} S_i)$ if $m \geq C_s \cdot \log \frac{P(N)}{\varepsilon}$, with

$$C_s \geq \max\{C'\} \cup \{C^i \mid D_i \in \mathcal{C}\} \cup \{2C_{s_i}(1-\alpha)^{-1} \mid D_i \in \mathcal{C}\}.$$

This concludes the proof because $S^{(\text{core})} = \{\mathcal{C}\} \cup (\bigcup_{D_i\in\mathcal{C}} S_i)$ by the monotonicity assumption. □

8.8 Proof of Lemma 5

Lemma 5. Given any fixed subset $\mathcal{D}$ of data inputs, we can compute in $O(|S^{(\text{ad})}| + \sum_{j=1}^k |A_j|) = O(N \cdot |S^{(\text{ad})}|)$-time the set of accounts $\{A_j \in \mathcal{A} \mid \mathcal{D} \subseteq A_j\}$ and so, $\{D_i' \notin \mathcal{D} \mid \frac{|\{A_j\in\mathcal{A} | \mathcal{D}\cup\{D_i'\}\subseteq A_j\}|}{|\{A_j\in\mathcal{A} | \mathcal{D}\subseteq A_j\}|} \geq x\}$. As a result, Lines 1-7 (til the first for-loop) can be executed in $O(|\mathcal{C}| \cdot N \cdot |S^{(\text{ad})}|) = O(|\mathcal{I}| \cdot N|S^{(\text{ad})}|)$-time. Moreover, at each step of the second for-loop it holds that S, S_i are subsets of $\mathcal{P}(\mathcal{I})$ and so, the merge $S \cup S_i$ can be executed in $O(|\mathcal{I}|2^{|\mathcal{I}|})$-time. Let us finally denote by $T_{\mathcal{I}}$ an upper-bound on the computational cost of any recursive call to the algorithm.

We have that GSI can be executed in $O(|\mathcal{I}| \cdot (N \cdot |S^{(\text{ad})}| + |\mathcal{I}|2^{|\mathcal{I}|} + T_{\mathcal{I}}))$-time. By induction, the time-complexity is $O(|\mathcal{I}|! \cdot N \cdot |S^{(\text{ad})}| + \underbrace{\sum_{j=1}^{|\mathcal{I}|-1} \frac{|\mathcal{I}|!}{(|\mathcal{I}|-j)!}(|\mathcal{I}|-j+1)2^{|\mathcal{I}|-j+1}}_{\Gamma(|I|)})$.

This concludes the proof as we have:

$$\Gamma(|I|) = \sum_{j=1}^{|\mathcal{I}|-1} \frac{|\mathcal{I}|!}{j!}(j+1)2^{j+1} \leq 2 \cdot |\mathcal{I}|! \left[\sum_{j=0}^{\infty}(j+1)\frac{2^j}{j!}\right] \leq 6e^2 \cdot |\mathcal{I}|!$$ □

8.9 Proof of Proposition 3

Proposition 3. Let $\mathcal{S}^{(core)} = \{D_i \mid \exists \mathcal{C} \in S^{(\text{core})} \text{ s.t. } D_i \in \mathcal{C}\}$, and let $\mathcal{S} = \{D_i \mid \frac{|\{A_j \in S^{(\text{ad})} | D_i \in A_j\}|}{|S^{(\text{ad})}|} \geq x\}$. By Lemma 4, there is C' such that $\forall \varepsilon > 0$, for all polynomial P, we have $\mathcal{S} \subseteq \mathcal{S}^{(core)}$ with probability $1 - \frac{\varepsilon}{P(N)}$ whenever $m \geq C' \cdot \log \frac{P(N)}{\varepsilon}$. Applying this argument recursively, we obtain that the depth of the recursive calls is upper-bounded by lr and so, that we also have $\mathcal{I} \subseteq \mathcal{S}^{(core)}$ with probability $1 - \frac{\varepsilon}{P(N)}$ whenever $m \geq C'(1-\alpha)^{-lr} \cdot \log \frac{P(N)}{\varepsilon}$. In such case, our set-intersection algorithm can be implemented to run in $O(|\mathcal{I}|! \cdot N \cdot |S^{(\text{ad})}|) = O\left((lr)! \cdot Nm\right)$-time by Lemma 5.

The expected running-time is therefore upper-bounded by an $O\left(\left[\left(1 - \frac{\varepsilon}{P(N)}\right)(lr)! + \frac{\varepsilon}{P(N)} N!\right] Nm\right)$. By setting $\frac{\varepsilon}{P(N)} = \frac{1}{N!}$, we conclude that it is $O\left((lr)! \cdot Nm\right)$ whenever $m = \Omega\left(N \log N\right)$. □

8.10 Proof of Lemma 6

Lemma 6. When $l = 1$ one can easily see that $\varphi_{1,r}$ is strictly increasing on this interval and computes its limit as x approaches 1. A similar argument holds for $r = 1$.

Whenever $r > 1$ and $l > 1$, introducing the new variable $z = (1-x)^{1/l}$ we first observe:

$$\varphi_{l,r}(z) = f_l(z) \cdot f_r(1-z)\,, \text{ where } f_n(z) = \frac{z^n}{1-z^n}.$$

This symmetry immediately implies that $M_{l,r} = M_{r,l}$. Note that the form of the function also directly yields that

$$M_{\max(l,r),\max(l,r)} \leq M_{l,r} \leq M_{\min(l,r),\min(l,r)}\,.$$

We have $\varphi'_{l,r}(z) = f'_l(z) \cdot f_r(1-z) - f_l(z) \cdot f'_r(1-z)$, and observe that this derivative becomes null whenever we have $f'_l(z)/f_l(z) = f'_r(1-z)/f_r(1-z)$. Moreover, it holds that

$$f'_n(z) = -\frac{lz^{n-1}}{(1-z^n)^2} \quad \text{hence} \quad f'_n(z)/f_n(z) = \frac{n}{z(1-z^n)}$$

so that the condition is $\frac{l}{z(1-z^l)} = \frac{r}{(1-z)(1-(1-z)^r)}$ which yields the value of z reaching the maximum.

To conclude, we just need to observe that there is a unique solution in $]0;1[$. We can immediately observe, when $r > 1$ and $l > 1$ that the product $f_l(z) \cdot f_r(1-z)$ has null limits on both sides, and a derivative that is positive near 0^+ and 1^-. Since its third derivative is strictly positive, its second derivative increases and can only be null once. We deduce that the derivative cannot cancel twice between 0 and 1 since it would create two inflection points.

Finally, when $r = l = n$, since the product is symmetric in z and it has a unique maximum on $]0;1[$ it has to be in $z = \frac{1}{2}$ which yields the result. □

Appendix N

A theory for ad targeting identification

A theory for ad targeting identification

Abstract

The problem of learning juntas has been studied under different notions of learning. We here study a new model, where the goal is “exact” learning (with high probability) of a given Boolean function with membership queries. The main novelty in the model is that queries are subject to asymmetric classification noise and limited cross-unit effects. Furthermore, it extends (and is inspired by) the theory behind two already well established *web transparency* tools. Such tools aim to put emphasis on any form of misuse of our personal data by the institutions and companies on-line. However, they have so far accounted only for targeting on a *monotone* function, with the constrictive assumption that users are targeted *independently* the one from the other. In contrast with prior work, we prove that *any* function can be learnt in this extended model — conditioned on one assumption about the noise, that will be proved to be necessary. More precisely, we show that for any k, the function can be learnt in $N^{\mathcal{O}(k)}$-time and polylog(N) queries with k-juntas as hypotheses. Our algorithms build upon some variation of a known greedy heuristic which reduces to Set Cover in order to infer the relevant variables. Finally, we show that there is a given (monotone) 2-junta which cannot be learnt within our model when it is made no assumption about the noise.

Keywords: web transparency; negative targeting; cross-unit effect; exact learning; juntas.

1 The model

1.1 Targeting functions

Our problem formulation extends the one in [7]. So, in particular, it differs from (but can be easily shown to be equivalent to) standard terminology in the literature of Boolean function learning. Let $\mathcal{D} = \{D_1, D_2, \ldots, D_N\}$ be a set of N inputs representing individual information from a given user (typically, emails in an account, see also [4]). Our main objective is to identify how these inputs affect a given output of interest (say, an ad or a recommendation).

In order to achieve the goal, we here assume that each output is affected through an unknown targeting function f_{output}, that we simply denote by f in the following. More precisely, let any $\mathcal{C} \subseteq \mathcal{D}$ be called a combination. The targeting function f is a mapping from the family of all combinations to the Boolean set $\{0; 1\}$. By convention, $f(\mathcal{C}) = 1$ indicates that an account *exactly* containing the inputs in $\mathcal{C}$ is targeted, and we denote $f(.) = 0$ if the ad is untargeted. In particular unlike [5], we do not assume here that f is *monotone* (*i.e.*, $\overline{f(\mathcal{C}) = 1 \text{ and } \mathcal{C} \subseteq \mathcal{C}' \not\Longrightarrow f(\mathcal{C}') = 1}$). Hence, the targeting function f can be any Boolean formula with a subset of $\mathcal{D}$ as its variables. However in practice, we assume that f only depends on a small number k of inputs, with k being a universal constant. Such targeting functions are called k-juntas in the literature [3]. We are particularly interested in how the value of k affects the complexity of the targeting detection and identification problems, *i.e.*, what is their parameterized complexity ?

In this note, we adopt the classical approach in order to learn the targeting function f, that is, we seek to learn the class $\mathcal{S}^{(\text{in})}$ of all combinations $\mathcal{C}$ such that $f(\mathcal{C}) = 1$.

1.2 Outcome properties

In order to learn the targeting function, we are bound to rely on experiments — to see how it reacts to various inputs. For instance, in [7] these experiments consist in collecting the ads for Gmail accounts with different subsets of emails. We model this as an oracle from function learning theory [1], denoted by $\mathcal{O}_f$. Formally, $\mathcal{O}_f$ is a membership oracle with (asymmetric) classification noise. That is, it outputs the Boolean $f(\mathcal{C})$ for any combination $\mathcal{C}$ with some probability to flip the result. Unlike prior work [2], we do not assume the classification noise to be symmetric, *i.e.*, the oracle may flip the result with some propability *depending on the combination.* Nonetheless, we will assume a few properties for the noise distribution. To our best knowledge, the following assumptions that are made on this probability have not been studied before in the literature.

Histories. Experiments in [9] have evidenced that the noise distribution is subject to cross-unit effects. So, in order to handle with these correlations, we find it more suitable to generalize our oracle $\mathcal{O}_f$ so that it can take *families of combinations* as inputs. More precisely, let a family be any vector of combinations, denoted by $\mathcal{F} = \langle A_1, A_2, \ldots, A_t \rangle$. The outcome $\mathcal{O}_f(\mathcal{F})$ is simply defined as the binary vector $\mathcal{O}_f(\mathcal{F}) = \langle \mathcal{O}_f(A_1), \mathcal{O}_f(A_2), \ldots, \mathcal{O}_f(A_t) \rangle$. Furthermore, let the pair $\mathrm{H}_{\mathcal{F}} = (\mathcal{F}; \mathcal{O}_f(\mathcal{F}))$ be the history of f.

As usual, let $\mathcal{F}_{-i} = \langle A_1, \ldots, A_{i-1}, A_{i+1}, \ldots, A_t \rangle$. We will assume that each individual outcome $\mathcal{O}_f(A_i)$ may be correlated to the partial history $\mathrm{H}_{\mathcal{F}_{-i}}$. However, it may and must be the case that some natural properties hold independently from any history, that we now detail as follows:

Assumption 1 (targeting lift)**.** *There exists a universal constant $\varphi \in]0;1[$, called the targeting lift and such that for any $\mathcal{C}_0, \mathcal{C}_1$ with $f(\mathcal{C}_0) = 0, f(\mathcal{C}_1) = 1$:*

$$\mathbb{P}r[\mathcal{O}_f(A_i) = 1 \mid A_i = \mathcal{C}_0, \mathrm{H}_{\mathcal{F}_{-i}}] < \varphi \cdot \mathbb{P}r[\mathcal{O}_f(A_i) \mid A_i = \mathcal{C}_1, \mathrm{H}_{\mathcal{F}_{-i}}].$$

Assumption 1 is local and it simply ensures that it is more likely for $\mathcal{O}_f$ to output 1 on accounts A_i within scope, that is, for which $f(A_i) = 1$. In particular, it implies that the targeting function f is related to the outcome we study. Note that a similar assumption was made in [5, 7], but in the less realistic case when no cross-unit effect occurs, and so, each account is targeted independently. However, the following two global assumptions are new (if there is no cross-unit effect then they can be proven to be true by using standard concentration inequalities and independence, see [7]).

Assumption 2 (polynomial-growth)**.** *There exist positive universal constant α, β, γ with $\alpha \leq 1$ and such that:*

$$\mathbb{P}r[\sum_{i=1}^{t} \mathcal{O}_f(A_i) < \left(\beta \cdot |\mathcal{F} \cap \mathcal{S}^{(in)}|^{\alpha}\right)] \leq e^{-\gamma \cdot t}$$

We properly state with Assumption 2 that there must be a significant fraction of the account population *within scope* being targeted, except on some small event with low probability like, for instance, when the targeting campaign runs out of budget. Note that in [5], it was assumed that there is some minimum *constant* probability p_{in} for an account within scope to be targeted, so, Assumption 2 was satisfied for $\alpha = 1$. By considering the case $\alpha \leq 1$, we may consider the case when this minimum probability slowly tends to zero, say, $p_{in} \sim p_o / \log^{\mathcal{O}(1)}(N)$ where p_0 is a constant. This case was observed to happen in practice [7].

Assumption 3 (noninterference)**.** *Let the targeting function f only depend on inputs in $V \subseteq \mathcal{D}$. Furthermore, let $A'_i = A_i \cap V$ and let $\mathcal{F}' = \langle A'_1, \ldots, A'_t \rangle$.*

$$\mathbb{P}r[\mathcal{O}_f(\mathcal{F})] = \mathbb{P}r[\mathcal{O}_f(\mathcal{F}')].$$

Finally, we formalize with Assumption 3 that none of the input that does not affect the targeting can impact on the outcome.

1.3 Experiments and random families

The model in Section 1.2 supports *adaptive queries*. However in practice, the methodologies for web transparency [9] recommend to use so-called "exchangeable" accounts in the experiments. In particular, one experimental design used in practice [4, 7] is to populate each account randomly so that an input independently appears with same probability — that will be taken equal to 1/2 in the remaining of the paper. So, we will constrain our queries on pairwise independent random accounts in the following. We will name a random Bernouilli family any family of such random accounts.

2 Preliminaries

Prior work [5, 7] has made extensive use of concentration inequalities in the analysis of the algorithms, *i.e.*, Chernoff bounds. Standard bounds apply to the sum of *independent* variables, so, they cannot be used in our setting directly. The following is a tedious (but classical) analysis where we show how to adapt Chernoff bounds to our needs.

Lemma 1. *Let $X_1, \ldots, X_m$ be random Boolean variables satisfying:*

$$p_{\min} \le \mathbb{P}r[X_i = 1 \mid X_1, \ldots, X_{i-1}] \le p_{\max}$$

for some constant $p_{\min}, p_{\max}$. Then the following hold for any $0 < \delta < 1$:

$$\mathbb{P}r[\sum_{i=1}^{m} X_i \ge (1+\delta) \cdot p_{\max} \cdot m] \le e^{-\delta^2 m p_{\max}/3}$$

$$\mathbb{P}r[\sum_{i=1}^{m} X_i \le (1-\delta) \cdot p_{\min} \cdot m] \le e^{-\delta^2 m p_{\min}/2}$$

Proof. By symmetry, we will only consider the first inequality. Let $t > 0$. Let us show that:

$$\mathbb{E}[\Pi_{i=1}^m e^{t \cdot X_i}] \le \left(p_{\max}(e^t - 1) + 1\right)^m .$$

The proof is by induction. By the hypothesis,

$$\mathbb{E}[e^{t\cdot X_m} \mid X_1, \ldots, X_{m-1}] = e^t \cdot \mathbb{P}r[X_m = 1 \mid X_1, \ldots, X_{m-1}] + 1 \cdot \mathbb{P}r[X_m = 0 \mid X_1, \ldots, X_{m-1}] \le p_{\max}(e^t - 1) + 1,$$

that is the base case. Suppose for the induction hypothesis that:

$$\mathbb{E}[\Pi_{j=i+1}^m e^{t\cdot X_j} \mid X_1, \ldots, X_i] \le \left(p_{\max}(e^t - 1) + 1\right)^{m-i} .$$

Then by the law of total probability:

$$\begin{aligned}\mathbb{E}[\Pi_{j=i}^m e^{t\cdot X_j} \mid X_1, \ldots, X_{i-1}] = e^t \cdot \mathbb{P}r[X_i = 1 \mid X_1, \ldots, X_{i-1}] \cdot \mathbb{E}[\Pi_{j=i+1}^m e^{t\cdot X_j} \mid X_1, \ldots, X_{i-1}, X_i = 1] \\ + 1 \cdot \mathbb{P}r[X_i = 0 \mid X_1, \ldots, X_{i-1}] \cdot \mathbb{E}[\Pi_{j=i+1}^m e^{t\cdot X_j} \mid X_1, \ldots, X_{i-1}, X_i = 0]\end{aligned}$$

$$\le \left(\mathbb{P}r[X_i = 1 \mid X_1, \ldots, X_{i-1}] \cdot (e^t - 1) + 1\right) \cdot \left(p_{\max}(e^t - 1) + 1\right)^{m-i} \le \left(p_{\max}(e^t - 1) + 1\right)^{m-i+1} ,$$

which proves the induction hypothesis. The remaining of the proof is now classical computation of Chernoff Bound. By Markoff inequality:

$$\begin{aligned}\mathbb{P}r[\sum_{i=1}^{m} X_i \ge (1+\delta) \cdot p_{\max} \cdot m] &= \mathbb{P}r[e^{t\cdot\sum_{i=1}^m X_i} \ge e^{t\cdot(1+\delta)\cdot p_{\max}\cdot m}] \le \mathbb{E}[e^{t\cdot\sum_{i=1}^m X_i}]/e^{t\cdot(1+\delta)\cdot p_{\max}\cdot m} \\ &= e^{-t\cdot(1+\delta)\cdot p_{\max}\cdot m} \cdot \mathbb{E}[\Pi_{i=1}^m e^{t\cdot X_i}] \le e^{-t\cdot(1+\delta)\cdot p_{\max}\cdot m} \cdot \left(p_{\max}(e^t - 1) + 1\right)^m \\ &\le e^{-t\cdot(1+\delta)\cdot p_{\max}\cdot m} \cdot e^{p_{\max}(e^t-1)\cdot m} = e^{p_{\max}\cdot m\cdot\left(e^t - 1 - t\cdot(1+\delta)\right)}\end{aligned}$$

Finally, set $t = \ln(1+\delta)$. One obtains:

$$\mathbb{P}r[\sum_{i=1}^{m} X_i \geq (1+\delta)\cdot p_{\max}\cdot m] \leq \left(\frac{e^{\delta}}{(1+\delta)^{1+\delta}}\right)^{mp_{\max}} \leq e^{-\delta^2 mp_{\max}/3}.$$

□

3 Building block algorithm: the case k=1

We first describe a simple algorithm with 1-juntas as hypotheses. A simpler variation of the following Algorithm 1 is the core algorithm of the Xray prototype [7]. Here, we extend the algorithm to the case of negative targeting, and we prove its correctness under our more general assumptions.

```
Input: a family $\mathcal{F}$; threshold parameters $x, y$.
Output: intersecting families $S_x, S_y$.
$S_x \leftarrow \{D_j \in \mathcal{D} \mid D_j$ appears in $\geq x \cdot |\mathcal{F}|$ accounts in $\mathcal{F}\}$ ;
$S_y \leftarrow \{D_j \in \mathcal{D} \mid D_j$ appears in $\leq y \cdot |\mathcal{F}|$ accounts in $\mathcal{F}\}$ ;
```

Algorithm 1: Set-intersection algorithm.

The reader may observe that Algorithm 1 requires two parameters x, y as inputs. For simplicity, we will assume that a good estimate on the *targeting lift* (Assumption 1) is given, and we will show in the following that the latter information is enough in order to tune x, y. Nonetheless, we point out that finding these two parameters in practice may be cumbersome. We refer the reader to [6, 7] for experimental and theoretical methods in order to tune x, y.

Lemma 2. *Fix any polynomial P. Let $\mathcal{B}$ be a random Bernouilli family. There is a constant $a_{x,y}$ such that if $y < 1/2 < x$, $\mathcal{F}$ contains the targeted accounts in $\mathcal{B}$ and has size $|\mathcal{F}| \geq a_{x,y} \cdot \log(2 \cdot P(N) \cdot N/\varepsilon)$, then the following holds with probability $\geq 1 - \varepsilon/P(N)$: the targeting function f depends on any input in S_x or S_y.*

Proof. Set $a_{x,y} = \frac{6}{(\min\{1-2y, 2x-1\})^2}$. We will identify $\leq N$ events so that, if it is the case that f does not depend on some input in $S_x \cup S_y$, then one of these events must fail. So, in order to prove the lemma, we will prove that each event fails with probability $\leq \varepsilon/(P(N)\cdot N)$ — in which case, it is easy to conclude by taking a union bound.

Before this, we claim that every input D_j of which the targeting function f does not depend on appears in the combinations of $\mathcal{F}$ *independently* and with probability 1/2. Our proof is combinatorial. Let $I \subseteq \{1, \ldots, |\mathcal{B}|\}$ be fixed. The set I will denote the indices of combinations $A_i \in \mathcal{B}$ that are targeted, *i.e.*, $\mathcal{O}_f(A_i) = 1$ if and only if $i \in I$. For any $i \in I$, let X_i be the random Boolean variable denoting whether $D_j \in A_i$. In order to prove the claim, we must prove that variables X_i are mutually independent. So, let $J \subset I$ and $i \in I \setminus J$. Let us fix X_q for every $q \in J$. Finally, consider the set Ω_J of all histories $(\mathcal{B}, \mathcal{O}_I)$ satisfying: $\mathcal{O}_I$ is the binary vector with its nonzero entries indexed by I, and for every $q \in J$, $D_j \in A_q$ if and only if $X_q = 1$. Since $h_i : \langle A_1, \ldots, A_{i-1}, A_i, A_{i+1}, \ldots, A_{|\mathcal{B}|}\rangle \to \langle A_1, \ldots, A_{i-1}, A_i \Delta\{D_j\}, A_{i+1}, \ldots, A_{|\mathcal{B}|}\rangle$ is one-to-one, there is half of the histories in Ω_J that satisfy X_i. Furthermore, since f does not depend on D_j, for any $(\mathcal{B}, \mathcal{O}_I) \in \Omega_J$, $\mathbb{P}r[\mathcal{O}_f(\mathcal{B}) = \mathcal{O}_I] = \mathbb{P}r[\mathcal{O}_f(h_i(\mathcal{B})) = \mathcal{O}_I]$ by Assumption 3. As a result, $\mathbb{P}r[X_i \mid X_{q_1}, \ldots, X_{q_{|J|}}] = 1/2$, with $J = \{q_1, \ldots, q_{|J|}\}$, that proves the claim.

Finally, for every irrelevant input D_j (there are $\leq N$ such inputs), since $|\mathcal{F}|$ is large enough we have by Chernoff bound (applying Lemma 1 with $p_{\min} = p_{\max} = 1/2$) that with probability $\geq 1 - \varepsilon/(P(N)\cdot N)$ the irrelevant input D_j appears in a fraction $y < . < x$ of the accounts in $\mathcal{F}$. □

By Lemma 2, every input detected by the Set-intersection algorithm is relevant. However, the main drawback with the above Algorithm 1 is that it may fail in identifying *all* the relevant inputs for the targeting. We now prove that Algorithm 1 can be used in order to learn the targeting function f, in the special case when it depends on a unique input (either positively, or negatively).

Theorem 1. *Set $\varphi/(1+\varphi) < y < 1/2 < x < 1/(1+\varphi)$. Furthermore, fix any polynomial Q. Let $\mathcal{B}$ be a random Bernouilli family of size $|\mathcal{B}| = m$.*

There is a constant $b_{x,y}$ such that if $m \geq b_{x,y} \cdot \log^{1/\alpha}(8 \cdot Q(N) \cdot N/\varepsilon)$ and $\mathcal{F}$ contains the targeted accounts in $\mathcal{B}$, then the following holds with probability $\geq 1 - \varepsilon/Q(N)$:

- $S_x = \{D_j\},\ S_y = \{\}$ *if* $f : \mathcal{C} \to \mathbb{I}_{\{D_j \in \mathcal{C}\}}$*;*
- $S_x = \{\},\ S_y = \{D_j\}$ *if* $f : \mathcal{C} \to \mathbb{I}_{\{D_j \notin \mathcal{C}\}}$*.*

Proof. Let $a_{x,y}$ be the constant defined in Lemma 2. Set $b_1 = 12$, $b_2 = 1/\gamma$, $b_3 = 4\left(\frac{a_{x,y}}{\beta}\right)^{1/\alpha}$, $b_4 = 4\left(\frac{3}{\beta\cdot(1-x(1+\varphi))^2}\right)^{1/\alpha}$ and $b_5 = 4\left(\frac{3\varphi^2}{\beta\cdot(y-\varphi(1-y))^2}\right)^{1/\alpha}$. Finally, set $b_{x,y} = \max_{1\leq i\leq 5} b_i$.

By symmetry we only need to consider the case when $f : \mathcal{C} \to \mathbb{I}_{\{D_j \in \mathcal{C}\}}$ for some fixed j. In this case, since $\mathcal{B}$ is a random Bernouilli family, $\mathbb{E}[|\mathcal{B}\cap\mathcal{S}^{(\text{in})}|] = |\mathcal{B}|/2$. Thus, by Chernoff bound, since $m \geq b_1 \cdot \log(8 \cdot Q(N)/\varepsilon)$ we have that $|\mathcal{B}\cap\mathcal{S}^{(\text{in})}| \geq |\mathcal{B}|/4$ with probability $\geq 1 - \varepsilon/(4\cdot Q(N))$. Furthermore, by Assumption 2, since $m \geq b_2 \cdot \log(8\cdot Q(N)/\varepsilon)$ we have that $|\mathcal{F}| \geq \beta \cdot (|\mathcal{B}\cap\mathcal{S}^{(\text{in})}|)^\alpha$ with probability $\geq 1 - \varepsilon/(4\cdot Q(N))$.

First, let us show that irrelevant inputs can be ignored. Since we can assume that $|\mathcal{F}| \geq \beta\cdot(b_3/4)^\alpha \cdot \log(8\cdot Q(N)\cdot N/\varepsilon)$, it follows that $|\mathcal{F}| \geq a_{x,y} \cdot \log(8\cdot Q(N)\cdot N/\varepsilon)$ with probability $\geq 1 - \varepsilon/(2\cdot Q(N))$. Furthermore, setting $P(N) = 4\cdot Q(N)$, one obtains by Lemma 2 that with probability $\geq 1-\varepsilon/(4\cdot Q(N))$, either $D_j \in S_x$ or $S_x = \emptyset$, similarly either $D_j \in S_y$ or $S_y = \emptyset$.

Second, let $\mathcal{F} = \langle A_{i_1}, \ldots, A_{i_t}\rangle$. Define X_l to be the random Boolean variable denoting whether $D_j \in A_{i_l}$. We will prove that $\mathbb{P}r[X_l = 1 \mid X_1,\ldots,X_{l-1}] \geq 1/(1+\varphi)$. To prove it, fix $I \subseteq \{1,\ldots,|\mathcal{B}|\}$, with $|I| = t$, that will represent the indices of the combinations $A_{i_l} \in \mathcal{B}$ that are within $\mathcal{F}$. Let $i_l \in I$ and let $X_1,\ldots,X_{l-1}$ be fixed. Consider the set Ω of all histories $(\mathcal{B},\mathcal{O}_I)$ where $\mathcal{O}_I$ denotes the binary vector with its nonzero entries being indexed by I and for any $p < l$, $D_j \in A_{i_p}$ if and only if $X_p = 1$. Since $h_l : \langle A_1,\ldots,A_{i_l-1},A_{i_l},A_{i_l+1},\ldots,A_m\rangle \to \langle A_1,\ldots,A_{i_l-1},A_{i_l}\Delta\{D_j\},A_{i_l+1},\ldots,A_m\rangle$ is one-to-one, there is half of the histories in Ω satisfying X_l. Furthermore, for any $(\mathcal{B},\mathcal{O}_I)$ satisfying X_l, by Assumption 1:

$$\frac{\mathbb{P}r[\mathcal{O}_f(\mathcal{B}) = \mathcal{O}_I]}{\mathbb{P}r[\mathcal{O}_f(h_l(\mathcal{B})) = \mathcal{O}_I]} = \frac{\mathbb{P}r[\mathcal{O}_f(A_{i_l}) = 1 \mid D_j \in A_{i_l}, \mathrm{H}_{\mathcal{B}_{-i_l}} = \mathcal{O}_{I-i_l}]}{\mathbb{P}r[\mathcal{O}_f(A_{i_l}) = 1 \mid D_j \notin A_{i_l}, \mathrm{H}_{\mathcal{B}_{-i_l}} = \mathcal{O}_{I-i_l}]} > 1/\varphi.$$

As a result, $\mathbb{P}r[X_l = 1 \mid X_1,\ldots,X_{l-1}] \geq 1/(1+\varphi)$, that proves the claim. By Lemma 1 (with $p_{\min} = 1/(1+\varphi)$), since we can assume that $|\mathcal{F}| \geq \beta\cdot(b_4/4)^\alpha\cdot\log(8\cdot Q(N)/\varepsilon)$ one obtains that $D_j \in S_x$ with probability $\geq 1-\varepsilon/(4\cdot Q(N))$. Therefore, we can prove Theorem 1 simply by taking a union bound. □

4 Application: targeting identification

Equipped with Algorithm 1, we will show how it can be used as a routine in order to learn *any* targeting function f with k-juntas as hypotheses. Our algorithm proceeds in two main steps. It first computes the (at most k) relevant inputs of which f depends on, that is the dominant part of the complexity of our algorithm (Section 4.1). Then, it guesses from these inputs the truth table of f (Section 4.2). Furthermore, we will show that the second step requires an additional hypothesis about the noise, that will be proved to be necessary in Section 5.

4.1 Finding the relevant inputs

The relevant inputs will be inferred by virtually "fixing" $k-1$ inputs from the set $\mathcal{D}$. Such removal will reduce the problem to the identification of a given 1-junta, and so, Algorithm 1 can be used. This is formalized with Algorithm 2.

```
Input: a family $\mathcal{F}$; a lower-bound $lb$; threshold parameters $x, y$.
Output: the set of relevant inputs $V$.
$V \leftarrow \{\}$ ;
foreach $\langle \mathcal{C}_{in}, \mathcal{C}_{out} \rangle$ with $|\mathcal{C}_{in}| + |\mathcal{C}_{out}| \leq k-1$ do
    $\hat{\mathcal{F}} \leftarrow \{A_p \in \mathcal{F} \mid \mathcal{C}_{in} \subseteq A_p$ and $A_p \cap \mathcal{C}_{out} = \emptyset\}$ ;
    if $|\hat{\mathcal{F}}| \geq lb$ then
        $(S_x, S_y) \leftarrow$ Set-intersection($\hat{\mathcal{F}}; x, y$) ;
        $\hat{S} \leftarrow (S_x \cup S_y) \setminus \mathcal{C}_{in}$ ;
        $V \leftarrow V \cup \hat{S}$ ;
    end
end
```

Algorithm 2: Inference algorithm for the relevant inputs.

Theorem 2. *Set $\varphi/(1+\varphi) < y < 1/2 < x < 1/(1+\varphi)$. Furthermore, fix any polynomial R. Let $\mathcal{B}$ be a random Bernouilli family of size $|\mathcal{B}| = m$.*

There are constant $a_{x,y}, c_{x,y}$ such that if:

- *f is a k-junta;*
- *$lb = a_{x,y} \cdot \log\left(3 \cdot 2^k \cdot R(N) \cdot N^k/\varepsilon\right)$;*
- *$m \geq c_{x,y} \cdot \log^{1/\alpha}\left(3 \cdot k \cdot 2^{k+2} \cdot R(N) \cdot N^k/\varepsilon\right)$, and $\mathcal{F}$ contains the targeted accounts in $\mathcal{B}$;*

then Algorithm 2 is correct with probability $\geq 1 - \varepsilon/R(N)$.

Proof. Let $a_{x,y}, b_{x,y}$ as defined in Lemma 2 and Theorem 1. Set $c_{x,y} = 3 \cdot 2^{k+2} \cdot b_{x,y}$. Finally, let $\langle \mathcal{C}_{in}, \mathcal{C}_{out} \rangle$ be fixed, with $|\mathcal{C}_{in}| + |\mathcal{C}_{out}| \leq k-1$.

Define $\hat{\mathcal{B}} \subseteq \mathcal{B}$ as the family of all combinations that both contain $\mathcal{C}_{in}$ and do not intersect $\mathcal{C}_{out}$. Let $\hat{\mathcal{D}} = \mathcal{D} \setminus (\mathcal{C}_{in} \cup \mathcal{C}_{out})$. Furthermore, let $\hat{f}(\hat{\mathcal{C}}) = f(\hat{\mathcal{C}} \cup \mathcal{C}_{in})$ and $\hat{\mathcal{O}}_f(\hat{\mathcal{C}}) = \mathcal{O}_f(\hat{\mathcal{C}} \cup \mathcal{C}_{in})$ for every combination $\hat{\mathcal{C}} \subseteq \hat{\mathcal{D}}$. In order to reuse the results from Section 3, we will base on the property that $\hat{\mathcal{O}}_f$ "almost" behaves like an oracle for the targeting function $\hat{f}$. That is, it satisfies Assumptions 1 and 2 (trivially), but it only satisfies Assumption 3 partially. More precisely, if f (and not $\hat{f}$) only depends on some inputs in $\hat{V} \cup \mathcal{C}_{in} \cup \mathcal{C}_{out}$, then Assumption 3 applies for $\hat{V}$. So, applying Lemma 2 to $\hat{\mathcal{B}}$, since lb is large enough and $\hat{\mathcal{O}}_f$ satisfies the above above weaker version of Assumption 3, one obtains that f depends on any input in $\hat{S}$ with probability $\geq 1 - \varepsilon/(3 \cdot 2^{k-1} \cdot R(N) \cdot N^{k-1})$. By taking a union bound over all possible pairs $\langle \mathcal{C}_{in}, \mathcal{C}_{out} \rangle$, it follows that f depends on any input in V with probability $\geq 1 - \varepsilon/(3 \cdot R(N))$.

In order to complete the proof of the theorem, let D_j be any input on which f depends on. Since D_j is relevant, there is a bipartition $\langle \mathcal{C}_{in}, \mathcal{C}_{out} \rangle$ of the relevant inputs from $\mathcal{D} \setminus D_j$ so that $f(\mathcal{C}_{in} \cup \{D_j\}) \neq f(\mathcal{C}_{in})$. So, let us fix any such bipartition $\langle \mathcal{C}_{in}, \mathcal{C}_{out} \rangle$. In such case, $\hat{f}$ is a 1-junta that only depends on D_j, furthermore $\hat{\mathcal{O}}_f$ satisfies Assumption 3 for $\hat{f}$. The average size of $\hat{\mathcal{B}}$ is $|\mathcal{B}|/2^{k-1}$. So, by Chernoff bound (with $\delta = 1/2$), $\hat{\mathcal{B}}$ has size $\geq b_{x,y} \cdot \log^{1/\alpha}\left(3 \cdot k \cdot 2^{k+2} \cdot R(N) \cdot N^k/\varepsilon\right)$ with probability $\geq 1 - \varepsilon/(3 \cdot k \cdot R(N))$. In such case, by Theorem 1, D_j is placed in $\hat{S}$ with probability $\geq 1 - \varepsilon/(3 \cdot R(N) \cdot k)$. So, by taking a union bound over the relevant inputs, every input on which f depends on is in V with probability $\geq 1 - 2\varepsilon/(3 \cdot R(N))$. □

4.2 Filtering routine

Suppose that we are given the relevant inputs for the targeting function f. In order to learn $\mathcal{S}^{(\text{in})}$, it suffices to learn all the subsets $\mathcal{C}$ on these (at most k) inputs so that $f(\mathcal{C}) = 1$. Intuitively, this can be achieved by comparing any two combinations $\mathcal{C}_0, \mathcal{C}_1$ and testing whether containing one of these two subsets, say, $\mathcal{C}_1$, increases the chance to be targeted (compared to $\mathcal{C}_0$). On may expect that the latter certifies $f(\mathcal{C}_1) = 1$ and $f(\mathcal{C}_0) = 0$. Algorithm 3 (introduced next) builds upon this intuition.

```
**Input**: a set of inputs $V$; a family $\mathcal{F}$; a threshold parameter $t$.
**Output**: the class $\mathcal{T}_k$ of all bipartitions $\langle \mathcal{C}_{in}, \mathcal{C}_{out} \rangle$ of $V$ s.t. $\langle \mathcal{C}_{in}, \mathcal{C}_{out} \rangle \in \mathcal{S}^{(\mathrm{in})}$.
$k \leftarrow |V|$ ;
Partition $\mathcal{F}$ into $\mathcal{F}_1, \mathcal{F}_2, \ldots, \mathcal{F}_{2^k}$ s.t.:
    • $\forall 1 \leq i < 2^k,\ |\mathcal{F}_i| \geq |\mathcal{F}_{i+1}|$ ;
    • $\forall A_p, A_q \in \mathcal{F},\ A_p \cap V = A_q \cap V \iff A_p, A_q \in \mathcal{F}_i$ for some $i$;
for $i \in \{1, \ldots, 2^k\}$ do
    $V_i \leftarrow A_p \cap V$ with $A_p \in \mathcal{F}_i$ ;
end
$i_{\lim} \leftarrow \min\{1 \leq i \leq 2^k \mid |\mathcal{F}_i| \geq t \cdot |\mathcal{F}_{i+1}|\}$;
$\mathcal{T}_k \leftarrow \{\langle V_i, V \setminus V_i \rangle \mid 1 \leq i \leq i_{\lim}\}$ ;
```

Algorithm 3: Recognition algorithm for the targeting function.

It turns out that subtle complications occur which may prevent Algorithm 3 to be correct with high probability. These can be best defined by introducing a new parameter, that we define next.

Definition 1. *The oracle has* positive variance ψ *if for any family* $\mathcal{F} = \langle A_1, \ldots, A_t \rangle$ *the following holds for any* $\mathcal{C}_1, \mathcal{C}'_1 \in \mathcal{S}^{(in)}$*:*

$$\mathbb{P}r[\mathcal{O}_f(A_i) = 1 \mid A_i = \mathcal{C}_1, \mathrm{H}_{\mathcal{F}_{-i}}] \geq \psi \cdot \mathbb{P}r[\mathcal{O}_f(A_i) = 1 \mid A_i = \mathcal{C}'_1, \mathrm{H}_{\mathcal{F}_{-i}})].$$

We will show in Section 5 that it is, roughly, the comparison between the positive variance and the *targeting lift* (cf. Assumption 1) that determines what can be learnt within our model.

Theorem 3. *Suppose that the oracle has positive variance* $1 \geq \psi > \varphi$*, where* φ *denotes the targeting lift. Set* $1/\psi < t < 1/\varphi$*, and let* $\mathcal{B}$ *be a random Bernouilli family of size* m*.*

There is a constant d_t *such that if* f *is a* k*-junta that exactly depends on the* k *inputs in* V*,* $m \geq d_t \cdot \log^{1/\alpha}\left(3 \cdot 2^{2k+1}/\varepsilon\right)$*, and* $\mathcal{F}$ *contains the targeted accounts in* $\mathcal{B}$*, then Algorithm 3 outputs* f *with probability* $\geq 1 - \varepsilon$*.*

Proof. Set $d_1 = 12, d_2 = \frac{1}{\gamma}$ and $d_3 = 2^{k+1} \cdot \left(\frac{3 \cdot (1+t)^2}{\beta \cdot (1+\varphi) \cdot (1-t\varphi)^2}\right)^{1/\alpha}, d_4 = 2^{k+1} \cdot \left(\frac{3 \cdot (1+t)^2}{\beta \cdot (1+\psi) \cdot (t\psi-1)^2}\right)^{1/\alpha}$. Finally, set $d_t = \max_{1 \leq i \leq 4} d_i$.

Fix any pair $V_i, V_j \subseteq V$ so that $f(V_i) = 1$ (there are $\leq 4^k$ such pairs). Define $\mathcal{B}_i$, resp. $\mathcal{B}_j$, as the subfamily of all accounts $A_p \in \mathcal{B}$ so that $A_p \cap V = V_i$, resp. $A_p \cap V = V_j$. Since $\mathbb{E}[|\mathcal{B}_i|] = |\mathcal{B}|/2^k$ and $m = |\mathcal{B}|$ is large enough, by Chernoff bound (Lemma 1 with $\delta = 1/2$), we have that $|\mathcal{B}_i| \geq |\mathcal{B}|/2^{k+1}$ with probability $1 - \varepsilon/(3 \cdot 4^k)$. The latter implies by Assumption 2, $|\mathcal{F}_i| \geq \beta(\max\{d_3, d_4\}/2^{k+1})^{\alpha} \cdot \log\left(3 \cdot 2^{2k+1}/\varepsilon\right)$ with probability $\geq 1 - \varepsilon/(3 \cdot 4^k)$. We will show that, with high probability, $|\mathcal{F}_i| \geq t \cdot |\mathcal{F}_j|$ if and only if $f(V_j) = 0$, that will prove the theorem.

Denote by $\langle A_{p_1}, A_{p_2}, \ldots, A_{p_s} \rangle$ the subfamily of all accounts in $\mathcal{F}_i \cup \mathcal{F}_j$. Let X_l be the random Boolean variable denoting whether $A_{p_l} \in \mathcal{F}_i$. Fix the set of indices I of all accounts within $\mathcal{B}_i \cup \mathcal{B}_j$. Similarly, fix the subset $J \subseteq I$ of the s accounts within $\mathcal{F}_i \cup \mathcal{F}_j$, and fix the variables $X_1, X_2, \ldots, X_{l-1}$. Consider the set Ω of the histories $(\mathcal{B}, \mathcal{O})$ satisfying:

- all the entries of $\mathcal{O}$ that are indexed by J are nonzero (there may be other nonzero entries);
- all the entries of $\mathcal{O}$ that are indexed by $I \setminus J$ are equal to zero;
- for every $A_p \in \mathcal{B}$, we have that $A_p \in \mathcal{F}_i \cup \mathcal{F}_j$ if and only if $p \in I$;

- for every $1 \leq q \leq l-1$, $A_{p_q} \in \mathcal{F}_i$ if and only if $X_q = 1$.

Let $h_l : \langle A_1, \ldots, A_{p_l-1}, A_{p_l}, A_{p_l+1}, \ldots, A_m \rangle \to \langle A_1, \ldots, A_{p_l-1}, A'_{p_l}, A_{p_l+1}, \ldots, A_m \rangle$ where $A_{p_l} \setminus V = A'_{p_l} \setminus V$ and $\{A_{p_l} \cap V, A'_{p_l} \cap V\} = \{V_i, V_j\}$. Since $(\mathcal{B}, \mathcal{O}) \to (h_l(\mathcal{B}), \mathcal{O})$ is one-to-one, there is half of the histories in Ω which satisfy X_l.

On the one direction, assume $f(V_j) = 0$. For every $(\mathcal{B}, \mathcal{O}) \in \Omega$ such that X_l is satisfied, by Assumption 1:

$$\frac{\mathbb{P}r[\mathcal{O}_f(\mathcal{B}) = \mathcal{O}]}{\mathbb{P}r[\mathcal{O}_f(h_l(\mathcal{B})) = \mathcal{O}]} = \frac{\mathbb{P}r[\mathcal{O}_f(A_{p_l}) = 1 \mid A_{p_l} \cap V = V_i, \mathrm{H}_{\mathcal{B}-p_l} = \mathcal{O}_{-p_l}]}{\mathbb{P}r[\mathcal{O}_f(A_{p_l}) = 1 \mid A_{p_l} \cap V = V_j, \mathrm{H}_{\mathcal{B}-p_l} = \mathcal{O}_{-p_l}]} > 1/\varphi.$$

As a result, $\mathbb{P}r[X_l = 1 \mid X_1, \ldots, X_{l-1}] \geq 1/(1+\varphi) > t/(1+t)$. By Lemma 1 (with $p_{\min} = 1/(1+\varphi)$), since $|\mathcal{F}_i| \leq |\mathcal{F}_i| + |\mathcal{F}_j|$ is large enough, we have that that $|\mathcal{F}_i| \geq \frac{t}{1+t} \cdot (|\mathcal{F}_i| + |\mathcal{F}_j|)$ with probability $\geq 1 - \varepsilon/(3 \cdot 4^k)$, and so, $|\mathcal{F}_i| \geq t \cdot |\mathcal{F}_j|$ with high probability.

On the other direction, assume $f(V_j) = 1$. For every $(\mathcal{B}, \mathcal{O}) \in \Omega$ such that X_l is satisfied, by Definition 1:

$$\frac{\mathbb{P}r[\mathcal{O}_f(\mathcal{B}) = \mathcal{O}]}{\mathbb{P}r[\mathcal{O}_f(h_l(\mathcal{B})) = \mathcal{O}]} = \frac{\mathbb{P}r[\mathcal{O}_f(A_{p_l}) = 1 \mid A_{p_l} \cap V = V_i, \mathrm{H}_{\mathcal{B}-p_l} = \mathcal{O}_{-p_l}]}{\mathbb{P}r[\mathcal{O}_f(A_{p_l}) = 1 \mid A_{p_l} \cap V = V_j, \mathrm{H}_{\mathcal{B}-p_l} = \mathcal{O}_{-p_l}]} \leq 1/\psi.$$

As a result, $\mathbb{P}r[X_l = 1 \mid X_1, \ldots, X_{l-1}] \leq 1/(1+\psi) < t/(1+t)$. By Lemma 1 (with $p_{\max} = 1/(1+\psi)$), since $|\mathcal{F}_i| \leq |\mathcal{F}_i| + |\mathcal{F}_j|$ is large enough, we have that that $|\mathcal{F}_i| < \frac{t}{1+t} \cdot (|\mathcal{F}_i| + |\mathcal{F}_j|)$ with probability $\geq 1 - \varepsilon/(3 \cdot 4^k)$, and so, $|\mathcal{F}_i| < t \cdot |\mathcal{F}_j|$ with high probability. $\square$

Note that in [7], the oracle has positive variance 1. Therefore, it follows from Theorem 3 that *any* targeting function is learnable in this simpler model.

Furthermore, we notice that Algorithm 3 (or slight variations of it) can be proved correct under other assumptions that are similar in spirit as Definition 1. For instance, the oracle has *negative variance* ψ' if for any for any family $\mathcal{F} = \langle A_1, \ldots, A_t \rangle$ the following holds for any $\mathcal{C}_0, \mathcal{C}'_0 \notin \mathcal{S}^{(\mathrm{in})}$:

$$\mathbb{P}r[\mathcal{O}_f(A_i) = 1 \mid A_i = \mathcal{C}_0, \mathrm{H}_{\mathcal{F}_{-i}}] \geq \psi' \cdot \mathbb{P}r[\mathcal{O}_f(A_i) = 1 \mid A_i = \mathcal{C}'_0, \mathrm{H}_{\mathcal{F}_{-i}})].$$

When the oracle has negative variance $\psi' > \varphi$ the targeting function can be learnt by replacing line 3 in Algorithm 3 with $i_{\lim} \leftarrow \max\{1 \leq i \leq 2^k \mid |\mathcal{F}_i| \geq t \cdot |\mathcal{F}_{i+1}|\}$. Nonetheless, it remains elusive to learn the targeting function *without* any additional information. We will explain in the subsequent section why no such algorithm exists.

5 Impossibility results

Intuitively, the targeting function f can be learnt only if the *targeting lift* can be detected (cf. Assumption 1). Our additional assumptions on the positive, resp. negative, variance in Section 4.2 are ways to detect the lift using a simple leftmost, resp. rightmost, approach. In the general case when no such assumption holds, ambiguity may occur that prevents from detecting f with high certainty.

Proposition 1. *It is impossible to learn the targeting function f in general. In particular, there is a given monotone 2-junta that cannot be learnt even if the targeting lift is arbitrarily small.*

Proof. In order to prove the result, we will construct an oracle $\mathcal{O}_f$ that satisfies Assumptions 1, 2 and 3 for two distinct targeting functions. The latter is enough to prove the proposition since in such case, $\mathcal{O}_f$ could be used in our model for any of the two functions, and so, these cannot be distinguished with high probability. More precisely, fix $0 < p_0 < 1/5$. Let us define $\mathcal{O}_f$ such that for any combination $\mathcal{C}$:

$$\mathbb{P}r[\mathcal{O}_f(\mathcal{C}) = 1] = p_0 \cdot (1 + 2 \cdot \mathbb{I}_{\{D_1 \in \mathcal{C}\}} + 2 \cdot \mathbb{I}_{\{D_2 \in \mathcal{C}\}}).$$

Since every combination has positive probability to be targeted and the above oracle considers the combinations independently, by Chernoff bound, $\mathcal{O}_f$ satisfies Assumption 2 with $\alpha = 1$ for any targeting function. Furthermore, $\mathcal{O}_f$ satisfies Assumption 3 for any targeting function that only depends on the two inputs D_1, D_2. In particular, let $f_1(\mathcal{C}) = \max\{\mathbb{I}_{\{D_1 \in \mathcal{C}\}}, \mathbb{I}_{\{D_2 \in \mathcal{C}\}}\}$ and let $f_2(\mathcal{C}) = \mathbb{I}_{\{D_1 \in \mathcal{C}\}} \cdot \mathbb{I}_{\{D_2 \in \mathcal{C}\}}$. These two functions are monotone. In fact, they are linear combinations since $f_1(\mathcal{C}) = 1 \iff \mathbb{I}_{\{D_1 \in \mathcal{C}\}} + \mathbb{I}_{\{D_2 \in \mathcal{C}\}} \geq 1$, and similarly $f_1(\mathcal{C}) = 1 \iff \mathbb{I}_{\{D_1 \in \mathcal{C}\}} + \mathbb{I}_{\{D_2 \in \mathcal{C}\}} \geq 2$. For both functions, the oracle $\mathcal{O}_f$ satisfies Assumption 1 with any targeting lift $\varphi > 1/2$.

Finally, note that in order to extend this negative result to lifts arbitrarily smaller than 1/2, one may just consider a slightly more complex oracle for the above two functions f_1, f_2, namely:

$$\mathbb{P}r[\mathcal{O}_f(\mathcal{C}) = 1] = q_0^{3 - \mathbb{I}_{\{D_1 \in \mathcal{C}\}} - \mathbb{I}_{\{D_2 \in \mathcal{C}\}}},$$

for some nonzero probability q_0 that can be taken arbitrarily small. □

We point out that the negative result of Proposition 1 applies to the particular case when the targeting function is a linear combination of inputs. Hence, it applies to the theory behind the tools XRay [7] and Sunlight [8], that assume the targeting function is monotone or a linear combination of inputs respectively.

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