New structure learning algorithms and evaluation methods for large dynamic Bayesian networks

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JURY

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Declaration of originality: I hereby declare that this thesis is based on my own work and has not been submitted for any other degree or professional qualification, except when otherwise stated. Much of the work presented here has appeared in previously published conference and workshop papers. The chapters discussing the Benchmarking dynamic Bayesian Networks structure learning, DMMHC approach and evaluating its performance on real data are based on [100, 101]. Where reference is made to the works of others, the extent to which that work has been used is indicated and duly acknowledged in the text and bibliography.

Ghada TRABELSI BEN SAID (November, 2013)

DEDICATION

There are a number of people without whom this thesis might not have been written, and to whom I am greatly indebted.

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Abbreviations and Acronyms

AIC	Akaike Information Criterion
BIC	Bayesian Information Criterion
BD	Bayesian Dirichlet
BDe	Bayesian Dirichlet Equivalent
BN	Bayesian Network
CPC	set of Parents Children candidates
CPC_t	set of Parents Children candidates in t time slice
CP_{t-1}	set of Parent candidates in t-1 time slice
CPDAG	Complete Partially Directed Acyclic Graph
CC_{t+1}	set of Children candidates in t+1 time slice
DAG	Directed Acyclic Graph
DBN	Dynamic Bayesian Network
DMMHC	Dynamic Max Min Hill Climbing
DMMPC	Dynamic Max Min Parents Children
DSS	Decision support System
EM	Expectation Maximization
GS	Greedy Search
G_0	Initial network
$G_{\rightarrow}$	Transition network
HBN	Hierarchical Bayesian Netxork
IC, PC	Inductive/Predictive Causation
KDD	knowledge Data Discovery
KL-divergence	Kullback-Leibler divergence
MB	Markov Blanket
MCMC	Monte Carlo Markov Chain
MDL	Minimum Description Length
MIT	Mutual Information test
MMH	Max Min Heuristic
MMHC	Max Min Hill Climbing
MMPC	Max Min Parents Children

MWST	Maximum Weight Spanning Tree
Ne_0	set of neigherbood in time slice 0
Ne_+	set of neigherbood in time slice t $\geq$ 1
PDAG	Partially Directed Acyclic Graph
$PDAG_k$	Partially Directed Acyclic Graph with knowledge
SA	Simulated Annuling
SHD	Structural hamming Distance
SHD(2-TBN)	Structural hamming Distance for 2-TBN
SGS	Spirtes, Glymour & Scheines
RB	Reseau Bayésien
RBD	Reseau Bayésien Dynamique
2-TBN	two-slices Temporal Bayes Net

Résumé

La plupart des techniques de fouille des données utilisent des algorithmes qui fonctionnent sur des données fixes non temporelles. Cela est dû à la difficulté de la construction de ces modèles au niveau de l'exploitation des données temporelles (que certains qualifient comme complexes) qui sont délicates à manipuler. Ainsi peu des travaux proposent des algorithmes standards pour l'extraction des connaissances à partir de données multidimensionnelles et temporelles contrairement aux données statiques.

Dans plusieurs domaines tels que celui de la santé les données concernant un individu sont saisies à des moments différents d'une manière plus ou moins périodiques. Ainsi, dans ce domaine le temps est un paramètre important. Nous avons cherché à simplifier cette dimension (le temps) en utilisant un ensemble de techniques complémentaires de fouilles des données.

Dans ce contexte, la présente thèse présente deux contributions : l'extraction des modèles de connaissances en utilisant les réseaux bayésiens dynamiques (RBD) comme étant une technique de fouille de données et l'évaluation de ces modèles temporels (dynamiques).

L'apprentissage de structure dans les Réseaux Bayésiens (RB) est un problème d'optimisation combinatoire. En ce qui concerne la dépendance temporelle, les réseaux bayésiens sont changés par les réseaux bayésiens dynamiques. L'intégration du terme " temporel " rend l'apprentissage de structure dans les RBD plus compliqué. Nous sommes ainsi obligés de chercher l'algorithme le plus adéquat et le plus rapide pour résoudre ce problème.

Dans les développements récents, les algorithmes d'apprentissage de structure dans les modèles graphiques temporels basés sur les scores sont utilisés par plusieurs d'équipes de chercheurs dans le monde entier. Néanmoins, il existe quelques algorithmes d'apprentissage de structure des RB qui incorporent la méthode de recherche locale qui permet un meilleur passage à l'échelle. Cette méthode de recherche locale combine les algorithmes d'apprentissage basés sur les scores et ceux basés sur les contraintes. Cette méthode hybride, peut être utile pour être appliquer sur les réseaux bayésiens dynamiques pour l'apprentissage de structure. Nous avons pu par cette méthodes de rendre l'apprentissage de structure dans les RBD plus pratique et diminuer l'espace de recherche de solutions dans les RBD qui est qualifié par

sa complexité à cause de la temporalité. Nous avons aussi proposé une approche pour l'évaluation des modèles graphiques temporels (construits lors de l'étape de l'apprentissage de structure).

L'apprentissage de structure pour les RB statiques est bien étudié par plusieurs groupes de recherches. Nombreuses approches concernant ce sujet sont proposées et l'évaluation de ses algorithmes se fait par l'utilisation des différents standards Benchmarks et mesures d'évaluations.

A notre connaissance, toutes les études qui s'intéressent à l'apprentissage de structure pour les RBDs utilisent ses propres réseaux, techniques d'évaluations et indicateurs de comparaison. Ainsi l'accès aux bases de données et aux codes sources de ces algorithmes n'est pas toujours possible.

Pour résoudre ce problème, nous avons proposé une nouvelle approche pour la génération des grands benchmarks standards pour les RBD. Cette approche se base sur le Tiling avec une métrique permettant d'évaluer la performance des algorithmes d'apprentissage de structure pour les RBDs de type 2-TBN.

Nous avons obtenu des résultats intéressants. Le premier fournit un outil de génération des larges benchmarks pour l'évaluation des réseaux bayésiens dynamique. Le deuxième, consiste à une nouvelle mesure pour évaluer la performance des algorithmes d'apprentissage de structure. Comme troisième résultat, nous avons montré dans la partie expérimentale que les algorithmes DMMHC développés sont plus perfermants que les autres algorithmes d'apprentissage de structure pour les RBDs existants.

Abstract

Most of data mining techniques use algorithms that work on fixed non-temporal data. This is due to the difficulty of the construction of these models in exploitating temporal data (described as complex) which are difficult to handle. A small number of works that proposed algorithms to extract knowledge from temporal and multi-dimensional data differently from the static ones.

In many fields such as health, data about an individual are captured at different times on a more or less regular basis. Thus, in this field, time is an important parameter. Using a set of complementary data mining techniques, we tried to solve this persisting problem.

In this context, this thesis presents two fundamental contributions: the extraction of knowledge models using dynamic bayesian networks (DBNs) as a data mining technique and techniques for the evaluation of these temporal (dynamic) models.

The structure learning in the bayesian networks (BNs) is a combinatorial optimization problem. Regarding the time dependence, the Bayesian networks are changed by Dynamic Bayesian Networks (DBNs). The inclusion of the term "Time" makes the learning structure more complicated. We are thus obliged to seek for the most appropriate algorithm and the fastest way to solve this problem.

In recent developments, the structure learning algorithms in temporal graphical models based on the scores are used by many research teams around the world. However, there are some BNs structure learning algorithms that incorporate local search methods that provide a better scalability. This local search method is hybrid, i.e it combines the learning algorithms based on the scores and the learning algorithms based on constraints. This method can be useful to be applied to the Dynamic Bayesian Networks for learning structure. Relying on this method we tried to make the learning structure of DBNs more convenient and reduce its complexity caused by temporality.

The other problem that arises is the evaluation of these temporal graphical models (built by the structure learning step). The structure learning for static BN has been well studied by several research groups. Many approaches have been proposed on this topic. The evaluation of their algorithms is done by the use of different standards Benchmarks and evaluation measures.

As far as we know, all studies on DBNs structure learning use their own net-

works and indicators of comparison. In addition, the access to the datasets and to the source code is not always possible. To solve this problem, we proposed a new approach for the generation of large standard benchmarks for DBNs which is based on the Tiling with a metric used to evaluate the performance of structure learning algorithms for DBNs (2-TBN).

We obtained interesting results, first we provided a tool for benchmarking dynamic Bayesian network structure learning algorithms. Second, we proposed a novel metric for evaluating the structure learning algorithms performance. As a third result, we showed in the experimental results that the DMMHC algorithms achieve better performance than the other existing structure learning for DBNs.

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Introduction

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1.1 Research context

Time is an important factor in several domains as medicine, finance and industry. It is one of the important problems in machine learning. Machine Learning is the study of methods for programming computers to learn. Computers are used to perform a wide range of tasks, and for most of these it is relatively easy for programmers to design and implement the necessary software. However, there are many tasks for which this is difficult or impossible. These can be divided into four general categories.

- Tasks for which there exist no human experts.
- Tasks where human experts exist, but where they are unable to explain their expertise.
- Tasks with rapidly-changing phenomena.
- Tasks where applications that need to be customized for each user separately.

Machine learning addresses many of the same research questions as the fields of statistics, data mining, but with differences of emphasis. Statistics focuses on understanding the phenomena that have generated the data, often with the goal of testing different hypotheses about those phenomena. Data mining seeks to find patterns in the data that are understandable by people [26].
Most of studies use data mining techniques for the training of fixed data and the extraction of the static knowledge models. Among these models we find the probabilistic graphical model, commonly used in probability theory, statistics, Bayesian statistics and machine learning.

Graphical models are a marriage between probability theory and graph theory. They provide a natural tool for dealing with two problems that occur throughout applied mathematics and engineering, uncertainty and complexity, and in particular they are playing an increasingly important role in the design and analysis of machine learning algorithms. Fundamental to the idea of a graphical model is the notion of modularity, a complex system is built by combining simpler parts. Probability theory provides the glue whereby the parts are combined, ensuring that the system as a whole is consistent, and providing ways to interface models to data. The graph theoretic side of graphical models provides both an intuitively appealing interface by which humans can model highly-interacting sets of variables as well as a data structure that lends itself naturally to the design of efficient general-purpose algorithms [32].

Bayesian networks [78, 48, 52] are a kind of the probabilistic graphical models. They are frequently used in the field of Knowledge from Data Discovery (KDD). A Bayesian network is a directed acyclic graph whose nodes represent variables and directed arcs denote statistical dependence relations between variables, and a probability distribution is specified over these variables. Dynamic systems model-

ing has resulted an extension of the BN called Dynamic Bayesian networks (DBN) [23, 73]. In order to exploit relational models from time-series data (called discovery task), it is natural to use a dynamic Bayesian network (DBN). DBN is a directed graphical model whose nodes are across different time slices, to learn and reason dynamic systems. DBNs model a temporal process using a conditional probability distribution for each node and a probabilistic transition between time slices [113].

Learning a BN from observational data is an important problem that has been studied extensively during the last decade. The construction of these models can be acheieved either by using expertise, or from data. Many studies have been conducted on this topic, leading to different approaches:

- Methods for the discovery of conditional independence in the data to reconstruct the graph
- Methods for optimizing an objective function called score
- Methods for the discovery of local structure around a target variable to reconstruct the global structure of the network

Most of the studies have been limited to the structure learning of Bayesian networks in the static cases. There are a few algorithms for DBN structure learning [35, 50]. Most of these algorithms use a conventional method based on scores. Indeed, the addition of the time dimension further complicated the search space of solutions.

In the remainder of this thesis, we focus on the interest of hybrid approaches (the local search identification and global optimisation) in the dynamic case, which could more easily take into account the temporal dimension of our models.

Moreover, we noticed that the static BN structure learning is a well-studied domain. Many approaches have been proposed and the quality of these algorithms has been studied over a range of different standard networks and methods of evaluation. To our knowledge, all studies about DBN structure learning use their own benchmarks and techniques for evaluation. The problem in the dynamic case is that we don't find previous works that provide details about used networks and indicators of comparison. In addition, access to the datasets and the source code is not always possible. In this thesis, we also focus on solving the evaluation problem in dynamic case.

Our contribution consists to answer these issues:

1. Can we prove that the hybrid learning allows scaling in the dynamic case?

2. How can we evaluate this approach to justify the efficiency and scalability of our approch?

1.2 Thesis overview

The structure of the thesis is organized around three intertwined topics, see Figure 1.1.

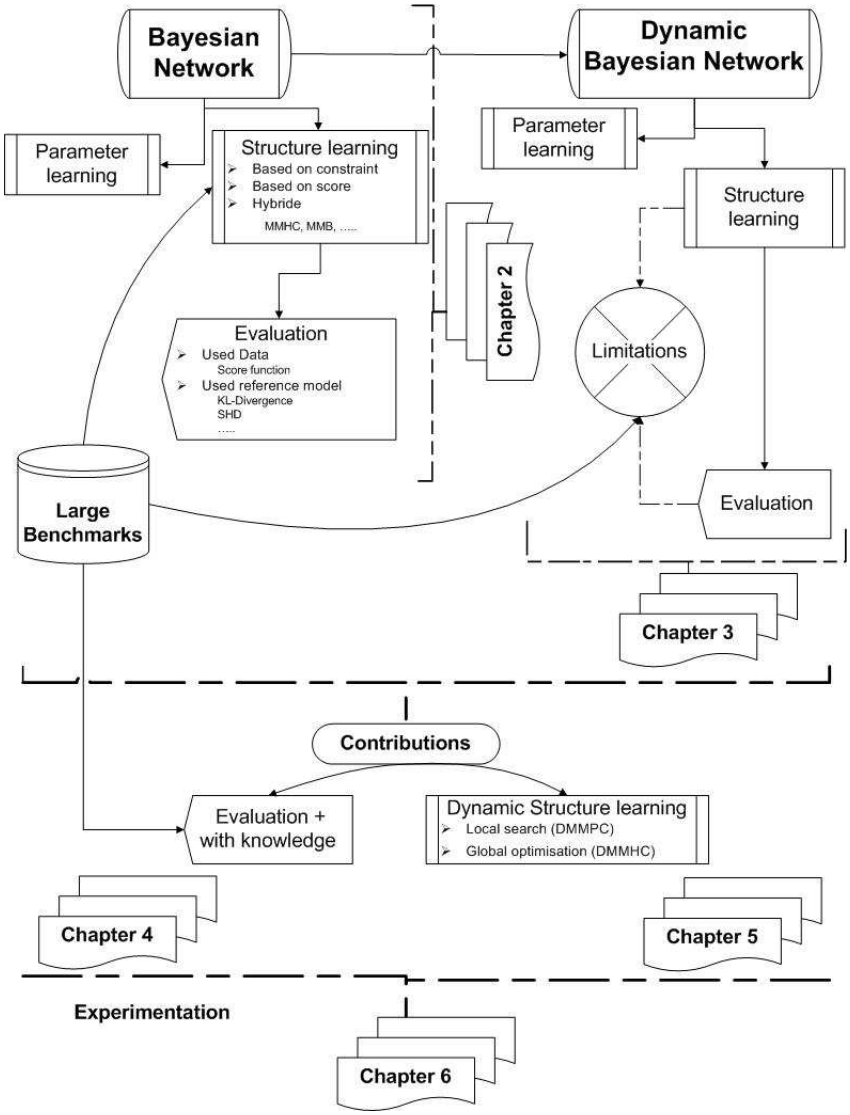

Figure 1.1: Thesis overview and interdependencies between chapters

Chapters 2 and 3 review the scientific background and establish the terminology required to discuss the structure learning for Bayesian Networks, thus providing the basis for the subsequent chapters of this thesis. It starts off by reminding some of the basic notations and definitions that are commonly used in the Bayesian Network literature.

Moreover, In chapter 3, we present the difference between the static Bayesian networks and their extension called dynamic bayesian networks when the time dimension is added. The two chapters are end up with an overview of the existing approaches for benchmarking static and dynamic bayesian networks and evaluating the structure learning algorithms in literature.

Chapter 4 is dedicated for our contributions. Initially, we show a description of our Benchmarking algorithms. The first one generates large dynamic bayesian with (2-TBN) form. The second is an extension of the structural hamming distance algorithm for the evaluation in the dynamic case. We also provide some experimental validation to justify the performance and utility of our first contributions.

Chapter 5 describes our new algorithm for DBN structure learning based on hybrid method. In this chapter, we give three (naïve, optimized and simplified) versions of our algorithm with the different necessary demonstrations. The chapter ends with the Time complexity of the algorithms and a toy example that presents the construction of structure learning proposed by our algorithms applied on simple Network.

Chapter 6 gives the different experiments achieved to show the performance of DMMHC algorithm in many levels as the quality and computational complexity of the algorithm for learning structure. In this chapter, we present the experimental protocol used in this thesis project. After that, we try to represent the obtained results and to compare the results given by the GS and SA algorithms with those given by naïve and optimized versions of our DMMHC. Also an interpretation and discussion of these results are achieved. In addition, we present a comparaison between our simplified DMMHC and the structure learning algorithms applied on a reduced search speace (2-TBN without intra-slice edges). Additional evidence of the scalability of DMMHC is found in the final section of this chapter.

Chapter 7 concludes the thesis summarizing the major results that we obtained. In addition, we tried to identify some perspectives for future research.

1.3 Publications

The following parts of this work have previously been published in different international journals and conferences:

- The contribution presented in chapter 4 was summarized in an article published in the proceedings of ICMSAO 2013 conference [100].
- The contribution presented in chapter 5 was summarized in an article published in the proceedings of IDA 2013 conference [101].
- Other application contributions not described in this thesis, were made by our research group in REGIM lab (Tunisia), have been the object of two scientific publications in Data Mining Workshops (ICDMW), 2012 IEEE 12th International Conference [63] and International Journal of Advanced Research in Artificial Intelligence [64]. In these works, we discussed the use of different data mining techniques as the dynamic Bayesian Networks and 3D visualization in Dynamic Medical Decision Support System.

I

State of the art

2

Bayesian Network and structure learning

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2.1 Introduction

Knowledge representation and reasoning from these representations have given birth for many models. Probabilistic graphical models, and more specifically the Bayesian networks, initiated by Judea Pearl in the 1980s, have proven to be useful tools for the representation of uncertain knowledge, and reasoning from incomplete information. Afterwards many studies such as [78, 59, 49, 52] introduced Bayesian probabilistic reasoning formalism.

In this thesis we are interested in Bayesian network learning. Learning Bayesian network consists of two phases: parameter learning and structure learning. There are three types of approaches for the structure learning: methods based on identification of conditional indepedence, methods based on the optimization of a score and hybrid methods (cf. Figure 2.1).

To hightlight the benefits of structure learning algorithms, we have to evaluate the quality of the Bayesian networks obtained by these learning algorithms. Many evaluation metrics are used in research. Some of them are characterized by the use of data as the score-based method. Some others are characterized by the use of a reference model. In our context, we are interested in the evaluation techniques using a reference model with a large number of variables.

This chapter reviews basic definitions and notations of classical Bayesian network and conditional independence. Section 2.2 introduces some notations and definitions of BN. Section 2.3 provides an overview of the static Bayesian networks structure learning. Based on this background, Section 2.4 is devoted to the evalution of Bayesian networks structure. Finally, in this chapter we present the existing approaches used to evaluate these structure learning algorithms on large benchmarks.

2.2 Bayesian Network definition

2.2.1 Description example [75]

The presence or absence of a disease in a human being has a direct influence on whether a test for that disease turns out positive or negative. We would use Bayes' theorem (cf. theorem 2.2.1) to compute the conditional probability of an individual to have a disease when a test for the diseaseturns out to be positive.

Let's consider the situation where several features are related through inference chains. For example, whether or not an individual has a history of smoking has a

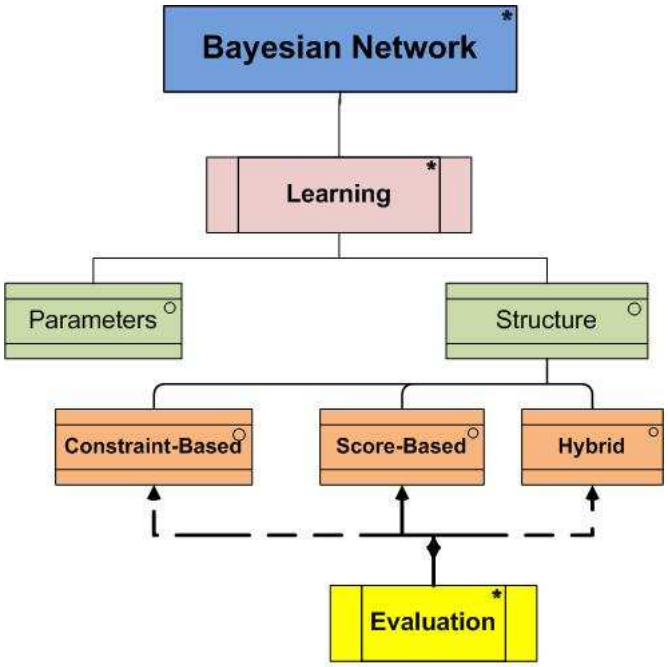

Figure 2.1: The different concepts presented in chapter 2

direct influence both on whether or not that individual has bronchitis and on whether or not that individual has lung cancer. In turn, the presence or absence of each of these diseases has a direct influence on whether or not the individual experiences fatigue.

Also, the presence or absence of lung cancer has a direct influence on whether or not a chest X-ray is positive. We would want to determine, for example, the conditional probabilities of both of bronchitis and of lung cancer when it is known that the individual smokes, is fatigued, and has a positive chest X-ray. Yet bronchitis has no direct influence (indeed no influence at all) on whether a chest X-ray is positive. Therefore, these conditional probabilities cannot be computed using a simple application of Bayes' theorem. There is a straightforward algorithm for computing them, but the probability values it requires are not ordinarily accessible;

Bayesian networks were developed to address these difficulties. By exploiting conditional independencies entailed by influence chains, it is able to represent a large instance in a Bayesian network using little space. We are also often able to perform probabilistic inference among the features in an acceptable period of time. In addition, the graphical nature of the Bayesian networks gives a much better intuitive grasp of the relationships among the features.

Figure 2.2 shows a Bayesian network representing the probabilistic relationships among the above discussed features. The values of the features in that network are represented in table 2.1

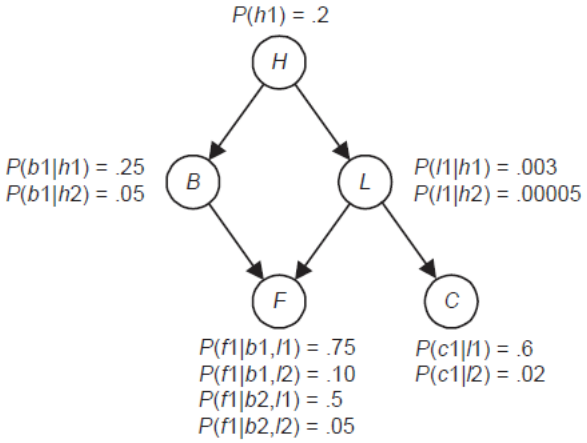

Figure 2.2: Example of Bayesian Network

Feature	Value	When the Feature Takes this Value
H	h1	There is a history of smoking
	h2	There is no history of smoking
B	b1	Bronchitis is present
	b2	Bronchitis is absent
L	l1	Lung cancer is present
	l2	Lung cancer is absent
F	f1	Fatigue is present
	f2	Fatigue is absent
C	c1	Chest X-ray is positive
	c2	Chest X-ray is negative

Table 2.1: The values of the features

2.2.2 Basic concepts

In this section, we give some basic concepts related to the Bayesian network used in our approach:

Definition 2.2.1 *Let X and Y be two sets of random variables, given that the probability of Y is different from zero, the conditional probability of X is defined by:*

$$P(X|Y) = \frac{P(X;Y)}{P(Y)} \tag{2.1}$$

Theorem 2.2.1 *(Bayes' theorem) [7]*
Let X and Y two sets of random variables, the Bayes' theorem determines the conditional probability of X given Y based on the probabilities of X, Y and Y given X, with the following formula:

$$P(X|Y) = \frac{P(Y|X).P(X)}{P(Y)} \tag{2.2}$$

Definition 2.2.2 *(Independence)*
Let X and Y two sets of random variables, X and Y are independent, denoted $<X \perp Y>$*, if and only if* $P(X|Y) = P(X)$.

Definition 2.2.3 *(Conditionally independent)*
Let X, Y, and Z be any three subsets of random variables. X and Y are said to be conditionally independent given Z (noted $Ind_P(X;Y \mid Z)$*) if* $P(X \mid Y, Z) = P(X \mid Z)$ *whenever* $P(Y,Z) > 0$.

Definition 2.2.4 *(directed graph)*
A directed graph G can be defined as an ordered pair that consists of a finite set V of nodes and an irreflexive adjacency relation E on V. The graph G is denoted as (V,E) . For each $(x,y) \in E$ *we say that there is an arc (directed edge) from node x to node y. In the graph, this is denoted by an arrow from x to y and x and y are called the start point and the end point of the arrow respectively. We also say that node x and node y are adjacent or x and y are neighbors of each other and node y and node x are adjacent or y and x are neighbors of each other. x is also called a parent of y and y is called a child of x. By using the concepts of parent and child recursively, we can also define the concept of ancestor and descendent. We also call a node that does not have any parent a root node. By irreflexive adjacency relation we mean that for any* $x \in V$ *,* $(x,x) \notin E$ *, i.e., an arc cannot have a node as both its start point and end point.*

Definition 2.2.5 *(Path)*
A path in a directed graph is a sequence of nodes from one node to another using the arcs.

Definition 2.2.6 *(directed path and cycle)*
A directed path from X_1 *to* X_n *in a DAG G is a sequence of directed edges* $X_1 \rightarrow X_2 \ldots \rightarrow X_n$*. The directed path is a cycle if* $X_1 = X_n$ *(i.e. it begins and ends at the same variable).*

Definition 2.2.7 *(A directed acyclic graph)*
A DAG is a Directed Acyclic (without cycles) Graph (See Figure 2.4.a).

Definition 2.2.8 *(d-separation)*
Let S be a trail (that is, a collection of edges which is like a path, but each of whose edges may have any direction) from node u to v. Then S is said to be d-separated by a set of nodes Z if and only if (at least) one of the following holds:

1. *S contains a chain,* $x \leftarrow m \leftarrow y$*, such that the middle node m is in Z,*
2. *S contains a fork,* $x \leftarrow m \rightarrow y$*, such that the middle node m is in Z, or*

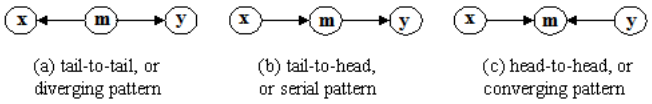

Figure 2.3: Patterns for paths through a node

3. *S contains an inverted fork (or collider), $x \rightarrow m \leftarrow y$, such that the middle node m is not in Z and no descendant of m is in Z.*

The graph patterns of "tail-to-tail", "tail-to-head" and "head-to-head" are shown in Figure 2.3. Thus u and v are said to be d-separated by Z if all trails between them are d-separated. If u and v are not d-separated, they are called d-connected.

Definition 2.2.9 *(D-separation for two sets of variables)*
Two sets of variables X and Y are d-separated by Z in a graph G (noted $Dsep_G(X;Y \mid Z)$) if and only if $\forall\ u \in X$ and $\forall\ v \in Y$, every tail from u to v d-separated by Z.

2.2.3 Bayesian Network definition

Definition 2.2.10 *(Markov condition) [78]*
The Markov condition can be stated as follows: Each variable X_i is conditionally independent of all its no-descending, knowing the state of his parents, $Pa(X_i)$.

$$Ind_P(X_i; NoDesc(X_i) \mid Pa(X_i)). \tag{2.3}$$

$$P(X_i|Pa(X_i); NoDesc(X_i)) = P(Xi|Pa(X_i)) \tag{2.4}$$

Definition 2.2.11 *(Bayesian Network) [75]*
Let P be a joint probability distribution of the random variables in some set V, and G = (V, E) be a DAG. We call (G,P) a Bayesian network if (G,P) satisfies the Markov condition. P is the product of its conditional distributions in G, and this is the way P is always represented in a Bayesian network.
A Bayesian Network B=(G,θ) is defined by:

- *G=(V,E) directed graph without circuit whose vertices are associated with a set of random variables $X = X_1,...,X_n$, there is a bijection between X and V (i.e. $X_i \longleftrightarrow V_i$) and E is the set of arcs representing the conditional independence between variables,*
- *$\theta = P(X_i|Pa(X_i))$, all probabilities of each node X_i conditional on the state of its parents $Pa(X_i)$ in G.*

Pearl et al. [78] have also shown that the Bayesian networks allow us to represent compactly the joint probability distribution over all variables:

$$P(X_1, X_2, ..., X_n) = \prod_{i=1}^{n} P(X_i|Pa(X_i)) \tag{2.5}$$

This decomposition of a global function, into a product of local terms depending only on the same node and its parents in the graph, is a fundamental property of Bayesian networks.

Theorem 2.2.2 *[93]*
In a BN, two nodes are d-separated by Z, they are also conditionally independent by Z.

$$Dsep_G(X; T|Z) = Ind_P(X; T|Z) \tag{2.6}$$

The graphical part of the Bayesian network indicates the dependencies (or independence) between variables and provides a visual tool for knowledge representation to make it more comprehensible to its users. In addition, the use of probabilities allows taking into account the uncertainty in quantifying the dependencies between variables.

2.2.4 Markov equivalence classes for directed Acyclic Graphs

There may be many DAGs associated to BNs that determine the same dependence model. Thus, the family of all DAGs with a given set of vertices is naturally partitioned into Markov-equivalence classes, with each class being associated with a unique independence model (See Figure 2.4.c).

Definition 2.2.12 *(Markov Equivalence) [77, 75, 104]*
Two DAGs G_1 and G_2 on the same set of nodes are Markov Equivalent if for every three mutually disjoint subsets A, B, C $\subseteq$ V, $Desp_{G1}$(A,B | C) $\Leftrightarrow$ $Desp_{G2}$(A,B | C).

Theorem 2.2.3 *(Verma and Pearl, 1991) [109]*
Two DAGs are equivalent if and only if they have the same skeleton and the same V-structures.

Definition 2.2.13 *(Patterns) [69]*
The pattern for a partially directed graph G is the partially directed graph which has the identical adjacencies as G and which has an oriented edge A $\rightarrow$ B if and only if there is a vertex C $\notin$ adj(A) such that A $\rightarrow$ B and C $\rightarrow$ B in G. Let pattern (G) denote the pattern for G. A triple (A, B, C) is an unshielded collider in G if and only if A $\rightarrow$ B, C $\rightarrow$ B and A is not adjacent to B (V-structure). It is easy to show

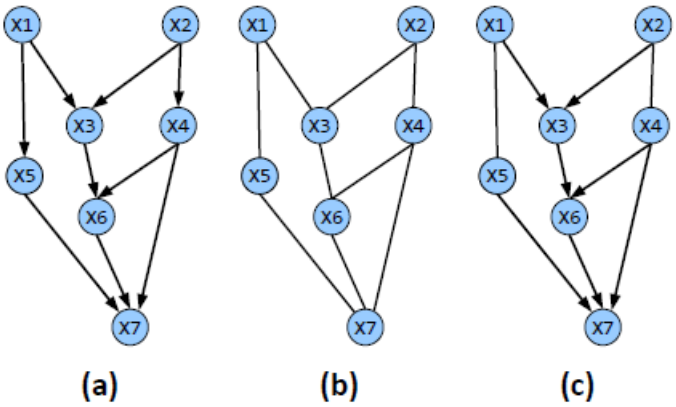

Figure 2.4: (a) Example of DAG, (b) the skeleton relative to the DAG and (c) an example of a PDAG [70]

that two directed acyclic graphs have the same pattern if and only if they have the same adjacencies and same unshielded colliders.

Theorem 2.2.4 *(Verma and Pearl, 1991) [109]*
Two directed acyclic graphs G and G' are Markov equivalent if and only if pattern(G) = pattern(G1).

Definition 2.2.14 *(Completed PDAG (CPDAG))*
The completed PDAG corresponding to an equivalence class is the PDAG consisting of a directed edge for every compelled edge in the equivalence class, and an undirected edge for every reversible edge in the equivalence class. An arc is said to be reversible if its reversion leads to a graph which is equivalent to the first one. An arc is said to be compelled if it is not reversible.

Several researchers, including [109, 69, 14], present rules based algorithms that can be used to implement DAG-to-CPDAG. The idea of these implementations is as follows. First, they undirect every edge in a DAG, except for those edges that participate in a v-structure. Then, they repeatedly apply one of a set of rules that transform undirected edges into directed edges. Meek proves that the transformation rules are sound and complete. That is, once no rule matches on the current graph, that graph must be a completed PDAG [69] (see Figures 2.5 R1, R2 and R3). We can notice that Chickering proposed an optimized implementation for this phase (PDAG determination) [14]. A CPDAG of graph G is the representation of all graphs equivalent to G.

Definition 2.2.15 *(Dependency model) [69]*
A dependency model is a list M of conditional independence statements of the form $A \perp B|S$ where A, B, and S are disjoint subsets of V

Definition 2.2.16 *(complete causal explanation) [69]*
A directed acyclic graph G is a complete causal explanation of $\boldsymbol{M}$ *if-and only if the set of conditional independence facts entailed by G is exactly the set of facts in* $\boldsymbol{M}$.

Meek proposed some orientation rules to find a partially directed graph whose adjacencies are the same as any complete causal explanation for M and whose edges are directed if and only if every complete causal explanation for M has the edges oriented.

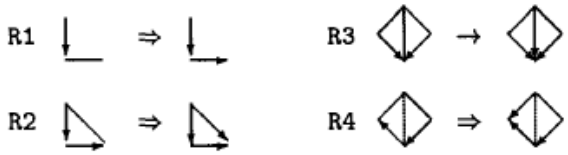

Figure 2.5: Orientation rules for patterns [69]

Let K be a set of background knowledge. K is a pair (F, R) where F is the set of directed edges which are forbidden, R is the set of directed edges which are required.

Definition 2.2.17 *(*$CPDAG_K$ *with Knowledge)*
A $CPDAG_K$ *of graph G representing all equivalent graphs of G and consistent with a set of knowledge K defining the priori.*

When proposing a first algorithm to determine the PDAG of a given graph, [69] Meek also proposed a way to take into account prior background knowledge.

This solution is decomposed into three phases. The first phase consists in determining the PDAG. As we mentioned before, this step can be solved by keeping the skeleton of the given DAG, and its V-structures, and then applying recursively a set of three rules R_1, R_2, and R_3 (Figure 2.5) in order to infer all the edge orientations compatible with the initial DAG.

The second phase consists in comparing this PDAG with the prior knowledge. If some information are conflicting, the algorithm turns out to be an error. The final step consists in iteratively adding the prior knowledge (edges) not present in the PDAG and applying again the previous recursive orientation rules in order to infer all the new edge orientations induced by the addition of the prior knowledge.

Meek demonstrates that another rule R_4 (figure 2.5) is needed in order to complete the three previous ones when we add the prior knowledge for the model.

2.3 Bayesian network structure learning

In recent years there has been a growing interest in the structure learning of the Bayesian networks from data [42, 77, 11, 75, 104]. There are three approaches for

finding a structure. The first approach poses learning as a constraint satisfaction problem. In this approach, we try to identify the properties of conditional independence among the variables in the data. This is usually done using a statistical hypothesis test, like the χ^2 test. We then build a network that exhibits the observed dependencies and independencies.

The second approach poses learning as an optimization problem. We start by defining a statistically motivated score that describes the fitness of each possible structure from the observed data. The learner's task is then to find a structure that maximizes the score. In general, this is an NP-hard problem [11], and thus we need to resort to heuristic methods. Although the constraint satisfaction approach is efficient, it is sensitive to failures in independence tests. Thus, the common opinion is that the optimization approach is a better tool for learning structure from a little amount of data.

The third approach, named hybrid methods, can solve this problem by the combination of the two previous ones. Local search methods are dealing with local structure identification and global model optimization constrained with these local information. These methods are able to scale distributions with more than thousands of variables.

Generally, people face the problem of learning BNs from training data in order to apply BNs to real-world applications. Typically, there are two categories in learning BNs, one is to learn BN parameters when a BN structure is known, and another is to learn both BN structures and parameters. We notice that, learning BN parameters can be handled with complete and incomplete data. This kind of learning is not as complicated as learning a BN structure. In this thesis, we focus on structure learning with complete data, as we recommend to read appendix A before reading this section.

2.3.1 Constraint-Based Learning

The idea of constraint-based structure learning is to know how to construct the structure of Bayesian network if we can perform independence test ($A \perp B|C$).

Constraint-based methods employ the conditional independence tests to first identify a set of conditional independence properties, and then attempts to identify the network structure that best satisfies these constraints corresponding to a CPDAG.

Fast [29] describes the constraint identification as "the process of learning the skeleton and separating sets from the training data. Due to limited size of the training data, this process is inherently error-prone. The goal of constraint identification is to efficiently identify the independence assertions while minimizing the number of constraints that are inaccurate. Constraint identification algorithms appearing in

the literature can be differentiated by three different design decisions: (1) the type of independence test used, (2) the ordering heuristic and other algorithmic decisions, and (3) the technique used to determine the reliability of the test".

This first family of structure learning approaches for BN, often called search under constraints, is derived from the work of Pearl's team and Spirtes' team. The most popular constraint-based algorithms are IC [78], SGS and PC [77, 104] algorithms. Three of them try to d-separate all the variable pairs with all the possible conditional sets whose sizes are lower than a given threshold. They are based on the same principle:

- build an undirected graph containing the relationships between variables, from conditional independence tests
- detect the V-structures (also using conditional independence tests)
- propagate the orientation of some arcs with meek's rules in section 2.2.4
- randomly direct some other edges in the graph without changing its CPDAG
- take into account the possible artificial causes due to latent variables.

One problem with constraint-based approaches is that they are difficult to reliably identify the conditional independence properties and to optimize the network structure [67].

The constraint-based approaches lack an explicit objective function and they do not try to directly find the global structure with maximum likelihood. So they do not fit in the probabilistic framework.

This kind of approach rely on quite heavy assumptions such as the faithfulness and correctness of the independence tests. In contrast, score-based algorithms search for the minimal model among all Bayesian networks.

2.3.2 Score-Based Learning

Unlike the first family of methods that construct the structure with the use of conditional independence between variables, this approach tries to define scoring function that evaluates how well a structure matches the data and to identify the graph with the highest score. These approaches are based on several scores such as BIC [87], AIC [2], MDL [57], BD [17], BDe [42]. All these scores are approximation of the marginal likelihood P(D|G) [18].

The score-Based methods are feasible in practice if the score should be locally decomposable. This score is expressed as the sum of local scores at each node. There is also the problem of search space of bayesian networks to find the best structure. The main problem with these approaches is that, it is NP-hard to compute the optimal structure using bayesian scores [11]. There are several algorithms for structure learning based on BN scores as MWST [15], K2 [17], and GS. Some proposed algorithms work in a small space such as trees [15], polytrees [15] and

hypertrees [94].

In this section, we present details of the Greedy search (GS) and Similated Annealing (SA) as we will compare them later with our algorithms because their extentions in dynamic case and their code sources (softwares) are available on the internet.

Greedy search algorithm This algorithm (algorithm 1) follows the heuristic problem solving of making the locally optimal choice at each step with the hope of finding a global optimum. It is initialized by a network G_0. It collects all possible simple graph operations (e.g., edge addition, removal or reversal) that can be performed on the network without violating the constraints (e.g., introducing a cycle), we use for this the Generate neighborhood algorithm (algorithm 2). Then, it picks the operation that increases the score of the network the most (This step can be repeated if the network can still be improved or the maximal number of interactions haven't been reached).

Algorithm 1 GS(G_0)

Require: initial graph (G_0)
Ensure: BN structure (DAG)

$G \leftarrow G_0$
$Test \leftarrow$ True
$S \leftarrow$ Score(G,D)
while $Test$=True **do**
  $N \leftarrow$ Generate_neighborhood(G, $\emptyset$)
  G_{max}= arg max$_{F \in N}$Score(F,D)
  if Score(G_{max},D) > S **then**
    G $\leftarrow$ G_{max}
    S $\leftarrow$ Score(G_{max},D)
  else
    $Test \leftarrow$ False
  end if
end while
return the DAG G found

Algorithm 2 Generate_neighborhood(G,G_c)

Require: current DAG (G); undirected graph of constraints (G_c)
Ensure: set of neighborhood DAGs (N)

$N \leftarrow \phi$
for all $e \in G$ **do**
  N $\leftarrow$ N $\bigcup$ ($G \setminus$\{e\}) % delete_edge(e)
  if acyclic($G \setminus$\{e\}$\bigcup$ invert(e)) **then**
    N $\leftarrow$ N $\bigcup$ ($G \setminus$\{e\}$\bigcup$ invert(e)) % invert_edge(e)
  end if
end for
for all $e \in G_c$ And $e \notin G$ **do**
  if acyclic($G \bigcup$\{e\}) **then**
    N $\leftarrow$ N $\bigcup$ ($G \bigcup$\{e\}) % add_edge(e)
  end if
end for

Simulated annealing algorithm (SA) This is another generic metaheuristic for the global optimization problem of locating a good approximation to the global optimum of a given function in a large search space. It can be used when the search space is discrete. the goal of this method is to find an acceptable good solution in a fixed amount of time, rather than the best possible one.

the SA algorithm can be seen as the previous GS algorithm where we replace step 8 by a softer comparison where we allow score decrease in the first iterations of the algorithm and we become more and more strict over the iterations.

2.3.3 Hybrid method or local search

Algorithm 3 MMHC(D)

Require: Data (D)
Ensure: BN structure (DAG)

1: $G_c \leftarrow \phi$
2: $G \leftarrow \phi$
3: $S \leftarrow 0$
% Local identification
4: **for all** $X \in \mathbf{X}$ **do**
5: CPC_X=MMPC(X, D)
6: **end for**
7: **for all** $X \in \mathbf{X}$ And $Y \in CPC_X$ **do**
8: $G_c \leftarrow G_c \bigcup$ (X,Y)
9: **end for**
% Greedy search (GS) optimizing score function in DAG space
10: G $\leftarrow$ GS(G_c)
11: return the DAG G found

Algorithm 4 MMPC(T, D)

Require: target variable (T); Data (D)
Ensure: neighborhood of T (CPC)

1: $ListC$ =$\mathbf{X} \setminus \{T\}$
2: $CPC = \overline{\text{MMPC}}(T, D, ListC)$
% Symmetrical correction
3: **for all** $X \in CPC$ **do**
4: **if** $T \notin \overline{\text{MMPC}}(X, D, \mathbf{X} \setminus \{X\})$ **then**
5: $CPC = CPC \setminus \{X\}$
6: **end if**
7: **end for**

Local search algorithms are hybrid BN structure learning methods dealing with local structure identification and global model optimization constrained with these local information.

Several local structure identifications have been proposed. They were dedicated to discover the candidate Parent-Children (PC) set of a target node such as the Max-Min Parent Children (MMPC) algorithm [102] or the Markov Blanket (MB) i.e. parents, children and spouses, of the target node [105, 85]. If the global structure

identification is the final goal, Parent-Children identification is sufficient in order to generate a global undirected graph which can be used as a set of constraints in the global model identification. For instance, the recent Max-Min Hill-Climbing algorithm (MMHC) (cf. algorithm 3) proposed by Tsamardinos [104] combines the local identidication provided by Max-Min Parent Children (MMPC) algorithm and a global greedy search (GS) where the neighborhood of a given graph is generated with the following operators: add_edge is restricted to edges discovered in the local search identification phase (if the edge belongs to the set of constraints and if the resulting is acyclic DAG) (see algorithm 3), delete_edge and invert_edge (if the resulting is acyclic DAG) (see algorithm 2).

The MMPC local structure identification, described in Algorithm 4, is decomposed into two tasks, the neighborhood identification itself ($\overline{\text{MMPC}}$), completed by a symmetrical correction (X belongs to the neighborhood of T if the opposite is also true). The neighborhood identification ($\overline{\text{MMPC}}$), described in Algorithm 5, uses the Max-Min Heuristic defined in Algorithm 6 in order to iteratively add (forward phase) in the candidate Parent-Children set (neighborhood) of a target variable T the variable the most directly dependent on T conditionally to its current neighborhood (line 1 in algorithm 6). This procedure can potentially add some false positives which are then deleted in the backward phase. Dependency is measured with an association measurement function $Assoc$ like χ^2, mutual information or G^2.

Algorithm 5 $\overline{\text{MMPC}}(T, D, ListC)$

Require: target variable (T); Data (D); List of potential candidates ($ListC$)
Ensure: neighborhood of T (CPC)

1: $CPC = \emptyset$
   % Phase I: Forward
2: **repeat**
3: $< F, assocF >=$ MaxMinHeuristic$(T, CPC, ListC)$
4: **if** $assocF \neq 0$ **then**
5: $CPC = CPC \bigcup \{F\}$
6: $ListC = ListC \setminus \{F\}$
7: **end if**
8: **until** CPC has not changed or $assocF = 0$ or $ListC = \emptyset$
   % Phase II: Backward
9: **for all** $X \in CPC$ **do**
10: **if** $\exists S \subseteq CPC$ **and** $assoc(X; T|S) = 0$ **then**
11: $CPC \setminus \{X\}$
12: **end if**
13: **end for**

Algorithm 6 MaxMinHeuristic$(T, CPC, ListC)$

Require: target variable (T); current neighborhood (CPC); List of potential candidates ($ListC$)
Ensure: the candidate the most directly dependent to T given CPC (F) and its association measurement ($AssocF$)

1: $assocF = max_{X \in ListC} Min_{S \subseteq CPC} Assoc(X; T|S)$
2: $F = argmax_{X \in ListC} Min_{S \subseteq CPC} Assoc(X; T|S)$

2.3.4 Learning with large number of variables

Bayesian network learning is a useful tool for exploratory data analysis. However, applying Bayesian networks to the analysis of large-scale data, consisting of thousands of variables, is not straight forward because of the heavy computational burden in learning and visualization. Some studies have focused on this problem to solve it through different approaches.

Friedman et al [33] introduce an algorithm that achieves faster learning from massive datasets by restricting the search space. Their iterative algorithm named "Sparse Candidate" restricts the parents of each variable to belong to a small subset of candidates. They then search for a network that satisfies these constraints. The learned network is then used to select better candidates for the next iteration. This algorithm is based on 2 steps: the first step is named restrict based on data D and B_{n-1} network, the selected candidates for X_i's parents include X_i's current parents. This requirement (restrict step) implies that the winning network B_n is a legal structure in the n+1 iteration. Thus, if the search procedure at the second step named maximize also examines this structure, it must return a structure that scores at least as well as B_n. The stopping criteria for the algorithm is when Score(B_n)=Score(B_{n-1}).

Steck and Jaakkola [96] look at active learning in domains with a large number of variables. They developed an approach to unsupervised active learning which is tailored to large domains. The computational efficiency crucially depends on the properties of the measure with respect to which the optimal query is chosen. The standard information gain turns out to require a committee size that scales exponentially with the size of the domain (the number of random variables). Also, they propose a new measure, which they term "average KL divergence of pairs" (KL2). It emerges as a natural extension to the query by the committee approach [30]. The advantages of this approach are illustrated in the context of recovering (regulatory) network models. The regulatory network involves 33 variables, 56 edges, and each variable was discretized to 4 states.

In 2006, Hwangand et al [44] proposed a novel method for large-scale data analysis based on hierarchical compression of information and constrained structural learning, i.e., hierarchical Bayesian networks (HBNs). The HBN can compactly visualize global probabilistic structure through a small number of hidden variables, approximately representing a large number of observed variables. An efficient learning algorithm for HBNs, which incrementally maximizes the lower bound of the likelihood function, is also suggested. They propose a two-phases learning algorithm for hierarchical Bayesian networks based on the above decomposition. In the first phase, a hierarchy for information compression is learned. After building the hierarchy, they learn the edges inside a layer when necessary by

the second phase. The effectiveness of their method is demonstrated by the experiments on synthetic large-scale Bayesian networks and a real-life microarray dataset. All variables were binary and local probability distributions were randomly generated. In this work, they show the results on two scale-free and modular Bayesian networks, consisting of 5000 nodes. Training datasets having 1000 examples.

Tsamardinos et al. [104] present an algorithm for the Bayesian network structure learning, called Max-Min Hill-Climbing (MMHC) described in the previous section. They show the ability of MMHC to scale up to thousands of variables. Tsamardinos brought the evidence of the scalability of MMHC by a reported experiment in Tsamardinos et al. [102] (for example MMPC was run on each node and reconstructed the skeleton of a tiled-ALARM network with approximately 10,000 variables from 1000 training instances).

De Campos et al [20] propose a new any-time exact algorithm using a branch-and-bound (B&B) approach with caches. Scores are computed during the initialization and a poll is built. Then, they perform the search over the possible graphs iterating over arcs. Although iterating over orderings is probably faster, iterating over arcs allows us to work with constraints in a straight forward way. Because of the B&B properties, the algorithm can be stopped at any-time with a best current solution found so far and an upper bound to the global optimum, which gives a kind of certificate to the answer and allows the user to stop the computation when she believes that the current solution is good enough. They show also empirically the advantages of the properties and the constraints, and the applicability of their presented algorithm that integrates parameter and structural constraints with large data sets (up to one hundred variables), that cannot be handled by other current methods (limited to around 30 variables), in a way to guarantee global optimality with respect to the score function.

2.4 Evaluation of Bayesian Network structure learning algorithms

2.4.1 Evaluation metrics

In the previous sections, we presented some bayes Net structure learning algorithms. In this section we present methods that evaluate the quality of the Bayesian network obtained by the structure learning algorithms.

There are two scenarios for the evaluation of a structure learning algorithm:

– Given a theoretical BN $B_0 = (G_0 ; \theta_0)$ and data D generated from the BN, the measures evaluate the quality of the algorithm by comparing the quality of the learned graph $B = (G,\theta)$ and that of the theoretical network B_0 with the

use of data

– the measure evaluates the quality of the algorithm by comparing the structure G of the learned graph and the structure G_0 of the theoretical graph.

To this end we notice that it would be better to compare the equivalence classes given by the original and learned BN. A BN obtained from the data is identified by its equivalence class. The best BN is obtained if we find that the CPDAG of the generated network is equal to that of the learned BN. So, all evaluation metrics must use the equivalence class to compare between the BNs for better evaluation. There are several measures proposed in the literature for the evaluation of structure learning algorithms [76].

Score-based method

To evaluate a structure learning algorithm, many studies use a comparision between the score fuction of the learned graph and the original graph. The learning algorithm is good if S(B,D) $\backsimeq$ S (G_0,D) where S is a score among the scores given in the previous section 2.3.2.

An advantage of this approach is that it takes into account Markov equivalence to evaluate the structure. this metric gives the best results if there is large learned dataset.

However, the use of score functions to evaluate the learning structure algorithms can produce some problems. For example, if the data are limited, it is possible to obtain a graph G with the same score as G0, but that is not in the same equivalence class.

Kullback-Leibler divergence-based method

The Kullback-Leibler (KL) divergence is a fundamental equation of information theory that quantifies the proximity of two probability distributions [86]. It is a non-symmetric measure of the difference between the probability distributions of a learned network P and the probability distributions of a target network Q. Specifically, the Kullback-Leibler divergence of Q from P, denoted D_{KL}(P | Q), is a measure of the information lost when Q is used to approximate P: KL measures the expected number of extra bits required to encode samples from P when using a code based on Q, rather than using a code based on P. Typically P represents the ”true” distribution of data, observations, or a precisely calculated theoretical distribution. The measure Q typically represents a theory, a model, a description, or an approximation of P.

If the variables are discrete, this divergence is defined by:

$$D_{KL}(P \mid Q) = \sum_{x=\chi} P(x) \log \frac{P(x)}{Q(x)} \tag{2.7}$$

D_{KL} is non-negative (≥ 0), not symmetric in P and Q, zero if the distributions match exactly, it can potentially equal infinity.

This metric is important when the network is used for inference. However, the KL-divergence is not directly penalized for extraneous edges and parameters [104]. There are situations where the KL divergence has limitations. In fact, the computational complexity is exponential to the number of variables. In this case, the principle of sampling can be used to reduce this complexity.

Sensitivity and specificity-based method

Sensitivity and specificity are statistical measures of the performance of a binary classification test, also known as classification function in statistics [29].

Sensitivity measures the proportion of actual positives which are correctly identified. Specificity measures the proportion of negatives which are correctly identified.

Given the graph of the theoretical network $G_0 = (V, E_0)$ and the graph of the learned network $G = (V, E)$, The sensitivity-specificity-based method begins by calculating the following indices:

- TP (true positive) = number of edges present in both G_0 and G
- TN (true negative) = number of edges absent in both G_0 and G
- FP (false positive) = number of edges present in G, but not in G_0
- FN (false negative) = number of edges absent in G, but not in G_0

Then, the sensitivity and specificity can be calculated as follows:

$$Sensitivity = \frac{TP}{TP+FN}$$
$$Specificity = \frac{TN}{TN+FP}$$

These measures are easy to calculate. They are often used in the literature. However, the differences in orientation between the two graphs in the same equivalence class are counted as errors.

Distance-based method

Tsamardinos et al. [104] have proposed an adaptation of the usual Hamming distance between graphs taking into account the fact that some graphs with different orientations can be statistically indistinguishable. As graphical models of independence, several equivalent graphs will represent the same set of dependence / independence properties. These equivalent graphs (also named Markov or likelihood equivalent graphs) can be summarized by a partially DAG (PDAG) (section 2.2.4). This new structural Hamming distance (SHD) compares the structure of the

PDAG of the learned and the original networks as described in algorithm 7 in order to compare only the orientations that are really statistically distinguishable.

As in the sensitivity and specificity, the advantage of this approach is the simplicity of calculation. This method also takes into account the Markov equivalence and it can run with a large number of variables.

As mentioned before, structure learning is a difficult task. Some works propose to use prior knowledge in order to limit the search space, for instance by declaring some forbidden or required edges in the final graph [21]. When dealing with PDAGs, the previous SHD measure takes into account only the information from the learning data, forgetting that some orientations have been provided by prior knowledge.

Algorithm 7 Structural Hamming distance [104]

Require: Learned PDAG H; Original PDAG G
Ensure: SHD value
1: $SHD = 0$
2: **for all** edge E different between H and G **do**
3: **if** (E is missing in H) or (E is extra in H) or (E is uncorrectly oriented in H) **then**
4: SHD=SHD+1
5: **end if**
6: **end for**

2.4.2 Generating large Benchmarks

As mentioned in section 2.4, the evaluation tasks need a reference model (is either a known graph or a randomly generated one). To evaluate the structure learning algorithms we must have different benchmarks that we use to construct the learned structures from data and compare them to the reference model. In this thesis we focus on the large benchmarks.

The constraint-based learning and score-based learning approaches are usually validated on benchmark models with a small number of variables (e.g., less than 100 variables). In literature, there are few standard benchmarks with a large size that are not very used in research. The most known large datasets are Andes (223 nodes) [16]; Pigs(442 nodes)(Created by Claus S. Jensen on the basis of a data base from Soren Andersen (Danske Slagterier, Axeltorv Copenhagen)); Link (724 nodes) [49] and Munin (1041 nodes) [3].

As existing BN benchmarks are limited in their number of variables, some researchers proposed generating BNs by controlling their size and/or complexity. We can decompose these works into two families. The first allows to randomly generate large benchmarks. The seconds permits to generate large benchmarks from known graphs.

As an example of the first familly Ide et al.'s work [45], it presented methods for the generation of random BN by generating uniformly distributed samples of

directed acyclic graphs. They develop a uniform generation of multi-connected and single-connected networks for a given number of nodes. Some studies use the generation of random graphs. These kinds of generation have some disatvantages. These graphs can have some repeated substructure. In addition some characteristics can be missed.

Generating a very large BN randomly is not very realistic. In many large applications, the global model can be decomposed in coherent repeated subgraphs. In the second familly, they chose the reference model as multi-copies of the original standard model. Tsamardinos et al, in [95], have proposed a novel algorithm and software for the generation of an arbitrary large BN (e.g., graphical models representation and joint probability distributions) by tiling smaller real-world known networks (tiles). The complexity of the final model is controlled by two parameters : the number of tiling n and the connectivity parameter c which determines the maximum number of connections between one node and the next tile. In literature, to solve the problems given by generation of random BN, most of the studies [104, 22, 39] use tiling to generate large benchmarks and use them for the validation of their learning algorithms. In these works, they use tiling of small standard Benchmarks as (Asia, Alarm and Hailfinder) by tiling the original structure 3, 5 and 10 times.

As far as we know, the tiling technique is the best and most useful algorithm for simulating large BNs. In fact, during our research, we have found that the Tiling was used in many studies, such as to compare different Markov Blanket learning algorithms in large (5000 variables) networks [105, 102]; or to compare many BN learning algorithms in [104, 6, 56, 39], and to examine the time efficiency and quality of a local BN learning algorithm to reconstruct local regions in a large (10000 variable) network in [104].

2.5 Conclusion

In this chapter, we proceeded by presenting the concepts of Bayesian networks, then we reviewed the different structure learning methods of these models. We also addressed the question of evaluation for these learning algorithms.

We have seen that the hybrid method for learning the BN perform better than others techniques based on constraints or on score on the level of scalability and complexity of algorithms.

Section 2.4 presented an overview of the evaluation methods. The score-based method takes into account the equivalence of Markov during the evaluation. But if the data were reduced, it would be difficult to distinguish two different networks by their scores. Other methods based on reference model are also able to take into

account Markov equivalence, though the calculation is costly when the number of variables is important.

In the next chapter we will introduce an extension of the Bayesian networks named Dynamic Bayesian Network. This kind of model is a special Bayesian Network, which is used with dynamic stochastic process models [73].

3

Dynamic Bayesian Networks and structure learning

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3.1 Introduction

It is natural to use a dynamic Bayesian network (DBN), a directed graphical model whose nodes are across different time slices, to learn and reason about dynamic systems. DBN model is a temporal process and use a conditional probability distribution for each node and a probabilistic transition between time slices.

It is generally assumed that a DBN model structure and parameters do not change over time, i.e., the model is time-invariant [73]. Learning a DBN model from data aims to find the best model of the unknown probability distribution underlying the temporal process on the basis of a random sample of a finite size, i.e. the learning data.

As the static case, the learning dynamic Bayesian network consists of two phases: learning of the parameters and the learning of the structure. In the dynamic context most of the structure learning methods for DBN are based on the optimization of a score and deal with small dimension of benchmarks. Some recent works use hybrid methods (local search identification and global optimisation). However, this kind of methods deals with large dimension of benchmarks on a ”simplified” search space.

As mentioned in Chapter 2, all studies try to evaluate their structure learning algorithms through some evaluation techniques. Many studies tried to know the goodness of their methods with the help of a scoring criterion, which is not the best way as we presented in section 2.4.1.

This chapter deals with basic definitions and notations of dynamic (temporal) Bayesian networks. Section 2.2 introduces some DBN notations and definitions. Section 2.3 provides an overview of the dynamic Bayesian networks structure learning. And as in the previous chapter, section 2.4 presents some techniques for the evaluation of Bayesian networks structure. Also, in this section we present what the existing approaches used to evaluate these structure learning algorithms on small and large Benchmarks. Finally, we try to enumerate the different limitations of the structure learning and evalution.

3.2 Dynamic Bayesian Network Definition

3.2.1 Representation

A dynamic Bayesian network (DBN) is a probabilistic graphical model devoted to represent sequential systems. More precisely, a DBN defines the probability distribution of a collection of random variables $\mathbf{X}[t]$ where $\mathbf{X} = \{X_1 \dots X_n\}$ is the set of variables observed along discrete time t [23, 73].

In this work, we consider the special class of DBNs mentioned in the previous paragraph, namely the 2-Time slice Bayesian Networks (2T-BN) (cf. Figure 3.1).

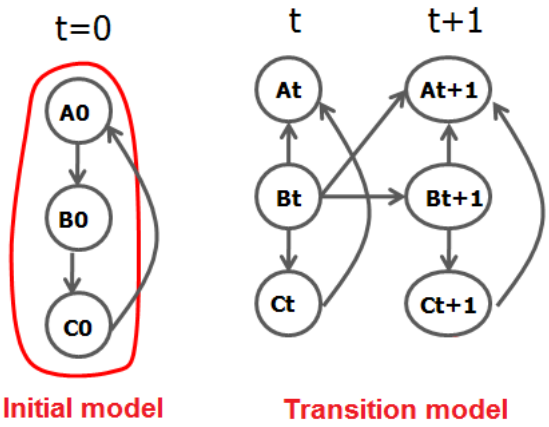

Figure 3.1: A structure of 2-TBN Bayesian network

3.2.2 Different forms of K-TBN

2-TBN

To represent a DBN, we don't need the entire unrolled DBN. This kind of model represents a process that is stationary and Markovian. (1) Stationary: the node relationships within a time-slice t and the transition function from time-slice t to time-slice t+1 do not depend on t. Therefore, we only need the initial time-slice; (2) Markovian: the transition function depends only on the immediately-preceding time-slice and not on any previous time-slices (e.g., no arrows go from time-slice t to time-slice t+2). Therefore, the set of nodes in a time-slice d-separate the past from the future.

A 2T-BN is a DBN which satisfies the Markov property of order 1 $\mathbf{X}[t-1] \perp \mathbf{X}[t+1] \mid \mathbf{X}[t]$. As a consequence, a 2T-BN is described by a pair $(M_0, M_{\rightarrow})$.

M_0 (**initial model**) is a BN representing the initial joint distribution of the process $P(\mathbf{X}[t=0])$ and consisting of a direct acyclic graph (DAG) G_0 containing the variables $\mathbf{X}[t=0]$ and a set of conditional distributions $P(X_i[t=0] \mid pa_{G_0}(X_i))$ where $pa_{G_0}(X_i)$ are the parents of the variable $X_i[t=0]$ in G_0.

$M_{\rightarrow}$ (**transition model**) is another BN representing the distribution $P(\mathbf{X}[t+1] \mid \mathbf{X}[t])$ and consisting of a DAG $G_{\rightarrow}$ containing the variables in $\mathbf{X}[t] \cup \mathbf{X}[t+1]$ and a set of conditional distributions $P(X_i[t+1] \mid pa_{G_{\rightarrow}}(X_i))$ where $pa_{G_{\rightarrow}}(X_i)$ are the parents of the variable $X_i[t+1]$ in $G_{\rightarrow}$, parents which can belong to time t or $t+1$. $M_{\rightarrow}$ is a two slice temporal Bayesian network (2TBN) that defines the transition

model p($X_t|X_{t-1}$) as follows:

$$p(Z_t|Z_{t-1}) = \prod_{t=1}^{N} p(Z_t^i|Pa(Z_t^i)) \tag{3.1}$$

The joint probability distribution for a sequence of length T can be obtained by unrolling the 2TBN network:

$$p(Z_{1:T}) = \prod_{t=1}^{T} \prod_{i=1}^{N} p(Z_t^i|Pa(Z_t^i)) \tag{3.2}$$

An example of 2-TBN structure, as one dynamic Bayesian network form, is presented in figure 3.2.

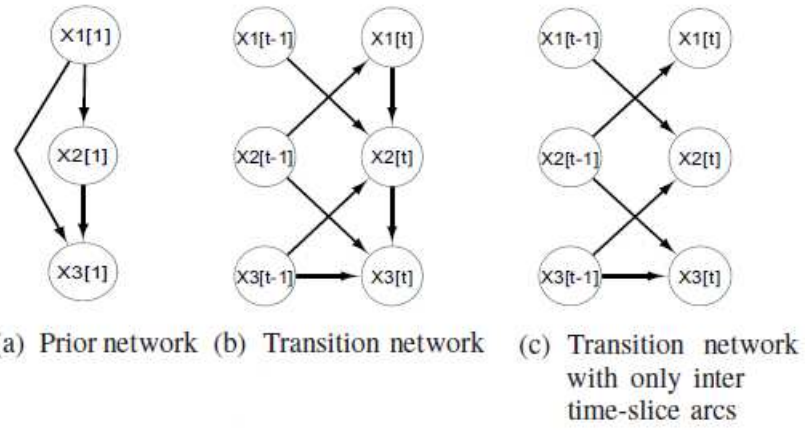

Figure 3.2: An example of 2-TBN Bayesian network [110]

k-TBN

Murphy's definition of DBNs is sufficient for modeling first-order Markov processes. However, there are others extensions for modeling temporal processes. It is possible to model k-1th-order Markov processes. This extension can be useful when modeling physiological processes at a small time-scale. For example when devising a DBN model that catches the dynamics of the human cardiovascular system for every 50[ms] [47]. In such temporal models, assuming a first-order process is not sufficient enough.

For M_0 (**initial model**) is a DBN representing the initial joint distribution of the process $P(\mathbf{X}[t = 0], ..., \mathbf{X}[t = k - 2])$.

For $M_{\rightarrow}$ (**transition model**), the extension of Murphy's definition to the following: B is not defined as a 2-TBN, but as a k-TBN that defines the transition model

p($Z_t|Z_{t-1}$,Z_{t-2}, . . . ,Z_{t-k}) for a k-1th-order Markov process.

$$p(Z_t|Z_{t-1}, Z_{t-2}, ..., Z_{t-k}) = \prod_{i=1}^{N} p(Z_t^i|Pa(Z_t^i)) \tag{3.3}$$

The equation 3.3 is essentially the same as equation 3.1, but for the set of parents which is not restricted to nodes in the previous or current time-slice, but can also contain nodes in time-slices further in the past. In this definition, the joint distribution for a sequence of length T can be obtained by unrolling the k-TBN and then multiplying all the CPTs. Again this equation is similar to equation 3.2.

$$p(Z_{1:T}) = \prod_{t=1}^{T} \prod_{i=1}^{N} p(Z_t^i|Pa(Z_t^i)) \tag{3.4}$$

Definition 3.2.1 *(Temporal arc)*
A temporal arc is an arc between a parent node and a child node with an index that denotes the temporal order or time-delay k > 0. A parent and a child node can be the same node.

An example of second-order DBN according to the k-TBN visualization is shown in figure 3.3 This example of DBN is relatively simple, but imagine specifying a DBN model with many variables and different temporal orders per time-slice.

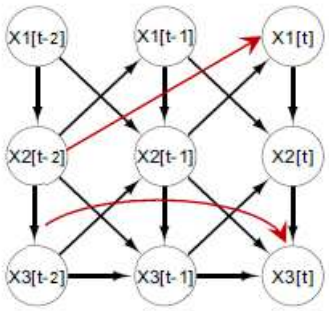

Figure 3.3: An example of k-TBN visualization of a second-order DBN (k=3) using t = 3 time-slices

Simplified k-TBN

In general, the transition networks may contain both inter and intra time slice arcs, as we presented in the previous figures 3.2 and 3.3.But some works have further restricted the transition network to contain only inter-time slice arcs, as illustrated in figures 3.2.c and 3.4 [27, 114, 110]. These models only capture the time delayed interactions between the variables while overlooking all the instantaneous interactions. The applicability of DBN models with only inter-time slice arcs largely depends on the nature of the interactions, and the time granularity, i.e., the

data sampling rate. Researchers use this kind of model in many fields as biological systems [27], genetics [110], nuclear translocation and turnover of the regulatory protein [83].

This kind of model is restricted in such a way that it contains only inter-time slice arcs that provides an important algorithmic advantage: there exist polynomial time algorithms for learning this class of DBN. So, with this model we can reduce the space search which is NP-hard in the DBN structure learning due primarily to temporal dimension.

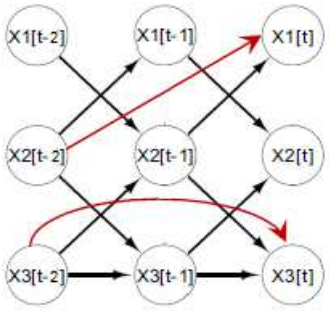

Figure 3.4: Simplified k-TBN

Other DBN forms

There are many studies using other kinds of DBN. Dynamic Bayesian networks (DBN) are a class of graphical models that has become a standard tool for modeling various stochastic time-varying or non-stationary phenomena [62].

The first kind is named non-Stationary DBN. In this model, an important assumption of the traditional DBN structure learning is that the data are generated by a stationary process, an assumption that is not true in many important settings. Non-stationary dynamic Bayesian networks represent a new framework for studying problems in which the structure of a network is evolving over time [62].

Robinson et al. [84] present also this class of graphical model called a non-stationary dynamic Bayesian network, in which the conditional dependence structure of the underlying data-generation process is allowed to change over time.

Wang and al. [113] propose another form (autoDBN) to learn DBNs with changing structures from multivariate time series. In auto-DBN, segmentation of time series is achieved first through detecting geometric structures transformed from time series, and then model regions are found from the segmentation by designed finding strategies.

Song and al. [91] propose time-varying dynamic Bayesian networks (TV-DBN) for modeling the structurally varying directed dependency structures underlying non-stationary biological/neural time series.

3.3 Dynamic Bayesian Network structure learning

The existing techniques for learning DBNs are mostly straightforward extensions of the techniques for learning BNs [73]. In this thesis, we only focus on the structure learning in DBN. Before explaining the structure learning in a DBN, We mentioned that to achieve parameter learning, we can use the techniques discussed in Appendix A. In this case, we just comment on two points that are applicable specifically to dynamic systems: (1) Parameters must be tied across time-slices, so we can model sequences of unbounded length; (2) The parameters, π, for $P(X_1)$ are usually taken to represent the initial state of the dynamic system [73].

3.3.1 Principle

As in Murphy's definition, the structure learning of a DBN has some assumptions must be respected:

- Learning the intra-slice connectivity, which must be a DAG,
- Learning the inter-slice connectivity, which is equivalent to the variable selection problem, since for each node in slice t, we must choose its parents from slice t-1.
- If we assume the intra-slice connections to be fixed, this means that structure learning for DBNs reduces to feature selection (simplified search space). If the system is fully observed (complete data), we can apply standard feature selection algorithms, such as forward or backwards stepwise selection, or the leaps and bounds algorithm [73].

When the system is partially observed (incomplete data), the structure learning becomes computationally intensive. One practical approach is the structural EM (SEM) algorithm [31].

3.3.2 Structure learning approaches for 2-TBN and k-TBN models

Friedman et al. [32] have shown that this task can be decomposed in two independent phases: learning the initial graph G_0 as a static BN structure with a static dataset corresponding to $\mathbf{X}[t = 0]$ and learning the transition graph $M_{\rightarrow}$ with another "static" dataset corresponding to all the transitions $\mathbf{X}[t] \cup \mathbf{X}[t + 1]$. They then proposed to apply usual score-based algorithms such as greedy search (GS) in order to find both graphs. Learning dynamic Bayesian network structures provides a main mechanism for identifying conditional dependencies in time-series data.

[35] developed another evolutionary approach for 2T-BN structure learning. In this work, The DBN structure learning based on BOA consists of two parts. The first part is to obtain the structure and parameters of the DBN in terms of a good

solution, and the second part is to produce new groups according to the obtained DBN structure. Wang and al. [112] also look at using evolutionary computation in 2T-BN structure learning by incorporating sampling methods.

Some other research work in structure learning propose their own algorithm for learning in such domains as the medicine, biology, geometry. Rajapakse et al. [82] use the dynamic Bayesian networks (DBN) and a Markov chain to model fMRI time-series and thereby determine temporal relationships of interactions among brain regions. Experiments on synthetic fMRI data demonstrate that the performance of the DBN is comparable to Granger causality mapping (GCM) in determining the structure of linearly connected networks.

Pena et al. [81] study cross-validation as a scoring criterion for learning dynamic Bayesian network models that can be well generalized. they argue that cross-validation is more suitable than the Bayesian scoring criterion as one of the most common interpretations of generalization.

Aydin and al. [5] present a secondary structure prediction method that employs dynamic Bayesian networks and support vector machines. This work is applied on biology.

All these approaches are validated on small benchmark models (with about 10 variables). In a more general context, due to inherent limitations of score-based structure learning methods, all these methods will have a very high complexity if the number of variables increases.

3.3.3 Structure learning approaches for simplified ”k-TBN and 2-TBN” models

Dojer [27] offers an algorithm for learning an optimal network structure. It works in polynomial time for both MDL and BDe scores. His method is addressed to the case when the benchmark is small and there is no need to examine the acyclicity of the graph. According to Dojer, the second assumption is satisfied in the DBN case. In fact, as he mentioned in his work, A DBN describes a stochastic evolution of a set of random variables over discretized time. Therefore conditional distributions refer to random variables in neighboring time points. The acyclicity constraint is relaxed, because the”unrolled” graph is always acyclic.

In 2009, Wilczynski et al. [114] implemented and ran the previous Dojer’s algorithm. He presented in a BNFinder software, which allows the Bayesian network reconstruction from experimental data. It supports dynamic Bayesian networks.

Vinh et al. dealt particularly with the problem of learning the globally optimal structure of a dynamic Bayesian network (DBN) [111]. They said that the MIT (Mutual Information Test) is better for evaluating the goodness-of-fit of the DBN structure than the other popular scoring metrics, such as BIC/MDL, K2 and BD,

and the well-known constraint-based PC algorithm.

Vinh et al. [110] propose another score based algorithm without equicardinality assumptions named MIT-global. Also, they propose another contribution in this work consist of a hybrid method with local Blanket identification (MIT-MMMB). They show that the local search MIT-MMMB and global-MIT have similar results better than advanced score based algorithm (simulated annealing). The MIT based on MMMB try to identify the Markov Blanket MB but in a restricted subclass of 2T-BNs named simplified 2-TBN (cf. figure 3.2.c) or kT-BNs (cf. figure 3.3). This assumption permits to simplify both the MB discovery and the global optimization but it is not able to identify the intra-time dependencies.

3.3.4 Structure learning approaches for other forms of DBN models

Tucker et al. have developed an evolutionary algorithm which exploits certain characteristics of the MTS process in order to generate good networks as quickly as possible. They compare this algorithm to other standard learning algorithms that have traditionally been used for static Bayesian networks but adapted for DBNs [108].

The work of Wyncoop and al.[115] addresses the problem of learning dynamic Bayesian network (DBN) models to support the reinforcement of learning. It focuses on the learning regression tree (context-specific dependence) models of the conditional probability distributions of the DBNs. In this study, they introduce a regression tree algorithm in which each leaf node is modeled as a finite mixture of deterministic functions. This mixture is approximated via a greedy set cover.

In the work of Wang et al. [113], the auto-DBN model permits a segmentation of time series achieved first through detecting geometric structures transformed from time series, and then the model regions are found from the segmentation by designed finding strategies; in each found model region, a DBN model is established by existing structure learning methods; Finally, a model revisiting is developed to refine model regions and improve DBN models. These techniques provide a special mechanism to find accurate model regions and discover a sequence of DBNs with changing structures, which are adaptive to changing relations between multivariate time series.

Robinson et al. [84] define the non-stationary DBN model, present an MCMC sampling algorithm to efficiently learn the structure of an nsDBN and the times of non-stationarities (transition times) under different assumptions, and demonstrate the effectiveness of the algorithm on simulated data.

3.4 Evaluation of DBN structure learning algorithms

All works for structure learning in literature develop an experimental study to present the goodness of their DBN structure learning algorithms . There are popular tools for the evaluation of the learning from time-series data. In this section we present the existing methods to evaluate structure learning algorithms for the DBN.

3.4.1 Benchmarks

The first step to evaluate the performance of these algorithms is to assemble different standard benchmarks. In Pena's work [81], the authors involve learning databases of different sizes sampled from a partial model of the transcriptional regulatory network of Saccharomyces cerevisiae. The model involves 30 transcription or (variables) factors and 56 interactions (dependences) between them.

In [50], the authors ran experiments with their DBN learning approach in the coffee task [9] (containing 6 variables), Taxi task [25] (containing 10 variables), and a simplified autonomous guided vehicle (AGV) task [38] (containing 20 variables).

Gao et al. [35] select DBNs that have 8 variables to match the database as an optimization object. They use the database from BNT Structure Learning Package [61].

Rajapakse et al. [82] illustrate their method with experiments on synthetic data as well as on two real fMRI datasets from fMRI Data Center, Dartmouth College (fMRIDC, 2004) (containing 5 variables).

Wang et al. [113] use a real data set, it is about the interest rates of Australia, France, UK and US in 240 months from July 1980 to June 2000 [65] with three variables. Another real data set is about daily stock prices of ten aerospace companies from January 1988 to October 1991 [1] with six variables.

Song [91] conducted 3 experiments using synthetic data, gene expression data and EEG signals. they generate 8 different anchor transition matrices $A_1{}^t$: : : $A_8{}^t$, each of which corresponds to a random graph of node size n=50 and average in degree of 2 (they have also experimented with n = 75 and 100 which provides similar results).

Finally in Hwang's work [43], the writers gathered video data recorded at several intersections and used them to detect accidents at different intersections which have different traffic flows and intersection designs. A total of 70 video scripts are used in the experiments, containing 33 accidents, 10 situations similar to accidents, and 27 normal situations. The model studied in this work contains 10 variables.

Although all the works interested in DBN structure learning generally use small benchmarks size, there are some other recent works as try to improve this disadvantage of the DBN structure learning. They use large benchmarks to run their

algorithms.

Dojer [27] tested the time complexity of learning an optimal dynamic BN on microarray experiments data of Arabidopsis thaliana (≈23 000 genes). The running time computed was about 48 hours for the MDL score and 170 hours for the BDe score.

In order to judge the performance of their software, [114] have compared it to the Banjo library. As a realistic dataset, we have chosen the dataset attached as an example to the Banjo package, consisting of 20 variables and 2000 observations, published by Smith et al. [90].

Vinh et al [111] employ several synthetic data sets generated by different data generation schemes that have been used in some previous studies. As a realistic number of samples for microarray data, they generated data sets of between 30 and 300 samples. With the ground-truth network available, they count the number of true positive (TP), false positive (FP), true negative (TN) and false negative (FN) edges, and report two network quality metrics, namely sensitivity and specificity.

In 2012, Vin et al. [110] proposed a study where the experimental study has been conducted with about 1595 variables.

3.4.2 Evaluation metric

We remark in this study that, like the static BNs, the structure learning for DBNs studies use the score functions or comparison between graphs to evaluate the performance of algorithms. Contrary to the static BN, that has many metrics used for evaluation as we mentioned in section 2.4. Also, in DBNs studies, we didn't find standard metrics that can be used as the SHD in tthestatic case.

[50] compared their active learning scheme with passive learning . In this case, they use the BIC and BDe scores to detect most of the refinements necessary to learn the true DBN model.

[35] used fitness function for a DBN, there exist two structure measure scales, namely, Bayesian Dirichlet metric (BD) and Bayesian information metric (BIC). In their paper, they use BD to measure network.

[82] used the square error e^2 between the true connectivity structure C= $\{c_{ij}\}$ and the estimated structure $= \{¢_{ij}\}$ is measured by the square error between the elements of the matrices defining the structures:

$$e^2 = \frac{1}{2n^2} \sum_{i=1}^{n} \sum_{j=1}^{n} (c_{ij} - ¢_{ij})^2 \tag{3.5}$$

the elements c and ¢ were scaled to the range [0,1] for comparison purposes with other approaches

Song et al evaluate the performance using an F1 score, which is the harmonic

mean of sensitivity and scores call-function in retrieving the true time-varying network edges [91].

In [43] they used the fitness function as a metric to evaluate the performance of population for the given problem. Fitness function, therefore, evaluates the suitability of a dynamic Bayesian network structure.

As we mentioned above most of theworks use score functions for the evaluation step. However, there are a few works that use large datasets to evaluate their approaches. They use some other techniques of evaluation. Dojer and Wilczynski [27, 114] use computation running time as measure. Vinh et al. in [111] use three features: the percent sensitivity, the percent imprecision and the running time. Vinh et al. in [110] use node degree or connectivity degree distribution and runtime to compare the performance of their algorithms to others algorithms.

We remark that all these studies used the running time as a common metric for the evaluation. This is explained by the fact that in high dimension it is not enough to show the reliability of system but the time is an important factor for the evaluation process.

3.5 Conclusion

In this chapter, after presenting the key concepts of Dynamic Bayesian network, we reviewed the different structure learning studies of these models in literature. We also addressed the topic of how the different works proceded to evaluate their learning algorithms.

In section 2.4, we focused on presenting an overview of the evaluation methods. The important conclusion reached in this study, is that the structure learning in the dynamic Bayesian Network has many disatvantages. This conclusion was given by many points:

Firstly, most of the works use networks with a small number of variables. This choice is explained by the fact that all works for learning structure are based on score and we showed previously that these methods of learning can't achieve a good performance when we increase the number of variables. we noted in previous section that the score function takes into account the equivalence of Markov in the evaluation. If an algorithm returns a graph G equivalent to G_0, both structures have the same score. This advantage is also a disadvantage, since if there is little data, it is possible to obtain a graph G with the same score G_0, but that is not in the same equivalence class. We think that this choice was taken by all these studies because of all the limitations mentioned before.

Secondly, all the studies about the DBN structure learning use their own benchmarks and techniques for evaluation. The problem in the dynamic case is that we

don't find previous works that provide details about the used networks and indicators of comparison. In addition, the access to the datasets and the source code is not always possible.

The last point, concerns the way of dealing with high dimension. The existing works, such as Vinh et al. [110], consider a restricted subclass of 2T-BN (eg. they learn only the inter-slice connectivity and ignore the intra-slice connectivity).

In the remaining chapters we will describe our contributions at the level of learning the DBN structure using the hybrid methods and we developed some techniques to evaluate these learning algorithms. These techniques are standard, and can be used with any other technique and on any standard large Benchmark. Also, they allow the amelioration of the evaluation quality with the insertion of a priori knowledge.

II

Contributions

4

Benchmarking dynamic Bayesian networks

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4.1 Introduction

During the last two decades, there has been an increasing interest in the Bayesian Network (BN) formalism [78, 42]. The BNs have been recognized as one of the most successful complete and consistent formalisms for the acquisition and representation of knowledge and for reasoning from incomplete and/or uncertain data. This success is due to the following factors: (1) their mathematical bases are rigorously justified; (2) they deal in an innate way with uncertainty (modeled as a joint probability distribution); (3) they are understandable (graphical representation); and (4) they take advantage of locality both in knowledge representation and during inference.

Learning the graphical part (i.e. the structure) of these models from data is an NP-hard problem. Many studies have been conducted on this subject [12, 11, 13]. Most of these works and their result interpretations use standard networks and common performance indicators, such as the approximation of the marginal likelihood of the obtained model or comparison of the resulting graph to the original graph given in benchmarking tasks with the help of the Structural Hamming Distance (SHD) proposed by Tsamardinos [104].

Dynamic Bayesian networks (DBNs) are a general and flexible model class for the represention of complex stochastic temporal processes [73]. Some structure learning algorithms have been proposed, adapting principles already used in ”static” BNs. Comparing these algorithms is a difficult task because the evaluation techniques and/or the reference networks used differ across research works. The evaluation of these algorithms is also often restricted to networks with a small number of variables. However, with the static BNs, the evaluation was carried out using a large number of variables.

In this chapter, we highlight our two major contributions: section 4.2 presents an algorithm for generating large 2-TBN networks (which could be used as standard 2-TBN benchmarks) using the tiling approach (see section 2.4.2) in the dynamic case; section 4.3 presents an algorithm for the evaluation of a 2-TBN structure learning algorithm adapting the SHD measure (section 2.4.1) no more correct with temporal networks. Finally, we show in section 4.4 some validation examples to prove the advantages of our methods. Our work can be a useful tool for benchmarking any 2-TBN structure learning algorithm in a common framework.

4.2 Generation of large k-TBN and simplified k-TBN

4.2.1 Principle

In order to generate a large k-TBN or a simplified model, we propose generating two models M_0 and $M_{\rightarrow}$ from an initial static benchmark BN M.

First we use the Tsamardinos' work for the generation of realistic large bayesian networks by tiling (section 2.4.2). We have used tiling approach because in the case of k-TBN (M_0 and $M_{\rightarrow}$) can be seen as a model obtained by one first tiling to generate M_0 from M and another one to generate $M_{\rightarrow}$ from M_0 when it is assumed that all the "intra slices" dependencies (dependencies between the variables in the same time slice) can be found at any time and the "inter slices" dependencies (dependencies between the variables in the successive time slices) can be repeated all the time.

In the case simplified k-TBN, we start with an empty model M. The tiling algorithm prevents the construction of "intra slices" dependencies and allows the "inter slices" dependencies. Our method consists in generating a large initial model M_0 and its conditional probability distribution by tiling n copies of the initial model M. Then we use tiling again to generate $M_{\rightarrow}$ and the transition probability distribution by tiling k copies of M_0.

Our suggestion is described in Algorithm 8. The complexity of the final k-TBN can be controlled by changing the number of tiling copies and the intra-connectivity c_i (used to generate M_0) or the temporal connectivity c_t (used to generate temporal edges).

Algorithm 8 Generation of large k-TBNs (**TileBN for kT-BN**)

Require: BN M, number of copies n, intra-connectivity c_i, temporal connectivity c_t
Ensure: Return initial M_0 and transition models $M_{\rightarrow}$
1: M_0 = bn_tiling(M,n,c_i)
2: $M_{\rightarrow}$ = bn_tiling(M_0,k,c_t)

4.2.2 Tiling the initial model

In this first step of generation, the algorithm needs to enter a Bayesian network BN M with a number n of tiles desired as an input and BN_1;: : : ;BN_n and an integer-valued connectivity parameter c_i controlling the number of introduced edges as an output of the algorithm. The algorithm returns the initial model characterized by a large Bayesian network consisting of tiles with the new edges between tiles. The joint probability distribution of the tiles is preserved. Also, our algorithm adds the number of level used for tiling as an optional parameter (cf. figure 4.1) (i.e. we give

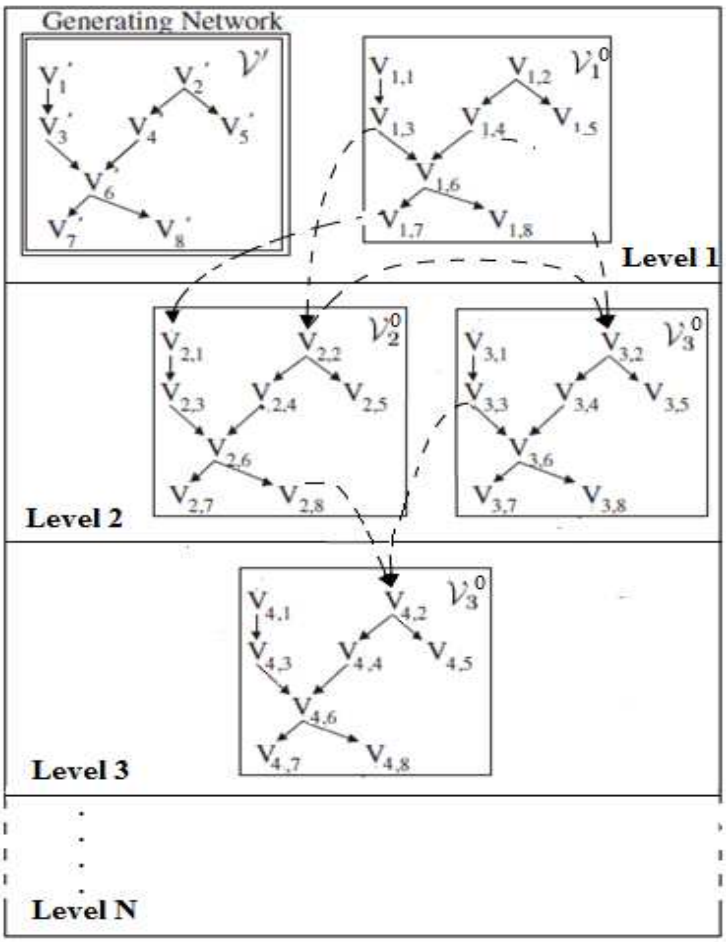

Figure 4.1: An example output of the initial model generation algorithm. The generating network is ASIA benchmark [59] shown in the top left of the figure.

N as number of levels and for each level we give the number of tiles n, and as result we have automatically a large network with N*n tiles).

There are tow changes in the case of the simplified k-TBN to construct the initial model: (1) the initial model M is an empty graph; (2) and the connectivity parameter c_i is equal to zero. With these constraints, we are sure that the initial model M_0 couldn't contain intra-slice edges.

4.2.3 Tiling the transition model

The second step is to generate the transition model. It is applied for k-TBN and simplified k-TBN in the same way. The algorithm needs to enter the initial model as input. It provides k copies (i.e. c_t= k for example, c_t=2 when the model is 2-TBN) of the initial graph with interconnections between them. These interconnections are the temporal relationships between nodes in t and t+1 time slices.

The interconnections must satisfy the property requirements of the tile algorithm in static and temporal cases. The tiles are topologically sorted according to their index and time, i.e., tile N_{j-1} is lower in the order than tile N_j and tile N_j^t is lower

in the order than tile N_j^{t+1}. Just as in the static case, TileBN for 2-TBN uses the number of the randomly selected interconnecting edges between the network in t-1 time slice and network in t time slice. TileBN for 2-TBN may add the edge $V_{p,k}^{t-1} \rightarrow V_{q,j}^{t}$ if the following four requirements are satisfied:

1. $p \neq q$, i.e., the edge goes from a variable to another belonging to a tile downstream (not allowed any cycle) [106]. This requirement is always checked because $V_{p,k}$ is in time slice t-1 and $V_{q,j}$ is in time slice t.
2. $Pa_j = \phi$;, i.e., the node $V_j^{'}$ of the generating network that corresponds to the endpoint of the edge $V_{t-1,j}$ is a minimal node in the generating network (it has no parents) [106].
3. If there exists another edge $V_{p',k'}^{t} \rightarrow V_{q,j'}^{t}$ to the same tile q then $j = j^{'}$, i.e., for each tile q only one minimal node can receive tile interconnecting edges. The second and third requirements will be used to determine the probabilistic properties of the output network [106].
4. All the interconnections go from a variable in t-1 to a variable in t (not allowed to invert any temporal edges).

We notice that the first three requirements are satisfied in the static case, i.e., we use these proprieties to construct the initial model. However, the last requirement is used when the algorithm links between BN_t and BN_{t+1}.

The DBN definition is unrolled for k + 1 time-slices where k denotes the temporal order of the Markov process. The DBN needs to be unrolled for this number of time-slices, because in the resulting unrolled network every CPD that needs to be learned will be represented with at least one copy (see appendix B algorithm 15).

4.3 Evaluation of k-TBN generated by data and prior knowledge

4.3.1 Principle

As 2-TBNs are defined by two graphs G_0 and $G_{\rightarrow}$, we propose to evaluate the structural difference between the theoretical 2-TBN and a learned one by the pair of the structural Hamming distance for the corresponding initial and transition graphs as described in algorithm 9.

As seen in section 2.4 (SHD method), taking into account Markov equivalence by comparing PDAGs is important for the BN structure learning evaluation, but it's not sufficient for DBNs. Some temporal information (a priori knowledge) is used for 2-TBN structure learning and can be lost by reasoning with PDAGs.

In the case of 2-TBN, two different models are learnt. The first one M_0 doesn't model temporal information, so the usual Tsamardinos' SHD (cf. section 2.4. algorithm 7) can be used.

The transition model $M_{\rightarrow}$ represents the dependency relations between nodes of the same slice t or between the nodes of slices t and $t+1$. In fact, here we have an important background (temporal) knowledge, edges between time slices are directed from t to $t+1$. We then propose to adapt the Tsamardinos' SHD in order to deal with this additional knowledge as proposed in definition 2.2.17 for BNs. One temporal correction is applied for each PDAG in order to obtain a corrected PDAG_k compatible with the prior knowledge. The structural Hamming distance is then computed between these PDAG_ks.

Algorithm 9 Structural Hamming distance for 2-TBNs

Require: Learned PDAG H_0; Learned PDAG $H_{\rightarrow}$; Original PDAG G_0; Original PDAG $G_{\rightarrow}$
Ensure: SHD values for initial and transition graphs
1: H_k=$H_{\rightarrow}$
2: G_k=$G_{\rightarrow}$
% calculate SHD_0
3: SHD_0=SHD(H_0,G_0)
% Temporal correction for $G_{\rightarrow}$
4: Select randomly an undirected temporal edge from $G_{\rightarrow}$
5: Orient this temporal edge in G_k
6: Recursively apply the Meek rules in G_k
7: If there exist any unprocessed temporal edge then repeat 4, 5, 6.
% Temporal correction for $H_{\rightarrow}$
8: Select randomly an undirected temporal edge from $H_{\rightarrow}$
9: Orient this temporal edge in H_k
10: Recursively apply the Meek rules in H_k
11: If there exist any unprocessed temporal edge then repeat 8, 9, 10.
% Calculate $SHD_{\rightarrow}$
12: $SHD_{\rightarrow}$=SHD(H_k,G_k)
% calculate SHD in 2-TBN
13: SHD = (SHD_0,$SHD_{\rightarrow}$)

PDAG with knowledge

The PDAG definition (see definition.2.2.12) is not sufficient when the DAGs are 2T-BN. As we mentioned before, a 2T-BN contains intra-connections and inter-connections. The second type of edges can be not oriented and therefore lose some information when we search the Markov Equivalence class (PDAG). However, we know that all temporal edges are oriented as the direction of time, i.e. the temporal edge is from a node in t to a node t+1. So, with this knowledge, we can orient some other edges in PDAG and we named this new PDAG with temporal correction PDAG_k.

To establish this PDAG_k building method we inspired by the temporal correction from the solution proposed by Meek to solve the following problem that there is a complete causal explanation for M that are the causal relationships common to every

complete causal explanation consistent with respect to the background knowledge K?

To construct this PDAG$_k$ graph we have to follow three steps. (1) Construct the PDAG, for this step we have used the Meek approach optimized by Chickering (cf. section 2.2.4); (2) insert the temporal knowledge K, using the solution proposed by Meek to insert the background knowledge (the set of directed edges which are forbidden, the set of directed edges which are required). (3) apply Meek's four orientation rules (described in definition 2.2.17)

Proposition 4.3.1 *(PDAG with temporal knowledge) [100]*
Two 2T-BN structures are said to be equivalent if the set of distributions and temporal constraints that can be represented with one of those structures is identical to the set of distributions and temporal constraints that can be represented with the other.

We notice that, we can use the same principal to calculate the SHD for k-TBN, but we have to respect the definitions of intial and transition networks.

SHD(2T-BN) advantages

As we previously presented, the SHD for 2T-BN is a measure inspired from SHD metric in the static case. So, all the SHD advantages are advantages characterizing the SHD(2T-BN). In addition, the new SHD has other advantages when it is used in the temporal (dynamic) case.

SHD advantages in the static context:

- It uses a reference model to evaluate contrary to the evaluation techniques that use data. These are not reliable when there is little data;
- It is defined by the distance between two PDAGs and not between two DAGs; With this method the problem of differences in orientation between the two graphs in the same equivalence class are counted as errors is removed;
- It uses the hamming distance, which is simple to compute. It can maintain its performance when the number of variables is large;
- It doesn't use certain assumptions or conditions in calculating;

SHD advantages in the temporal context:

- It inserts the priori knowledge;
- It can run with large Dynamic Bayesian network;
- It uses the equivalence class to evalute, contrary to other metrics used in structure learning DBN studies (mentionned in section 3.4.2) as the method based on sensitivity and specificity;
- It uses the temporal correction to construct PDAG$_k$ (see section 2.2.17;

4.4 Validation examples

4.4.1 2-TBN Benchmark generation

Implementation

The TileBN algorithm is implemented in Mathworks Matlab and is published as part of the Causal Explorer system [1]. The input BN is specified in HUGIN format, and a simple parser was written to read HUGIN BNs in a custom Matlab format.

The measure of evaluation used by many BN learning algorithm is plotted over several networks. Specifically, the following networks were used in the analysis, listed in order to increase the number of variables (number of variables given in parenthesis): Asia(8), Child (20), Insurance (27), Mildew (35), Alarm (37), Barley (48), and HailFinder (56). These BN learning algorithms are compared to different networks that contain 1, 3, 5, and 10 tiles of the original networks mentioned previously.

For our implementation, we decided that the initial network M is provided in Hugin [2] format readable by several BN software such as Genie/Smile [3] or Matlab toolboxes such as Causal Explorer [4].

As we mentioned previously, our method is inspired from tiling BN of Tsamardinos. So, we implement our method on the same tool used by tiling approach which is matlab *(causal explorer)* but we used some other tools as genie/smile. The implementation details of our method are shown in appendix B.

As Causal Explorer also proposes an implementation of bn_tiling(), this function allows generating a tiled standard network consisting of N copies of tiles with given connectivity parameter. We implemented our 2-TBN benchmark generation in Matlab using this function, and added another function in order to export an unrolled 2-TBN model in Hugin format. This exported 2-TBN function can then be used by several softwares for data generation and structure learning.

Toy example

Figure 4.2 illustrates our algorithm with ASIA [59] generating network, tiled 3 times for the initial model, with a maximum connectivity equal to 3. As we can see, we are now able to generate realistic 2-TBNs with very large domains by choosing any static and well-known benchmarks and controlling the complexity by increasing the number of tiles.

We recommend the reader to consult our Web page for Dynamic Bayesian

1. http://www.dsl-lab.org/causal explorer
2. http://www.hugin.com/
3. http://genie.sis.pitt.edu/
4. http://www.dsl-lab.org/causal_explorer/index.html

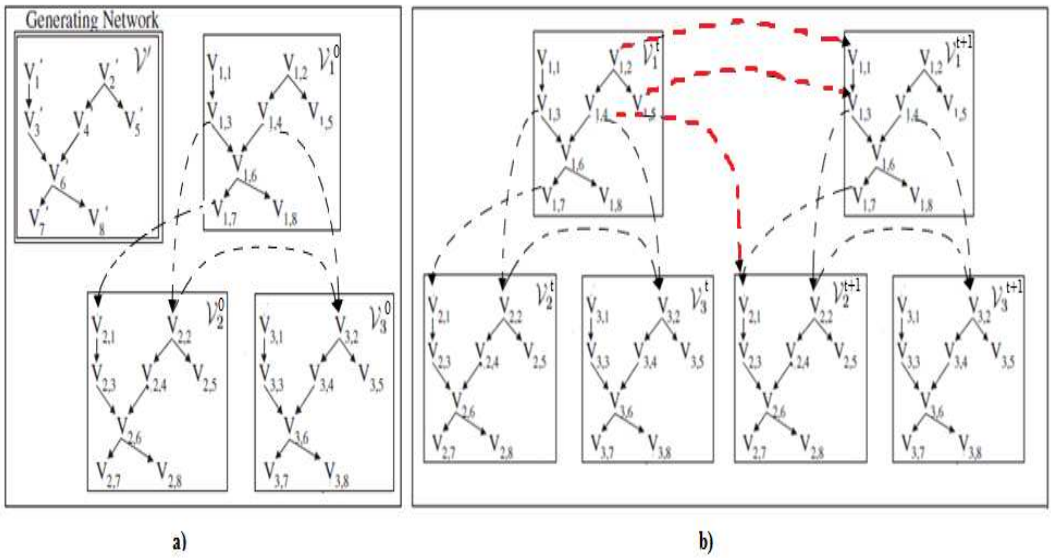

Figure 4.2: An example output of the 2-TBN generation algorithm. The generating network is ASIA benchmark [59] shown in the top left of figure a). a) The output of the initial network consists of three tiles of Asia with the addition of several intraconnecting edges shown with the dashed edges. b) The transition network output together with several added interconnecting edges are shown with the dashed red edges.

Networks	# vars	# edges	Temporal edges	# states (min-Max)	# parents (min-Max)	# neighbors (min-Max)
Asia_G_0	8	8		2-2	0-2	1-4
Asia_$G_{\rightarrow}$	16	21	5	2-2	0-3	1-5
Alarm_G_0	37	46		2-4	0-4	1-6
Alarm_$G_{\rightarrow}$	74	110	18	2-4	0-4	1-7
Hailfinder_G_0	56	66		2-11	0-4	1-7
Hailfinder_$G_{\rightarrow}$	112	156	24	2-11	0-4	1-17
Win95pts_G_0	76	112		2-2	0-7	1-10
Win95pts_$G_{\rightarrow}$	156	256	41	2-2	0-7	1-10
Andes_G_0	223	338		2-2	0-6	1-12
Andes_$G_{\rightarrow}$	446	820	144	2-2	0-6	1-12
Link_G_0	724	1125		2-4	0-3	1-17
Link_$G_{\rightarrow}$	1448	2530	280	2-4	0-4	1-17

Table 4.1: Generated benchmarks for Dynamic Bayesian Network

Network benchmarking (https://sites.google.com/site/dynamicbencmharking/). We present all standard large benchmarks for DBN that were constructed by our method for tempral tiling (see table 4.1).

4.4.2 SHD for 2-TBN

Implementation

We have implemented the SHD measure algorithm in a static case as described in section 2.3.3. This algorithm is considered as the reference for evaluation in many studies for DBN structure learning. Moreover, this implementation allows to convert DAG into PDAG based on Chikering approach. We have also implemented our new algorithms (SHD(2-TBN) and DAG to $PDAG_k$) to evaluate the structure learning dynamic BN algorithm with the insertion the temporal correction.

We also implemented these algorithms in our structure learning platform in C++ using Boost graph [5] and ProBT [6] libraries. Experiments were carried out on a dedicated PC with Intel(R) Core(TM) 2.20 Ghz,64 bits architecture, 4 Gb RAM memory and under Windows 7.

Toy example

In Figure 4.3, we show the interest of the temporal correction proposed for the SHD in section 2.4. We can notice that the PDAG corresponding to each 2-TBN loses some temporal information by un-orienting some temporal edges (resp. 1 and 2 for 2-TBN_1 and 2-TBN_2).

Applying the structural Hamming distance without correction gives us a distance equal to 2 between transition graphs related to 2-TBN_0 and 2-TBN_1 (example (b) SHD calculated between $PDAG_0$ and $PDAG_1$). This distance takes into account the missing edge between C_{t+1} and D_{t+1} and the missing orientation of the temporal edge between D_t and D_{t+1}. This distance increases to 4 between 2-TBN_0 and 2-TBN_2 (example (c) SHD calculated between $PDAG_0$ and $PDAG_2$) because of the 2 modifications (one missing edge and one added), but also the 3 missing orientations in 2-TBN_0.

The application of our temporal correction orients the temporal edges in the corrected $PDAG_0$, $PDAG_1$ and $PDAG_2$,we respectively orient 1, 2 and 0 (caused by V-structures in 2-TBN_2) more edges in the transition graph $PDAG_k$ related to 2-TBN_0, 2-TBN_1 and 2-TBN_2.

Applying the SHD with correction gives us a distance equal to 1 between transition graphs related to $PDAG_k0$ and $PDAG_k1$, which corresponds to the ”true” missing edge, and a distance equal to 2 between transition graphs related to $PDAG_0$ and $PDAG_1$ (example (b)).

Applying the structural Hamming distance with correction gives us a distance equal to 1 between transition graphs related to $PDAG_k0$ and $PDAG_k2$, which cor-

5. http://www.boost.org/
6. http://www.probayes.com/index.php

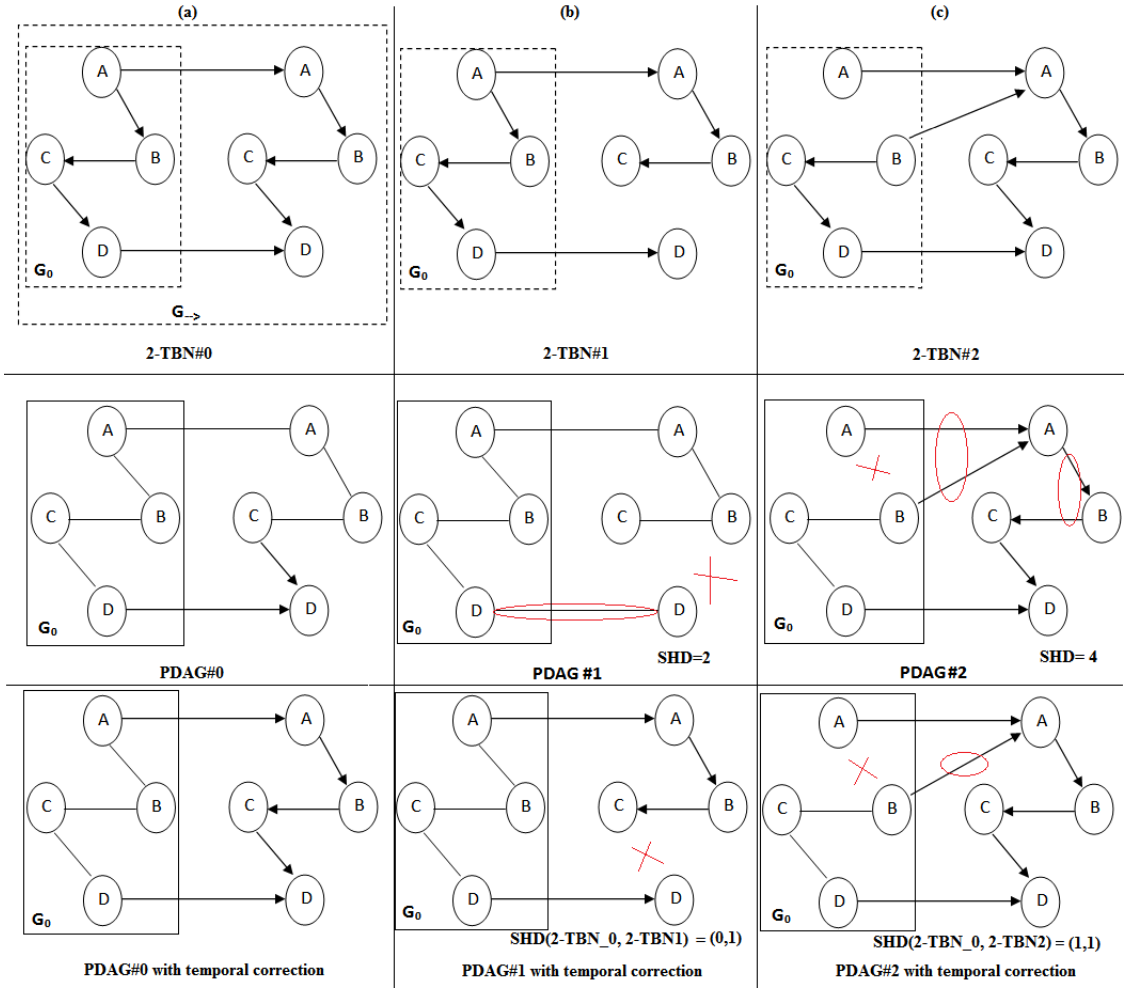

Figure 4.3: Examples of structural Hamming distance with or without temporal correction. A first 2-TBN and its corresponding PDAG and corrected PDAG_k are shown in (a). (b) and (c) show another 2-TBN and their corresponding PDAG, and the structural Hamming distance with the first model

responds to the "true" missing edge, and a distance equal to 4 between transition graphs related to $PDAG_0$ and $PDAG_2$ (example (c)).

As we can see in these toy examples, that our SHD with temporal correction is better in term of structural comparison of dynamic bayesian networks. The improvement is given by the integration of knowledge (temporal knowledge) in our metric.

4.5 Conclusion

We focused in this chapter on providing tools for benchmarking dynamic Bayesian network structure learning algorithms. Our first contribution is a 2-TBN generation algorithm inspired from the Tiling technique proposed by [95]. Our algorithm is able to generate large and realistic 2-TBNs that can, then, be used for sampling datasets. These datasets can then feed any 2-TBN structure learning algorithm.

Our second contribution is a novel metric for evaluating the performance of these structure learning algorithms, by correcting the Structural Hamming distance proposed by [104] in order to take into account temporal background information.

We have proposed a website by providing some 2-TBNs benchmarks (graphs and datasets) in order to afford common evaluation tools for every researcher interested in 2-TBN structure learning [7].

7. https://sites.google.com/site/dynamicbencmharking/

5

Dynamic Max Min Hill Climbing (DMMHC)

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5.1 Introduction

In this chapter, we focused on DBN structure learning with local search methods, by adapting the MMHC algorithm proposed by [104], one of the "state of the art" of this family algorithms . We believe that these local search algorithms can easily take into account the temporal dimension. Our objective is to propose a general structure learning algorithm that can work on 2-TBN models (with large search space) and use large benchmarks for validation tests.

We first present a version of DMMHC which is a simple adaptation of MMHC algorithm on 2-TBN models in section 5.2.1. Then, we optimized our approach by the use of temporal constraints in section 5.2.2. In addition we defined another version of the DMMHC that can run on simplified k-TBN models in section 5.4. We described, the complexity of each version of the DMMHC in section 5.5 and enumerated the advantages and disadvantages of our approach compared to others existing approaches in literature.

5.2 Dynamic Max Min Parents and children DMMPC

In 2T-BN models, temporality is limited by the first order Markov assumption. We think that local search algorithms can easily take into account this temporal constraint. We propose here a new DBN structure learning algorithm inspired from local search methods, by adapting the MMHC algorithm described in the previous section.

As seen in section 3.2, the 2-TBN structure is defined by two independent graphs G_0 and $G_{\rightarrow}$. Inspired from the MMHC algorithm detailed in section 2.3.3, our Dynamic MMHC algorithm proposes to identify independently these graphs by applying a greedy search algorithm (adapted by [32] for 2T-BN) constrained with local informations. This information is provided by the identification of the neighborhood Ne_0 (resp. Ne_+) of each node in G_0 (resp. $G_{\rightarrow}$).

By mimicking the procedure decomposition of MMHC described in section 2.3.3 , our local structure identification DMMPC will be decomposed into two tasks: the neighborhood identification itself ($\overline{\text{DMMPC}}$) completed by a symmetrical correction. We notice here that because of the non-symmetry of temporality, our local structure identification will be able to automatically detect some directed parent or children relationships if corresponding variables do not belong to the same time slice.

The following sub-sections described separately each of the proposed procedures, from the inner ones (the naive $\overline{\text{DMMPC}}$, the optimised $\overline{\text{DMMPC}}$ and DMMPC) to the final one (DMMHC).

5.2.1 Naïve $\overline{DMMPC}$ (neighborhood identification)

Our $\overline{\text{DMMPC}}$ algorithm consists of two phases detailed in Algorithm 10 dedicated to the identification of the neighborhood Ne_0 (resp. Ne_+) of a target variable T in G_0 (resp. $G_\rightarrow$).

Initial model $\mathbf{X}[0]$ and $\mathbf{X}[1]$ respectively denote the variables $\mathbf{X}$ for $t = 0$ and $t = 1$. We remind that the 2T-BN model is first-order Markov. Hence, it is possible that the neighborhood Ne_0 of a variable T in $\mathbf{X}[0]$ can belong to $\mathbf{X}[0]$ and $\mathbf{X}[1]$.

Let us define CPC_0 the parents or children of T in slice 0 and CC_1 the children of T in slice 1.

In $\overline{\text{DMMPC}}$, we propose to use the static MMPC algorithm with the candidate variables $ListC_0 = \mathbf{X}[0] \cup \mathbf{X}[1] \setminus \{T\}$ in order to identify Ne_0. Ne_0 contains variables included in $ListC_0$. We notice that, in this case, the MaxMinHeuristic function returns the maximum over all variables of the minimum association with T relative to Ne_0 (found), and the variable that belongs to $ListC_0$ that achieves the maximum. Because of temporal information, we will then be able to separate $Ne_0 = CPC_0 \cup CC_1$.

Transition model In the same way, $\mathbf{X}$[t-1], $\mathbf{X}[t]$ and $\mathbf{X}[t+1]$ respectively denote the variables $\mathbf{X}$ for times $t-1, t$ and $t+1$.

Ne_+ of a variable T in $\mathbf{X}[t]$ can belong to $\mathbf{X}[t-1]$, $\mathbf{X}[t]$ and $\mathbf{X}[t+1]$. So let us define CPC_t the parents or children of T in slice t, CC_{t+1} the children of T in slice $t+1$ and CP_{t-1} the parents of T in slice $t-1$

We propose to use the static MMPC algorithm with the candidate variables $ListC = \mathbf{X}[t-1] \cup \mathbf{X}[t] \cup \mathbf{X}[t+1] \setminus \{T\}$ in order to identify Ne_+ . We notice that, in this case, the MaxMinHeuristic function returns the maximum over all variables of the minimum association with T relative to Ne_+ (found), and the variable that belongs to $ListC$ that achieves the maximum. Because of temporal information, we will then be able to separate $Ne_+ = CPC_t \cup CC_{t+1} \cup CP_{t-1}$.

Algorithm 10 $\overline{\text{DMMPC}}(T, D)$

Require: target variable (T); Data (D)
Ensure: neighborhood of T in G_0 (Ne_0) and in $G_\rightarrow$ (Ne_+)

% search Ne_0 of T in $t = 0$
1: $ListC_0 = \mathbf{X}[0] \setminus \{T\} \bigcup \mathbf{X}[1]$
2: $Ne_0 = \overline{\text{MMPC}}(T, D, ListC_0)$
% search Ne_+ of T in $t > 0$
3: $ListC = \mathbf{X}[t-1] \bigcup \mathbf{X}[t] \setminus \{T\} \bigcup \mathbf{X}[t+1]$
4: $Ne_+ = \overline{\text{MMPC}}(T, D, ListC)$

5.2.2 Optimized $\overline{DMMPC}$ (Neighborhood identification)

The purpose of the following subsection is to redefine the previous method by reducing the computational complexity result of section 5.2.1. To this end, we relied on some properties:

- 2-TBN model is a first Markov order: the neighborhoods of a node in t time slice belongs to 3 time slices (t-1, t, t+1).
- The orientations of all temporal edges are from t-1 to t time slices or from t to t+1 time slices.
- The identification of these neighborhoods can be done in 3 steps: identification of CPC_t then CP_{t-1} then CC_{t-1} (this property is proposed by this thesis, we give its proof later in the appendix C)

Initial model As mentioned in section 3.2.2, the initial model is a static BN representing the initial joint distribution of the process P(X[t = 0]) and consisting of a direct acyclic graph (DAG) G0 containing the variables X[t = 0].

In this case, it is not needful to identify the temporal dependences (with X[t = 1]) which concern only the transition model. For this reason, we propose in this optimized version using the static MMPC algorithm with the candidate variables ListC0 = X[0]\{T} (instead of X[0] ∪ X[1]\{T}) in order to restrict this step to the identification of the neighborhoods Ne_0 of a variable T in this specific time slice X[0].

Transition model In this case, X[t-1], X[t] and X[t+1] respectively denote the variables X for times t-1; t and t+1. Let us define CPC_t the parents or children of T in slice t, CC_{t+1} the children of T in slice t + 1 and CP_{t-1} the parents of T in slice t - 1. According to the proposition 5.2.1 (the proof of this propostion given by the appendix C), contrary to the naive method we will separate the set of Ne_+ on CPC_t, CC_{t+1} and CP_{t-1} of a variable T in X[t]. Our algorithm tries to find the candidate parents and/or children through separate steps.

In the first step, we start by a forward phase that searches for the candidates that belong to CPC_t using the static MMPC algorithm with the candidate variables $ListC_t$ =X[t]\{T}. We notice that, the MaxMinHeuristic function returns the maximum over all variables of the minimum association with T relative to CPC_t (found), and X the variable that belongs to $ListC_t$ that achieves the maximum. The second Backward phase will reveal if there is any independence between every S variable in CPC_t and T knowing all subsets in CPC_t, and if it is true, this phase will remove S from the CPC_t as a false positive.

In the second step, we start by a forward phase that searches the candidates that belong to CP_{t-1} using the static MMPC algorithm with the candidate variables

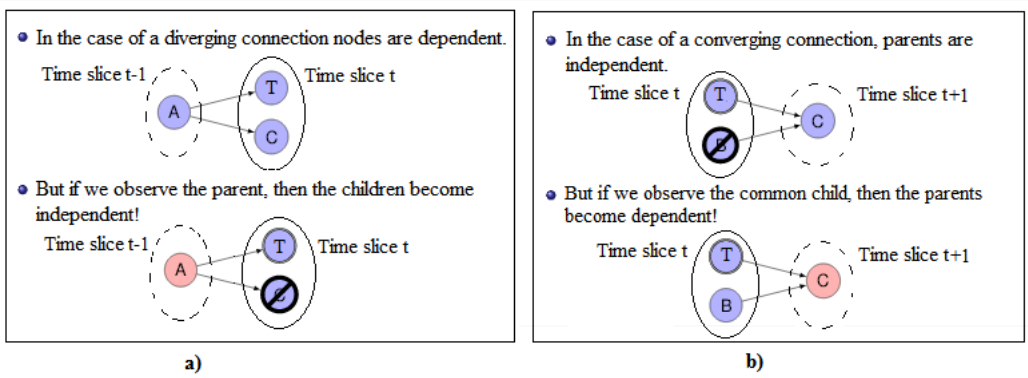


Figure 5.1: Conditional dependence. (a) divergence case. (b) convergence case

$ListC_{t-1}$ =X[t-1]. We notice that, the MaxMinHeuristic function returns the maximum over all variables of the minimum association with T relative to $CPC_t \cup CP_{t-1}$ (found), and X the variable that belongs to $ListC_{t-1}$that achieves the maximum. The second phase will discover if there are an independence between every variable A∈CP_{t-1} or C≠T∈CPC_t and T knowing all subset in $CPC_t \cup CP_{t-1}$ (divergence case), and if it is true, this phase will remove A or C respectivly from the CP_{t-1} or CPC_t as a false positive dependence (cf. figure 5.1.a).

In the third step, we start by a forward phase that searches the candidates that belong to CC_{t+1} using the static MMPC algorithm with the candidate variables $ListC_{t+1}$=X[t+1]. We notice that, the MaxMinHeuristic function returns the maximum over all variables of the minimum association with T relative to $CPC_t \cup CC_{t+1}$ (found), and X the variable that belongs to $ListC_{t+1}$ that achieves the maximum. The second phase will discover if there are an independence between every C variable in CC_{t+1} and T knowing all subsets in $CPC_t \cup CC_{t+1}$ (convergence case), and if it is true, this phase will remove C from the CC_{t+1} as a false positive dependence (cf. figure 5.1.b).

Proposition 5.2.1 *Let T be a target variable and D the learning data, if we consider having an infinite amount of data or results of statistical tests given by an oracle, we claim that our OptimisedDMMPC algorithm will identify the same neighborhood than the Naive one, in a reduced number of iterations.*

In the $\overline{DMMPC}$ algorithm, there are two principal phases (Forward and Backward). We can show that the number of iterations in Forward and Backward steps are smaller for our optimised algorithm. This reduction was obtained by some optimisations (in red in the following equations) used in algorithm 11 and proved in appendix C.

$$Forward\_NaiveDMMPC(\max_{X \subset V_t \setminus T \cup V_{t+1} \cup V_{t-1}} MinAssoc(X;T|CPC_t \cup CC_{t+1} \cup CP_{t-1})) \quad (5.1)$$

$$\backsimeq Forward\_optimisedDMMPC(\max_{X \subset V_t \setminus T \cup V_{t+1} \cup V_{t-1}} MinAssoc(X;T|CPC_t \cup CC_{t+1} \cup CP_{t-1})) \quad (5.2)$$

$$\backsimeq CPC_t\_found \bigcup CC_{t+1}\_found \bigcup CP_{t-1}\_found \tag{5.3}$$

Where
Forward_optimisedDMMPC($\max_{X \subset V_t \setminus T} MinAssoc(X; T | CPC_t\_found)$) = CPC_t_found
Forward_optimisedDMMPC($\max_{X \subset V_{t+1}} MinAssoc(X; T | CPC_t\_found \cup CC_{t+1}\_found)$)
= CC_{t+1}_found
Forward_optimisedDMMPC($\max_{X \subset V_{t-1}} MinAssoc(X; T | CPC_t\_found \cup CP_{t-1}\_found)$)
= CP_{t-1}_found

And

$$Backward\_NaiveDMMPC(Assoc_{X \in CPC_t \cup CC_{t+1} \cup CP_{t-1}}(X; T | S \subset CPC_t \cup CC_{t+1} \cup CP_{t-1})) \tag{5.4}$$

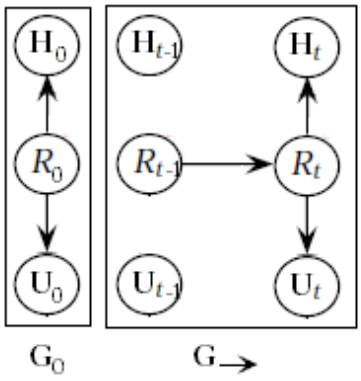
$$\backsimeq Backward\_optimisedDMMPC(Assoc_{X \in CPC_t \cup CC_{t+1} \cup CP_{t-1}}(X; T | S \subset CPC_t \cup CC_{t+1} \cup CP_{t-1})) \tag{5.5}$$

$$\backsimeq CPC_t \bigcup CC_{t+1} \bigcup CP_{t-1} \tag{5.6}$$

Where
Backward_optimisedDMMPC($\text{Assoc}_{X \in CPC_t\_found}(X; T | S \subset CPC_t\_found)$) = CPC_t
Backward_optimisedDMMPC($\text{Assoc}_{X \in CC_{t+1}\_found}(X; T | S \subset CPC_t\_found \cup CC_{t+1}\_found)$)
= CC_{t+1}
Backward_optimisedDMMPC($\text{Assoc}_{X \in CP_{t-1}\_found}(X; T | S \subset CPC_t\_found \cup CP_{t-1}\_found)$)
= CP_{t-1}

5.2.3 Toy example (naive $\overline{DMMPC}$ vs optimised $\overline{DMMPC}$)

In this section, we provide an example trace of $\overline{\text{DMMPC}}$ with a toy example, the extended Umbrella network shown in figure 5.2.



P(Height$_t$)		
Rain$_t$	top	low
True	0.7	0.001
False	0.3	0.999

P(Unbrella$_t$)		
Rain$_t$	True	False
True	0.9	0.2
False	0.1	0.8

P(Rain$_t$)		
Rain$_{t-1}$	True	False
True	0.7	0.01
False	0.3	0.99

Rain$_0$	
True	0.7
False	0.3

Figure 5.2: The extended Umbrella DBN

The dataset D is sampled from this network, with 20.000 time sequences of 8 time slices. The $Assoc$ function used for independence measurement is the χ^2 test with $\alpha = 0.05$.

Figure 5.3 describes how the naive approach deals with each iteration involved in Ne_+ identification for target node R_t. We can see that the naive $\overline{\text{DMMPC}}$ progressively discovers the right neighborhood and is able at the end to separate the candidate parents (in blue) in slice $t-1$, the candidate parents or children (in red) in slice t and the candidate children (in green) in slice $t+1$.

As proposed by [104], two optimizations are performed in order to control the algorithm complexity (estimated here by the number of calls to the $Assoc$ function). The first, in MaxMinheuristic (MMH) corresponds to the fact that one part of the $Assoc$ calls at iteration has already been computed in the previous iteration and can be saved. This optimization can be seen in iteration 2 where only 7 $Assoc$ calls have been performed. The same optimization can be achieved in all the next iterations. The second optimization corresponds to the fact that if one variable in $ListC$ reaches a minimal $Assoc$ value equal to zero for a given conditioning set, then it will get this minimal association for all the other iterations. We can then discard this variable from $ListC$ and save some other $Assoc$ calls in the next iterations. This "filtering step" is illustrated in iteration 4 where H_{t-1} and U_{t-1} get a minimal association equal to zero and are discarded of $ListC$ in iteration 5.

In figure 5.4 we show that the optimized $\overline{DMMPC}$ can discover the right neighborhood in CPC_t, CP_{t-1} and CC_{t+1} for target node R_t. In the previous paragraph, we mentioned that two optimizations are performed in order to control the algorithm complexity of the naïve method. In this optimized method (section 5.2.2), we added another optimization. To search for the neighborhood in CPC_t for target node R_t, we only need to use the variables in the t time slice ($ListC_t$). So, the number of the Assoc calls is minimized. This optimization can be seen in iterations 1 and 2 where respectively only 2 and 1 Assoc calls have been computed. However, in the naïve method the iterations 1 and 3 make respectively 8 and 7 Assoc calls. We can see this optimization in all iterations involved in CP_{t-1} and CC_{t+1} identification for the target node R_t.

5.2.4 Symmetrical correction

As its static counterpart, DMMPC algorithm described in algorithm 12 has to perform a symmetrical correction. Because of the non-symmetry of temporality, we have to adapt this correction. When $t = 0$, we have to apply the symmetrical correction on CPC_0 and CC_1 separately because for all $X \in CC_1$, X doesn't belong to slice $t = 0$ but in slice $t = 1$ and its temporal neighborhoods are given by $Ne_+(X)$. The DMMPC algorithm needs as inputs the result of (naïve or optimized) $\overline{DMMPC}$. In the case of initial model, the symmetrical correction is as follows.

1. Divide the Ne_0 into two subsets CPC_0 and CC_1
2. For all $\text{X} \in \text{X}[0]$ and $\text{X} \in \text{CPC}_0(\text{T})$, find if $\text{T} \notin \text{CPC}_0(\text{X})$ then X is removed

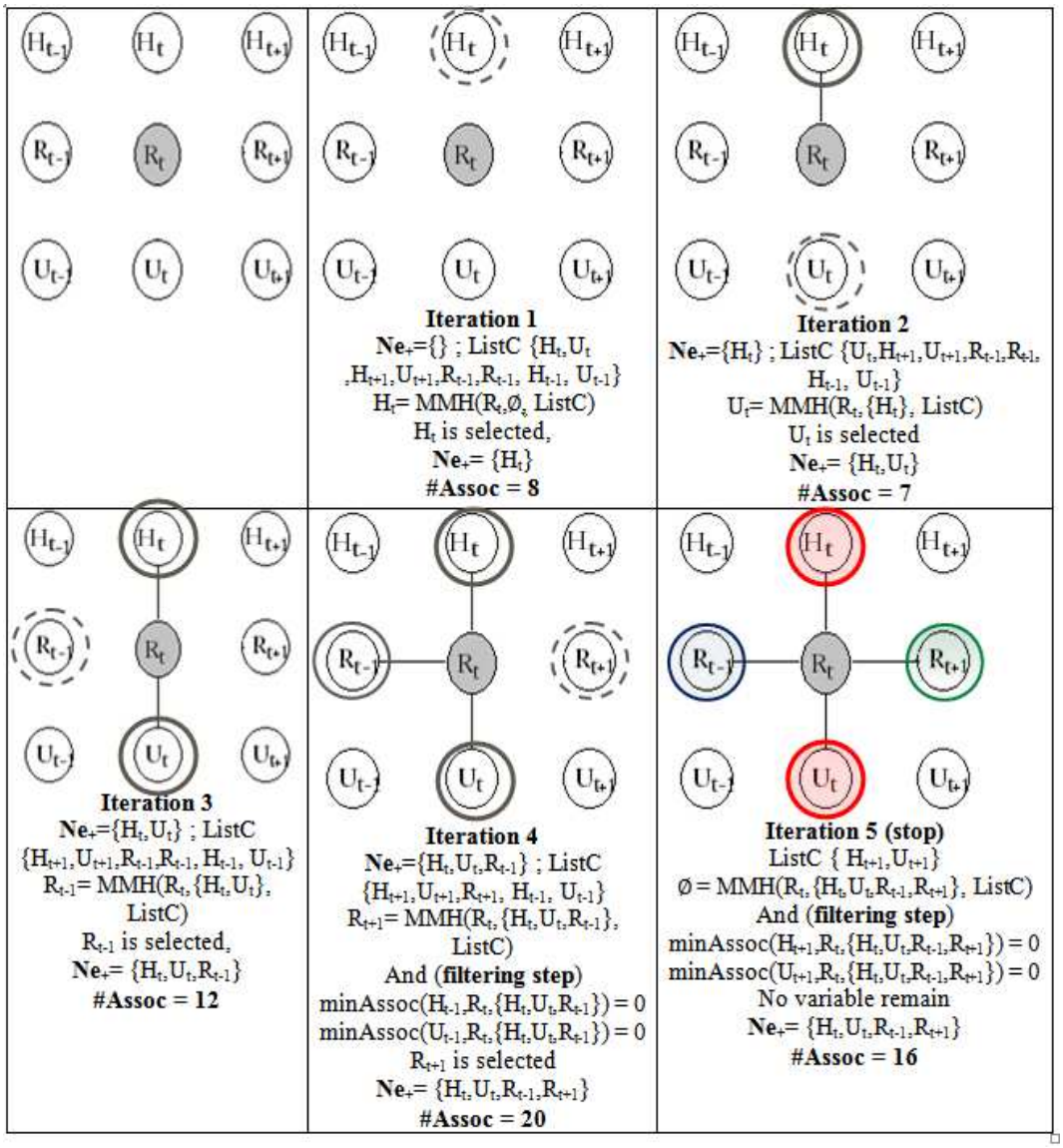


Figure 5.3: Example trace of naive $\overline{DMMPC}$

from $CPC_0(T)$.

3. For all $X \in X[1]$ and $X \in CC_1(T)$, find if $T \notin Ne_+(X)$ then X is removed from $CC_1(T)$. It uses Ne_+, because X belongs to the time slice 1>0 and the set of all parents and children of X exists in Ne_+.

In the case of transition model, the symmetrical correction is as follows.

1. The separation of the subsets CPC_t,CC_{t+1} and CP_{t-1} is not used.
2. For all $X \in Ne_+(T)$, finds if $T \notin Ne_+(X)$ then X is removed from $Ne_+(T)$.
3. Divide the Ne_+ into three subsets CPC_t, CP_{t-1} and CC_{t+1} depending on their membership to the time slices respectively t, t-1, t+1.

5.3 Dynamic Max Min Hill-Climbing DMMHC

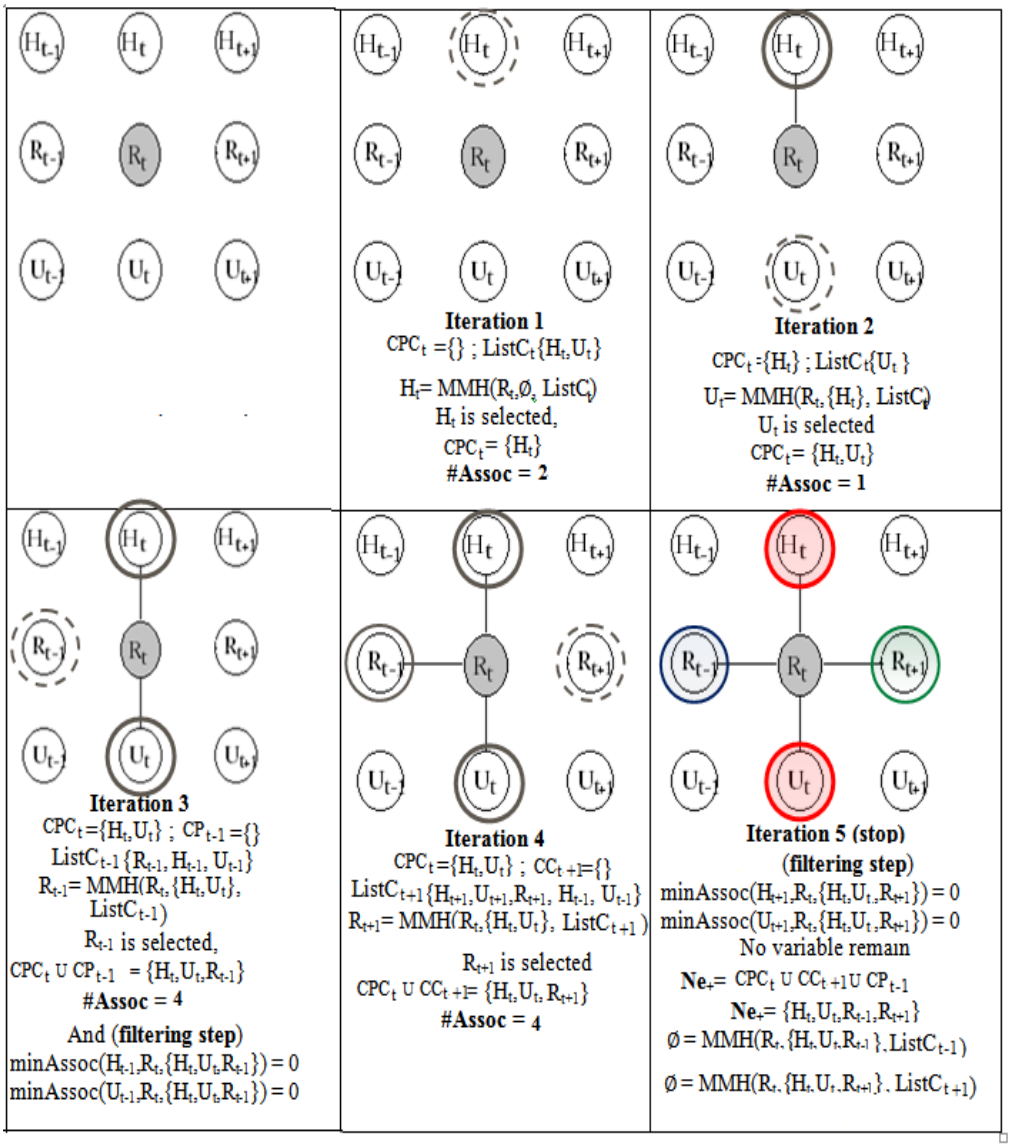


Figure 5.4: Example trace of optimised $\overline{DMMPC}$

This phase is dedicated to the global model optimization. Our Dynamic MMHC algorithm described in Algorithm 13 proposes to identify independently the graphs given by the DMMPC phase by applying a greedy search algorithm (adapted by [32] for a 2-TBN) constrained with local information. This information is provided by the identification of the neighborhood Ne_0 (resp. Ne_+) of each node in G_0 (resp. $G_{\rightarrow}$).

As its static counterpart, DMMHC will consider adding an edge during the greedy search, if and only if the starting node is in the neighborhood of the ending node. G_0 learning only concerns the variables in slice $t = 0$, so we can restrict the add_edge operator only to variables found in a CPC_0 of another variable.

$G_{\rightarrow}$ is a graph with variables in slices $t-1$ and t but this graph only describes the temporal dependencies between $t-1$ and t and "inner" dependencies in t. So we also restrict our operators in order to consider adding edges with these constraints

and we don't authorize reversing the temporal edges.

5.4 DMMHC for simplified 2-TBN

In simplified kT-BN , the temporality is constrained by the k order Markov assumption. There are two cases for this model when k=2 and k≥3. The first case is the simplified k-TBN. It allows representing the transition network with only the inter-connectivity between t-1 and t time slices and we can apply the first order Markov assumption in this model. We used this case in our work DMMHC for simplified 2-TBN. The second case represents the transition network with the inter-connectivity between t-s and t time slices where k > s.

We think that our DMMHC algorithm can easily take into account these temporal constraints. We propose here an extension of DMMHC named simplified DMMHC for 2-TBN structure learning.

As seen in section 3.2, the 2-TBN simplified structure focuses only on $G_{\rightarrow}$. This kind of model is limited to contain only inter time slice arcs. Inspired by DMMHC algorithm, our new simplified DMMHC algorithm proposes to identify $G_{\rightarrow}$ graph by applying the different phases of DMMHC shown in the previous sections.

Neighborhood identification In the first phase of neighborhood identification, we need only to identify the Ne+ for all variables T in t time slice. As we previously defined the set of Ne+(T)=CP_{t-1}(T) $\bigcup$ CPC_t(T) $\bigcup$ CC_{t+1}(T). In the simplified 2-TBN we have many properties to define (figure 5.5):

1. we don't need to identify the CPC_t(T) candidates because we are interested in the inter connectivity only.
2. we don't need to identify the CC_{t+1}(T) candidates because if X ∈ CC(T) ⇒ T ∈ CP(X) where X in t time slice (the temporal symmetrical correction result).
3. Ne_+(T)= CP_{t-1}(T) $\bigcup$ CPC_t(T) $\bigcup$ CC_{t+1}(T). We notice that with the use of the properties 1 and 2 ⇒ Ne_+(T)= CP_{t-1}(T).
4. To identify all X in CP_{t-1}(T), we need to compute the MaxMinAssoc(X; T|CP_{t-1} $\bigcup$ CPC_t). We suggested below the proposition 5.4.1 to facilate the computation (the proof of this propostion given by the appendix C):
5. The Backward phase of DMMHC allows to detect any false positives depending on the structure. But after the Forward phase we musn't find any one. So we can remove the Backward phase in DMMHC simplified.

Proposition 5.4.1 *Let V_{t-1} the set of variables for time slice t-1 and $X \in V_{t-1}$.*

$$\max_X \min Assoc(X; T|Ne_+(T)) = \max_X \min Assoc(X; T|CP_{t-1}) = \max_X Assoc(X; T|\emptyset) \tag{5.7}$$

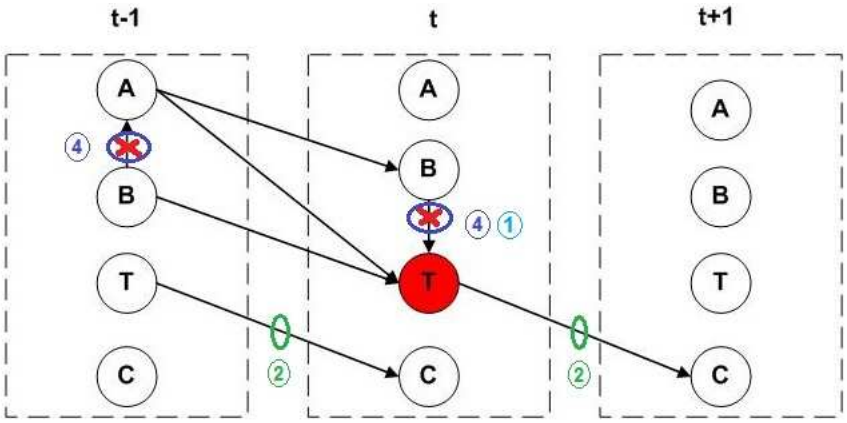


Figure 5.5: Example trace of simplified $\overline{DMMPC}$

Symmetrical correction Contrarily to its static and dynamic counterpart, the simplified DMMPC algorithm doesn't need to perform a symmetrical correction. (1) in this case, DMMHC doesn't look for any CPC_t candidates. (2) Because of the non-symmetry of temporality, we have to adapt this correction. But, we assume that in propriety (2) in neighborhood identification the $CC_{t+1}(T)$ is defined by $CP_{t-1}(X)$ where $X \in CC_{t+1}(T)$.

DMMHC In the naïve and optimized cases, DMMHC applies a greedy search algorithm constrained with local informations. In the naïve and optimized DMMPC, contrary to the edges existing in intra-time slice, all temporal edges are oriented by DMMPC. DMMHC uses the results of DMMPC as inputs and orients the undirected edges. In the case of simplified 2-TBN model, we need only to identify the temporal edges, so all edges in the graph are oriented by the DMMPC algorithm and we don't need to use the DMMHC to orient other edges. However we need the DMMHC to delete the false temporal edges.

5.5 Time complexity of the algorithms

In this section, we calculated the time complexity of our algorithm. First we remind how the time complexity of MMPC was calculated in the static case. According to [104] the number of independence tests for all variables with the target conditioned on all subsets of CPC (target parents and children set) is bound by $O(|V|.2^{|CPC|})$, where $|V|$ represents the number of all variables in the Bayesian network and $|CPC|$ is the number of all variables in the parents/children target set. The overall cost of identifying the skeleton of the BN is $O(|V|^2\ 2^{|PC|})$, where PC is the largest set of parents and children overall variables in V.

Naive DMMHC In our dynamic (temporal) case, as for the static, we first identify the number of tests in $\overline{DMMPC}$. In this part we have two cases to present (i.e. t=0 and t>0). For t=0, $\overline{DMMPC}$ will calculate the association of all variables in time slices t=0 and t=1 with target in slice t=0 conditioned on all subset of Ne_0 (in the worst case). Thus, the number of tests in the case t=0 is bounded by $O(|2V|.2^{|Ne_0|})$, where V is the set of all variables in a time slice. For t>0 case, the number of tests is bounded by $O((|3V|.2^{|Ne_+|})$, because $\overline{DMMPC}$ calculates the association of all variables in three time slices t, t-1, t+1 with the target in slice t conditioned on all subsets of Ne_+ (in the worst case).

We sum up, the total number of tests in both phases at $t = 0$ and $t > 0$ is bounded respectively by $O(|2V|.2^{|Ne_0|})$ and $O(|3V|.2^{|Ne_+|})$. Thus, the total number of tests in both phases is bounded by $O(|3V|.2^{|Ne_+|})$. The overall cost of identifying the skeleton of the initial and transition models in dynamic Bayesian network (i.e., calling DMMPC with all targets in G_0 and $G_{\rightarrow}$) is $O(|3V|^2.2^{|Ne|})$, where Ne is the largest set of neighborhood (in t and t+1 and t-1) over all variables in the time slice t.

Optimised DMMHC For the optimized DMMPC, we start with t=0, DMMPC will calculate the association of all variables in time slices t=0 with target in slice t=0 conditioned on all subsets of CPC_0 (in the worst case). Thus, the number of tests in the case t=0 is bounded by $O(|V|.2^{|CPC_0|})$, where V is the set of all variables in a time slice. For t≥1 case, the number of tests is bounded by $O(|V|.2^{|CPC_t|}+|V|.2^{|CPC_t|+|CP_{t-1}|}+|V|.2^{|CPC_t|+|CC_{t+1}|})$, because DMMPC calculates the association of all variables in t or in t-1 or t+1 with the target in slice t conditioned on all subsets respectively of CPC_t or $CPC_t \cup CP_{t-1}$ or $CPC_t \cup CC_{t+1}$ (in the worst case).

To recapitulate, the total number of tests in both phases at t = 0 and t > 0 is bounded respectively by $O(|V|.2^{|CPC|})$ and $O(|V|.2^{2|CPC|})$, where CPC is the largest set of neighborhood in one time slice (t or t+1 or t-1) over all variables in t (i.e. $|Ne| \simeq 3*|CPC|$). Thus, the total number of tests in both phases is bounded by $O(|V|.2^{2|CPC|})$. The overall cost of identifying the skeleton of initial and transition models in dynamic Bayesian network (i.e., calling DMMPC with all targets in G_0 and $G_{\rightarrow}$) is $O(|V|^2.2^{2|CPC|})$.

Simplified DMMHC The simplified DMMHC deals with the transition model only. $\overline{DMMPC}$ calculated the association of all variables in time slice t-1 with target in slice t conditioned on empty set (in all cases). Thus, the number of tests in the case t is bounded by O(N), where N is the set of all variables in a time slice.

We assume that, since we don't need to use the symmetrical correction and DMMHC, the overall cost of identifying the skeleton of transition model in dynamic Bayesian network (i.e., calling $\overline{DMMPC}$ with all targets in $G_{\rightarrow}$) is $O(N^2)$.

5.6 Related work

Many approaches for structure learning in DBN [32, 107, 108, 35, 112] are validated on benchmark models with about 10 variables. In a more general context, due to inherent limitations of the score-based structure learning methods, all these methods will have a very high complexity if the number of variables increases.

With the help of a local search, DMMHC is able to limit the search space in the final global optimization (GS). In this way, we can theoritically work in high dimensions like MMHC with static BNs. We can say that our approach outperforms the other approaches based on score, because contrary to these last kind of approaches, DMMHC can deal with large dimension and on complete search space.

Another way to deal with scalability is to restrict the class of 2T-BN by only considering parents of $X_i[t]$ in time slice t-1 (for 2T-BN) or any previous time slice (for kT-BN).

Dojer [27] proposes a score based method named polynomial time algorithm for learning this class of DBN (with BDe and MDL scores). Vinh et al. [111] proposed another polynomial time algorithm in the same context (equicardinality requirement) with other scoring function (MIT). Also, the authors proposed another contribution in this work consisting of a hybrid method with local Blanket identification (MIT-MMMB).

DMMHC and MIT based MMMB are both hybrid methods with local search and global optimization. When DMMHC tries to identify the candidate parents/children CPC set of a target variable in a 2T-BN, MIT based MMMB tries to identify the (more complex) Markov Blanket MB but in a restricted subclass of 2T-BNs. On the one hand, this assumption allows to simplify both MB discovery and global optimization. On the other hand, contrary to DMMHC, MIT based MMMB is not able to identify the intra-time dependencies. So, the hybrid method doesexist in literature and it can deal with large dimension but it is executed on simplified search space. In addition, we have proposed another version of DMMHC which can work on this kind of models.

5.7 Conclusion

In this chapter, we proposed a new 2T-BN structure learning algorithm dealing with large networks. Inspired from the MMHC algorithm proposed by [104] for static BNs, our DMMHC algorithm is a local search algorithm dealing with local structure identification (DMMPC) and global model optimization constrained with this local information.

We have shown that the local structure identification can easily take into account the temporal dimension in order to provide some additional information about tem-

porality that can then be used with a greedy search in order to learn the global structure, the initial model G_0, and the transition one $G_{\rightarrow}$. As far as we know, no method capable to learn 2-TBN models with such approaches has been proposed previously.

We also presented an optimisation for our DMMHC named optimised DMMHC. It is a local improvement of our algorithm. We think that our scalability can be improved during the local structure identification using temporality constraints in $\overline{\text{DMMPC}}$ in order to decrease the number of $Assoc$ calls and consequently decrease the running time that we will demonstrate in the next chapter dealing with our experimentation.

Furthmore, in this chapter, we suggested a new version of DMMHC, which work on simplified 2-TBN without intra-connectivity edges. We compared all the versions of DMMHC (naive DMMHC, optimised DMMHC and simplified DMMHC) for 2T-BN structure learning in terms of complexity and showed that we are able to decrease the complexity with the use of temporal constraints.

Algorithm 11 $\overline{\text{DMMPC}}$optimised(T, D)

Require: target variable (T); Data (D)
Ensure: neighborhood of T in G_0 (Ne_0) and in $G_{\rightarrow}$ (Ne_+)

% search Ne_0 of T in $t = 0$
1: $ListC_0 = \mathbf{X}[0] \setminus \{T\}$
2: $Ne_0 = \overline{\text{MMPC}}(T, D, ListC_0)$
% search Ne_+ of T in $t > 0$
3: $CPC_t = \emptyset$ % parents children candidates for T in slice t
4: $CP_{t-1} = \emptyset$ % only parents candidates for T in slice t-1
5: $CC_{t+1} = \emptyset$ % only children candidates for T in slice t+1
% search Ne_+ of T in t, $t+1$ and $t-1$
6: $ListC_t = \mathbf{X}[t] \setminus \{T\}$
7: $ListC_{t+1} = \mathbf{X}[t+1] \setminus \{T\}$
8: $ListC_{t-1} = \mathbf{X}[t-1] \setminus \{T\}$
% search CPC_t
% Phase I: Forward
9: **repeat**
10: $\prec F, assocF \succ$ = MaxMinHeuristic($T, CPC_t, ListC_t$)
11: **if** $assocF \neq 0$ **then**
12: $CPC_t = CPC_t \bigcup \{F\}$
13: $ListC_t = ListC_t \setminus \{F\}$
14: **end if**
15: **until** CPC_t has not change or $assocF = 0$ or $ListC_t = \emptyset$
% Phase II: Backward
16: **for all** $X \in CPC_t$ **do**
17: **if** $\exists S \subseteq CPC_t$ **and** $assoc(X; T|S) = 0$ **then**
18: $CPC \setminus \{X\}$
19: **end if**
20: **end for**
% search CP_{t-1}
% Phase I: Forward
21: **repeat**
22: $\prec F, assocF \succ$ = MaxMinHeuristic($T, CPC_t \cup CP_{t-1}, ListC_{t-1}$)
23: **if** $assocF \neq 0$ **then**
24: $CP_{t-1} = CP_{t-1} \bigcup \{F\}$
25: $ListC_{t-1} = ListC_{t-1} \setminus \{F\}$
26: **end if**
27: **until** CP_{t-1} has not change or $assocF = 0$ or $ListC_{t-1} = \emptyset$
% Phase II: Backward
28: **for all** $X \in CPC_t \cup CP_{t-1}$ **do**
29: **if** $\exists S \subseteq CPC_t \cup CP_{t-1}$ **and** $assoc(X; T|S) = 0$ **then**
30: $CP_{t-1} \setminus \{X\}$ or $CPC_t \setminus \{X\}$
31: **end if**
32: **end for**
% search CC_{t+1}
% Phase I: Forward
33: **repeat**
34: $\prec F, assocF \succ$ = MaxMinHeuristic($T, CPC_t \cup CC_{t+1}, ListC_{t+1}$)
35: **if** $assocF \neq 0$ **then**
36: $CC_{t+1} = CC_{t+1} \bigcup \{F\}$
37: $ListC_{t+1} = ListC_{t+1} \setminus \{F\}$
38: **end if**
39: **until** CC_{t+1} has not change or $assocF = 0$ or $ListC_{t+1} = \emptyset$
% Phase II: Backward
40: **for all** $X \in CC_{t+1}$ **do**
41: **if** $\exists S \subseteq CPC_t \cup CC_{t+1}$ **and** $assoc(X; T|S) = 0$ **then**
42: $CC_{t+1} \setminus \{X\}$
43: **end if**
44: **end for**
45: $Ne_+ = CPC_t \bigcup CP_{t-1} \bigcup CC_{t+1}$

Algorithm 12 DMMPC(T, D)

Require: target variable (T); Data (D)
Ensure: neighborhood of T in G_0 (Ne_0) and $G_{\rightarrow}$ (Ne_+)

$Ne_0 = \overline{\text{DMMPC}}(T, D,).Ne_0$
$Ne_+ = \overline{\text{DMMPC}}(T, D).Ne_+$
% symetrical correction Ne_0 of T in $t = 0$
$CPC_0 = Ne_0 \bigcap \mathbf{X}[0]$
$CC_1 = Ne_0 \bigcap \mathbf{X}[1]$
for all $X \in CPC_0$ **do**
  if $T \notin \overline{\text{DMMPC}}(X, D).Ne_0$ **then**
    $CPC_0 = CPC_0 \setminus \{X\}$
  end if
end for
for all $X \in CC_1$ **do**
  if $T \notin \overline{\text{DMMPC}}(X, D).Ne_+$ **then**
    $CC_1 = CC_1 \setminus \{X\}$
  end if
end for
$Ne_0 = CPC_0 \bigcup CC_1$
% symetrical correction Ne_+ of T in $t > 0$
for all $X \in Ne_+$ **do**
  if $T \notin \overline{\text{DMMPC}}(X, D).Ne_+$ **then**
    $Ne_+ = Ne_+ \setminus \{X\}$
  end if
end for
$CPC = Ne_+ \bigcap \mathbf{X}[t]$
$CC = Ne_+ \bigcap \mathbf{X}[t+1]$
$CP = Ne_+ \bigcap \mathbf{X}[t-1]$

Algorithm 13 DMMHC(D)

Require: Data D
Ensure: G_0 and $G_{\rightarrow}$
% Restrict
% Construction initial model G_0
for all $X \in \mathbf{X}[0]$ **do**
  CPC_X=DMMPC(X, D).CPC_0
  CC_X=DMMPC(X, D).CC_1
end for
% Greedy search (GS)
Only try operator add_edge $Y \rightarrow X$ if $Y \in CPC_X$
% Construction transition model
for all $X \in \mathbf{X}[t]$ **do**
  CPC_X=DMMPC(X, D).CPC
  CC_X=DMMPC(X, D).CC
  CP_X=DMMPC(X, D).CP
end for
% Greedy search (GS)
Only try operator add_edge $Y \rightarrow X$ if $Y \in CPC_X$ and $\{X, Y\} \in \mathbf{X}[t]$
Only try operator add_edge $X \rightarrow Y$ if $Y \in CC_X$ and $X \in \mathbf{X}[t]$ and $Y \in \mathbf{X}[t+1]$
Don't try operator reverse_edge $X \rightarrow Y$ if $Y \in CC_X$ and $X \in \mathbf{X}[t]$ and $Y \in \mathbf{X}[t+1]$

Algorithm 14 $\overline{\text{DMMPC}}$simplified(T, D)

Require: target variable (T); Data (D)
Ensure: neighborhood of T in $G_{\rightarrow}$ (Ne_{+})

% search Ne_{+} of T in $t > 0$
1: $CP_{t-1} = \emptyset$ % only parents candidates for T in slice t-1
% search Ne_{+} of T in $t - 1$
2: $ListC_{t-1} = \mathbf{X}$[t-1]\ {T}
% search CP_{t-1}
% Phase I: Forward
3: **repeat**
4: $< F, assocF >$ = MaxAssoc(T, {}, $ListC_{t-1}$)
5: **if** $assocF \neq 0$ **then**
6: $CP_{t-1} = CP_{t-1} \bigcup \{F\}$
7: $ListC_{t-1} = ListC_{t-1} \setminus \{F\}$
8: **end if**
9: **until** CP_{t-1} has not change or $assocF = 0$ or $ListC_{t-1} = \emptyset$
10: $Ne_{+} = CP_{t-1}$

6

Experimental study

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6.1 Introduction

The experimental study presented in this chapter covered many points that presented in the previous chapters of our contributions. In this chapter, we were justified our theoretical ideas by real experiments. First, in section 6.2, we described our experimental protocol. We explained the steps used to prepare the necessary elements to run the experiments concerning the structure learning algorithms, the small and large benchmarks used for evaluation and finally the different metrics used to compare between different techniques presented in this thesis.

In section 6.3, we performed some experiments with our methods and others techniques existing in literature on the same context, and we showed the different results with their corresponding interpretations.

After that, in section 6.4 we mainly focused on the application of simplified DMMHC to one biological and genetic task on simplified search space. We compared our DMMHC algorithms with others tools available in the internet as Banjo, BNFinder, etc... Finally, section 6.5 is dedicated to a scalability comparison of all versions of DMMHC.

6.2 Experimental protocol

6.2.1 Algorithms

We have implemented the Greedy Search (GS) for 2T-BN as described in section 3.2. This algorithm is considered as the reference algorithm for DBN structure learning. We have also implemented our proposal, DMMHC, described in chapter 5. We can notice here that our algorithm uses a constrained greedy search, whereas the original MMHC algorithm proposes to use a Tabu search.

We can notice that the MMHC implementation available in our platform employs a chi-square test based on the χ^2 statistics. Our implementation also uses a standard formula to compute the degree of freedom instead of the heuristic proposed in the original publication [103]. These differences may also explain some of the discrepancy found when we are trying to reproduce the results from the literature.

In the greedy search, we used the BIC score function. χ^2 independence test is used with $\alpha = 0.05$.

Experiments were carried out on a dedicated PC with Intel(R) Core(TM) 2.20 Ghz, 64 bits architecture, 4 Gb RAM memory and under Windows 7.

Networks	# vars	# edges	Temporal edges	# states (min-Max)	# parents (min-Max)	# neighbors (min-Max)
Asia_G_0	8	8		2-2	0-2	1-4
Asia_$G_{\rightarrow}$	16	21	5	2-2	0-3	1-5
Alarm_G_0	37	46		2-4	0-4	1-6
Alarm_$G_{\rightarrow}$	74	110	18	2-4	0-4	1-7
Hailfinder_G_0	56	66		2-11	0-4	1-7
Hailfinder_$G_{\rightarrow}$	112	156	24	2-11	0-4	1-17
Win95pts_G_0	76	112		2-2	0-7	1-10
Win95pts_$G_{\rightarrow}$	156	256	41	2-2	0-7	1-10
Andes_G_0	223	338		2-2	0-6	1-12
Andes_$G_{\rightarrow}$	446	820	144	2-2	0-6	1-12
Link_G_0	724	1125		2-4	0-3	1-17
Link_$G_{\rightarrow}$	1448	2530	280	2-4	0-4	1-17

Table 6.1: Characteristics of 2T-BNs (G_0, $G_{\rightarrow}$) generated from 6 usual static BNs (Asia, Alarm, Hailfinder, Win95pts, Andes, Link)

6.2.2 Benchmarks

Contrary to the static BN, evaluating a DBN structure learning algorithm is more difficult. One reason is the unavailability of standard benchmarks, except for instance some reference networks with a small number of variables (less than 10), such as Umbrella and Water [1].

In chapter 4, we provided tools for benchmarking dynamic Bayesian network structure learning algorithms by proposing a 2T-BN generation algorithm, able to generate large and realistic 2T-BNs from existing static BNs. We used these tools to generate 2T-BNs from 6 well-known static BNs (Asia, Alarm [8], Hailfinder [49], Win95pts, Andes [16] and Link). Details about these networks are given in table 6.1

For each of these 2T-BNs, we have respectively generated 2.000, 5.000 and 10.000 sequences of length equal to 6, which corresponds to datasets of size 2.000, 5.000 and 10.000 for G_0 structure learning and 5x2.000, 5x5.000 and 5x10.000 for $G_{\rightarrow}$ structure learning. Each data generation was also repeated 3 times for each network.

6.2.3 Performance indicators

The studies about DBN structure learning use different indicators to argue about the reliability of their proposals.

In chapter 4, we proposed a new metric to evaluate the performance of these structure learning algorithms, by correcting the existing Structural Hamming distance in order to take into account temporal background information. As 2T-BNs

1. http://www.cs.huji.ac.il/ galel/Repository/Datasets/water/water.html

Networks	GS[34]	GTT[22]	GS(G_0)	MMHC[34]	DMMHC(G_0)
Alarm	47	44	40	24	27
Hailfinder	**114**	48	54	**88**	46
Link				687	650

Table 6.2: SHD comparison with existing static structure learning approaches ([34],[22]), for Alarm, Hailfinder and Link benchmarks with 5000 samples.

are defined by two graphs G_0 and $G_{\rightarrow}$, the distance between one theoretical 2T-BN and the learnt one is defined as the pair of the structural Hamming distances for initial and transition graphs.

The running time was also measured. Experiments were canceled when computations were not completed within 48 hours.

6.3 Empirical results and interpretations on complete search space

6.3.1 Initial validation

To carry out comparisons with other the existing algorithms, Murphy [74] lists over 50 software packages available for different applications of Bayesian networks. However, as we mentioned in chapter III, there are few free softwares able to infer the structure of static and dynamic Bayesian networks from data, which are:

- Banjo package [2]: Bayesian Network Inference with Java Objects
- Bayes Net Toolbox [72] for Matlab with an extension for dynamic Bayesian networks inference using MCMC.
- BNFinder package [114]: exact and efficient method for learning Bayesian networks

Learning the initial model for our proposed algorithm is very similar to the static structure learning. As we created our 2T-BN benchmarks from usual static BNs, we can compare the results of our implementations to static ones. [34] provides one comparative study involving GS and MMHC for Alarm, Hailfinder and Link benchmarks with 5000 samples, with BDeu score (and similar results for BIC score). [22] provides SHD results for Alarm and Hailfinder with 5000 samples for another structure learning algorithm, Greedy Thick Thinning (GTT) [19], a two-phase hill-climbing heuristic algorithm.

Table 6.2 summarizes the structure Hamming distance obtained for 3 different hill-climbling algorithms and 2 implementations of MMHC, in about the same contexts (5000 samples). We can observe that our implementation gives similar results as concurrent ones for Alarm and Link benchmarks. Some strange results occur

2. http://www.cs.duke.edu/ amink/software/banjo/

Networks	DMMHC G_0			GS G_0		
	2000	5000	10000	2000	5000	10000
Asia	**6**±2	**5**±1	4±1	**5**±2	**4**±2	**2**±1
Alarm	**33**±3	**27**±3	**22**±3	43±7	40±3	35±5
Hailfinder	**48**±1	**46**±1	**40**±1	55±1	54±7	48±5
Win95pts	**86**±3	**74**±3	**64**±1	102±11	93±5	85±15
Andes	**132**±11	**110**±9	**94**±3	-	-	-
Link	**698**±13	**650**±8	**598**±10	-	-	-

Table 6.3: Average±standard deviation of SHD obtained by GS and DMMHC in G_0

for Hailfinder benchmark. [34] reports SHD results equal to 114 (resp. 88) for GS (resp. MMHC) and our implementation obtains 54 (resp. 46) when [22] obtains 48. A deeper study was conducted in order to understand this phenomenon. The definition of the SHD in the original publication is different than the one employed here. It is defined as the number of operations "add/remove undirected edge", "add/remove arrowhead of an edge" required to make two CPDAGs become the same. Thus, if CPDAG G1 contains a directed edge and CPDAG G2 does not contain the edge their SHD is increased by 2: one operation to insert the missing edge and one operation to direct it. In this thesis, the SHD metric employed would increase by 1 instead. This does not present a problem with the empirical evaluation but it is better to note it. It could also explain why there is a discrepancy in the results on the Hailfinder network between the published SHD obtained by MMHC on the same network and the one reproduced by our used SHD.

6.3.2 DMMHC versus dynamic GS and SA

Tables 6.3 and 6.4 present the average results obtained by GS and DMMHC algorithms with respect to the sample sizes. This table describes the results for the initial model and transition model corresponding to six (small and large) benchmarks (Asia, Alarm, Hailfinder, Win95pts, Andes, Link). We can notice that for every benchmark, DMMHC algorithm obtains better SHD than GS. except for Asia where the results are similar for G_0.

Table 6.5 shows the running time measured for DMMHC and GS algorithms for each experimental context. We can observe than DMMHC overperforms GS running time. This situation is really significant even for benchmarks with a small number of variables. We can then notice that, unlike GS, DMMHC is able to provide results in a decent time for large benchmarks (Andes and Link).

Figure 6.1 presents the average results of SHD and running time obtained by GS and DMMHC algorithms with respect to the sample sizes. This figure describes the results for the initial model corresponding to six (small and large) benchmarks (Asia, Alarm, Hailfinder, Win95pts, Andes, Link).

Networks	DMMHC $G_{\rightarrow}$			GS $G_{\rightarrow}$		
	2000	5000	10000	2000	5000	10000
Asia	**4**±0	**4**±0	**4**±0	19±2	22±6	22±5
Alarm	**35**±2	**29**±1	**26**±3	115±6	107±2	101±3
Hailfinder	**46**±1	**45**±1	**45**±1	129±9	122±12	118±8
Win95pts	**153**±0	**153**±0	**153**±0	238±20	224±18	217±23
Andes	**155**±0	**134**±2	**124**±3	-	-	-
Link	**804**±60	**720**±45	**589**±12	-	-	-

Table 6.4: Average±standard deviation of SHD obtained by GS and DMMHC in $G_{\rightarrow}$

Networks	DMMHC G_0			GS G_0		
	2000	5000	10000	2000	5000	10000
Asia	**0,8**±0	**1**±0,3	**29**±3	4±0.3	5±0,5	112±2
Alarm	**12**±1	**17**±1	**22**±2	293±40	343±20	430±26
Hailfinder	**20**±1	**37**±5	**46**±1	1070±161	995±162	1318±222
Win95pts	**30**±0	**43**±6	**63**±10	3492±328	5153±229	6545±1961
Andes	**593**±51	**603**±26	**775**±87	-	-	-
Link	**1153**±122	**1525**±153	**1836** ±112	-	-	-

Table 6.5: Average±standard deviation running time for DMMHC and GS in G_0

Networks	DMMHC $G_{\rightarrow}$			GS $G_{\rightarrow}$		
	2000	5000	10000	2000	5000	10000
Asia	**126**±11	**409**±40	**831**±58	260±8	917±68	1564±308
Alarm	**346**±65	**383**±16	**911**±64	1448±545	2206±272	5094±1338
Hailfinder	**755**±170	**1629**±35	**2145**±144	5225±1058	20789±3121	40210±6335
Win95pts	**792**±145	**1736**±46	**4143**±87	35318±3760	72653±6912	102851±7012
Andes	**12996**±131	**23755**±623	**62149**±3883	-	-	-
Link	**68156**±2963	**149773**±3310	**263624**±7518	-	-	-

Table 6.6: Average±standard deviation running time for DMMHC and GS in $G_{\rightarrow}$

Figure 6.2 compares the results of SHD(2-TBN) in dynamic GS and DMMHC for a transition graph corresponding to benchmarks used before. For all the sample sizes 2000, 5000 and 10000, the DMMHC always outperforms GS for 2-TBN in terms of quality (construction transition network) (cf. Figure 6.2). Also, we notice that GS couldn't deal with large dimension benchmarks. The obtained results are only for Asia, Alarm, Hailfinder and Win95pts datasets. However, DMMHC could be run on all benchmarks of different complexities with reasonable time whether for the initial network (cf. figure 6.1) or the transition network (cf. figure 6.4).

In figure 6.3 between the results of SHD(2-TBN) in SA algorithm, provided by Banjo tools, and those of the DMMHC for transition graph corresponding to benchmarks used before. For all sample sizes 2000, 5000 and 10000, the DMMHC outperforms SA in terms of quality (construction transition network) (cf. Figure 6.3). We also remark that SA couldn't deal with two benchmarks (Hailfinder and Link). The obtained results are only for Asia, Alarm, Win95pts and Andes datasets. However, DMMHC could be run on all benchmarks with different complexities

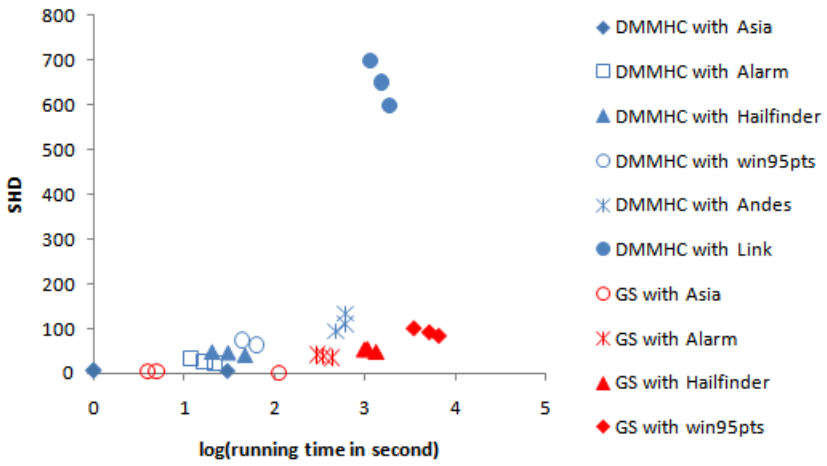

Figure 6.1: Average SHD vs running time obtained by GS and DMMHC with respect to sample size in initial graph

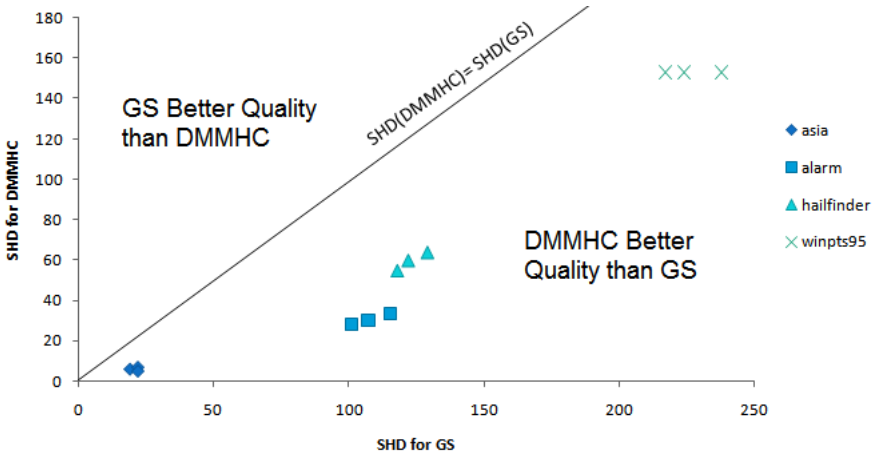

Figure 6.2: Average SHD(DMMHC) vs SHD(GS) with respect to sample size in transition graph

Networks	DMMHC $G_{\rightarrow}$			SA $G_{\rightarrow}$		
	2000	5000	10000	2000	5000	10000
Asia	**4**±0	**4**±0	4±0	17±0	14±2	**3**±0
Alarm	**35**±2	**29**±1	**26**±3	118±5	112±3	76±7
Hailfinder	**46**±1	**45**±1	**45**±1	-	-	-
Win95pts	**153**±0	**153**±0	**153**±0	266±20	264±4	256±13
Andes	**155**±0	**134**±2	**124**±3	592±10	563±24	551±19
Link	**804**±60	**720**±45	**589**±12	-	-	-

Table 6.7: Average±standard deviation of SHD obtained by SA and DMMHC in $G_{\rightarrow}$

with reasonable time whether for the initial network (cf. figure 6.1) or the transition network (cf. figure 6.4).

We also notice that SA algorithm couldn't deal with hailfinder and link 6.7, the first execution (hailfinder benchmark) has stopped because the maximum number

of states that a variable can assume is limited to 7 in banjo tools however, Hailfinder dataset contains variables with more than 7 states. The second execution (link benchmark) has stopped because Banjo has run out of available memory (link contains about 1500 variables with more than 10000 sequences).

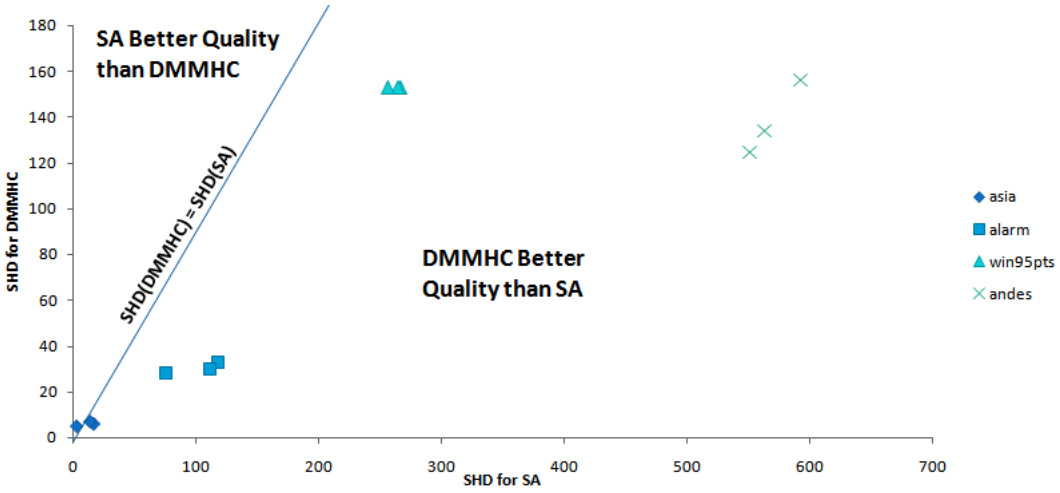

Figure 6.3: Average SHD(DMMHC) vs SHD(SA) with respect to sample size in transition graph

From these results, we can see that the DMMHC is an efficient algorithm for 2T-BN structure learning. The quality of the learned structure is better than for our reference algorithm (2T-BN greedy search) with a better scalability: the results are obtained in a lower running time. In addition, the DMMHC can successfully manage high dimensional benchmarks such as 2T-BN generated from Andes and Link (cf. figure 6.9).

The comparison with the existing works is a difficult task because the works about 2T-BN structure learning deal with specific benchmarks or a specific evaluation metric, as reported in [100].

It is the first time that the existing static benchmarks have been extended for 2T-BN structure learning. It is also the first time that the Structural Hamming distance has been used for 2T-BN, with a temporal correction as described in [100]. For these reasons, comparisons with the existing results obtained by concurrent 2T-BN structure learning algorithms are not possible. We intend to disseminate our benchmarks and performance indicators in order to propose a unified evaluation framework for 2T-BN structure learning.

6.3.3 Naive versus optimized DMMHC

In this part of experimentations we present only the results obtained by the naïve and optimized DMMHC in the transition model. In fact, we remark that there is not a big difference or change between the results of the naive DMMHC and the

Networks	naiveDMMHC $G_{\rightarrow}$			optimisedDMMHC $G_{\rightarrow}$		
	2000	5000	10000	2000	5000	10000
Asia	**4**±0	**4**±0	**4**±0	**6**±2	7±0	**5**±2
Alarm	**35**±2	**29**±1	**26**±3	**33**±0	**30**±2	28±2
Hailfinder	**46**±1	**45**±1	**45**±1	64±4	60±8	55±2
Win95pts	**153**±0	**153**±0	**153**±0	**153**±0	**153**±0	**153**±0
Andes	**155**±0	**134**±2	**124**±3	**156**±2	**134**±1	**125**±2
Link	**804**±60	**720**±45	**589**±12	**815**±48	728±56	**591**±24

Table 6.8: Average±standard deviation SHD for naive and optimised DMMHC in $G_{\rightarrow}$

Networks	naiveDMMHC $G_{\rightarrow}$			optimisedDMMHC $G_{\rightarrow}$		
	2000	5000	10000	2000	5000	10000
Asia	126±11	409±40	831±58	**62**±10	**202**±21	**419**±26
Alarm	346±65	383±16	911±64	**216**±36	**312**±8	**638**±23
Hailfinder	**755**±170	**1629**±35	**2145**±144	743±87	2549±76	4695±118
Win95pts	792±145	1736±46	4143±87	**488**±8	**1137**±60	**2968**±384
Andes	12996±131	23755±623	62149±3883	**10607** ±476	**19090**±2405	**35832**±3160
Link	68156±2963	149773±3310	336879±12589	**63401**±2596	**141325**±5967	**283819**±10221

Table 6.9: Average±standard deviation running time for naive and optimised DMMHC in $G_{\rightarrow}$

optimized DMMHC in the initial model. This is explained by the use of a small number of variables which makes the difference between the number of calls to the assoc function in the naïve and optimized approaches limited.

Table 6.8 presents a comparison of SHD(2T-BN) average results obtained by the naive and the optimised DMMHC algorithms with respect to the sample sizes. This table describes only the results for the transition model corresponding to six (small and large) benchmarks (Asia, Alarm, Hailfinder, Win95pts, Andes, Link). We can notice that for every benchmark, the two versions of DMMHC algorithm obtain in almost all the cases similar SHD results. Apart from, for Hailfinder benchmarks, the naïve DMMHC algorithm obtains better SHD than the optimized version with a difference in interval [8, 15].

Similarly, Table 6.9 shows the running time measured for the naive and optimized DMMHC algorithms for each experimental context. We can observe that the optimized version outperforms the naïve one in terms of running time. This situation is really significant even for benchmarks with a small number of variables. But, we can also notice that the more the number of variables increases, the running time differences between the naïve and the optimized versions are important. We can then notice that, unlike the GS, the two versions of the DMMHC are able to provide results in an acceptable time for large benchmarks (Andes and Link).

In figure 6.4, we present all SHD(2-TBN) results obtained for the transition model in terms of both time and quality. We remark that the results of SHD for the naive and the optimized DMMHC are similar in most of the several benchmarks with different complexity and sample sizes. However, the optimized DMMHC out-

performs the naïve DMMHC in terms of running time. In addition, we can see that the results of the naive and the optimized DMMHC are better than those of the dynamic GS in terms of both accuracy (SHD(2-TBN)) and complexity (running time).

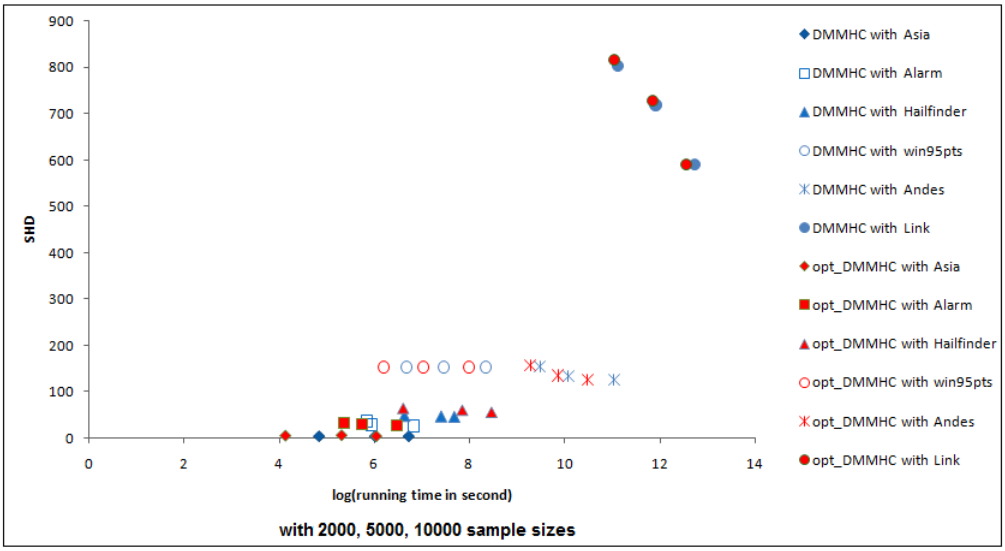

Figure 6.4: Average SHD vs running time obtained by naive and optimised DMMHC with respect to sample size in transition graph

We have demonstrated in sections 5.2.3 and 5.5 that, the optimized version of the DMMHC performs the calls of assoc function and minimizes the complexity of the algorithm. And we have demonstrated these optimizations theoretically. Now, we try to prove them with experimentally. According to the two previous paragraphs, we can summarize that, the optimized version permits to learn large model in a shorter running time than other algorithms for DBN structure learning. In addition, this optimization maintains the quality of the algorithm for the learning structure. We present this improvement in tables 6.8, 6.9 and figure 6.4 showing the different results of SHD(2T-BN) for transition graph given by dynamic GS, naive and optimised DMMHC.

6.4 Empirical results and interpretations on simplified search space

6.4.1 Simplified 2-TBN with small benchmark

Our aim is to provide an algorithm which could be used for different applications of a large dynamic Bayesian network reconstruction. In order to assess the performance of our software, we have first compared it to the Banjo library. As a realistic dataset, we have chosen the dataset attached as an example to the Banjo

package, consisting of 20 variables and 2000 observations, published by Smith et al. [90] (available in BNFinder tutorial [3]). The results of both techniques are discussed below:

We notice that in this part of work both techniques(simplfied DMMHC and GS (used in Banjo tool) are used as inputs of the minimum and maximum Markov lag, and in this example both are equal to 1, which means that no links between nodes of Markov lag 0 are allowed (i.e. we use the simplified 2-TBN "no intra-slice edges" in model).

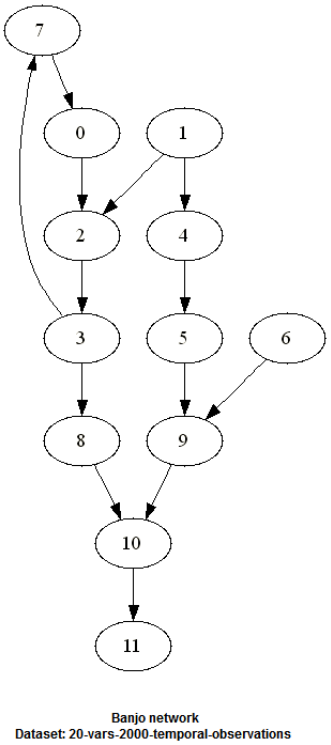

Figure 6.5: Network reconstruction results for GS algorithm of Banjo tool. The used benchmark is the biological dataset 20 variables and 2000 observations

Banjo uses a setting file where we can change any parameter (or input) for algorithms. We modified the provided settings file to allow a run (of 15 minutes), Greedy searcher as structure learning algorithms and made a few other changes. The result of this algorithm is presented in figure 6.5.

we note that, this figure presents a path (7→0→2→3→7) which is not a cycle, but shows temporal dependence between two nodes in different time slices (For example $7 \rightarrow 0 \iff 7_{t-1} \rightarrow 0_t$ and $3 \rightarrow 7 \iff 3_{t-1} \rightarrow 7_t$).

As mentioned before, the DMMHC uses χ^2 independence test with $\alpha = 0.05$. Also, it uses greedy search GS algorithm if it can give a better network score. The GS uses the BIC score function. The result of this algorithm is presented in figure 6.6.

3. http://bioputer.mimuw.edu.pl/software/bnf/tutorial.php

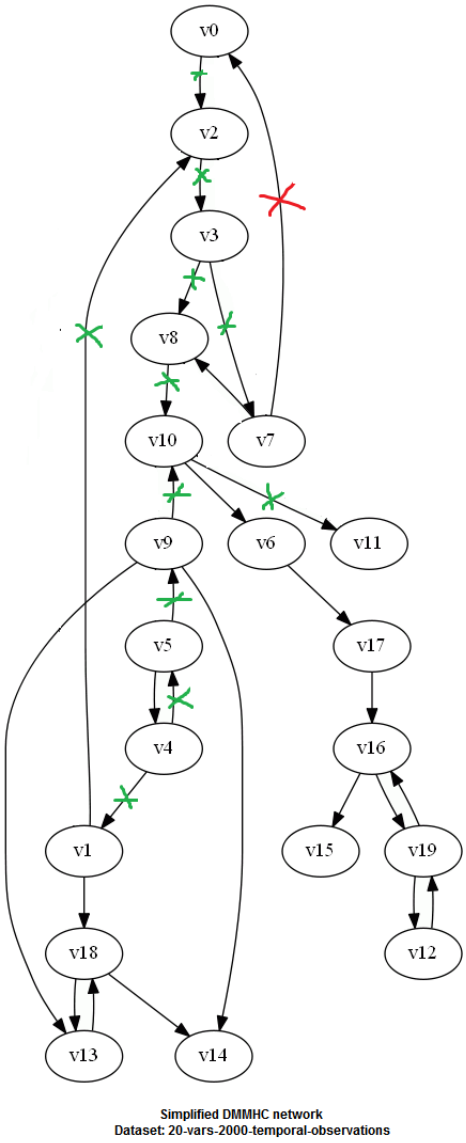

Figure 6.6: Network reconstruction results for simplified 2-TBN DMMHC. The used benchmark is the biological dataset 20 variables and 2000 observations.

Figures 6.5 and 6.6 show that the DMMHC and the Banjo tool are able to identify the same temporal edges (12 edges, the green cross present the same temporal edges identified by simplified DMMHC and GS in Banjo), there is only one edge (from 0 to 7 presented by the red cross) is inversed. Besides, the simplified DMMHC discover other temporal edges (for 12,...,19 nodes) but we can not prove if these edges are truly or falsely identified because we don't find the generating (original) network with which we can compare the other learned graphs. We think that the comparison between both techniques is not precise, however we can say that the DMMHC is able to discover a 2-TBN model by simplifying the search space.

6.4.2 Simplified 2-TBN with large benchmark

Cyanothece genetic network

The second test for our simplified DMMHC algorithm on a large dimension as the cyanobacterial genetic network was of great interest. For more details of this dataset it is recommended to read [97, 98, 110].

Vinh et al. [110] used transcriptomic data from two previous studies [97, 98]. They analyzed the same set of 1595 genes which presents a fold-change superior to 2.5 states for one variable. In addition, they also included a variable that represents the relevant environmental condition, namely light, that takes binary values (L/D). Gene expression data were discretized using 3-state quantile discretization. After the changes made on the data set by Vinh, we obtained a set of 1595 columns and 24 sequences.

For this large network, the two methods (DMMHC and Vinh's algorithm) set the significance level of $\alpha = 0.9999$. Every method took a reasonably small amount of time to learn this network, i.e., Banjo was set to run for 1 hour and DMMHC was set to run for 2 hours. The networks learned by the MIT-based global and local algorithms are presented in figure 6.7(a,b) [110]. The networks learned by DMMHC and Banjo algorithms are presented in figure 6.7(c,d). DMMHC generated a small network and was able to identify many edges. We think that this result is attributed to the small number of sequences and it is insignificant to learn 1595 variables with very small number of sequences.

We remark that in the overall network structure the majority of nodes have only a few connections and a small number of hubs (i.e. node with many connections) that have many connections. The node degree in a scale-free network is calculated according to a powerlaw distribution, $P(x) \propto x^{-\gamma}$.

For the networks reconstructed by the MIT-based global and local MMMB algorithms, the scale parameters, estimated via linear regression on the log-log node degree distribution plot, are respectively $\gamma_1 = 2.33$ and $\gamma_2 = 2.35$, falling well within the typical range. Furthermore, the coefficients of determination are respectively $R_1^2 = 0.90$ and $R_2^2 = 0.93$, indicate very good fits. The node degree distributions of various reconstructed networks are shown in figure 6.8.

However, for the networks reconstructed by DMMHC, the scale parameter is γ=1.7 and the determination coefficient is $R^2 = 0.95$. The Banjo reconstructed network is presented in Figure 6.7(c). It exhibits a radically different structure as compared to the networks reconstructed by the other algorithms in figure 6.8. A linear regression on the log-log node degree distribution plot yields $\gamma = 1.41$ and $R^2 = 0.358$, clearly indicating a large deviation from a scale-free topology [110]. In addition, Vinh plots the degree distribution for a random graph with the same number of nodes and connections as in the Banjo reconstructed network. It is noted that

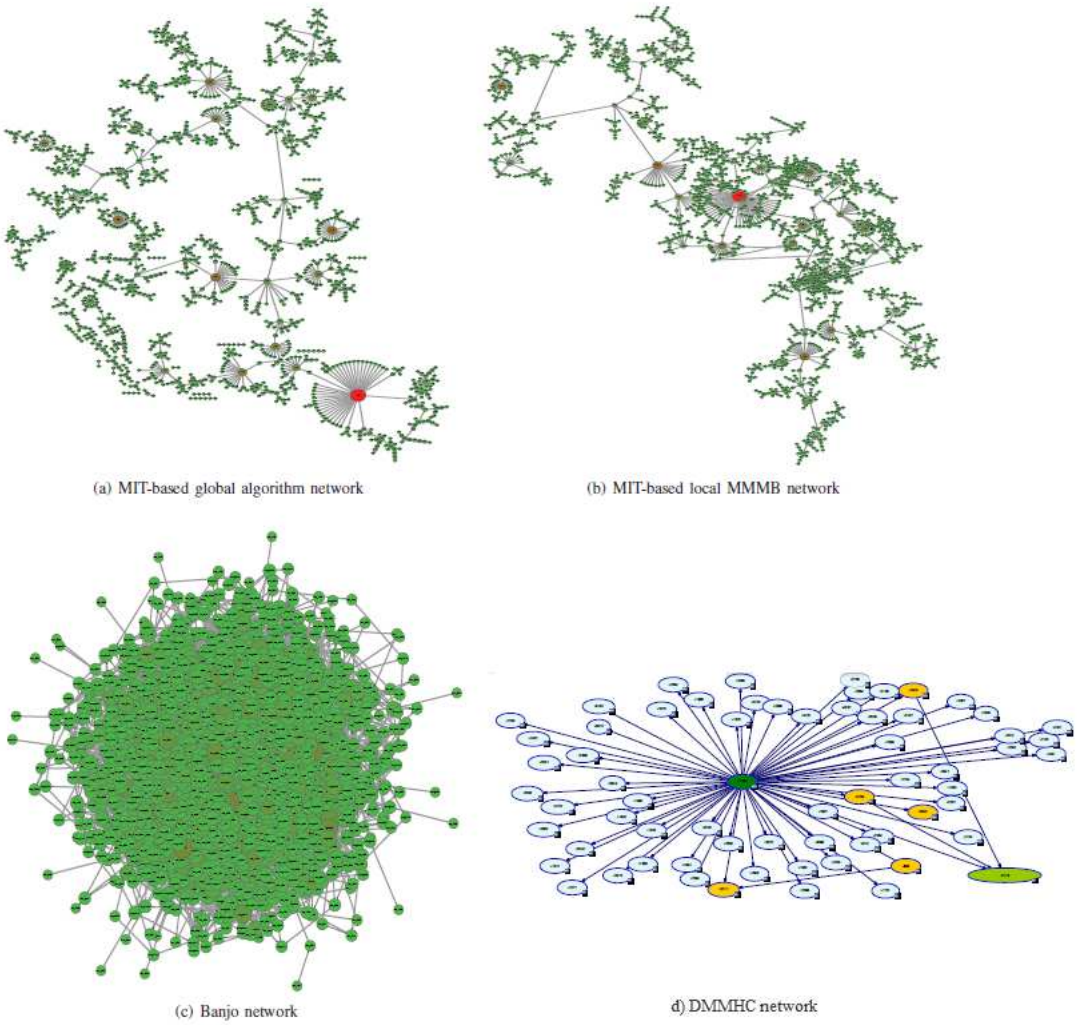

Figure 6.7: Network reconstruction results for MIT-based global, MIT-based MMMB, Banjo [110] and DMMHC from Cyanothece genetic benchmarks

the node degree distributions of the Banjo network and the random graph are very similar.

6.5 Comparison between all DMMHC versions

An evidence of the scalability of DMMHC is found in the previous experiments (section 6.3.2, 6.3.3 and 6.4.1). We gave a summary of all these experimens in figure 6.9. Naive, optimized and simplified DMMPCs were run on each node and reconstructed the skeleton of a tiled-LINK networks with approximately more than one thousand variables from the 10,000 training instances using the same hardware as above in respectivly 4 days, 3 days and 1 day of a single-CPU time.

Figure 6.9 illustrates the ability of the DMMHC to scale up to thousands of variables. We present in this figure, the behavior or the variation of running time

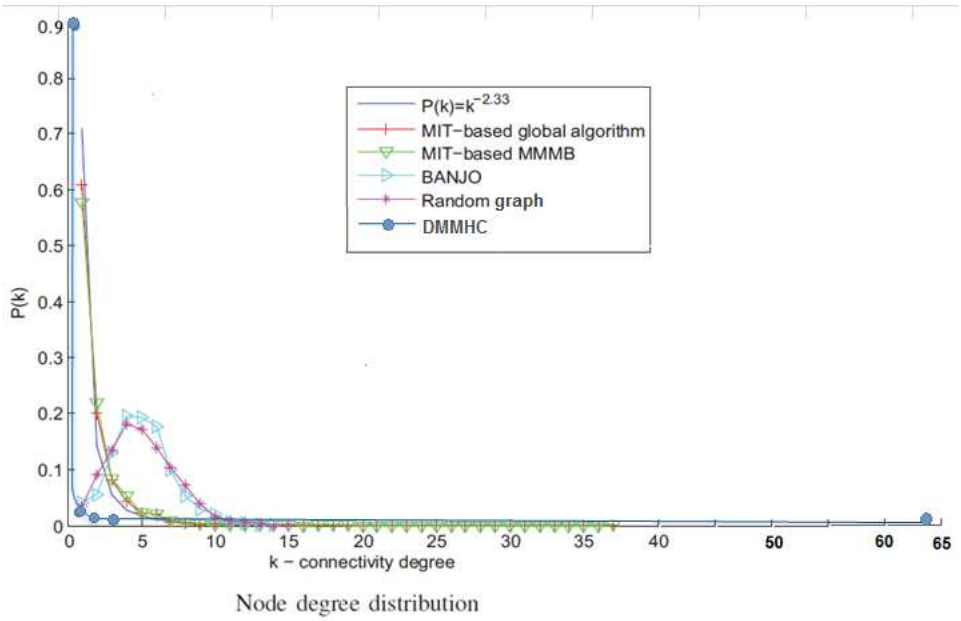

Figure 6.8: Network reconstruction results

with the number of variables on different benchmarks for all versions of DMMHC. In this figure, the X axis presents the number of variables and the Y axis presents the logarithmic function of running time.

The complexity variation of all DMMHC versions is different from the exponential function. These results were demonstrate theoretically in section 5.5, and now, we demonstrate this advantage experimentally. We calculated the different Asymptote equations eq1, eq2 and eq3 respectivly for the naive DMMHC, the optimised DMMHC and the simplified DMMHC variations. We noticed that the asymptote equations are different from the exponential function.

$$equation1 : Ln(T) = a_1 N + b_1 = 0,125N + 650 \tag{6.1}$$

$$equation2 : Ln(T) = a_2 N + b_2 = 0,125N + 600 \tag{6.2}$$

$$equation3 : Ln(T) = a_3 N + b_3 = 0,125N + 450 \tag{6.3}$$

where T is the running time and N the number of variables.

We would like to remind that, in section 5.5, we said that the complexity of the optimized DMMHC is lower than that of the naive DMMHC and the simplified DMMHC complexity is lower than that of the optimized DMMHC one. This remark is well presented in figure 6.9.

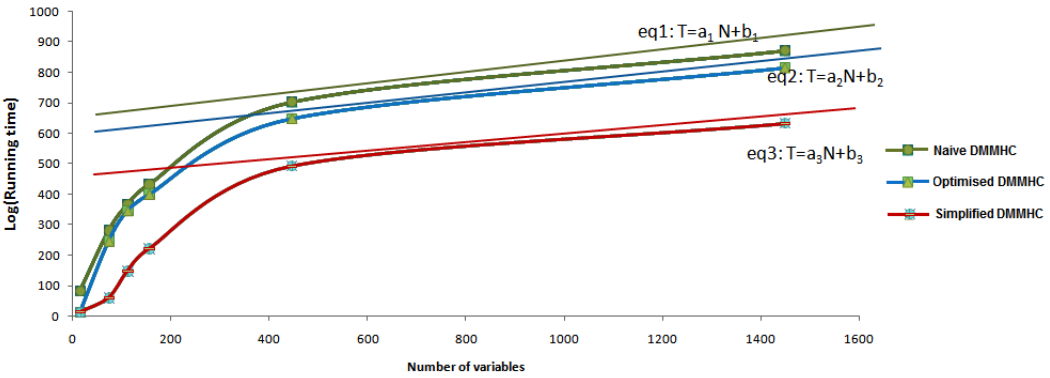

Figure 6.9: Complexity of all DMMHC versions

6.6 Conclusion

The experimental results, provided in this chapter, show that the proposed DMMHC algorithms achieve a better performance than the other existing structure learning for DBN such as Greedy Search or the Simulated Annuling algorithms.

The proposed approach was tested through real and standard benchmarks created by our evaluation techniques for a dynamic case. Also, we validated the DMMHC on a real biology field (Cyanothece genetic network). Nevertheless, the main problem is that there is no commonly accepted benchmark that can be used to learn with a large number of instances (i.e. Cyanothece genetic benchmark contains only 24 instances) that can lead to more rigorous results.

7

Conclusion

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7.1 Summary

In the different sections of this thesis work, we discussed in (the chapter 2 and chapter 3), the problem of representation the Probabilistic graphical Models (PGM), especially in the Bayesian networks and their extension Dynamic BN.

In **chapter 2**, we present the key concepts of Bayesian networks, structure learning methods of these models and all techniques used to evaluate these learning algorithms. We concluded in this chapter that the hybrid method for learning the BN performed better than the techniques based on constraints or those based on score. We also noted that most of the studies use the methods based on the score for evaluation, although this kind of method has disadvantages when the data size is reduced and the calculation is costly when the number of variables is important.

In the same way, in **chapter 3**, we present the key concepts of the dynamic bayesian network and the different structure learning studies of these models. We also addressed to a discussion of the different elaborated works to evaluate their DBN structure learning algorithms.

For these approaches, there are many weaknesses as they use their oun evaluation Benchmarks and techniques to evaluate. In addition, we don't find any online availbale structure learning algorithm software for DBN, that can be compared to our methods. The important conclusions that can be drawn from this study is that the most of the studies use networks with small number of variables and score based techniques for evaluation. This makes the comparison between our study and other works more difficult.

In the chapters 4 and 5, we tried to solve the problems mentioned in the previous chapters. In **chapter 4**, we focused on solving the problem of evaluation for the temporal graphical model as the DBN and especially the 2T-BN models. We also introduced, tow contributions: the first is a large 2-TBN generation algorithm inspired from the Tiling technique; the second is a novel metric to evaluate the performance of DBN structure learning algorithms. It is inspired from the Structural Hamming distance used in the static case, but it takes into account temporal background information.

In **chapter 5**, we developed a novel approach for DBN structure learning named DMMHC. It is a hybrid method that uses a local search algorithm dealing with local structure identification (DMMPC) and global model optimization constrained with the local information (DMMHC). We demonstrated that this approach can easily take into account the temporal dimension in order to provide some additional information about temporality that can then be used with a greedy search in order to learn the global structure the initial model G_0 and the transition one $G_{\rightarrow}$. As far as we know, no method able to learn dynamic network models with such approaches has been proposed previously.

To analyze and validate the merits of our proposed and used methods, we carried out some experiments, detailed in **chapter 6**, on standard large benchmarks constructed with our method described in chapter 4. These benchmarks are derived from the standard benchmarks used in the evaluation of structure learning methods in a static case as Asia, alarm, hailfinder ...

The results have shown the significance of our novel algorithms for dynamic Bayesian network structure learning on the level of scalability, complexity, running time and accuracy (quality of construction models).

7.2 Applications

Since the sixties, saving the multi-dimensional and temporal data has increased in many fields. "Time" is an important concept in medical care [79, 89]. Several studies done in the medical field for the evaluation of the nosocomial infections (IN) predominance and the factors associated to its presence [37, 40]. In our future studies, we are interested in solving this problem through the prediction of the prognostic patient's cases. Our system, named Decision Support System Nosocomial Infection (**DSS-NI**), enables to predict their cases relying on the patient's history and medical treatment during his hospital stay. This work is important since physiciens complain about incomplete and irregular data structure, which makes their job more difficult. As a result, the predictions are judged to be poor in question of the extracted knowledge [55, 60, 66, 99].

Nosocomial infections (NIs) continue to be a major problem. It causes high morbidity and mortality. Consequently, it increases the length of hospitalization and the cost of treatment. The supervision of NIs is an essential part of the infection control program. Therefore, prevention is better than cure for our patients. Successful infection control measures depend on education at the level of healthcare workers (HCWs), surveillance of the prevalent microorganisms and their antimicrobial resistance patterns, and an efficient interdisciplinary collaboration. The supervision activities are part of infection control efforts to improve the quality of hospital care. Most of the research on the controls of the NI concentrate on the acquisition of this supervision. Since a hospitalization may end up with the patient's death.

In the decision support analysis initialized by Morton and Keen [88, 53], most of the studies used in this domain are limited to the static aspect as the static Bayesian Networks [4, 68]. This is insufficient for a dynamic decision making as in the medical field. The dynamic processes which advance over time, known as Markov decision processes, are used as the basis for prediction models. The techniques such as decision-trees [71], neural networks [116], association rule, Hidden Makov models [28, 46] and (dynamic) Bayesian networks [10, 32, 66, 79], developed by the

artificial intelligence community, have become popular prediction models. Markov models have been used in various medical applications. For instance, in medical artificial intelligence (AI) Markov models often have a complex and multivariate state representation. The models are represented as a dynamic Bayesian network DBN [79], in this thesis we justify our choice to use this existing technique to provide Markov models with multivariate and complex state descriptions of medical data. Our objective is to extract models that can identify temporal patterns, predict the daily prognostic of the patient's state and test clinical hypotheses. Furthermore, our models should be able to detect the future probable presence of a nosocomial infection at ICU for tow levels 1) the processes regarding the eventual outcome of ICU (to die or to survive), 2) and the processes related to the development of the patient's state (acquisition of NI) during of his/her hospitalization period.

The results of this thesis are relevant to these processes and demonstrate the induction, inference, evaluation, and use of these models in practice data concerning patients admitted to the ICU of Habib Bourguiba hospital (Sfax, Tunisia). The Intensive Care Unit of the CHU Habib Bourguiba of Sfax contains 22 beds in 11 boxes of 2 beds. Each box is thus made up of 2 beds separated by a care zone containing all that a nurse needs (compress, gloves, serum, drugs, etc.) to deal with his/her 2 patients. A nurse is responsible for the care of 2 patients. The majority of the patients admitted in ICU are known as "heavy" because they require a 24h/24h care. They are often connected to machines (artificial respirator, electrocardiogram, electric syringe, etc.) and/or connected to catheters (venous catheters, urinary probe, thoracic drain...). These patients are often in a very delicate health situation. They are vulnerable to new germs entering their bodies. For each appearance of infection either nosocomial or not, it is necessary to send a blood sample to the laboratory to carry out a antibiogram. According to the antibiogram result, an antibiotherapie is prescribed. The problem of the antibiotherapie is that a germ can be sensitive to the antibiotic during the first period and resisting a few weeks or months later. This sensitivity can be different from an individual to another [64].

7.3 Limitations

Despite our multiple attempts to take into account all interactions that can occur between the DBN structure learning and evaluation techniques, we still face a few difficulties to justify the performance of our techniques. In our experiments we compared our algorithms to only the GS and the SA algorithms. This is not enough to show the utility of our approach applied on large benchmarks.

As a second limitation, we should point out that the DBN and more generally BN also led to create a decision extension called influence diagrams (ID) [54] that

can solve the decision problems. It is possible to distinguish the variables on which it is possible to act, with respect to other contextual variables. Thus we can act on the costs of each decision or utility with respect to each context. In this thesis, we don't have enough time to achieve this final part of the study.

The third limitation, is that in our experiment we did not use real data. For two raisons: (1) First we didn't have enough time to make experiments using data generated from standard benchmarks and data from a real dataset. (2) The medical database provided by Habib Bouguiba hospital is not well prepared for use in experiments due to the small base size (less than 1000 cases and less than 100 variables). However, we need thousands of variables to apply our learning algorithms.

7.4 Issues for future researches

Our main immediate perspective is to introduce some local improvements on our algorithm. Our framework offers several opportunities for future research. Among this, we believe that all the theoretical properties and experimentation results should be extended. We have identified several perspective ideas:

1. Our next step in this direction is the adaptation of the structural Hamming distance in order to take into account any background knowledge (forbidden edges, required ones, partial ordering, ...).
2. We think that the quality of the structure reconstruction can be improved during the global optimization using a more evolved meta-heuristic such as a Tabu search instead of a standard hill-climbing algorithm.
3. We plan to extend our dynamic approach with the use of others local identification methods such as PCD algorithm [80] that can correct it under faithfulness assumption.
4. Develop the structure learning algorithm for duration graphical model (DGM) relying on what we have reached in this thesis.
5. Extend our approach for learning the dynamic models to a decisional task with the use of influence diagram (ID) and dynamic decision models (DDM).
6. Apply the algorithms developed before for a decision support task in the medical field. Indeed, the currently developed system, for ICU Habib Bourguiba hospital of Sfax, to predict the occurrence of nosocomial infections (NI) is based on the dynamic bayesian network. This system gives only the scores for predicting occurrence of IN without proposing any decision. Our major goal is to develop a decision support system to fight against the NI in the ICU of Habib Bourguiba Hospital of Sfax.

A

Bayesian Network and Parameter learning

Here we are looking for estimating the probability distributions from available data. The estimation of the probability distributions, parametric or not, is a vast and complex subject. We describe here the most commonly used methods in the Bayesian networks, as the data are complete, for more information, we advise to read [51, 41].

A.1 From completed data

A.1.1 Statistical Learning

In the case where all variables are observed, the easiest and most used method is the statistical estimate. It estimates the probability of an event by the frequency of occurrence of the event in the database. This approach, called maximum likelihood (ML). It is defined by:

$$\hat{P}(X_i = x_k | Pa(X_i) = x_j) = \frac{N_{i,j,k}}{\sum_k (N_{i,j,k})} \tag{A.1}$$

Where $N_{i,j,k}$ is the number of events in the data base, for which the variable X_i is in the state x_k and its parents are in the configuration x_j .

A.1.2 Bayesian Learning

The Bayesian estimation follows a different principle. It consists in finding the most likely parameter thetta as the data were observed using the a priori knowledge over the parameters (e.g. maximum a posteriori (MAP) estimation). If we assume that each $P(X_{i,j} \mid Pa(X_i))$ follows a multinomial distribution, the conjugate distribution follows a Dirichlet distribution with the parameters $\alpha_{i,j,k}$

$$\hat{\theta}^{MAP}_{i,j,k}(X_i = x_k | Pa(X_i) = x_j) = \frac{N_{i,j,k} + \alpha_{i,j,k} - 1}{\sum_k (N_{i,j,k} + \alpha_{i,j,k} - 1)} \tag{A.2}$$

$\alpha_{i,j,k}$ are the parameters of the Dirichlet distribution associated with the prior probability $P(X_i = x_k \mid Pa(X_i) = x_j)$.

A.2 From incomplete data

A.2.1 Nature of the missing data and their treatment

The real-world data usually contains missing entries. We need to deal with incomplete data sets that looks like the following (example A.1):

X1	X2	X3	X1	X2	X3
1	1	1	2	1	1
2	?	1	?	1	1
1	2	1	?	?	?

where ? indicates missing values.

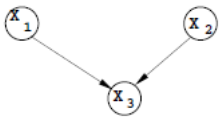

Figure A.1: Example of BN structure

To deal with the missing values, we need to make the follwing assumptions:

- MCAR (Missing Completely At Random): the actual value of X and the event X-is-missing are independent on data.
- MAR (Missing At Random): the actual value of X and the event X-is-missing are conditionally independent given other observed variables.
- NMAR (Not Missing At Random): the actual value of X and the event X-is-missing are conditionally independent given other observed and missing variables.

The situations MCAR and MAR are the easiest to solve, because the observed data contain all the information necessary to estimate the distribution of the missing data.

When the missing data are MCAR, the earliest and simplest approach is the analysis of complete examples. This method tried to estimate the parameters from completed data sets of all the examples fully observed in the observed data.

Many methods attempt to estimate the parameters of a model from data in MAR. For example, we can cite the sequential updating [92], Gibbs sampling [36], and the expectation maximization algorithm (EM) [58].

A.2.2 EM algorithm

One algorithm for parameters learning from incomplete data: The expectation-maximization (EM) algorithm. Developed in the Statistics community (Dempster et al. 1977)[24]. Adapted for Bayesian networks by Lauritzen (1994) [58].

It is an iterative algorithm.

- Starts with an initial estimation θ_0.
- At each iteration t:
  - Expectation: Complete the data set based on θ_t.
  - Maximization: Re-estimate parameters using the completed data set, obtaining θ_{t+1}.

B

Benchmarking the dynamic bayesian network

B.1 BNtiling for 2-TBN implementation

Our approach is based on five steps: (1) generating a standard BN; (2) tiling the BN; (3) conversting the BN to DBN with the determined number of time slices; (4) constructing the initial and transition models of DBN; (5) generating of data for the new DBN; the benchmarking for 2T-BN process is described as follows:

1. Building a Bayesian network with HUGIN format (.net)
2. Generating data file from the network with .dat format used the geniesmile tools.
3. Converting the generated data on matlab format and save them in a data file (.mat)

data=data_converter_hugin('../Data/network.dat', '../Data/ network.net');

4. Use the "bn_tiling" process to generate the new network R1 with N copies of the original network

network_filename='../Data/network.net';
dataset_filename='../Data/data.mat';
*nodes=bn_tiling(network_filename, dataset_filename, nbr_variables*N, 2);*

Remark: N represents the number of copies "tile" in R1. This command does not give R1 in HUGIN format, so we have to create a method that allows the construction of the new network with new transformations.

data=data_converter_hugin('../Data/ data.dat', '../Data/ network.net');

5. Extract all the characteristics of R1 and nodes (name, parents, table of probabilities)
6. Generate the Dynamic Bayesian network R2 from network R1.
   – Building the DBN with K time slices:

   Hugin_DBN(nodes, N, K);

   – Building the initial and transition model by :

   Hugin_Net(nodes,1); % the initial model
   Hugin_Net(nodes,2); % the transition model
7. Generate the new database from R2 dynamic network used the *geniesmile* tools.

B.2 Generating large Dynamic Bayesian Networks

Algorithm 15 Generating large Dynamic Bayesian Networks

Require: DAG M, number of copies (n), number of time slices (k)
Ensure: Return initial and transition models (M_{i0}, $M_{i\rightarrow}$), and DBN B_i with N time slices

```
1: B_i is empty graph
2: Generate Dataset D for M
3: Create a large Bayesian network M_i with n copies of M by tiling
4: M_i0 = M_i
5: Generate Dataset D_i for M_i
   % add priori Knowledges (Temporal dependencies)
6: Create M_i→ with 2 copies of M_i by tiling
7: 2-TBN model = (M_i0, M_i→)
8: for all i≥0 and i≤k do
9:     add M_i→ to B_i
10: end for
11: Return B_i
```

C

DMMHC: Dynamic Max Min Hill Climbing

C.1 Proofs of propositions used by DMMHC

C.1.1 Proof proposition 5.2.2:

Let V_i , V_{i+1} et V_{i-1} be the variable sets respectively of time slices i, i+1 and i-1. Let Ne_+ be the set of candidates parents/children of variable $T \in V_i$ (noted $Ne_+ = CPC_i \bigcup CC_{i+1}) \bigcup CP_{i-1}$).

1. $\forall \mathbf{X} \in \mathbf{V}_i \setminus \mathbf{T}$
   Let p a be path from T to X through the node $m \in V_{i+1}$ and k its child ($k \in V_{i+1}$)
   Because of temporality, there is at least one V-structure in the path p and m is its well (middle node), so p contains at least one convergence: $X \rightarrow m \leftarrow T$.

   (a) If $m \notin CC_{i+1}$ and $k \notin CC_{i+1}$ then the path p is blocked by $CC_{i+1} \Rightarrow Indp(X ;T \mid CC_{i+1})$

   (b) If $m \in CC_{i+1}$ then the path p is active by CC_{i+1} and we have $dep(X ;T \mid m)$ but this dependance is indirect between X and T, so it will be removed in Phase II (Backward) of our algorithm and hence $\Rightarrow Indp(X ;T \mid CC_{i+1})$

   (c) If $m \notin CC_{i+1}$ and $k \in CC_{i+1}$ then there is at least one V-structure in the path p' and k is its middle node $X \rightarrow k \leftarrow T \Rightarrow Indp(X ;T \mid CC_{i+1})$

Let p be a path from T to X through the node m $\in V_{i-1}$

(a) If m $\in CP_{i-1}$ then, because of temporality, there is at least a divergence in the path p, so the path p is blocked by $CP_{i-1} \Rightarrow$ Indp(X ;T | CP_{i-1})
Hence $\forall$ X $\in V_i \setminus$, $\text{Min}_{(Z \subseteq CP_{i-1})}$ Assoc(X ;T | Z) = 0

we conclude that $\forall$ Z $\subseteq V_{i+1} \Rightarrow$ Indp(X ;T | Z) $\Rightarrow$ Indp(X ;T | CC_{i+1}))
Hence $\forall$ X $\in V_i \setminus$, $\text{Min}_{(Z \subseteq CC_{i+1})}$ Assoc(X ;T | Z) = 0
Hence $\text{Max}_{X \in V_i \setminus T} \text{Min}_{(Z \subseteq Ne_+)}$Assoc(X;T | Z)
=$\text{Max}_{X \in V_i \setminus T} \text{Min}_{(Z \subseteq CPC_i \cup CC_{i+1} \cup CP_{i-1})}$Assoc(X;T | Z)
= $\text{Max}_{X \in V_i \setminus T}$\{$\text{Min}_{(Z \subseteq CPC_i)}$Assoc(X;T | Z),$\text{Min}_{(Z \subseteq CC_{i+1})}$Assoc(X;T | Z),$\text{Min}_{(Z \subseteq CP_{i-1})}$Assoc(X;T | Z) \}
= $\text{Max}_{X \in V_i \setminus T}$\{$\text{Min}_{(Z \subseteq CPC_i)}$Assoc(X;T | Z), 0,0\}
= $\text{Max}_{X \in V_i \setminus T} \text{Min}_{(Z \subseteq CPC_i)}$Assoc(X;T | Z)

2. $\forall$ **X** $\in$ **V**$_{i+1}$
Our model is the first Markov-order P(X_t | $X_{1:t-1}$) = P(X_t | X_{t-1})
Hence $\text{Max}_{X \in V_i \setminus T} \text{Min}_{(Z \subseteq Ne_+)}$Assoc(X;T | Z)
=$\text{Max}_{X \in V_i \setminus T} \text{Min}_{(Z \subseteq CPC_i \cup CC_{i+1} \cup CP_{i-1})}$Assoc(X;T | Z)
=$\text{Max}_{X \in V_i \setminus T} \text{Min}_{(Z \subseteq CPC_i \cup CC_{i+1})}$Assoc(X;T | Z)

3. $\forall$ **X** $\in$ **V**$_{i-1}$
Let p be a path from X to T through tne node m $\in V_{i+1}$ and K its child (k $\in V_{i+1}$)
Because of temporality, there is at least one V-structure in the path p and m is its well (middle node), so p contains at least one convergence: X $\rightarrow$ m $\leftarrow$ T.

(a) If m $\notin CC_{i+1}$ et k $\notin CC_{i+1}$ then the path p is blocked by $CC_{i+1} \Rightarrow$ Indp(X ;T | CC_{i+1})

(b) If m $\in CC_{i+1}$ then the path p is active by CC_{i+1} and we have dep(X ;T | m) but this dependance is indirect between X and T, so it will be removed in Phase II (Backward) of our algorithm and hence $\Rightarrow$ Indp(X ;T | CC_{i+1})

(c) If m $\notin CC_{i+1}$ et k $\in CC_{i+1}$ then there is at least one V-structure in the path p' and k is its middle node X$\rightarrow$ k $\leftarrow$T $\Rightarrow$ Indp(X ;T | CC_{i+1})

We conclude that $\forall$ Z $\subseteq V_{i+1}$ we have Indp(X ;T | Z) $\Rightarrow$ Indp(X ;T | CC_{i+1}))
Hence $\forall$ X $\in V_i \setminus$, $\text{Min}_{(Z \subseteq CC_{i+1})}$ Assoc(X ;T | Z) = 0
Hence $\text{Max}_{X \in V_{i-1} \setminus T} \text{Min}_{(Z \subseteq Ne_+)}$Assoc(X;T | Z)
=$\text{Max}_{X \in V_{i-1}} \text{Min}_{(Z \subseteq CPC_i \cup CC_{i+1} \cup CP_{i-1})}$Assoc(X;T | Z)
= $\text{Max}_{X \in V_{i-1}}$\{$\text{Min}_{(Z \subseteq CPC_i)}$Assoc(X;T | Z),$\text{Min}_{(Z \subseteq CC_{i+1})}$Assoc(X;T | Z),$\text{Min}_{(Z \subseteq CP_{i-1})}$Assoc(X;T

| Z) }
= $\text{Max}_{X \in V_{i-1}}\{\text{Min}_{(Z \subseteq CPC_i)}\text{Assoc}(X;T \mid Z), 0, \text{Min}_{(Z \subseteq CP_{i-1})}\text{Assoc}(X;T \mid Z)\}$
= $\text{Max}_{X \in V_{i-1}}\text{Min}_{(Z \subseteq CPC_i \cup CP_{i-1})}\text{Assoc}(X;T \mid Z)$

C.1.2 Proof proposition 5.4.1:

As we know, in the Forward phase of DMMHC we need to calculate the assoc function. Function Assoc(X; T|Z) is an estimate of the strength of association (dependency) of X and T given Z. To identify all X in $CP_{t-1}(T)$, we need to compute the Assoc(X; T|$CP_{t-1} \bigcup CPC_t$) (see algorithm 12).

- in this case we don't have $CPC_t(T)$ candidates. So, we mustn't find any false positives depending on the structure Assoc(X; T|$CP_{t-1} \bigcup CPC_t$)= Assoc(X; T|CP_{t-1}) .
- we mustn't find any intra-connectivity in t-1 time slice. So, Assoc(X; T|$CP_{t-1} \bigcup CPC_t$)= Assoc(X; T|∅) where $X \in V_{t-1}$ and V_{t-1} is the set of all variables in t-1 time slice.

$$\max_{X \in V_{t-1}} \min Assoc(X;T|Z) = \max_{X \in V_{t-1}} \min_{S \subseteq Z} Assoc(X;T|S) \tag{C.1}$$

$$= \max_{X \in V_{t-1}} \min_{S \subseteq CP \bigcup CPC} Assoc(X;T|S) \tag{C.2}$$

$$= \max_{X \in V_{t-1}} \min_{S \subseteq \Phi} Assoc(X;T|S) \tag{C.3}$$

$$= \max_{X \in V_{t-1}} Assoc(X;T|\emptyset) \tag{C.4}$$

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PÔLE DE RECHERCHE ET D'ENSEIGNEMENT SUPÉRIEUR

UNIVERSITÉ DE NANTES

Thèse de Doctorat

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Nouveaux algorithmes d'apprentissage et méthodes d'évaluation pour les réseaux bayésiens dynamiques de grande dimension

New structure learning algorithms and evaluation methods for large dynamic Bayesian networks

Résumé
Les réseaux bayésiens dynamiques (RBD) sont une classe de modèles graphiques probabilistes qui est devenu un outil standard pour la modélisation de divers phénomènes stochastiques variant dans le temps. A cause de la complexité induite par l'ajout de la dimension temporelle, l'apprentissage de la structure DBN est une tâche très complexe. Les algorithmes existants sont des adaptations des algorithmes d'apprentissage de structure pour les RB basés sur score mais sont souvent limitées lorsque le nombre de variables est élevé. Une autre limitation pour les études d'apprentissage de la structure des RBD, ils utilisent leurs propres Benchmarks et techniques pour l'évaluation. Le problème dans le cas dynamique, nous ne trouvons pas de travaux antérieurs qui fournissent des détails sur les réseaux et les indicateurs de comparaison utilisés. Nous nous concentrons dans ce projet à l'apprentissage de la structure des RBD et ses méthodes d'évaluation avec respectivement une autre famille des algorithmes d'apprentissage de la structure, les méthodes de recherche locale, et une nouvelle approche de génération des grandes standard RBD et un métrique d'évaluation. Nous illustrons l'intérêt de ces méthodes avec des résultats expérimentaux.

Mots clés
Réseaux Bayésiens Dynamiques, les Modèles 2-TBN, apprentissage de structure, scalability, les méthodes de recherche locale, Benchmarking.

Abstract
Dynamic Bayesian networks (DBNs) are a class of probabilistic graphical models that has become a standard tool for modeling various stochastic time-varying phenomena. Probabilistic graphical models such as 2-Time slice BN (2TBNs) are the most used and popular models for DBNs. Because of the complexity induced by adding the temporal dimension, DBN structure learning is a very complex task. Existing algorithms are adaptations of score-based BN structure learning algorithms but are often limited when the number of variables is high. Another limitation of DBN structure learning studies, they use their own benchmarks and techniques for evaluation. The problem in the dynamic case is that we don't find previous works that provide details about used networks and indicators of comparison. We focus in this project on DBN structure learning and its methods of evaluation with respectively another family of structure learning algorithms, local search methods, known by its scalability and a novel approach to generate large standard DBNs and metric of evaluation. We illustrate the interest of these methods with experimental results.

Key Words
Dynamic Bayesian networks, 2-TBN models, structure learning, scalability, local search methods, Benchmarking.