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LEARNING BAYESIAN NETWORKS FROM INCOMPLETE DATABASES

by

M RAMONI and P SEBASTIANI

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Northampton Square London EC1V 0HB

Telephone 0171-477 8000



Learning Bayesian Networks from Incomplete Databases

Marco Ramoni Knowledge Media Institute The Open University Paola Sebastiani
Department of Actuarial Science and Statistics
City University

Abstract

Bayesian approaches to learn the graphical structure of Bayesian Belief Networks (BBNs) from databases share the assumption that the database is complete, that is, no entry is reported as unknown. Attempts to relax this assumption often involve the use of expensive iterative methods to discriminate among different structures. This paper introduces a deterministic method to learn the graphical structure of a BBN from a possibly incomplete database. Experimental evaluations show a significant robustness of this method and a remarkable independence of its execution time from the number of missing data.

Keywords: Uncertainty and Methods for Learning and Data Mining: Bayesian Belief Networks, Bayesian Learning, Missing Data, Model Selection.

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Address: Paola Sebastiani, Department of Actuarial Science and Statistics, The City University, Northampton Square, London EC1V 0HB, United Kingdom. PHONE: +44 (171) 477 8959, FAX: +44 (171) 477 8838, EMAIL: P.Sebastiani@city.ac.uk, URL: http://www.city.ac.uk/~sn303.

1. INTRODUCTION

A Bayesian Belief Network (BBN) [9] is a direct acyclic graph where nodes represent stochastic variables and arcs represent conditional dependencies among these variables. A conditional dependency links a *child* variable to a set of *parent* variables and is defined by the conditional distributions of the child variable given the configurations of its parent variables.

Although in their original concept BBNs were designed to rely on human experts to provide the graphical structure and assess the conditional probabilities, during the past few years an increasing number of efforts has been addressed toward the development of methods able to directly construct BBNs from databases. Early results in this quest were based on non Bayesian approaches [13], but a seminal paper by Cooper and Herskovitz [4] gave rise to a stream of research within a Bayesian framework [1, 7]. Along this approach, the learning process involves two main tasks: the induction of the graphical model best fitting the database and the extraction of the conditional probabilities defining the dependencies in the graphical model.

Methods to perform the first task, known as *model selection*, typically involve two components: a search procedure to explore the space of possible graphical models and a scoring metric to assess the goodness-of-fit of a particular model. Current approaches exploit heuristics to reduce the search space and use the scoring metric to drive the search process. Although the task of extracting a BBN from a database in known to be NP-Hard for the general case [2], under certain assumptions these methods are able to extract quite large BBNs from databases of thousands of cases. One of these assumptions is that the database is *complete*, that is, no entry in the database is reported as unknown.

The reason for this assumption is that a key step in the Bayesian learning process is the computation of the marginal likelihood of the database given a graphical model. This computation can be performed efficiently when the database is complete using exact Bayesian updating, but it becomes intractable when data are missing. Therefore, methods to approximate the marginal likelihood of the data have to be used. Current approaches [3] exploit the EM algorithm [5] or Markov Chain Monte Carlo methods, such as Gibbs Sampling [6]. The basic strategy underlying these methods is based on the Missing Information Principle [8]: fill in the missing observations on the basis of the available information. EM performs this task by replacing the missing entries with the maximum likelihood estimates extracted from the available data and proceeds by iteratively estimating and replacing until stability is reached within a certain threshold. Gibbs Sampling generates a value for the missing data from some conditional distributions and provides a stochastic estimation of the posterior probabilities. Unfortunately, these methods are usually highly resource demanding, their convergence rate may be slow, and their execution time heavily depends on the number of missing data.

Ramoni and Sebastiani [11] introduced a deterministic method to estimate the conditional probabilities defining the dependencies in a BBN which does not rely on the Missing Information Principle. This method, called Bound and Collapse (BC), starts by bounding the set of possible estimates consistent with the available observations in the database and then collapses the resulting interval to a point via a convex combination of the extreme estimates with weights depending on the assumed pattern of missing data. The intuition behind BC is that the information available in the database induces a set of possible estimates and that

the pattern of missing data can be used to select a single distribution within this set. The pattern of missing data may be either provided by an external source of information or may be estimated from the available information under the assumption that data are missing at random. Experimental evaluations [11] show clearly that the estimates provided by BC are very similar to those provided by Gibbs Sampling when data are missing at random, and they are more robust to departure from the true pattern of missing data. On the other hand, BC reduces the cost of estimating a conditional distribution to the cost of an exact Bayesian updating and a convex combination for each state of the distribution.

This paper describes how BC can be used to estimate the marginal likelihood of a database given a model thus extending the principle underlying BC from the task of learning the conditional probabilities to the task of extracting the graphical model of a BBN from an incomplete database. The reminder of this paper is structured as follows: Section 2 introduces the technical background, Section 3 describes the new method, Section 4 reports some results of a preliminary experimental evaluation, and Section 5 summarizes the relevant results.

2. BACKGROUND

A BBN is defined by a set of variables $\mathcal{X} = \{X_1, \ldots, X_I\}$ and a direct acyclic graph identifying a model \mathcal{M} of conditional dependencies among these variables. A conditional dependency links a *child* variable X_i to a set of parent variables Π_i , and is defined by the conditional distributions of the child variable given the configurations of its parent variables. We shall consider discrete variables only, and denote by c_i the number of states of X_i , and X_i the number of states of X_i . The model X_i yields a factorization of the joint probability of a particular set of values of the variables in X_i , say $X_i = \{x_{1k}, \ldots x_{Ik}\}$, as

$$p(\mathcal{X} = x_k | \mathcal{M}) = \prod_{i=1}^{I} p(X_i = x_{ik} | \Pi_i = \pi_{ij}, \mathcal{M}), \tag{1}$$

where π_{ij} is the state of Π_i in x_k . We will denote $X_i = x_{ik}$ by x_{ik} , and $\Pi_i = \pi_{ij}$ by π_{ij} .

Suppose we are given a database of n cases $\mathcal{D} = \{x_1, \ldots, x_n\}$ from which we wish to select a model \mathcal{M} of conditional dependencies among the variables in the database. We adopt a Bayesian approach, so that if $p(\mathcal{M})$ is our prior belief about a particular model \mathcal{M} , we can use the information in the database \mathcal{D} to compute the posterior probability of \mathcal{M} given the data:

$$p(\mathcal{M}|\mathcal{D}) = \frac{p(\mathcal{M}, \mathcal{D})}{p(\mathcal{D})},$$

and then we choose the model which has the highest posterior probability. When the comparison is between two rival models \mathcal{M}_1 and \mathcal{M}_2 with $p(\mathcal{M}_1) = p(\mathcal{M}_2)$, this is equivalent to choosing \mathcal{M}_1 if the Bayes factor:

$$\frac{p(\mathcal{D}|\mathcal{M}_1)}{p(\mathcal{D}|\mathcal{M}_2)} = \frac{p(\mathcal{M}_1, \mathcal{D})}{p(\mathcal{M}_2, \mathcal{D})},$$

is greater than one. It is well known [4], that $p(\mathcal{M}, \mathcal{D})$ can be easily computed if the conditional probabilities defining \mathcal{M} are regarded as random variables θ_{ijk} whose prior

distribution represents the observer's beliefs before seeing any data. The joint probability of a case x_k can then be written in terms of the random vector $\theta = \{\theta_{ijk}\}$ as: $p(x_k|\theta) = \prod_{i=1}^{I} \theta_{ijk}$. This parameterization of the probabilities defining \mathcal{M} allows us to write:

$$p(\mathcal{M}, \mathcal{D}) = p(\mathcal{M}) \int p(\theta|\mathcal{M}) p(\mathcal{D}|\theta) d\theta$$
 (2)

where $p(\theta|\mathcal{M})$ is the prior density of θ , and $p(\mathcal{D}|\theta)$ is the sampling model. A solution of (2) exists in closed form if: 1. The database is complete; 2. The cases are independent, given the parameter vector θ associated to \mathcal{M} ; 3. The prior distribution of the parameters is conjugate to the sampling model $p(\mathcal{D}|\theta)$; 4. The parameters are marginally independent.

Let $n(x_{ik}|\pi_{ij})$, $i=1,...,I,j=1,...,q_i,k=1,...,c_i$, be the frequency of cases in the database with $x_{ik}|\pi_{ij}$, so that $n(\pi_{ij})=\sum_{k=1}^{c_i}n(x_{ik}|\pi_{ij})$ is the frequency of cases with π_{ij} . Assumptions 1 and 2 lead to

$$p(\mathcal{D}| heta) = \prod_{i=1}^I \prod_{j=1}^{q_i} \prod_{k=1}^{c_i} heta_{ijk}^{n(x_{ik}|\pi_{ij})}.$$

A prior distribution on the parameters that satisfies 3 and 4 is a product of Dirichlet distributions. Thus, if we denote by $\theta_{ij} = (\theta_{ij1}, ..., \theta_{ijc_i})$ the vector of parameters associated to the conditional distribution of $X_i | \pi_{ij}$, we have $\theta_{ij} \sim D(\alpha_{ij1}, ..., \alpha_{ijc_i})$. The prior hyperparameters α_{ijk} can be regarded as frequencies of the imaginary cases needed to formulate the prior distribution. As a matter of fact, the marginal probability of $x_{ik} | \pi_{ij}$ is $\alpha_{ijk} / \alpha_{ij}$, and $\alpha_{ij} = \sum_{k=1}^{r_i} \alpha_{ijk}$ is the prior precision on θ_{ij} . Under the assumptions 1 – 4, the posterior distribution of θ is still a product of Dirichlet distributions [12], and

$$\theta_{ij}|\mathcal{D} \sim D(\alpha_{ij1} + n(x_{i1}|\pi_{ij}),...,\alpha_{ijc_i} + n(x_{ic_i}|\pi_{ij})).$$

Thus, the standard Bayesian estimate of $p(x_{ik}|\pi_{ij})$ is the posterior expectation of θ_{ijk} :

$$E(\theta_{ijk}|\mathcal{D}) = \frac{\alpha_{ijk} + n(x_{ijk}|\pi_{ij})}{\alpha_{ij} + n(\pi_{ij})},$$
(3)

and the posterior precision on θ_{ij} is $\alpha_{ij} + n(\pi_{ij})$. Furthermore, the integral (2) has the solution:

$$p(\mathcal{M}) \prod_{i=1}^{I} \prod_{j=1}^{q_i} \prod_{k=1}^{c_i} rac{\Gamma(lpha_{ij})\Gamma(lpha_{ijk} + n(x_{ik}|\pi_{ij}))}{\Gamma(lpha_{ij} + n(\pi_{ij}))\Gamma(lpha_{ijk})}$$

and therefore

$$p(\mathcal{D}|\mathcal{M}) = \prod_{i=1}^{I} \prod_{j=1}^{q_i} \prod_{k=1}^{c_i} \frac{\Gamma(\alpha_{ij})\Gamma(\alpha_{ijk} + n(x_{ik}|\pi_{ij}))}{\Gamma(\alpha_{ij} + n(\pi_{ij}))\Gamma(\alpha_{ijk})}$$
(4)

is the marginal likelihood of \mathcal{D} given \mathcal{M} . Note that $p(\mathcal{D}|\mathcal{M})$ depends on the updated hyperparameters of $\theta_{ij}|\mathcal{D}$, and the posterior precision on θ_{ij} . The probability (4) is the base for the algorithm proposed by Cooper and Herskovitz [4] to induce the model from a database. Suppose we have a partial order on the variables so that $X_i \prec X_j$ if X_i cannot be parent of X_j . Let \mathcal{P}_i be the set of current parents of X_i , thus \mathcal{P}_i is the empty set if X_i is a root

node. Then the local contribution of a node X_i and its parents Π_i to the joint probability of $(\mathcal{M}, \mathcal{D})$ is measured by

$$g(X_i, \mathcal{P}_i) = \prod_{j=1}^{q_i} \prod_{k=1}^{c_i} \frac{\Gamma(\alpha_{ij})\Gamma(\alpha_{ijk} + n(x_{ik}|\pi_{ij}))}{\Gamma(\alpha_{ijk})\Gamma(\alpha_{ij} + n(\pi_{ij}))}.$$
 (5)

The algorithm proceeds by adding a parent at a time and computing $g(X_i, \mathcal{P}_i)$. The set \mathcal{P}_i is expanded to include the parent nodes that give the largest contribution to $g(X_i, \mathcal{P}_i)$, and stops if the probability does not increase any longer. This greedy search strategy has been shown to be extremely cost-effective when the number of variables is large. When the database is complete, (4) can be efficiently computed using the hyper-parameters $\alpha_{ijk} + n(x_{ik}|\pi_{ij})$ and the precision $\alpha_{ij} + n(\pi_{ij})$ of the posterior distribution of θ_{ij} .

Suppose now that we are given the incomplete database $\mathcal{D}_i = \mathcal{D}_o \cup \mathcal{D}_m$, where \mathcal{D}_m denotes the part of \mathcal{D}_i with missing entries. The exact probability of $(\mathcal{M}, \mathcal{D}_i)$ is

$$p(\mathcal{M}, \mathcal{D}_i) = \sum_c p(\mathcal{M}, \mathcal{D}_i, \mathcal{D}_c) = \sum_c p(\mathcal{D}_i) p(\mathcal{M}, \mathcal{D}_c | \mathcal{D}_i)$$

where the sum is over all possible complete databases \mathcal{D}_c consistent with the available data. Clearly, as the number of missing entries increases, the exact calculation of $p(\mathcal{M}, \mathcal{D}_i)$ is infeasible, and some approximation is needed.

3. METHOD

In this section, we will show that it is possible to approximate the hyper-parameters of the posterior distributions of θ_{ij} , from which we derive an estimate of the marginal likelihood given in (4).

Let \hat{p}_{ijk} be an estimate of the posterior expectation of θ_{ijk} , and $\hat{\alpha}_{ij}$ be an estimate of the posterior precision of θ_{ij} . Then the distribution $D(\hat{\alpha}_{ij}\hat{p}_{ij1},...,\hat{\alpha}_{ij}\hat{p}_{ijc_i})$ will have precision $\hat{\alpha}_{ij}$ and expectation \hat{p}_{ijk} , $k=1,\cdots,c_i$. Thus a moment-matching approximation of the posterior distribution of θ_{ij} is:

$$\theta_{ij}|\mathcal{D} \sim D(\hat{\alpha}_{ij}\hat{p}_{ij1},...,\hat{\alpha}_{ij}\hat{p}_{ijc_i}).$$
 (6)

From (6) we can then derive an estimate of (4):

$$\hat{p}(\mathcal{D}|\mathcal{M}) = \prod_{i=1}^{I} \prod_{j=1}^{q_i} \prod_{k=1}^{c_i} \frac{\Gamma(\alpha_{ij})\Gamma(\hat{\alpha}_{ij}\hat{p}(x_{ik}|\pi_{ij}))}{\Gamma(\alpha_{ijk})\Gamma(\hat{\alpha}_{ij})}$$
(7)

which can be also used to extend the algorithm in [4] to incomplete databases by estimating (5) as:

$$\hat{g}(X_i, \mathcal{P}_i) = \prod_{j=1}^{q_i} \prod_{k=1}^{c_i} \frac{\Gamma(\alpha_{ij})\Gamma(\hat{\alpha}_{ij}\hat{p}(x_{ik}|\pi_{ij}))}{\Gamma(\hat{\alpha}_{ij})\Gamma(\alpha_{ijk})}.$$
(8)

Clearly the goodness of the approximation depends on the goodness of the estimates of \hat{p}_{ijk} and $\hat{\alpha}_{ij}$. In the reminder of this section we will show how to use the BC method to estimate the posterior expectation of θ_{ijk} , and the posterior precision of θ_{ij} .

| | case | X_1 | X_2 | X_3 | |
|-----------------------|--------|-------|------------------|-------------|---------|
| | x_1 | 1 | 2 | 2 | |
| | x_2 | 2 | ? | 1 | |
| | x_3 | ? | 1 | 2 | |
| | x_4 | ? | ? | 1 | |
| | x_5 | 1 | ? | ? | |
| | | 1 | | | , |
| $n^{\bullet}(x_{31} $ | (1,1)) | =2 | $n^{\bullet}(x)$ | $_{31} (1,$ | 2)) = 2 |
| $n^{\bullet}(x_{31} $ | (2,1)) | = 2 | $n^{\bullet}(x)$ | $_{31} (2,$ | 2)) = 2 |
| $n^{\bullet}(x_{32})$ | | | $n^{\bullet}(x)$ | $_{32} (1,$ | 2)) = 1 |
| $n^{\bullet}(x_{32})$ | (2,1)) | = 1 | $n^{\bullet}(x)$ | $_{32} (2,$ | 2)) = 0 |

Figure 1: Completions $n^{\bullet}(x_{3k}|x_1,x_2)$ consistent with the incomplete database.

3.1 POSTERIOR EXPECTATION

Let \mathcal{M} be a model of conditional dependencies, specifying for each X_i the parent variable Π_{ij} . BC estimates the conditional probabilities defining the dependencies in \mathcal{M} by first bounding the set of possible posterior distributions of θ_{ij} consistent with the database, and then collapsing the extreme distributions in one single Dirichlet using the assumed pattern of missing data.

Let $n^{\bullet}(x_{ik}|\pi_{ij})$ be the frequency of cases with $X_i = x_{ik}$, given the parent configuration π_{ij} , which have been obtained by completing the incomplete cases. A case may be incomplete because of either a missing observation in the parent configuration or a missing observation of the child variable. An example is given in Figure 1 for the model

$$egin{array}{ccccc} X_1 & & & & & & \\ & \searrow & & & & X_i & {
m binary}, & i=1,2,3. \\ X_2 & \longrightarrow & X_3 & & & & \end{array}$$

For each incomplete case, let ϕ_{ijk} be the probability of a completion:

$$\phi_{ijk} = p(x_{ik}|\pi_{ij}, X_i =?). \tag{9}$$

When data are missing at random, and therefore \mathcal{D}_o is a representative sample of the complete but unknown database \mathcal{D} , the probability of a completion can be estimated from \mathcal{D}_o as

$$\hat{\phi}_{ijk} = \frac{\alpha_{ijk} + n(x_{ik}|\pi_{ij})}{\alpha_{ij} + \sum_{h} n(x_{ih}|\pi_{ij})}.$$

In this case, the BC estimate $\hat{p}(x_{ik}|\pi_{ij}, \mathcal{D}_i, \phi_{ijk})$ of $E(\theta_{ik}|\mathcal{D}_i)$ becomes:

$$\sum_{l \neq k} \hat{\phi}_{ijl} p_{l\bullet}(x_{ik} | \pi_{ij}, \mathcal{D}_i) + \hat{\phi}_{ijk} p^{\bullet}(x_{ik} | \pi_{ij}, \mathcal{D}_i)$$
(10)

where

$$p^{\bullet}(x_{ik}|\pi_{ij},\mathcal{D}_i) = \frac{\alpha_{ijk} + n(x_{ik}|\pi_{ij}) + n^{\bullet}(x_{ik}|\pi_{ij})}{\alpha_{ij} + \sum_h n(x_{ih}|\pi_{ij}) + n^{\bullet}(x_{ik}|\pi_{ij})}$$

$$p_{l\bullet}(x_{ik}|\pi_{ij},\mathcal{D}_i) = \frac{\alpha_{ijk} + n(x_{ik}|\pi_{ij})}{\alpha_{ij} + \sum_h n(x_{ih}|\pi_{ij}) + n^{\bullet}(x_{il}|\pi_{ij})}.$$

The value $p^{\bullet}(x_{ik}|\pi_{ij}, \mathcal{D}_i)$ is the upper bound of $p(x_{ik}|\pi_{ij}, \mathcal{D}_i)$, which is achieved when all incomplete cases in the database which could be completed as $x_{ik}|\pi_{ij}$ are assigned to $x_{ik}|\pi_{ij}$, and the other incomplete cases are assigned to $x_{ih}|\pi_{il}$, any h, and $l \neq j$. Thus, each maximum probability $p^{\bullet}(x_{ik}|\pi_{ij}, \mathcal{D}_i)$ is obtained from a Dirichlet distribution

$$D_k(\alpha_{ij1} + n(x_{i1}|\pi_{ij}), \dots, \alpha_{ijk} + n(x_{ik}|\pi_{ij}) + n^{\bullet}(x_{ik}|\pi_{ij}), \dots, \alpha_{ijc_i} + n(x_{ic_i}|\pi_{ij}))$$

which identifies a unique probability $p_{k\bullet}(x_{il}|\pi_{ij}, \mathcal{D}_i)$ for the other states of the variable X_i given π_{ij} from which $p_{l\bullet}(x_{ik}|\pi_{ij}, \mathcal{D}_i)$ is obtained. The estimates $\hat{p}(x_{ik}|\pi_{ij}, \mathcal{D}_i, \phi_{ijk})$, $k = 1, ..., c_i$, so found define a probability distribution since $\sum_{k=1}^{c_i} \hat{p}(x_{ik}|\pi_{ij}, \mathcal{D}_i, \phi_{ijk}) = 1$.

1,..., c_i , so found define a probability distribution since $\sum_{k=1}^{c_i} \hat{p}(x_{ik}|\pi_{ij}, \mathcal{D}_i, \phi_{ijk}) = 1$.

As the number of missing entries in \mathcal{D}_i decreases, $p^{\bullet}(x_{ik}|\pi_{ij}, \mathcal{D}_i)$ and $p_{l^{\bullet}}(x_{ik}|\pi_{ij}, \mathcal{D}_i)$ approach $(\alpha_{ijk} + n(x_{ijk}|\pi_{ij}))/(\alpha_{ij} + n(\pi_{ij}))$ so that, when the database is complete, (10) returns the exact estimate $E(\theta_{ijk}|\mathcal{D}_i)$. As the number of missing entries increases then both $\hat{\phi}_{ijk}$ and the estimate (10) approach the prior probability α_{ijk}/α_{ij} , so that the estimation method is coherent and no updating is performed when data are totally missing.

If $n^{\bullet}(x_{ik}|\pi_{ij}) = n^{\bullet}_{ij}$, as for instance when data are missing only on the child variable, (10) simplifies to

$$\frac{\alpha_{ijk} + n(x_{ik}|\pi_{ij}) + \hat{\phi}_{ijk}n_{ij}^{\bullet}}{\alpha_{ij} + \sum_{h} n(x_{ih}|\pi_{ij}) + n_{ij}^{\bullet}},$$
(11)

which is a consistent estimate of the expected posterior expectation

$$\frac{\alpha_{ijk} + n(x_{ik}|\pi_{ij}) + n_{ij}^{\bullet}\phi_{ijk}}{\alpha_{ij} + \sum_{h} n(x_{ih}|\pi_{ij}) + n_{ij}^{\bullet}}$$

If $\alpha_{ijk} = 0$, then (11) is the classical maximum likelihood estimate of θ_{ijk} [8]. Experimental comparisons [11] have shown that, when data are missing at random, the estimates computed by the BC method are very close to those obtained by Gibbs Sampling, and are more robust to departures from the true pattern of missing data.

Although BC is able to incorporate the assumption that data are missing at random, in the general case it is not limited to it, since the parameters ϕ_{ijk} may be used to encode any pattern of missing data. For instance, when no information on the mechanism generating the missing data is available and therefore any pattern is equally likely, then $\phi_{ijk} = 1/c_i$. Furthermore, BC provides a new measure of the information available in the database when we consider that the extreme probabilities $p_{l\bullet}(x_{ik}|\pi_{ij},\mathcal{D}_i)$, $l=1,\cdots,c_i$ lead to a lower bound of $p(x_{ik}|\pi_{ij},\mathcal{D}_i)$ —that is, $p_{\bullet}(x_{ik}|\pi_{ij},\mathcal{D}_i)$ = $\min_{l}\{p_{l\bullet}(x_{ik}|\pi_{ij},\mathcal{D}_i)\}$ —and therefore the interval $[p_{\bullet}(x_{ik}|\pi_{ij},\mathcal{D}_i),p^{\bullet}(x_{ik}|\pi_{ij},\mathcal{D}_i)]$ contains all posterior estimates of θ_{ijk} that would be obtained from the possible completions of the database, thus providing a measure of the quality of information conveyed by \mathcal{D}_i about θ_{ijk} [10].

3.2 POSTERIOR PRECISION

The value in (10) is an estimate of $E(\theta_{ijk}|\mathcal{D}_i)$. We now derive an estimate of the posterior precision of θ_{ij} . Suppose we have $n(\pi_{ij})$ cases completely observed on π_{ij} , so that n-

| | Generating Structure | Variables | Cases |
|-----------------|--|--|-------|
| \mathcal{M}_1 | $X_1 	o X_2 	o X_3$ | $X_1(2)X_2(2) \ X_3(2)$ | 1000 |
| \mathcal{M}_2 | $X_1 	o X_2 	o X_3$ | $X_1(2)X_2(2) \ X_3(3)$ | 1000 |
| \mathcal{M}_3 | $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | $X_1(2)X_2(2) \ X_3(3) \ X_4(2)X_5(2)$ | 5000 |
| \mathcal{M}_4 | $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | $X_1(3)X_2(3) \ X_3(3) \ X_4(3)X_2(4)$ | 10000 |

Table 1: Generating structures used in the experimental evaluations. The number next to each variable reports the number of states.

 $\sum_{j} n(\pi_{ij})$ is the number of cases partially observed on the parent variable Π_i . Let $\theta_i = (\theta_{i1},...,\theta_{iq_i})$ be the parameters associated to the joint probability distribution of Π_i , and let $D(\beta_{i1},...,\beta_{iq_i})$ be the prior distribution, so that $\beta_i = \sum_j \beta_{ij}$ is the prior precision. If we knew the probability distribution of π_{ij} we could distribute the incomplete cases across the states of Π_i , so that the expected precision of the posterior distribution of θ_{ij} would be $\alpha_{ij} + n(\pi_{ij}) + p(\pi_{ij})(n - \sum_j n(\pi_{ij}))$. Thus if $\hat{p}(\pi_{ij}|\mathcal{D}_i)$ is an estimate of $p(\pi_{ij})$, an estimate of the posterior precision is

$$\hat{\alpha}_{ij} = \alpha_{ij} + n(\pi_{ij}) + \hat{p}(\pi_{ij}|\mathcal{D}_i)(n - \sum_i n(\pi_{ij})). \tag{12}$$

Clearly, $\hat{\alpha}_{ij}$ is the exact posterior precision when the database is complete and, as the number of missing entries increases, the accuracy of $\hat{\alpha}_{ij}$ heavily depends on $\hat{p}(\pi_{ij}|\mathcal{D}_i)$. We can apply the BC method to obtain the estimate $\hat{p}(\pi_{ij}|\mathcal{D}_i)$. When data are missing at random, the estimate of $\phi_{ij} = p(\Pi_i = \pi_{ij}|\Pi =?), j=1,...,q_i$, is

$$\hat{\phi}_{ij} = \frac{\beta_{ij} + n(\pi_{ij})}{\beta_i + \sum_h n(\pi_{ih})}.$$

We can then apply (10) to obtain

$$\hat{p}(\pi_{ij}) = \sum_{l \neq j=1}^{q_i} \hat{\phi}_{il} p_{l\bullet}(\pi_{ij} | \mathcal{D}_i) + \hat{\phi}_{ij} p^{\bullet}(\pi_{ij} | \mathcal{D}_i)$$

where

$$\begin{split} p^{\bullet}(\pi_{ij}|\mathcal{D}_i) &= \frac{\beta_{ij} + n(\pi_{ij}) + n^{\bullet}(\pi_{ij})}{\beta_i + \sum_h n(\pi_{ih}) + n^{\bullet}(\pi_{ij})} \\ p_{l\bullet}(\pi_{ij}|\mathcal{D}_i) &= \frac{\beta_{ij} + n(\pi_{ij})}{\beta_i + \sum_h n(\pi_{ih}) + n^{\bullet}(\pi_{il})}, \end{split}$$

with $n^{\bullet}(\pi_{ij})$ denoting the number of possible completions of the incomplete cases on π_{ij} . As the number of missing entries increases, the estimate $\hat{\alpha}_{ij}$ tends to $\alpha_{ij} + (\beta_{ij}/\beta_i)n$ so that

| % | Induced Model | $\hat{l}(\mathcal{D}_i \mathcal{M})$ | Time |
|-----|---|--------------------------------------|------|
| 100 | $X_1 \longrightarrow X_2 \longrightarrow X_3$ | 1437 | 12 |
| 80 | $egin{array}{ccc} X_2 & \longrightarrow & X_3 \ \uparrow & \nearrow & & & & \\ X_1 & & & & & & \end{array}$ | 1426 | 13 |
| 60 | $X_1 X_2 \longrightarrow X_3$ | 1446 | 11 |
| 40 | $X_1 \longrightarrow X_2 \longrightarrow X_3$ | 1447 | 12 |
| 20 | $X_1 \longrightarrow X_2 \longrightarrow X_3$ | 1414 | 12 |

Table 2: Models induced from the database generated from \mathcal{M}_1 for different percentages of available entries.

| % | $X_1 = 1$ | $X_2 = 1$ | $X_3 = 1$ |
|-----|-----------|-----------|-----------|
| 100 | 0.11 | 0.78 | 0.56 |
| 80 | 0.11 | 0.78 | 0.57 |
| 60 | 0.12 | 0.79 | 0.56 |
| 40 | 0.11 | 0.79 | 0.57 |
| 20 | 0.10 | 0.79 | 0.60 |

Table 3: Marginal probabilities induced for the structure \mathcal{M}_1 for different percentages of available entries

the cases are distributed according to the prior belief about the parameters defining the BBN.

4. EXPERIMENTAL EVALUATION

The aim of the experiments described in this Section is to evaluate the accuracy of the estimate (7) as the number of missing entries in the database increases.

4.1 MATERIALS AND METHODS

We considered four different models described in Table 1. From each of these models we generated a random sample of n cases, and applied the algorithm for the induction of the model from the data, using an initial order which was consistent with the generating structure, and assuming uniform prior distributions on the parameters. We then iteratively deleted 20% of the sample at random, until the database was empty. On each incomplete database we run our system to induce the model from the data. The algorithm takes as input a database together with a partial order on the variables occurring in it, and returns a BBN. The induction of the graphical model uses a greedy search strategy and replaces the measure (5) with the BC estimate (8). Once the graphical model has been chosen, the conditional probabilities are estimated using the BC method. This method was implemented in Common Lisp and the experiments were performed on a Macintosh 7500/100.

| | 100 | 80 | 60 | 40 | 20 |
|--------------------|-----|-----|-----|-----|-----|
| $g(X_1)$ | 356 | 353 | 367 | 350 | 324 |
| $g(X_2)$ | 531 | 526 | 519 | 512 | 506 |
| $g(X_3)$ | 690 | 692 | 689 | 689 | 678 |
| $g(X_2,X_1)$ | 519 | 512 | 520 | 511 | 483 |
| $g(X_3,X_1)$ | 691 | 692 | 692 | 684 | 667 |
| $g(X_3, X_2)$ | 562 | 560 | 560 | 586 | 607 |
| $g(X_3,(X_1,X_2))$ | 564 | 554 | 566 | 593 | 609 |

Table 4: Estimate of $-\log g(X_i,\Pi)$ for different percentages of available entries in the database generated from \mathcal{M}_1 .

| | 100 | 80 | 60 | 40 | 20 |
|---------------------------------------|------|------|------|------|------|
| X_1 X_3 X_2 | 1577 | 1570 | 1575 | 1552 | 1508 |
| $X_1 ightarrow X_3 X_2$ | 1579 | 1571 | 1578 | 1546 | 1491 |
| $X_1 X_2 	o X_3$ | 1450 | 1439 | 1446 | 1448 | 1437 |
| $X_1 	o X_3 \leftarrow X_2$ | 1452 | 1432 | 1452 | 1455 | 1438 |
| $X_1 \rightarrow X_2 X_3$ | 1565 | 1557 | 1576 | 1551 | 1485 |
| $X_2 \leftarrow X_1 \rightarrow X_2$ | 1566 | 1557 | 1578 | 1545 | 1469 |
| $X_1 \rightarrow X_2 \rightarrow X_3$ | 1437 | 1425 | 1447 | 1447 | 1414 |
| $X_1 \rightarrow X_2$ | | | | | |
| | 1439 | 1419 | 1452 | 1454 | 1416 |
| X_3 | | | | | |

Table 5: $-\log \hat{p}(\mathcal{D}_i|\mathcal{M})$ for all possible models consistent with $X_3 \prec X_2 \prec X_1$, for different percentages of available entries generated from \mathcal{M}_1 .

4.2 RESULTS AND DISCUSSION

Tables 2 and 6 show the models induced from the databases generated from the two models \mathcal{M}_1 and \mathcal{M}_2 , the estimates of $-\log p(\mathcal{D}_i|\mathcal{M})$ for different percentages of available entries, and the total run time, in seconds, taken to extract the graphical model and estimate the parameters of the BBN. Tables report $-\log \hat{p}$ as \hat{l} . The marginal probabilities are displayed in Tables 3 and 7. The initial order on the variables was in both cases $X_3 \prec X_2 \prec X_1$.

The models learned from the database generated from \mathcal{M}_1 are the correct ones when 40% and 20% of the entries in the database are available, and coherently the model of independence is induced from the empty database. With 60% and 80% of the entries, the induced models differ from the generating structure in one link. Run times show a remarkable independence from the percentage of missing data in the database.

Table 4 gives the estimates $-\log \hat{g}(X_i,\Pi_{ij})$ computed in each step of the algorithm. When 80% of the entries is available, $-\log \hat{g}(X_3,(X_1,X_2)=554$ and $-\log \hat{g}(X_3,X_2)=560$, so that the model induced from the incomplete database is $\exp(-554+560)=403.4$ times more likely than the generating structure, if we assume that the prior distribution on the eight possible models consistent with the order $X_3 \prec X_2 \prec X_1$ is uniform. The strong

| % | Induced Model | $\hat{l}(\mathcal{D}_i \mathcal{M})$ | Time |
|-----|--|--------------------------------------|------|
| 100 | $X_1 \longrightarrow X_2 \longrightarrow X_3$ | 1869 | 12 |
| 80 | $egin{array}{ccc} X_2 & \longrightarrow & X_3 \ \uparrow & \nearrow & & & & & & & & & & & & & & & & &$ | 1855 | 13 |
| 60 | $X_1 \longrightarrow X_2 \longrightarrow X_3$ | 1865 | 11 |
| 40 | $egin{array}{ccc} X_2 & \longrightarrow & X_3 \ \uparrow & \nearrow & & & & & & & & & & & & & & & & &$ | 1825 | 12 |
| 20 | $X_1 \longrightarrow X_2 \longrightarrow X_3$ | 1770 | 12 |

Table 6: Models induced from the database generated from \mathcal{M}_2 for different percentages of available entries.

evidence against the model used to generate the database can be due to the fact that $p(X_3=1|X_2=2)=0.1$ and $p(X_2=2)=0.77$ in the generating structure. In the complete database $n(X_3=1|X_2=2)=22$ which becomes 11 when 20% of entries are deleted, so that the small number of entries may cause the imprecision of the estimate $-\log \hat{p}(\mathcal{D}_i|\mathcal{M})$. The conditional probabilities estimated for the model selected are $p(X_3=1|X_1=1,X_2=1)=0.77$ and $p(X_3=1|X_1=2,X_2=1)=0.70$, $p(X_3=1|X_1=1,X_2=2)=0.12$ and $p(X_3=1|X_1=2,X_2=2)=0.11$, so that the estimate of the marginal probability of $X_3=1$ differs from the estimate obtained from the complete database by 1%. When 60% of the entries are available $-\log \hat{g}(X_2)=519$ and $-\log \hat{g}(X_2,X_1)=520$ so that the model induced from the data is only 2.7 times more likely than the generating structure. Again the marginal probabilities computed from the induced network are very similar to the marginal probabilities found in the model induced from the complete database: thus the choice of a slightly different model has little effect on the predicting power of the network.

Table 5 gives the estimate $-\log \hat{p}(\mathcal{D}_i|\mathcal{M})$ for the eight possible models consistent with the initial ordering of the variables. These estimates can be computed from the values in Table 4 by adding relevant terms. The estimates are very accurate until 40% of the entries are retained. When only 20% of the entries is available, the error of the estimate increases, but nonetheless the model induced from the database is equal to the generating structure. If we assume that the set of possible models is limited to the eight models consistent with the order $X_3 \prec X_2 \prec X_1$, and that they are a priori equally likely, then from the values in Table 5 we can compute the marginal probability of \mathcal{D} and of the four incomplete databases \mathcal{D}_i from which we can compute the posterior probabilities of all possible models. The posterior probability of the model induced from the database with 80% of the entries is 0.9987, against a probability 0.0012 for the generating structure. The other models have posterior probabilities near 0. With 60% of the entries, the posterior probability of the induced model is 0.6699, against 0.3258 for the generating structure.

Similar results are found for the models induced from the database generated from \mathcal{M}_2 . The models induced from the databases with 80% and 40% of the entries differs from the generating structure in one link, and they are respectively $\exp(-980 + 985) = 148$ and $\exp(-993 + 995) = 7.4$ more likely than the generating structure. The estimates of the

| % | $X_1 = 1$ | $X_2 = 1$ | $X_3 = 1$ | $X_3 = 2$ |
|-----|-----------|-----------|-----------|-----------|
| 100 | 0.11 | 0.78 | 0.25 | 0.30 |
| 80 | 0.12 | 0.78 | 0.23 | 0.30 |
| 60 | 0.12 | 0.79 | 0.23 | 0.29 |
| 40 | 0.12 | 0.79 | 0.23 | 0.28 |
| 20 | 0.10 | 0.81 | 0.19 | 0.30 |

Table 7: Marginal probabilities in the networks induced from the database generated from \mathcal{M}_2 for different percentages of available entries.

| % | Induced Model | $\hat{l}(\mathcal{D}_i \mathcal{M})$ | Time |
|-----|---|--------------------------------------|------|
| 100 | $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | 25024 | 183 |
| 80 | $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | 24673 | 191 |
| 60 | $\begin{array}{ccccc} X_5 & \longleftarrow & X_3 & & X_4 \\ & \swarrow & & \nearrow & \\ X_1 & \longrightarrow & X_2 & & \end{array}$ | 24871 | 187 |
| 40 | $\begin{array}{ccccc} X_5 & \longleftarrow & X_3 & \longrightarrow & X_4 \\ & \swarrow & & \nearrow & \\ X_1 & \longrightarrow & X_2 & & \end{array}$ | 24814 | 188 |
| 20 | $\begin{array}{ccccc} X_5 & \longleftarrow & X_3 & & X_4 \\ \uparrow & \swarrow & & \nearrow & \\ X_1 & \longrightarrow & X_2 & & \end{array}$ | 25112 | 185 |

Table 8: Models induced from the database generated from \mathcal{M}_3 for different percentages of available entries.

marginal probabilities are very similar to those obtained in the complete database, again showing that the consequence of a slightly different model has little effect on the reasoning process. The estimate of $-\log p(\mathcal{D}_i|\mathcal{M})$ is very accurate until the database contains 40% of the original entries. The total run times make even clearer that the source of complexity is the search space and the performances of the method remain insensitive to the number of missing data. This result is not surprising when we realize that the computational cost of BC does not depend on the number of missing data. The number of missing data affects only the storage procedure described in [10] but its effect is limited by taking advantage of the local independencies of the BBN and by using discrimination trees to store the counters of observed data and to keep track of the possible completions.

The models induced from the databases generated from \mathcal{M}_3 and \mathcal{M}_4 are given in Table 8 and 10, respectively. The initial order on the variables was in both cases $X_5 \prec X_4 \prec X_3 \prec X_2 \prec X_1$. The models induced from the complete database are equal to the generating

| % | $X_1 = 1$ | $X_2 = 1$ | $X_3 = 1$ | $X_4 = 1$ | $X_5 = 1$ |
|-----|-----------|-----------|-----------|-----------|-----------|
| 100 | 0.20 | 0.70 | 0.39 | 0.30 | 0.52 |
| 80 | 0.20 | 0.71 | 0.38 | 0.29 | 0.53 |
| 60 | 0.21 | 0.70 | 0.39 | 0.29 | 0.53 |
| 40 | 0.21 | 0.70 | 0.39 | 0.30 | 0.53 |
| 20 | 0.21 | 0.69 | 0.40 | 0.31 | 0.54 |

Table 9: Marginal probabilities in the networks induced from the database generated from \mathcal{M}_3 for different percentages of available entries.

structure for both \mathcal{M}_{\ni} and \mathcal{M}_{\triangle} , and coherently the empty structure is induced when data are totally missing. Table 9 displays the marginal probabilities computed in the networks induced from the incomplete databases generated by \mathcal{M}_{\ni} .

As the number of entries available decreases, at most two extra dependencies are induced from the database. The only exception is the model induced from the database generated from \mathcal{M}_4 with 80% of the entries available. In this case, four extra dependencies are learned, and the Bayes factor of the induced model against the generating structure is e^{13} . However the conditional probabilities learned are only slightly different, so that the estimates of the marginal probabilities are extremely robust thus limiting the effect in the subsequent reasoning process. The estimates of $-\log p(\mathcal{D}_i|\mathcal{M})$ are again extremely accurate.

5. CONCLUSIONS

Missing data represent a challenge for learning methods because they may affect their use in real-world applications, where databases are often incomplete. Current methods to learn BBNs from incomplete databases rely on iterative methods, such as EM or Gibbs Sampling, to obtain an approximate estimate of the marginal likelihood of the database given a graphical model, a fundamental step in the process of extracting the graphical structure of a BBN from a database. This paper introduced a deterministic method able to provide this estimation, using BC, and to extract the graphical structure from an incomplete database. In this way, BC can be used to both induce the graphical structure and assess the conditional probabilities of a BBN from an incomplete database. Preliminary experimental evaluations show a significant robustness of this method and a remarkable independence of its execution time from the number of missing data.

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| % | Induced Model | $\hat{l}(\mathcal{D}_i \mathcal{M})$ | Time |
|-----|--|--------------------------------------|------|
| 100 | $\begin{array}{ccccc} X_5 & \longleftarrow & X_3 & & X_4 \\ & \nwarrow & & \nearrow \\ X_1 & \longrightarrow & X_2 & \end{array}$ | 40125 | 275 |
| 80 | $egin{array}{ccccc} X_5 &\longleftarrow & X_3 \ \uparrow & \swarrow & \uparrow \ X_1 &\longrightarrow & X_2 \ & \searrow & \downarrow \ & & X_4 \ \end{array}$ | 39369 | 296 |
| 60 | $egin{array}{cccccccccccccccccccccccccccccccccccc$ | 42146 | 278 |
| 40 | $\begin{array}{cccc} X_5 & \longleftarrow & X_3 & & X_4 \\ & \swarrow & & \nearrow & \\ X_1 & \longrightarrow & X_2 & & \end{array}$ | 40132 | 289 |
| 20 | $egin{array}{ccccc} X_5 & \longleftarrow & X_3 & & X_4 \ & \nwarrow & \uparrow & \nearrow & \ X_1 & \longrightarrow & X_2 & & & \end{array}$ | 39952 | 285 |

Table 10: Models induced from the database generated from \mathcal{M}_4 for different percentages of available entries.

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