From Incomplete, Dynamic Data to Bayesian Networks

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Bayesian networks are a versatile and powerful tool to model complex phenomena and the interplay of their components in a probabilistically principled way. Moving beyond the comparatively simple case of completely observed, static data, which has received the most attention in the literature, in this paper we will review how Bayesian networks can model dynamic data and data with incomplete observations. Such data are the norm at the forefront of research and applications, and Bayesian networks are uniquely positioned to model them due to their explainability and interpretability.

Keywords — Bayesian networks, dynamic data, incomplete data, structure learning, inference

1 | INTRODUCTION

Bayesian networks (BNs; Koller and Friedman 2009) are graphical models in which the nodes of a directed acyclic graph (DAG) \( \mathcal{G} \) represent a set \( \mathbf{X} = \{X_1, \ldots, X_N\} \) of random variables describing some quantities of interest. The arcs connecting the nodes express direct dependence relationships, with graphical separation in \( \mathcal{G} \) implying conditional independence in probability. As a result, \( \mathcal{G} \) induces the factorisation

\[
P(\mathbf{X} | \mathcal{G}, \Theta) = \prod_{i=1}^{N} P(X_i | \Pi_{X_i}, \Theta_{X_i}) .
\]

in which the joint probability distribution of \( \mathbf{X} \) (with parameters \( \Theta \)) decomposes in one local distribution for each \( X_i \) (with parameters \( \Theta_{X_i}, \cup_{X_j \in \mathbf{X}} \Theta_{X_j} = \Theta \)) conditional on its parents \( \Pi_{X_i} \). Assuming \( \mathcal{G} \) is sparse\(^1\) BNs provide a compact representation of both low- and high-dimensional probability distributions.

\(^{1}\) There is no universally accepted threshold on the number of arcs for a DAG to be called "sparse"; typically it is taken to have \( O(cN) \) arcs, with \( c \) between 1 and 5.

\( \text{1} \)
BNs are also very flexible in terms of distributional assumptions; but while in principle we could choose any probability distribution for $X$, the literature has mostly focused on three cases for analytical and computational reasons. Discrete BNs [Heckerman et al. 1995] assume that both $X$ and the $X_i$ are multinomial random variables. Local distributions take the form

$$X_i \mid \Pi_{X_i} \sim \text{Mul} \left( \pi_{ik \mid j} \right), \quad \pi_{ik \mid j} = P \left( X_i = k \mid \Pi_{X_i} = j \right);$$

(2)

their parameters $\pi_{ik \mid j}$ are the conditional probabilities of $X_i$ given each configuration of the values of its parents, usually represented as a conditional probability table for each $X_i$. Gaussian BNs (GBNs; [Geiger and Heckerman 1994] model $X$ with a multivariate normal random variable and assume that the $X_i$ are univariate normals linked by linear dependencies. The parameters of the local distributions can be equivalently written [Weatherburn 1961] as the partial correlations $\rho_{X_i X_j \mid \Pi_{X_i \setminus X_j}}$ between $X_i$ and each parent $X_j$ given the other parents; or as the coefficients $\beta_{X_i}$ of the linear regression model

$$X_i = \mu_{X_i} + \Pi_{X_i} \beta_{X_i} + \varepsilon_{X_i}, \quad \varepsilon_{X_i} \sim N \left( 0, \sigma^2_{X_i} \right),$$

(3)

so that $X_i \mid \Pi_{X_i} \sim N \left( \mu_{X_i} + \Pi_{X_i} \beta_{X_i}, \sigma^2_{X_i} \right)$. Finally, conditional linear Gaussian BNs (CLGBNs; [Lauritzen and Wermuth 1989] combine discrete and continuous random variables in a mixture model:

- discrete $X_i$ are only allowed to have discrete parents (denoted $\Delta_{X_i}$), and are assumed to follow a multinomial distribution as in (2);
- continuous $X_i$ are allowed to have both discrete and continuous parents (denoted $\Gamma_{X_i}, \Delta_{X_i} \cup \Gamma_{X_i} = \Pi_{X_i}$), and their local distributions are

$$X_i \mid \Pi_{X_i} \sim N \left( \mu_{X_i, \delta_{X_i}} + \Pi_{X_i} \beta_{X_i, \delta_{X_i}}, \sigma^2_{X_i, \delta_{X_i}} \right)$$

which can be written as a mixture of linear regressions

$$X_i = \mu_{X_i, \delta_{X_i}} + \Pi_{X_i} \beta_{X_i, \delta_{X_i}} + \varepsilon_{X_i, \delta_{X_i}}, \quad \varepsilon_{X_i, \delta_{X_i}} \sim N \left( 0, \sigma^2_{X_i, \delta_{X_i}} \right)$$

against the continuous parents with one component for each configuration $\delta_{X_i}$ of the discrete parents $\Delta_{X_i}$. If $X_i$ has no discrete parents, the mixture reverts to a single linear regression like (3).

The task of learning a BN from a data set $D$ containing $n$ observations is performed in two steps:

$$P(G, \Theta \mid D) = P(G \mid D) \cdot P(\Theta \mid G, D).$$

Structure learning consists in finding the DAG $G$ that encodes the dependence structure of the data, thus maximising $P(G \mid D)$ or some alternative goodness-of-fit measure; parameter learning consists in estimating the parameters $\Theta$ given the $G$ obtained from structure learning. Both steps can integrate data with expert knowledge through the use of suitable prior distributions on $G$ and $\Theta$ (see for example Castelo and Siebes 2000; Mukherjee and Speed 2008; Druzdzel and van der Gaag 1995). If we assume that parameters in different local distributions are independent and that the data
contain no missing values \cite{Heckerman1995}, we can perform parameter learning independently for each $X_i$ because following \cite{Eckerman1995}

$$P(\Theta | G, \mathcal{D}) = \prod_{i=1}^{N} P(\Theta_{X_i} | \Pi_{X_i}, \mathcal{D}).$$

Furthermore, assuming $G$ is sparse, each local distribution $X_i | \Pi_{X_i}$ will involve only a few variables and thus will have a low-dimensional parameter space, making parameter learning computationally efficient.

On the other hand, structure learning is well known to be both NP-hard \cite{Chickering1994} and NP-complete \cite{Chickering1996}, even under unrealistically favourable conditions such as the availability of an independence and inference oracle \cite{Chickering2004}. This is despite the fact that if we take

$$P(G | \mathcal{D}) \propto P(G) P(\mathcal{D} | G),$$

again following \cite{Eckerman1995} we can decompose the marginal likelihood $P(\mathcal{D} | G)$ into one component for each local distribution

$$P(\mathcal{D} | G) = \int P(\mathcal{D} | G, \Theta) P(\Theta | G) d\Theta = \prod_{i=1}^{N} \int P(X_i | \Pi_{X_i}, \Theta_{X_i}) P(\Theta_{X_i} | \Pi_{X_i}) d\Theta_{X_i};$$

and despite the fact that each component can be written in closed form for discrete BNs \cite{Heckerman1995}, GBNs \cite{Geiger1994} and CLGBNs \cite{Battcher2001}. The same is true if we replace $P(\mathcal{D} | G)$ with frequentist goodness-of-fit scores such as BIC \cite{Schwarz1978}, which is commonly used in structure learning because of its simple expression:

$$\text{BIC}(G, \Theta | \mathcal{D}) = \sum_{i=1}^{N} \log P(X_i | \Pi_{X_i}, \Theta_{X_i}) - \frac{\log(n)}{2} |\Theta_{X_i}|.$$

Compared to marginal likelihoods, BIC also has the advantage that it does not depend on any hyperparameter, while converging to $\log P(\mathcal{D} | G)$ as $n \to \infty$. These score functions have two important properties:

- they allow local computations because, following \cite{Eckerman1995}, they decompose into one component for each local distribution;
- they take the same value for all the DAGs that encode the same probability distribution (score equivalence), which can then be grouped in equivalence classes \cite{Chickering1997}.

Structure learning via score maximisation is usually based on general-purpose heuristic optimisation algorithms, adapted to take advantage of these two properties to increase the speed of structure learning \cite{Scutari2019}. The most common are greedy search strategies such as hill-climbing and tabu search \cite{Russell2009} that employ local moves designed to affect only one or two local distributions in each iteration; other options explored in the literature include genetic algorithms \cite{Larrañaga1996} and ant colony optimisation \cite{Campos2002}. Learning equivalence classes directly (as opposed to DAGs) can be done along the same lines with the Greedy Equivalence Search (GES) \cite{Chickering2002} algorithm. Exact maximisation of $P(\mathcal{D} | G)$ and BIC has also become feasible in recent years.

\footnote{Interestingly, some relaxations of BN structure learning are not NP-hard; see for example \cite{Dojer2006} on learning the structure of causal networks.}

\footnote{All DAGs in the same equivalence class have the same underlying undirected graph and $v$-structures (patterns of arcs like $X_i \rightarrow X_j \leftarrow X_k$, with no arcs between $X_i$ and $X_k$).}
thanks to increasingly efficient pruning of the space of DAGs and tight bounds on the scores (Cussens, 2012; Suzuki, 2017; Scanagatta et al., 2015).

Another option for structure learning is using conditional independence tests to learn conditional independence constraints from \( \mathcal{D} \), and thus identify which arcs should be included in \( \mathcal{G} \). The resulting algorithms are called constraint-based algorithms, as opposed to the score-based algorithms we introduced in the previous paragraph; for an overview and a comparison of these two approaches see Scutari et al., 2018. Chickering et al. (2004) proved that constraint-based algorithms are also NP-hard for unrestricted DAGs; and they are in fact equivalent to score-based algorithms given a fixed topological ordering of the nodes in \( \mathcal{G} \) when independence constraints are assessed with statistical tests related to cross-entropy (Cowell, 2001).

Finally, once both \( \mathcal{G} \) and \( \Theta \) has been learned, we can answer queries about our quantities of interest using the resulting BN as our model of the world. Common types are conditional probability queries, in which we compute the posterior probability of some variables given evidence on others; and most probable explanation queries, in which we identify the configuration of values of some variables that has the highest posterior probability given the values of some other variables. The latter is especially suited to implement both prediction and imputation of missing data. These queries can be automated, for any given BN, using either exact or approximate inference algorithms that work directly on the BN without the need for any manual calculation; for an overview of such algorithms see Koller and Friedman (2009).

Given their ability to represent the word, to automatically answer arbitrary queries, and to combine data and expert knowledge in the learning process, BNs can model a wide variety of phenomena effectively. However, their applicability is not always apparent to practitioners in other fields due to the strong focus of the literature on the simple scenario in which data are static (as opposed to dynamic, that is, with a time dimension) and complete (as in, completely observed). However, dynamic data are central to a number of cutting-edge applications and research in fields as different as genetics and robotics; and incomplete data are a fact of life in almost any real-world data analysis. Hence, in Section 2 we will review the main definitions and properties of dynamic Bayesian networks, including a selection of popular probabilistic models they subsume and their applications. In Section 3 we will then review both structure and parameter learning in the presence of missing data, highlighting limitations and possible solutions depending on the patterns of missingness.

2 | Dynamic Bayesian Networks

Dynamic BNs (DBNs) (Murphy, 2002) combine classic (static) BNs and Markov processes to model dynamic data in which each individual is measured repeatedly over time, such as longitudinal or panel data. They have major applications in engineering (Pavlovic et al., 1999; Frigault et al., 2008), medicine (Hofheitner et al., 2012), genetics and systems biology (Perrin et al., 2003). The term “dynamic” in this context implies we are modelling a dynamic system, not necessarily that the network changes over time.

4 Confusingly, discrete BNs are sometimes called DBNs to be consistent with Gaussian BNs being called GBNs.
Definitions and Properties

For simplicity, let’s assume at first that we are operating in discrete time: our system consists of one set $X^{(t)}$ of random variables for each of $t = 1, \ldots, T$ time points. We can model it as a DBN with Markov process of the form

$$
P(X^{(0)} \ldots, X^{(T)}) = P(X^{(0)}) \prod_{t=1}^{T} P(X^{(t)} | X^{(t-1)}). \quad (6)
$$

where $P(X^{(0)})$ gives the initial state of the process and $P(X^{(t)} | X^{(t-1)})$ defines the transition between times $t - 1$ and $t$. We can model this transition with a 2-time BN (2TBN) defined over $(X^{(t-1)}, X^{(t)})$, in which we naturally assume that any arc between a node in $t - 1$ and a node in $t$ must necessarily be directed towards the latter following the arrow of time. When modelling $X^{(t)}$, the nodes in $X^{(t-1)}$ only appear in the conditioning; we take them to be essentially fixed and to have no free parameters, so we leave them as root nodes. After all, $X^{(t-1)}$ will be stochastic in $P(X^{(t-1)} | X^{(t-2)})$ and it would not be consistent with $6$ to treat $X^{(t-1)}$ as a stochastic quantity twice! Then, following $7$, we can write

$$
P(X^{(t)} | X^{(t-1)}) = \prod_{i=1}^{N} P(X^{(t)}_{i} | \Pi X^{(t)}_{i}), \quad (7)
$$

and we usually assume that the parameters associated with the local distributions do not change over time to make the process time-homogeneous.

These choices are motivated by computational and statistical simplicity: there is no intrinsic limitation in the construction of DBNs that prevents them from modelling dependencies that stretch further back in time or, for that matter, trends or seasonality. Grzegorczyk and Husmeier [2009] 2011, for instance, constructed non-stationary, non-homogeneous DBNs for modelling continuous data using change-points to capture different regimes in different time intervals; they balanced this increased flexibility by requiring $G$ to be the same for all regimes, allowing only the parameters of the local distributions to change. Similarly [Robinson and Hartemink, 2010] defined a non-stationary DBN with change-points and associated arc changesets, with truncated geometric priors on the size of the changesets, number of and interval between change-points; and Song et al. [2009] constructed DBNs that vary smoothly (not piece-wise) over time in both structure and parameters. Kim et al. [2004] introduced an even more flexible model that used spline regression with B-splines to identify $\Pi X^{(t)}$. Augmenting temporal (panel) data with non-temporal (cross-sectional) data for learning DBNs has also been explored by Lähdesmäki and Shmulevich [2008] using an score that approximates the resulting intractable likelihood.

Modelling DBNs as discrete time processes is likewise a choice motivated by mathematical simplicity. Nodelman et al. [2003] originally proposed a class of continuous-time DBNs (CTBNs) with independent exponential waiting times and discrete nodes; they are uniquely identifiable since all arcs are non-instantaneous, and they have a closed-form marginal likelihood as well. More recently, this work has been expanded in Liu et al. [2018] by replacing exponential waiting times with hypoexponentials to better reflect the behaviour of data in several domains. Discrete-time DBNs are certainly simpler than any of these CTBNs, but that mathematical simplicity comes with important practical consequences. Firstly, in order to work in discrete time we must choose a uniform time step (the length of time between $t - 1$ and $t$) for the whole DBN; but in many real-world phenomena different variables can have very different time granularities, and those time granularities may vary as well in the course of data collection, making any single choice for the time step inappropriate. Secondly, the choice of the time step may obscure the dynamics of the phenomenon. The implication of using discrete time is that we aggregate all the state changes in the DBN over the entire course of each time step. On the one hand, if variables evolve at slower pace than the time step we are forced to model the DBN...
as a higher-order Markov process\(^5\), resulting in a much more complex model. On the other hand, if variables evolve at a faster pace than time step, this averaging will effectively hide state changes and their interplay into a single summary statistic; hence the DBN will provide a very poor approximation of the underlying phenomenon. Furthermore, if we are unable to correctly identify the \( \Pi_{X_i(t)} \), \( X_i(t) \) may end up being recursively linked to the parents of the \( \Pi_{X_i(t)} \), resulting into dense DBNs that are much more complex than the real underlying phenomenon and that are difficult to learn from limited data.

A partial solution to the latter problem is to allow the parents \( \Pi_{X_i(t)} \) to be either in the same time or in the previous time point, modelling the DBN as a first-order Markov process. When observations represent average or aggregate measurements over a period of time (say, the 4th time point corresponds to the 4th week’s worth of data), it makes sense to allow instantaneous dependencies between variables in the same time point, since the instantaneousness of the dependence is just a fiction arising from our model definition. On the other hand, when observations actually correspond to instantaneous measurements (such as from synchronised sensors) only non-instantaneous dependencies are usually allowed in the model, on the grounds that conditioning event (\( \Pi_{X_i(t)} \)) should precede in time the conditioned event (\( X_i(t) \)). From a causal perspective, we can similarly argue that each of the \( \Pi_{X_i(t)} \) can only cause \( X_i(t) \) if it precedes \( X_i(t) \) in time; if that \( \Pi_{X_i(t)} \) is in the same time point as \( X_i(t) \) then what we are modelling is co-occurrence and not causation. This the core idea of *Granger causality* \(^{\text{Granger 1968}}\), which states that one time series (such as the \( \Pi_{X_i(t)} \)) can be said to have a causal influence on a second time series (such as the \( X_i(t) \)) if and only if incorporating past knowledge about the former improves predictive accuracy for the latter. Therefore, allowing instantaneous dependencies makes causal reasoning on the DBN markedly more difficult. The same is true for learning the structure of the DBN in the first place: learning a general BN is NP-hard \(^{\text{Chickering and Heckerman 1994, Chickering et al. 2004}}\), while learning a DBN containing only non-instantaneous dependencies is not \(^{\text{Dojer 2006}}\). Intuitively, the space of the possible DBNs is much smaller if we do not allow instantaneous dependencies because there are fewer candidate arcs that we can include, and because their directions are fixed to follow the arrow of time and Granger causality.

### 2.2 Models That Can Be Expressed as DBNs

DBNs have a strong expressive power, and they subsume and generalise a variety of classic models that have been studied individually in the literature. Here we will discuss three such models: hidden Markov models, vector autoregressive models and Kalman filters. Hidden Markov models and Kalman filters can be seen as particular instances of state-space models, and their DBN representations make clear the general relationship between these two classes of models. Representing these models as DBNs has advantages beyond making their comparison more convenient; it makes it possible to use the probabilistic machinery we covered in Sections 1 and 2.1 when more convenient or computationally efficient than the alternatives (as in the case of inference in hidden Markov models in \(^{\text{Murphy 2002}}\)). Some examples are shown in Figure 1 and will be illustrated below.

*Hidden Markov models* (HMMs; \(^{\text{Zucchini and MacDonald 2009}}\)) are one of the most widespread approaches to model phenomena with hidden state, that is, in which the behaviour of the observed variables \( X \) depends on that of one or more discrete latent variables \( Z \) as well as on other variables in \( X \). This scenario commonly arises when technical, economic or ethical considerations make it unfeasible to completely observe the underlying state of the phenomenon.

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\(^{5}\) A stochastic process is a Markov process of order \( L \) if \( X(t) \) depends only on \( X(t-1) \) \( \ldots \) \( X(t-L) \) and is independent from \( X(t-L-1) \) \( \ldots \) \( X(0) \). The higher the order, the further back in time the dependencies can reach.

\(^{6}\) This issue is often called entanglement.

\(^{7}\) Interestingly, when the number of available time points is small, inference based on DBNs is more accurate than methods directly based on Granger causality; but the opposite is true for longer time series \(^{\text{Luo and Feng 2009}}\).
of interest. Notable examples are imputation (Marchini and Howie 2010) and phasing in genome-wide association studies (Delaneau et al. 2012), due to limitations in the technology to probe and tag DNA; tracking animals in ecology (Patterson et al. 2008), where we can observe their movements using radio beacons but not their behaviour; and confirming mass migrations through history by combining archaeological artefacts and ancient DNA samples (Schifflers and Durbin 2014). Until the advent of deep neural networks, HMMs were also the choice model for speech (Gales and Young 2008) and handwriting recognition (Plotz and Fink 2009).

In DBN terms, a typical HMM model with $M$ latent variables can be written as

$$P\left(X^{(t)} | X^{(t-1)}, Z^{(t)}\right) = \prod_{i=1}^{N} P\left(X^{(t)}_{i} | \prod X^{(t)}_{i}, Z^{(t)}\right) \quad \text{and} \quad P\left(Z^{(t)}\right) = \prod_{j=1}^{M} P\left(Z^{(t)}_{j} | \prod Z^{(t)}_{j}\right), \quad (8)$$

with the restriction that the parents of $Z^{(t)}_{j}$ can only be other latent variables. Latent variables are assumed to be discrete; and in the vast majority of the literature observed variables are assumed to be discrete as well. Depending on the choice of $\prod Z^{(t)}_{j}$, we can obtain various HMM variants such as: hierarchical HMMs (Fine et al. 1998), in which each $Z^{(t)}_{j}$ is defined as an HMM itself to produce a multi-level stochastic model; and factorial HMMs (Ghahramani and Jordan 1996), in which the $X^{(t)}_{i}$ are driven by the configuration of a set of mutually independent $Z^{(t)}_{j}$ (shown in Figure 1, top-left panel).

**Vector auto-regressive models (VARs)** (Box et al. 2016) are a straightforward multivariate extension of univariate auto-regressive time series for continuous variables. As such, their major applications are forecasting in finance (Banbura...
and more recently in the analysis of fMRI data [Gates et al., 2009]. They are defined as
\[ X^{(t)} = A_1 X^{(t-1)} + \ldots + A_L X^{(t-L)} + \epsilon_t, \quad \epsilon_t \sim N(0, \Sigma), A_1, \ldots, A_L \in \mathbb{R}^{N \times N}, \]
for some fixed Markov order \( L \). We can rewrite \( 9 \) as
\[ X^{(t)} \mid X^{(t-1)}, \ldots, X^{(t-L)} \sim N \left( A_1 X^{(t-1)} + \ldots + A_L X^{(t-L)} , \epsilon_t \right) \]
and then restrict the parents of each \( X_i^{(t)} \) to those for which the corresponding regression coefficients in \( A_1, \ldots, A_L \) are not zero using the one-to-one correspondence between regression coefficients and partial correlations [Weatherburn, 1961]. Formally, \( X_j^{(t-1)} \in \Pi_{X_i^{(t)}} \) if and only if \( A_i[i, j] \neq 0 \), which makes it possible to write \( 9 \) in a similar form to \( 6 \) and obtain a Gaussian DBN. The same construction is used by [Song et al., 2009] for their non-homogeneous DBN models, which are parameterised as VAR processed and estimated using \( L_1 \)-penalised regressions. In the special case in which \( L = 1 \), VARs can be graphically represented in two equivalent ways shown in the bottom panels of Figure 1: an “unrolled” DBN in which each node corresponds to a single \( X_i^{(t)} \); and a more compact “rolled-up” DBN in which each node corresponds to a variable \( X_i \), an arc from \( X_i \) to \( X_j \) implies \( X_i^{(t-1)} \rightarrow X_j^{(t)} \). An arc from \( X_i \) to itself implies \( X_i^{(t-1)} \rightarrow X_i^{(t)} \) as a special case for \( i = j \).

Kalman filters (KFs; [Hamilton, 1994]) combine traits of both HMMs and VARs, as discussed in depth in [Roweis and Ghahramani, 1999] and [Ghahramani, 2001]: like VARs, they are linear Gaussian DBNs; but they also have latent variables like HMMs. They are widely used for filtering (that is, denoising) and prediction in GPS positioning systems [Work et al., 2008]; atmospheric modelling and weather prediction [Cassola and Burlando, 2012]; and seismology [Sakaki et al., 2010]. In their simplest form (see Figure 1 top-right panel), KFs include a layer of one or more latent variables that model the unobservable part of the phenomenon,
\[ Z^{(t)} = A Z^{(t-1)} + B U^{(t)} + \xi_t, \quad \xi_t \sim N(0, \Psi), A \in \mathbb{R}^{M \times M}, B \in \mathbb{R}^{M \times P} \]
feeding into one or more observed variables
\[ X^{(t)} = C Z^{(t)} + D U^{(t)} + \epsilon_t, \quad \epsilon_t \sim N(0, \Sigma), C \in \mathbb{R}^{N \times M}, D \in \mathbb{R}^{N \times P} \]
with independent Gaussian noise added in both layers. Both layers often include additional (continuous) explanatory variables \( U \) and can also be augmented with (discrete) switching variables to allow for different regimes as in [Grzegorczyk and Husmeier, 2009, 2011]. If we exclude the latter, the assumption is that the system is jointly Gaussian: that makes it possible to frame KFs as a DBN in the same way we did for VARs.

3 | BAYESIAN NETWORKS FROM INCOMPLETE DATA

The vast majority of the literature on learning BNs rests on the assumption that \( \mathcal{D} \) is complete, that is, a data set in which every variable has an observed value for each sample. However, in real-world applications we frequently have to deal with incomplete data; some samples will be completely observed while others will contain missing values for some of the variables. While it is tempting to simply impute the missing values as a preprocessing step, it has long been known that even fairly sophisticated techniques like hot-deck imputation are problematic in a multivariate setting [Kalton and...
FIGURE 2  BN representations of the MCAR (left), MAR (centre) and MNAR (right) patterns of missingness from [Rubin 1976] and [Little and Rubin 1987]. Shaded nodes and portion of nodes correspond to variables that are not observed in the data.

Kaspryzk [1986]. Just deleting incomplete cases can also bias learning, depending on how missing data are missing. [Rubin 1976] and [Little and Rubin 1987] formalised three possible patterns (or mechanisms) of missingness (illustrated in Figure 2):

- Missing completely at random (MCAR): when complete samples are indistinguishable from incomplete ones. In other words, the probability that a value will be missing is independent from both observed and missing values. For instance, in the left panel of Figure 2, both $X_2$ and $X_6$ are only partially observed; hence $X_2 = (X_2^O, X_2^M)$ and $X_6 = (X_6^O, X_6^M)$ where $X_2^O$ and $X_6^O$ are observed and $X_2^M$ and $X_6^M$ are missing. The patterns of missingness are controlled by $M_2$ (for $X_2$) and $M_6$ (for $X_6$) and are completely random; say, $M_2$ and $M_6$ are binary variables that encode the probability of two instruments (independently) breaking down and thus failing to measure $X_2$ and $X_6$ for some individuals.

- Missing at random (MAR): cases with incomplete data differ from cases with complete data, but the pattern of missingness is predictable from other observed variables. In other words, the probability that a value will be missing is a function of the observed values. An example is the central panel of Figure 2 compared to the left panel, we now know that the two instruments are likely to fail when (say) high values of $X_1$ (and $X_3$, in the case of $X_6$) are observed.

- Missing not at random (MNAR): the pattern of missingness is not random or it is not predictable from other observed variables; the probability that an entry will be missing depends on both observed and missing values. Common examples are variables that are missing systematically or for which the patterns of missingness depends on the missing values themselves. In the right panel of Figure 2 say that $X_2$ is censored (that is, it is never observed if its value is higher than a fixed threshold); but when $X_2$ is missing the probability that $X_6$ is missing (encoded by $M_6$) is also extremely high. Since we never observe $X_2$ when $X_6$ is missing, we are unable to correctly model this relationship; as far as we know both $X_2$ and $X_6$ may be missing due to some common external factor, since they appear to be missing together in the data.

MCAR and MAR are ignorable patterns of missingness; the probability that some item (in the data) is missing may depend on observed items but not on missing items, and thus can be properly modelled. If we denote with $\mathcal{D}^O$ and $\mathcal{D}^M$ the
observed and unobserved portions of \( D \), and we group all the binary missingness indicators \( M \) in \( M \) with parameters \( \Xi \), then we can write

\[
P(D, M | G, \Theta, \Xi) = P(D^O, D^M, M | G, \Theta, \Xi) = \int P(D^O, D^M | G, \Theta) P(M | D^O, D^M, G, \Xi) \, dD^M; \quad (10)
\]

if the missing data are MAR then \( M \) only depends on \( D^O \),

\[
P\left( M | D^O, D^M, G, \Xi \right) = P\left( M | D^O, G, \Xi \right);
\]

and if the missing data MCAR then \( M \) does not depend on either \( D^O \) or \( D^M \),

\[
P\left( M | D^O, D^M, G, \Xi \right) = P\left( M | G, \Xi \right).
\]

In both cases it is possible to model \( M \) from the available data. However, this is not the case for MNAR since \( M \) depends on the unobserved \( D^M \).

Modelling incomplete data is analytically intractable and computationally prohibitive compared to the complete data scenario: an exact analysis requires the computation of the joint posterior distribution of \( \Theta \) considering all possible completions of \( D \). However, completing \( D \) has a computational complexity that grows exponentially with the number of missing entries, since it involves finding the set of missing data completions with the highest probability given the observed data. Considering just the most probable completion can also induce over-confidence in the results of the analysis, since completed observations will have lower variability by construction; but full Bayesian inference averaging over all possible \( \Theta \) and completed \( D \) is so computationally challenging as to be unfeasible even in simple settings. Furthermore, this joint maximisation breaks the parameter independence assumption and makes it impossible to define decomposable scores for structure learning without resorting to some approximation.

### 3.1 Parameter Learning

Many approaches have been developed for parameter learning from incomplete data given a fixed, known structure\(^8\) ranging from iterative methods like Data Augmentation (DA;\cite{TannerWong1987} and the Expectation-Maximisation algorithm (EM;\cite{Lauritzen1995}), to methods based on probability intervals such as Bound and Collapse (BC;\cite{RamoniSebastiani1997} and uncertain probabilities (\cite{deCamposetal1994}). These methods usually assume missing data are MCAR or MAR to work on \( P(\Theta, D^M | G, D^O) \), and their accuracy decreases dramatically if that is not the case (\cite{SpiegelhalterCowell1992}; however, BC has been found to be robust also for MNAR data (\cite{Oniskoetal2002}) also noted that simple imputation approaches can perform well in learning the parameters of a BN given a fixed, sparse network structure, which further expands available options.

In the context of parameter learning, the EM algorithm retains its classic structure:

- the **expectation** (E) step consists in computing the expected values of the sufficient statistics (such as the counts \( n_{ijk} \) in discrete BNs, partial correlations in GBNs), using exact inference along the lines described above to make use of incomplete as well as complete samples;

- the **maximisation** (M) step takes the sufficient statistics from the E-step and estimates the parameters of the BN,

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\(^8\) Although almost all the literature specific to BNs assumes discrete data.
either using maximum likelihood or Bayesian posterior estimators.

The parameter estimates are then used in the next E-step to update the expected values of the sufficient statistics; repeated iterations of these two steps will in the limit return the maximum likelihood or maximum a posteriori estimates for the parameters. Using the notation of \[10\], the E-step is equivalent to computing \(E(D^M, D^O \mid \mathcal{G}, \Theta)\) and the M-step to maximising \(P(\Theta \mid \mathcal{G}, D^O, D^M)\).

DA is quite similar, but instead of converging iteratively to a single set of parameter estimates it uses Gibbs Sampling to generate values from the posterior distributions of both \(D^M\) and \(\Theta\). The two steps are as follows:

- in the imputation (I) step the data are completed with values drawn from the predictive distributions of the missing values;
- in the parameter (P) estimation step a parameter value is drawn from the posterior distribution of \(\Theta\) conditional on the completed data from the I-step.

More formally, we define the augmented parameter vector \(\{D^M, \Theta\}\) containing both the missing values and the parameters of the BN. Given an initial set of values, it updates each element of \(\{D^M, \Theta\}\) by sampling a new value for each missing value from \(P(D^M \mid D^H, \Theta)\), and by sampling a new value for each parameter from \(P(\Theta \mid \Theta_{-i}, D^M)\), each in turn. After an initial burn-in phase, this process will converge to its stationary distribution and return parameter realisations from the posterior distribution of \(\Theta\) conditional on the observed data. A similar Gibbs sampling approach has been proposed more recently by [Riegelsen, 2004]: it samples from a simpler, approximate predictive distribution and makes use of weights to implement an efficient importance sampling scheme. In addition, the weights make it possible to use samples generated in the burn-in phase as well as those from the stationary distribution of the Gibbs samples because they weight samples according to their estimated predictive accuracy.

Finally, BC and its successor the Robust Bayesian Estimator (RBE; [Ramoni and Sebastiani, 2001]) exploit the discrete nature of categorical variables to produce rough interval estimates of the conditional probabilities learned from incomplete variables, which are then reduced to point estimates either via a convex combination of the intervals’ bounds, expert knowledge or both. The first (bound) step, uses the fact that each \(\pi_{ik \mid j}\) can be bounded below by assuming that none of the missing values for \(X_j\) are completed with their \(k\)th value when the \(j\)th parent configuration is observed; and that \(\pi_{ik \mid j}\) can be bounded above by assuming that all missing values are completed with their \(k\)th value. This approach has the merit of not making any assumptions on the distribution of missing data. Furthermore, the width of each interval provides an explicit representation of the reliability of the estimates, which can be taken into account in inference and prediction. The second (collapse) step assumes missing data are MAR or MCAR to be able to compute the expected completions for incomplete samples, which are then used to compute the mean and variance of the \(\pi_{ik \mid j}\). Interestingly, the intervals from the bound step can be used to augment both EM and Gibbs sampling and obtain more precise inferences, but the predictive accuracy of RBE was shown to be superior to both in [Ramoni and Sebastiani, 2001]. A similar investigation in the context of BN classifiers can be found in [Peña et al., 2000]. A conceptually similar approach was also proposed by [Liao and Ji, 2009], which first used qualitative expert knowledge on the parameter values to bound them, and then estimated their values using convex optimisation embedded in the EM algorithm.

Note that we can work on latent variables using similar approaches as long as \(\mathcal{G}\) is fixed and we just need to learn \(\Theta\). A recent example is given in [Yamazaki and Motomura, 2019], who show it is possible to learn the domain of a latent discrete variable as well as the associated parameters as long as it has observed parents and children. Several other examples are discussed in the context of DBNs in [Murphy, 2002].
3.2 Structure Learning

Learning the structure of a BN from incomplete data is, in many respects, an extension of the techniques covered in Section 3.1. In its general form it is computationally unfeasible because we need to perform a joint optimisation over the missing values and the parameters to score each candidate network. Starting from (10), we can make this apparent by rewriting $P(D|G)$ as a function of $D^O, D^M$:

$$P(D|G) = P(D^O, D^M|G) = \int P(D^O, D^M|G, \Theta) P(\Theta|G) d\Theta =$$

$$= \int P(D^M|D^O, G, \Theta) P(D^O|G, \Theta) P(\Theta|G) d\Theta dD^M. \quad (11)$$

From this expression we can see that in order to maximise $P(D|G)$ we should jointly maximise the probability of the observed data $D^O$ and the probability of the missing data $D^M$ given the observed data, for each candidate $G$ and averaging over all possible $\Theta$. This gives us the maximum a posteriori solution to structure learning; a full Bayesian approach would require averaging over all the possible configurations of the missing data as well, leading to

$$P(D|G) = \int P(D^M|D^O, G, \Theta) P(D^O|G, \Theta) P(\Theta|G) d\Theta dD^M. \quad (12)$$

Compared to (11), (12) contains one extra dimension for each missing value (in addition to one dimension for each parameter in $\Theta$) and thus it is too high-dimensional to compute in practical applications. An additional problem is that, while $P(D^O|G, \Theta)$ decomposes as in (9), $P(D^M|D^O, G, \Theta)$ does not in the general case.

In order to sidestep these computational issues, the literature has pursued two possible approaches: iteratively completing and refining the data, an using standard algorithms and scores for complete data; or using scoring functions that approximate BIC and $P(D|G)$ but that are decomposable and can be computed efficiently even on incomplete data.

The Structural EM algorithm (SEM\cite{friedman1997}) is the most famous implementation of the first approach: it has important applications in phylogenetics \cite{friedman2002}, clinical record \cite{vanderheijden2014} and clinical trial analysis \cite{liew2019}. SEM makes structure learning computationally feasible by searching for the best structure inside of EM, instead of embedding EM inside a structure learning algorithm. It consists of two steps like the classic EM:

- in the E-step, we complete the data by computing the expected sufficient statistics using the current network structure;
- in the M-step, we find the structure that maximises the expected score function for the completed data.

Since the scoring in the M-step uses the completed data, structure learning can be implemented efficiently using standard algorithms. The original proposal by \cite{friedman1997} used BIC and greedy search; \cite{friedman1998} later extended SEM to a fully Bayesian approach based posterior scores, and proved the convergence of the resulting algorithm.

In fact, any combination of structure learning algorithm and score can be used in the M-step; most recently

\cite{friedman1997} This acronym is another source of confusion, since SEM can also stand for “structural equation models” which are closely related to BNs. See \cite{gupta2008} for a discussion of their similarities and differences.
Scanagatta et al. (2018) proposed learning BNs with a bounded-treewidth structure using their k-MAX algorithm and a variant of BIC. (This has the two-fold advantage of speeding up the M-step and of yielding BNs for which completing data in the E-step is relatively fast.) Singh (1997) proposed a similar approach based on DA, generating sets of completed data sets and averaging the resulting learned networks in each iteration. Myers et al. (1999b) also chose to iteratively learn both the network structures and the missing data at the same time, but did so using evolutionary algorithms and encoding both as "genes". Hence, the individuals in the population being evolved comprise both a completed data set and the associated BN. This was combined with Metropolis-Hastings to speed up learning as discussed in Myers et al. (1999a).

More recently, Adeel and de Campos (2017) proposed an exact learning algorithm that explicitly models the patterns of missingness with auxiliary variables, which are included as separate nodes in the BN rather than just being computational devices. Additionally, they showed that its computational complexity is the same as that of other exact learning algorithms for complete data; and they adapted the proposed algorithm into a (faster) heuristic that is then proven to be consistent.

The second group of approaches includes the variational-Bayesian EM from Beal and Ghahramani (2003) that maximises a variational approximation of $P(\mathcal{D} | \mathcal{G})$, which in turn is a lower bound to the true marginal likelihood. Balov (2013) proved that structure learning with BIC is not consistent even under MCAR, and suggested replacing it with node-average penalised log-likelihoods computed from locally complete observations. An alternative consists in using approximations based on mixtures of truncated exponentials, as was showcased in Fernández et al. (2010); they combined EM and DA to fit regression-like BNs with structures that resemble naive Bayes and tree-augmented naive Bayes classifiers, and approximating explanatory variables. Approachable introductions to this area of research are provided in Chickering and Heckman (1997) and Heckerman (1997), which describe the relationship between $P(\mathcal{D} | \mathcal{G})$, its Laplace approximation and BIC in mathematical detail.

4 | SUMMARY

In this paper we have reviewed the fundamental definitions and properties of BNs, and how BNs can be stretched to encode more complex probabilistic models than what might be apparent from reference material and most of the literature. Both have an overwhelming focus on the straightforward case in which the data being modelled are both static (that is, with no time dimension) and complete (that is, with no missing values). However, dynamic and incomplete data are central to many cutting-edge applications in research fields ranging from genetics to robotics; BNs can play an important role in many of these settings, as has been evidenced by the examples referenced in Sections 2 and 3. Given their expressive power, BNs also subsume several classic probabilistic models and can augment them with automatic reasoning capabilities through various kinds of queries that can be performed algorithmically. Much research has been and is being developed to adapt BNs to these applications and make them a competitive choice for modelling complex data.
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