# Beyond Uniform Priors in Bayesian Network Structure Learning

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# Abstract

Bayesian network structure learning is often performed in a Bayesian setting, evaluating candidate structures using their posterior probabilities for a given data set. Score-based algorithms then use those posterior probabilities as an objective function and return the maximum a posteriori network as the learned model. For discrete Bayesian networks, the canonical choice for a posterior score is the Bayesian Dirichlet equivalent uniform (BDeu) marginal likelihood with a uniform (U) graph prior, which assumes a uniform prior both on the network structures and on the parameters of the networks. In this paper, we investigate the problems arising from these assumptions, focusing on those caused by small sample sizes and sparse data. We then propose an alternative posterior score: the Bayesian Dirichlet sparse (BDs) marginal likelihood with a marginal uniform (MU) graph prior. Like U+BDeu, MU+BDs does not require any prior information on the probabilistic structure of the data and can be used as a replacement noninformative score. We study its theoretical properties and we evaluate its performance in an extensive simulation study, showing that MU+BDs is both more accurate than U+BDeu in learning the structure of the network and competitive in predicting power, while not being computationally more complex to estimate.

**Keywords:** Bayesian networks, structure learning, graph prior, marginal likelihood, discrete data.

#### 1. Introduction

Bayesian networks (BNs; Pearl, 1988; Koller and Friedman, 2009) are a class of probabilistic models composed by a set of random variables  $\mathbf{X} = \{X_1, \dots, X_N\}$  and by a directed acyclic graph (DAG)  $\mathcal{G} = (\mathbf{V}, A)$  in which each node in  $\mathbf{V}$  is associated with one of the random variables in  $\mathbf{X}$  (they are usually referred to interchangeably). The arcs in A express direct dependence relationships between the variables in  $\mathbf{X}$ ; graphical separation of two nodes implies the conditional independence of the corresponding random variables. In principle, there are many possible choices for the joint distribution of  $\mathbf{X}$ ; literature has focused mostly on discrete BNs (Heckerman et al., 1995), in which both  $\mathbf{X}$  and the  $X_i$  are multinomial random variables and the parameters of interest are the conditional probabilities associated with each variable, usually represented as conditional probability tables. Other possibilities include Gaussian BNs (Geiger and Heckerman, 1994) and conditional linear Gaussian BNs (Lauritzen and Wermuth, 1989).

The task of learning a BN from data is performed in two steps in an inherently Bayesian fashion. Consider a data set  $\mathcal{D}$  and a BN  $\mathcal{B} = (\mathcal{G}, \mathbf{X})$ . If we denote the parameters of the joint distribution of  $\mathbf{X}$  with  $\Theta$ , we can assume without loss of generality that  $\Theta$  uniquely identifies  $\mathbf{X}$  in the family of distributions chosen to model  $\mathcal{D}$  and write

$$\underbrace{P(\mathcal{B} \mid \mathcal{D}) = P(\mathcal{G}, \Theta \mid \mathcal{D})}_{\text{learning}} = \underbrace{P(\mathcal{G} \mid \mathcal{D})}_{\text{structure learning}} \cdot \underbrace{P(\Theta \mid \mathcal{G}, \mathcal{D})}_{\text{parameter learning}} . (1)$$

Structure learning consists in finding the DAG  $\mathcal{G}$  that encodes the dependence structure of the data. Three general approaches to learn  $\mathcal{G}$  from  $\mathcal{D}$  have been explored in the literature: constraint-based, score-based and hybrid. Constraint-based algorithms use conditional independence tests such as mutual information (Cover and Thomas, 2006) to assess the presence or absence of individual arcs in  $\mathcal{G}$ . Score-based algorithms are typically heuristic search algorithms and use a goodness-of-fit score such as BIC (Schwarz, 1978) or the Bayesian Dirichlet equivalent uniform (BDeu) marginal likelihood (Heckerman et al., 1995) to find an optimal  $\mathcal{G}$ . For the latter a uniform (U) prior over the space of DAGs is usually assumed for simplicity. Hybrid algorithms combine the previous two approaches, using conditional independence tests to restrict the search space in which to perform a heuristic search for an optimal  $\mathcal{G}$ . For some examples, see Aliferis et al. (2010), Larrañaga et al. (1997), Cussens (2011) and Tsamardinos et al. (2006).

Parameter learning involves the estimation of the parameters  $\Theta$  given the DAG  $\mathcal{G}$  learned in the first step. Thanks to the Markov property (Pearl, 1988), this step is computationally efficient because if the data are complete the global distribution of  $\mathbf{X}$  decomposes into

$$P(\mathbf{X} \mid \mathcal{G}) = \prod_{i=1}^{N} P(X_i \mid \Pi_{X_i})$$
(2)

and the local distribution associated with each node  $X_i$  depends only on the configurations of the values of its parents  $\Pi_{X_i}$ . Note that this decomposition does not uniquely identify a BN; different DAGs can encode the same global distribution, thus grouping BNs into equivalence classes (Chickering, 1995) characterised by the skeleton of  $\mathcal{G}$  (its underlying undirected graph) and its v-structures (patterns of arcs of the type  $X_j \to X_i \leftarrow X_k$ , with no arc between  $X_j$  and  $X_k$ ).

In the remainder of this paper we will focus on discrete BN structure learning in a Bayesian framework. In Section 2 we will describe the canonical marginal likelihood used to identify maximum a posteriori (MAP) DAGs in score-based algorithms, BDeu, and the uniform prior U over the space of the DAGs. We will review and discuss their underlying assumptions, fundamental properties and known problems. In Section 3 we will introduce a new posterior score, which we will call the Bayesian Dirichlet sparse (BDs) marginal likelihood with a marginal uniform (MU) prior, and the corresponding alternative set of assumptions. We will study its theoretical properties and we will show that it does not suffer from the same problems as U+BDeu when learning BNs from small and sparse samples. Based on the results of an extensive simulation study, in Section 4 we will show that MU+BDs is preferable to U+BDeu because it is more accurate in learning  $\mathcal G$  from the data; and because the resulting BNs provide predictive power that is at least as good as that of the BNs learned using U+BDeu. Proofs for all theorems are collected in Appendix A and detailed simulation results are reported in Appendix B.

# 2. U+BDeu: A Posterior Score Arising from Uniform Priors

Starting from (1), we can decompose  $P(\mathcal{G} \mid \mathcal{D})$  into

$$P(\mathcal{G} \mid \mathcal{D}) \propto P(\mathcal{G}) P(\mathcal{D} \mid \mathcal{G}) = P(\mathcal{G}) \int P(\mathcal{D} \mid \mathcal{G}, \Theta) P(\Theta \mid \mathcal{G}) d\Theta$$

where  $P(\mathcal{G})$  is the prior distribution over the space of the DAGs and  $P(\mathcal{D} | \mathcal{G})$  is the marginal likelihood of the data given  $\mathcal{G}$  averaged over all possible parameter sets  $\Theta$ . Using (2) we can then decompose  $P(\mathcal{D} | \mathcal{G})$  into one component for each node as follows:

$$P(\mathcal{D} | \mathcal{G}) = \prod_{i=1}^{N} P(X_i | \Pi_{X_i}) = \prod_{i=1}^{N} \left[ \int P(X_i | \Pi_{X_i}, \Theta_{X_i}) P(\Theta_{X_i} | \Pi_{X_i}) d\Theta_{X_i} \right].$$
 (3)

In the case of discrete BNs, we assume  $X_i \mid \Pi_{X_i} \sim Multinomial(\Theta_{X_i} \mid \Pi_{X_i})$  where the  $\Theta_{X_i} \mid \Pi_{X_i}$  are the conditional probabilities  $\pi_{ij} \mid_k = P(X_i = k \mid \Pi_{X_i} = j)$ . We then assume a conjugate prior  $\Theta_{X_i} \mid \Pi_{X_i} \sim Dirichlet(\alpha_{ijk}), \sum_{jk} \alpha_{ijk} = \alpha_i > 0$  to obtain the posterior  $Dirichlet(\alpha_{ijk} + n_{ijk})$  which we use to estimate the  $\pi_{ij} \mid_k$  from the counts  $n_{ijk}, \sum_{ijk} n_{ijk} = n$  observed in  $\mathcal{D}$ .  $\alpha_i$  is known as the *imaginary* or *equivalent sample size* and determines how much weight is assigned to the prior in terms of the size of an imaginary sample supporting it.

### 2.1 The Bayesian Dirichlet Equivalent Uniform Score (BDeu)

Further assuming positivity  $(\pi_{ij|k} > 0)$ , parameter independence  $(\pi_{ij|k}$  for different parent configurations are independent), parameter modularity  $(\pi_{ij|k}$  associated with different nodes are independent) and complete data, Heckerman et al. (1995) derived a closed form expression for (3), known as the Bayesian Dirichlet (BD) score:

$$BD(\mathcal{G}, \mathcal{D}; \boldsymbol{\alpha}) = \prod_{i=1}^{N} BD(X_i | \Pi_{X_i}; \alpha_i) = \prod_{i=1}^{N} \prod_{j=1}^{q_i} \left[ \frac{\Gamma(\alpha_{ij})}{\Gamma(\alpha_{ij} + n_{ij})} \prod_{k=1}^{r_i} \frac{\Gamma(\alpha_{ijk} + n_{ijk})}{\Gamma(\alpha_{ijk})} \right]$$
(4)

where  $r_i$  is the number of states of  $X_i$ ;  $q_i$  is the number of configurations of  $\Pi_{X_i}$ ;  $n_{ij} = \sum_k n_{ijk}$ ;  $\alpha_{ij} = \sum_k \alpha_{ijk}$ ; and  $\alpha$  is the set of the  $\alpha_i$ . For  $\alpha_{ijk} = 1$ ,  $\alpha_i = r_i q_i$  we obtain the K2 score from Cooper and Herskovits (1991); for  $\alpha_{ijk} = 1/2$ ,  $\alpha_i = r_i q_i/2$  we obtain the BD score with Jeffrey's prior (Suzuki, 2016); and for  $\alpha_{ijk} = \alpha/(r_i q_i)$ ,  $\alpha_i = \alpha$  we obtain the Bayesian Dirichlet equivalent uniform (BDeu) score from Heckerman et al. (1995), which is the most common choice used in score-based algorithms to estimate  $P(\mathcal{D} | \mathcal{G})$ . The corresponding posterior probability estimates of the  $\pi_{ij|k}$  are

$$p_{ij|k}^{(\alpha_i^*)} = \frac{\alpha_{ijk} + n_{ijk}}{\sum_{k=1}^{r_i} \alpha_{ijk} + n_{ijk}} = \frac{\alpha_i^* + n_{ijk}}{r_i \alpha_i^* + n_{ij}} \qquad \text{where } \alpha_i^* = \frac{\alpha}{r_i q_i}.$$
 (5)

It can be shown that BDeu is score equivalent (Chickering, 1995), that is, it takes the same value for DAGs that encode the same probability distribution; and that it is the only BD score with this property (Koller and Friedman, 2009, Theorem 18.4). The uniform prior over the parameters associated with each  $X_i \mid \Pi_{X_i}$  has been justified by the lack of

prior knowledge and widely assumed to be non-informative. It is typically used with small imaginary sample sizes such as  $\alpha=1$  as suggested by Koller and Friedman (2009) and Ueno (2010) so that it can be easily dominated by the data.

However, there is an increasing amount of evidence that these assumptions lead to a prior that is far from non-informative and that has a strong impact on the quality of the learned DAGs. Silander et al. (2007) showed via simulation that the MAP DAGs selected using BDeu are highly sensitive to the choice of  $\alpha$ . Even for "reasonable" values such as  $\alpha \in [1, 20]$ , they obtained DAGs with markedly different number of arcs, and they showed that large values of  $\alpha$  tend to produce DAGs with more arcs. This is counter-intuitive because larger  $\alpha$  would normally be expected to result in stronger regularisation and sparser BNs. Steck and Jaakkola (2003) similarly showed that the number of arcs in the MAP DAG is determined by a complex interaction between  $\alpha$  and  $\mathcal{D}$ ; in the limits  $\alpha \to 0$  and  $\alpha \to \infty$  it is possible to obtain both very sparse and very dense DAGs. (We informally define  $\mathcal{G}$  to be sparse if |A| = O(N), typically with |A| < 5N; a dense  $\mathcal{G}$ , on the other hand, has a relatively large |A| compared to N.) In particular, for small values of  $\alpha$  and/or sparse data (that is, discrete data for which we observe a small subset of the possible combinations of the values of the  $X_i$ ),  $\alpha_i^* \to 0$  and

$$BDeu(\mathcal{G}, \mathcal{D}; \alpha) \to \alpha^{d_{EP}^{(\mathcal{G})}}$$
(6)

where  $d_{\mathrm{EP}}^{(\mathcal{G})}$  is the effective number of parameters of the model, defined as

$$d_{\text{EP}}^{(\mathcal{G})} = \sum_{i=i}^{N} d_{\text{EP}}^{(X_i,\mathcal{G})} = \sum_{i=i}^{N} \left[ \sum_{j=1}^{q_i} \tilde{r}_{ij} + \tilde{q}_i \right], \quad \tilde{r}_{ij} = \sum_{k=1}^{r_i} \mathbb{1}_{\{x>0\}}(n_{ijk}), \quad \tilde{q}_i = \sum_{j=1}^{q_i} \mathbb{1}_{\{x>0\}}(n_{ij}), \quad \tilde{q}_i = \sum_{j=1}^{q_i} \tilde{q}_{ij} + \tilde{q}_i \right],$$

where  $\tilde{r}_{ij}$  is the number of positive  $n_{ijk}$  in the jth configuration of  $\Pi_{X_i}$  and  $\tilde{q}_i$  is the number of configurations in which at least one  $n_{ijk}$  is positive.

This was then used to prove that

$$\frac{\mathrm{P}(\mathcal{D} \mid \mathcal{G}^{+})}{\mathrm{P}(\mathcal{D} \mid \mathcal{G}^{-})} = \frac{\mathrm{BDeu}(X_{i} \mid \Pi_{X_{i}} \cup X_{l}; \alpha)}{\mathrm{BDeu}(X_{i} \mid \Pi_{X_{i}}; \alpha)} \to \begin{cases} 0 & \text{if } d_{\mathrm{EDF}} > 0\\ +\infty & \text{if } d_{\mathrm{EDF}} < 0 \end{cases}$$
(7)

for two DAGs  $\mathcal{G}^-$  and  $\mathcal{G}^+ = \mathcal{G}^- \cup \{X_l \to X_i\}$  that differ only by the inclusion of a single arc  $X_l \to X_i$ . The effective degrees of freedom  $d_{\text{EDF}}$  are defined as  $d_{\text{EP}}^{(\mathcal{G}^+)} - d_{\text{EP}}^{(\mathcal{G}^-)}$ . The practical implication of this result is that, if we use the Bayes factor in (7) for structure learning, a large number of zero-cell-counts will force  $d_{\text{EDF}}$  to be negative, which means the inclusion of additional arcs is favoured. But that in turn makes  $d_{\text{EDF}}$  even more negative, quickly leading to overfitting  $\mathcal{G}$ .

Furthermore, Steck and Jaakkola (2003) argued that BDeu can be rather unstable for "medium-sized" data and small  $\alpha$ , which is a very common scenario. Steck (2008) approached the problem from a different perspective and derived an analytic approximation for the "optimal" value of  $\alpha$  that maximises predictive accuracy, further suggesting that the interplay between  $\alpha$  and  $\mathcal{D}$  is controlled by the skewness of the  $P(X_i | \Pi_{X_i})$  and by the strength of the dependence relationships between the nodes. Skewed  $P(X_i | \Pi_{X_i})$  result in some  $\pi_{ij}|_k$  being smaller than others, which in turn makes sparse data sets more

likely; hence the problematic behaviour described in Steck and Jaakkola (2003) and reported above. Most of these results have been analytically confirmed more recently by Ueno (2010, 2011).

Finally, Suzuki (2016) studied the asymptotic properties of BDeu using BD with Jeffrey's prior as a term of comparison. He found that BDeu is not regular in the sense that it may learn DAGs in a way that does not respect the maximum entropy principle (Jaynes, 1957a,b) depending on the values of the underlying  $\pi_{ij|k}$ , even if the positivity assumption holds and if n is large. This agrees with the observations in Ueno (2010), who also observed that BDeu is not necessarily consistent for any finite n, but only asymptotically for  $n \to \infty$ .

### 2.2 The Uniform Graph Prior (U)

As far as  $P(\mathcal{G})$  is concerned, the most common choice is the uniform (U) distribution  $P(\mathcal{G}) \propto 1$ ; the space of the DAGs grows super-exponentially in N (Harary and Palmer, 1973) and that makes it extremely difficult to specify informative priors. Two notable examples are presented in Castelo and Siebes (2000) and Mukherjee and Speed (2008). Castelo and Siebes (2000) described a *completed prior* in which they elicitated prior probabilities for a subset of arcs and completed the prior to cover the remaining arcs with a discrete uniform distribution. So, if we denote

$$\overrightarrow{p_{ij}} = \mathrm{P}(\{X_i \to X_j\} \in A), \quad \overleftarrow{p_{ij}} = \mathrm{P}(\{X_i \leftarrow X_j\} \in A), \quad \overrightarrow{p_{ij}} = \mathrm{P}(\{X_i \to X_j, X_i \leftarrow X_j\} \not\in A)$$
(8)

with  $\overrightarrow{p_{ij}} + \overleftarrow{p_{ij}} + p_{ij}^{\circ} = 1$ , Castelo and Siebes (2000) proposed to elicitate the triplets  $(\overrightarrow{p_{ij}}, \overleftarrow{p_{ij}}, p_{ij}^{\circ}, p_{ij}^{\circ})$  for specific pairs of nodes  $(X_i, X_j)$ , and to assume  $\overrightarrow{p_{ij}} = \overleftarrow{p_{ij}} = p_{ij}^{\circ} = 1/3$  for the rest. Priors for distinct  $(X_i, X_j)$  were assumed to be independent and thus they can be combined in

$$P(\mathcal{G}) \propto \prod_{(i,j)} \overrightarrow{p_{ij}} \mathbb{1}_{\{\{X_i \to X_j\} \in A\}}(i,j) + \overleftarrow{p_{ij}} \mathbb{1}_{\{\{X_i \leftarrow X_j\} \in A\}}(i,j) + p_{ij}^{\circ} \mathbb{1}_{\{\{X_i \to X_j, X_i \leftarrow X_j\} \notin A\}}(i,j).$$

As an alternative, Mukherjee and Speed (2008) proposed an informative prior using a loglinear combination of arbitrary features  $f_i(\cdot)$  of  $\mathcal{G}$ ,

$$P(\mathcal{G}) \propto \exp\left(\lambda \sum_{i} w_i f_i(\mathcal{G})\right),$$

whose relative importance is controlled with some positive weights  $w_i$ . The hyperparameter  $\lambda$  was used to control the overall strength of the prior, much like the imaginary sample size in BDeu. While both approaches have been shown to improve the accuracy of structure learning, they require us to elicit substantial amounts of information from domain experts, which is notoriously challenging (Madigan and Raftery, 1994).

The uniform prior is at the opposite end of the spectrum, in that it does not have any free parameter and therefore does not require any prior elicitation. In our previous work (Scutari, 2013), we explored the first- and second-order properties of U and we showed that for each possible pair of nodes  $(X_i, X_j)$ 

$$\overrightarrow{p_{ij}} = \overleftarrow{p_{ij}} \approx \frac{1}{4} + \frac{1}{4(N-1)} \quad \text{and} \quad \overrightarrow{p_{ij}} \approx \frac{1}{2} - \frac{1}{2(N-1)}. \tag{9}$$

This prior distribution is asymptotically (marginally) uniform over both arc presence and direction: each arc is present in  $\mathcal{G}$  with probability  $^1/2$  and, when present, it appears in each direction with probability  $^1/2$  as  $N \to \infty$ . We also showed that two arcs are correlated if they are incident on a common node, with

$$COR(A_{ij}, A_{jk}) \approx 2 \left[ \frac{3}{4} - \frac{1}{4(N-1)} \right]^2 \left[ \frac{1}{4} + \frac{1}{4(N-1)} \right]$$

and  $COR(A_{ij}, A_{kl}) = 0$  otherwise, through exhaustive enumeration of all possible DAGs for  $N \leq 7$  and through simulation for larger N. This suggests that false positives (arcs that are incorrectly included in  $\mathcal{G}$ ) and false negatives (arcs that are incorrectly excluded from  $\mathcal{G}$ ) can potentially propagate through  $P(\mathcal{G})$ : for instance, if an arc is incorrectly included in  $\mathcal{G}$ , then arcs incident on the same head node are now more likely to be included, which increases the possibility of including further arcs in that part of  $\mathcal{G}$ . This in turn may cause further problems in  $P(\mathcal{D} \mid \mathcal{G})$ , since the number of parameters of the BN increases combinatorially with the number of parents of its nodes.

In order to prevent this from happening, many papers in the literature choose to put a hard limit on the maximum number of parents of each node (see, for instance, Friedman and Koller, 2003; Friedman et al., 1999). The prior then becomes

$$P(\mathcal{G}) \propto \begin{cases} 1 & \text{if } |\Pi_{X_i}| < m \text{ for all } X_i \\ 0 & \text{otherwise} \end{cases}$$

which strongly limits the space of the candidate DAGs by imposing a strong uniformity constraint on their structure if m is small (that is, all nodes have about the same small number of parents). Indeed, choosing too small a value for m has a strong negative impact on the accuracy of structure learning, as discussed by Elidan and Gould (2008). A "softer" alternative would be to use the classic variable selection prior (Scott and Berger, 2010) independently for each local distribution, that is

$$P(X_i \mid \Pi_{X_i}) = \prod_{j \neq i} \overrightarrow{p_{ij}} \mathbb{1}_{\{X_j \in \Pi_{X_i}\}}(j)$$

typically simplified to  $\overrightarrow{p_{ij}} = p_i$  or even  $\overrightarrow{p_{ij}} = p$  in practical use. This choice, however, is more problematic to use than the completed prior, because  $\overrightarrow{p_{ij}}$  and  $\overleftarrow{p_{ij}}$  are specified independently of each other (they are associated with different  $X_i \mid \Pi_{X_i}$ ); and because inclusion events are assumed to be independent for different nodes and for different parents of each node, but they are not  $(X_j \in \Pi_{X_i} \text{ implies } X_i \notin \Pi_{X_j})$ .

### 3. MU+BDs: A Posterior Score Arising from Piecewise Uniform Priors

It is clear from the literature review in Section 2 that assuming uniform priors for  $\Theta_{X_i} \mid \Pi_{X_i}$  and  $\mathcal{G}$  can have a negative impact on the quality of the DAGs learned using U+BDeu. Therefore, we propose a new score with an alternative set of assumptions: the *Bayesian Dirichlet sparse* (BDs) marginal likelihood with a marginal uniform (MU) prior.

### 3.1 The Bayesian Dirichlet Sparse (BDs) Marginal Likelihood

Firstly, we consider the marginal likelihood BDeu. Starting from (4) and (5), we can write it as

$$BDeu(\mathcal{G}, \mathcal{D}; \alpha) = \prod_{i=1}^{N} BDeu(X_i | \Pi_{X_i}; \alpha) = \prod_{i=1}^{N} \prod_{j=1}^{q_i} \left[ \frac{\Gamma(r_i \alpha_i^*)}{\Gamma(r_i \alpha_i^* + n_{ij})} \prod_{k=1}^{r_i} \frac{\Gamma(\alpha_i^* + n_{ijk})}{\Gamma(\alpha_i^*)} \right]. \quad (10)$$

If the positivity assumption is violated, the sample size n is small or the data are sparse, there may be configurations of some  $\Pi_{X_i}$  that are not observed in  $\mathcal{D}$ . In such cases,  $n_{ij} = 0$  and

$$\mathrm{BDeu}(X_i \mid \Pi_{X_i}; \alpha) = \prod_{j: n_{ij} = 0} \left[ \frac{\Gamma(r_i \alpha_i^*)}{\Gamma(r_i \alpha_i^*)} \prod_{k=1}^{r_i} \frac{\Gamma(\alpha_i^*)}{\Gamma(\alpha_i^*)} \right] \prod_{j: n_{ij} > 0} \left[ \frac{\Gamma(r_i \alpha_i^*)}{\Gamma(r_i \alpha_i^* + n_{ij})} \prod_{k=1}^{r_i} \frac{\Gamma(\alpha_i^* + n_{ijk})}{\Gamma(\alpha_i^*)} \right].$$

This implies that the effective imaginary sample size decreases as the number of unobserved parents configurations increases, since  $\sum_{j:n_{ij}>0}\sum_k \alpha_i^* \leqslant \sum_{j,k} \alpha_i^* = \alpha$ . As a result, the posterior estimates of  $\pi_{ij|k}$  gradually converge to the corresponding maximum likelihood estimates thus favouring overfitting and the inclusion of spurious arcs in  $\mathcal{G}$ . (The DAG that maximises the likelihood for any given data set is that that corresponds to the saturated model.)

Furthermore, the comparison between DAGs with different numbers of arcs may be inconsistent because of the different effective imaginary sample sizes used in the respective priors. This phenomenon is best illustrated by comparing the empirical estimator for Shannon entropy (Cover and Thomas, 2006) of  $X_i | \Pi_{X_i}$ , which uses  $p_{ij}|_k = n_{ijk}/n_{ij}$ , with that using the posterior estimates in (5). Consider, for instance, two DAGs  $\mathcal{G}^-$  and  $\mathcal{G}^+ = \mathcal{G}^- \cup X_l$  as in (7). According to the maximum entropy principle, we should prefer  $\mathcal{G}^+$  to  $\mathcal{G}^-$  if

$$H(X_i | \Pi_{X_i} \cup X_l) > H(X_i | \Pi_{X_i}), \qquad H(X_i | \Pi_{X_i}) = -\sum_{j=1}^{q_i} \sum_{k=1}^{r_i} p_{ij | k} \log p_{ij | k}$$

since in that case  $\mathcal{G}^+$  captures more information that  $\mathcal{G}^-$ . For sparse data, in practice we have

$$H(X_i | \Pi_{X_i}) = -\sum_{j: n_{ij} > 0} \sum_{k=1}^{r_i} p_{ij | k} \log p_{ij | k}$$

since the terms corresponding to unobserved parent configurations are assumed to be  $0 \log 0 = 0$  for continuity. If we replace the maximum likelihood estimates  $p_{ij \mid k}$  with the corresponding posterior estimates, which are what BDeu uses to evaluate candidate DAGs, we obtain the following.

**Theorem 1** In a Bayesian setting, the conditional entropy  $H(\cdot)$  of  $X_i \mid \Pi_{X_i}$  given a uniform Dirichlet prior with imaginary sample size  $\alpha$  over the cell probabilities is

$$H(X_i | \Pi_{X_i}; \alpha) = -\sum_{j: n_{ij} > 0} \sum_{k=1}^{r_i} p_{ij|k}^{(\alpha_i^*)} \log p_{ij|k}^{(\alpha_i^*)} \qquad with \qquad p_{ij|k}^{(\alpha_i^*)} = \frac{\alpha_i^* + n_{ijk}}{r_i \alpha_i^* + n_{ij}}.$$

 $and \ \mathrm{H}(X_i \,|\, \Pi_{X_i}; \alpha) < \mathrm{H}(X_i \,|\, \Pi_{X_i}; \beta) \ if \ \alpha < \beta \ and \ X_i \,|\, \Pi_{X_i} \ is \ not \ a \ uniform \ distribution.$ 

Therefore, in the posterior we prefer  $\mathcal{G}^+$  to  $\mathcal{G}^-$  if

$$H(X_i \mid \Pi_{X_i} \cup X_l; \alpha) > H(X_i \mid \Pi_{X_i}; \alpha).$$

Consider, for instance, a non-sparse model  $\mathcal{G}^-$  (all  $q_i'$  configurations of  $\Pi_{X_i}$  are observed) and a sparse model  $\mathcal{G}^+$  ( $\tilde{q}_i < q_i$  configurations of  $\Pi_{X_i} \cup X_l$  are observed). For continuity, if  $\alpha$  is small and  $\alpha_i^* \to 0$  we would expect that

$$\mathrm{H}(X_i \mid \Pi_{X_i} \cup X_l; \alpha) \approx \mathrm{H}(X_i \mid \Pi_{X_i} \cup X_l)$$
 and  $\mathrm{H}(X_i \mid \Pi_{X_i}; \alpha) \approx \mathrm{H}(X_i \mid \Pi_{X_i}),$ 

and that we would be consistent in our choice between  $\mathcal{G}^+$  and  $\mathcal{G}^-$ . Instead we prefer  $\mathcal{G}^+$  over  $\mathcal{G}^-$  if

$$H(X_i \mid \Pi_{X_i} \cup X_l; \alpha \tilde{q}_i/q_i) > H(X_i \mid \Pi_{X_i}; \alpha),$$

where  $H(X_i | \Pi_{X_i} \cup X_l; \alpha \tilde{q}_i/q_i) < H(X_i | \Pi_{X_i} \cup X_l; \alpha)$  since  $\tilde{q}_i < q_i$ . This argument complements that in Suzuki (2016) in the context of finite sample sizes and elucidates the underlying reason for the problematic behaviour of BDeu shown in that paper, which is made clear in the following theorem.

**Theorem 2** Let  $\beta_i^* = \beta/(r_i q_i) \to 0$  and let  $0 < \alpha < \beta$ . Then

$$\mathrm{BDeu}(X_i \mid \Pi_{X_i}; \alpha) < \mathrm{BDeu}(X_i \mid \Pi_{X_i}; \beta) \qquad if \ d_{\mathrm{EP}}^{(X_i, \mathcal{G})} > 0,$$

$$\mathrm{BDeu}(X_i \mid \Pi_{X_i}; \alpha) = \left(\frac{1}{r_i}\right)^{\tilde{q}_i} \qquad if \ d_{\mathrm{EP}}^{(X_i, \mathcal{G})} = 0.$$

Therefore, if  $d_{\rm EP}^{(X_i,\mathcal{G}^+)}>0$  and  $d_{\rm EP}^{(X_i,\mathcal{G}^-)}>0$  model selection is inconsistent because

$$\alpha \frac{\tilde{q}_i}{q_i} < \alpha \Rightarrow \begin{cases} H(X_i \mid \Pi_{X_i} \cup X_l; \alpha \tilde{q}_i/q_i) < H(X_i \mid \Pi_{X_i} \cup X_l; \alpha) \\ BDeu(X_i \mid \Pi_{X_i} \cup X_l; \alpha \tilde{q}_i/q_i) < BDeu(X_i \mid \Pi_{X_i} \cup X_l; \alpha) \end{cases}$$

for most finite sample sizes, since we may have a non-zero probability of comparing a pair of DAGs  $\mathcal{G}^+$  and  $\mathcal{G}^-$  for which at least one  $X_i$  has  $\tilde{q}_i < q_i$ . High-dimensional and sparse data sets are especially likely to produce such inconsistencies because we will evaluate more candidate DAGs in the course of structure learning and because zero-cell-counts will be more common.

We illustrate this phenomenon in the example below for non-singular local distributions  $(d_{\text{EP}}^{(X,\mathcal{G}^+)} > 0, d_{\text{EP}}^{(X,\mathcal{G}^-)} > 0)$  below.

**Example 1** Consider a simple example, inspired by that in Suzuki (2016), based on the data set  $\mathcal{D}_1$  and the DAGs  $\mathcal{G}^-$ ,  $\mathcal{G}^+$  shown in Figure 3.1. The conditional distributions for  $X \mid \Pi_X$  in  $\mathcal{G}^-$  and for  $X \mid \Pi_X \cup Y$  in  $\mathcal{G}^+$  both have positive empirical entropy. The sample frequencies  $(n_{ijk})$  for  $X \mid \Pi_X$  are:

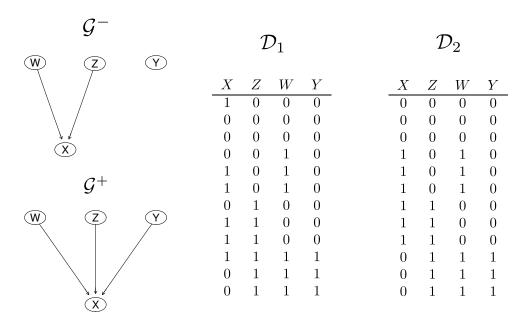


Figure 3.1: DAGs and data sets used in Examples 1 and 2. The DAGs  $\mathcal{G}^+$  and  $\mathcal{G}^-$  are used in both examples. The data set  $\mathcal{D}_1$  refers to Example 1, while  $\mathcal{D}_2$  refers to Example 1; the former is a modified version of the latter, which is originally from Suzuki (2016).

and those for  $X \mid \Pi_X \cup Y$  are as follows.

Therefore, the marginal likelihood for  $X \mid \Pi_X$  is estimated from a contingency table in which all parents configurations are observed in the data. On the other hand, we only observe 4 out of 8 parents configurations in the contingency table for  $X \mid \Pi_X \cup Y$ .

Even though  $X \mid \Pi_X$  and  $X \mid \Pi_X \cup Y$  have the same empirical entropy,

$$H(X | \Pi_X) = H(X | \Pi_X \cup Y) = 4 \left[ -\frac{1}{3} \log \frac{1}{3} - \frac{2}{3} \log \frac{2}{3} \right] = 2.546;$$

if  $\alpha=1$ ,  $\alpha_i^*=1/8$  for  $\mathcal{G}^-$  and  $\alpha_i^*=1/16$  for  $\mathcal{G}^+$ , so the posterior entropies are different:

$$\begin{split} \mathrm{H}(X\,|\,\Pi_X;1) &= 4\left[-\frac{1+1/8}{3+1/4}\log\frac{1+1/8}{3+1/4} - \frac{2+1/8}{3+1/4}\log\frac{2+1/8}{3+1/4}\right] = 2.580,\\ \mathrm{H}(X\,|\,\Pi_X\cup Y;1) &= 4\left[-\frac{1+1/16}{3+1/8}\log\frac{1+1/16}{3+1/8} - \frac{2+1/16}{3+1/8}\log\frac{2+1/16}{3+1/8}\right] = 2.564. \end{split}$$

Therefore,  $\mathcal{G}^-$  would be preferred over  $\mathcal{G}^+$ , and that is the decision that is reached using BDeu:

$$BDeu(X \mid \Pi_X; 1) = \left(\frac{\Gamma(1/4)}{\Gamma(1/4+3)} \left[ \frac{\Gamma(1/8+2)}{\Gamma(1/8)} \cdot \frac{\Gamma(1/8+1)}{\Gamma(1/8)} \right] \right)^4 = 3.906 \times 10^{-7},$$

$$BDeu(X \mid \Pi_X \cup Y; 1) = \left( \frac{\Gamma(1/8)}{\Gamma(1/8+3)} \left[ \frac{\Gamma(1/16+2)}{\Gamma(1/16)} \cdot \frac{\Gamma(1/16+1)}{\Gamma(1/16)} \right] \right)^4 = 3.721 \times 10^{-8}.$$

Like the posterior entropy, we note that BDeu takes different values for two local distributions,  $X \mid \Pi_X$  and  $X \mid \Pi_X \cup Y$ , that encode exactly the same information.

Structure learning is inconsistent also if at least one of the DAGs implies a singular and sparse local distribution (say,  $d_{\text{EP}}^{(X,\mathcal{G}^+)} = 0$  below) since in that case BDeu converges to a constant that does not depend on the data as  $\alpha_i^* \to 0$ , unlike the posterior conditional entropy.

**Example 2** Consider the second data set  $\mathcal{D}_2$  in Figure 3.1, originally from Suzuki (2016), and the same DAGs  $\mathcal{G}^-$  and  $\mathcal{G}^+$ . The sample frequencies for  $X \mid \Pi_X$  are:

and those for  $X \mid \Pi_X \cup Y$  are as follows.

The empirical entropy of X given its parents is equal to zero for both  $\mathcal{G}^+$  and  $\mathcal{G}^-$ , since the value of X is completely determined by the configurations of its parents in both DAGs. Again, the posterior entropies for  $\mathcal{G}^+$  and  $\mathcal{G}^-$  differ:

$$\begin{split} \mathrm{H}(X\,|\,\Pi_X;1) &= 4\left[-\frac{0+1/8}{3+1/4}\log\frac{0+1/8}{3+1/4} - \frac{3+1/8}{3+1/4}\log\frac{3+1/8}{3+1/4}\right] = 0.652,\\ \mathrm{H}(X\,|\,\Pi_X\cup Y;1) &= 4\left[-\frac{0+1/16}{3+1/8}\log\frac{0+1/16}{3+1/8} - \frac{3+1/16}{3+1/8}\log\frac{3+1/16}{3+1/8}\right] = 0.392. \end{split}$$

However, BDeu with  $\alpha = 1$  yields

$$\mathrm{BDeu}(X \mid \Pi_X; 1) = \left(\frac{\Gamma(1/4)}{\Gamma(1/4+3)} \left[ \frac{\Gamma(1/8+3)}{\Gamma(1/8)} \cdot \frac{\Gamma(1/8)}{\Gamma(1/8)} \right] \right)^4 = 0.0326,$$

$$\mathrm{BDeu}(X \mid \Pi_X \cup Y; 1) = \left(\frac{\Gamma(1/8)}{\Gamma(1/8+3)} \left[ \frac{\Gamma(1/16+3)}{\Gamma(1/16)} \cdot \frac{\Gamma(1/16)}{\Gamma(1/16)} \right] \right)^4 = 0.0441,$$

preferring  $\mathcal{G}^+$  over  $\mathcal{G}^-$  even though the additional arc  $Y \to X$  does not provide any additional information on the distribution of X, and even though 4 out of 8 conditional distributions in  $X \mid \Pi_X \cup Y$  are not observed at all in the data. In fact, both the empirical and the posterior entropies would lead to selecting  $\mathcal{G}^-$  over  $\mathcal{G}^+$  in this example.

To address these undesirable features of BDeu we propose to replace  $\alpha_i^*$  in (10) with

$$\tilde{\alpha}_i = \begin{cases} \alpha/(r_i \tilde{q}_i) & \text{if } n_{ij} > 0\\ 0 & \text{otherwise.} \end{cases} \quad \text{where} \quad \tilde{q}_i = \{ \text{number of } \Pi_{X_i} \text{ such that } n_{ij} > 0 \}. \tag{11}$$

Note that (11) is still piece-wise uniform, but now  $\sum_{j:n_{ij}>0}\sum_k \tilde{\alpha}_i = \alpha$  so the effective imaginary sample size is equal to  $\alpha$  even for sparse data. Intuitively, we are defining a uniform prior just on the conditional distributions we can estimate from  $\mathcal{D}$ , thus moving from a fully Bayesian to an empirical Bayes score. Plugging (11) in (4) we obtain BDs:

$$BDs(X_i | \Pi_{X_i}; \alpha) = \prod_{j: n_{ij} > 0} \left[ \frac{\Gamma(r_i \tilde{\alpha}_i)}{\Gamma(r_i \tilde{\alpha}_i + n_{ij})} \prod_{k=1}^{r_i} \frac{\Gamma(\tilde{\alpha}_i + n_{ijk})}{\Gamma(\tilde{\alpha}_i)} \right], \tag{12}$$

and we can write

$$BDs(X_i | \Pi_{X_i}; \alpha) = BDeu(X_i | \Pi_{X_i}; \alpha q_i / \tilde{q}_i).$$
(13)

The relationship between BDeu and BDs for small and large imaginary sample sizes and for large sample sizes is as follows.

**Theorem 3** If  $\alpha_i^* \to 0$ , then

$$BDs(X_i | \Pi_{X_i}; \alpha) = BDeu(X_i | \Pi_{X_i}; \alpha) \cdot \left(\frac{q_i}{\tilde{q}_i}\right)^{d_{EP}^{(X_i, \mathcal{G})}}.$$

**Theorem 4** BDs is equivalent to BDeu if at least one the following conditions holds:

- 1.  $n \to \infty$  and the positivity assumption holds;
- 2.  $\alpha \to \infty$ .

We can interpret  $q_i/\tilde{q}_i$  as an adaptive regularisation hyperparameter that corrects for  $X_i | \Pi_{X_i}$  that are not fully observed in  $\mathcal{D}$ , which typically correspond to  $X_i$  with a large number of incoming arcs; or equivalently as a finite sample correction for BDeu. We can also link BDs to posterior entropy by defining

$$\widetilde{\mathrm{H}}(X_i \mid \Pi_{X_i}; \alpha) = -\sum_{i: n_{i,i} > 0} \sum_{k=1}^{r_i} p_{ij \mid k}^{(\tilde{\alpha}_i)} \log p_{ij \mid k}^{(\tilde{\alpha}_i)} \qquad \text{with} \qquad p_{ij \mid k}^{(\tilde{\alpha}_i)} = \frac{\tilde{\alpha}_i + n_{ijk}}{r_i \tilde{\alpha}_i + n_{ij}}.$$

as we did for BDeu in Theorem (1). Since now the imaginary sample size is equal to  $\alpha$  even when some  $n_{ij} = 0$ , model selection is again consistent as we can see by revisiting Examples 1 and 2.

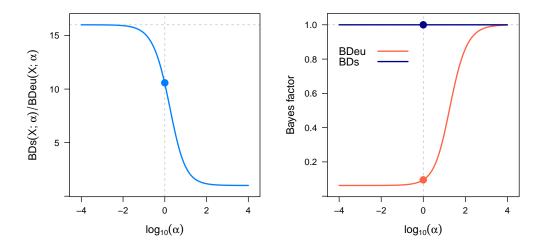


Figure 3.2: The ratio between  $BDs(X | \Pi_X \cup Y; \alpha)$  and  $BDeu(X | \Pi_X \cup Y; \alpha)$  (left panel) from Example 1; and the Bayes factors for  $\mathcal{G}^+$  versus  $\mathcal{G}^-$  computed using BDeu and BDs (right panel; in orange and dark blue, respectively). The bullet points correspond to the values observed for  $\alpha = 1$ .

**Example 1 (Continued)** Consider again the data set  $\mathcal{D}_1$ . BDs does not suffer from the bias arising from  $\tilde{q}_i < q_i$  and it correctly assigns the same score to both networks

$$BDs(X | \Pi_X; 1) = BDs(X | \Pi_X \cup Y; 1) = 3.906 \times 10^{-7}$$

following the maximum entropy principle, and

$$\tilde{H}(X \mid \Pi_X; 1) = \tilde{H}(X \mid \Pi_X \cup Y; 1) = 2.580.$$

We can also verify that the limit results in Theorems 3 and 4 hold for  $\mathcal{G}^+$  (BDeu and BDs are identical for  $\mathcal{G}^-$ ), as shown in the left panel Figure 3.2:

$$\lim_{\alpha_i^* \to 0} \frac{\operatorname{BDs}(X \,|\, \Pi_X \cup Y; \alpha)}{\operatorname{BDeu}(X \,|\, \Pi_X \cup Y; \alpha)} = \left(\frac{8}{4}\right)^{d_{\operatorname{EP}}^{(X, \mathcal{G}^+)}} = 16, \quad \lim_{\alpha_i^* \to \infty} \frac{\operatorname{BDs}(X \,|\, \Pi_X \cup Y; \alpha)}{\operatorname{BDeu}(X \,|\, \Pi_X \cup Y; \alpha)} = 1,$$

where  $d_{\text{EP}}^{(X,\mathcal{G}^+)} = 8 - 4 = 4$ . Furthermore,

$$H(X \mid \Pi_X) < H(X \mid \Pi_X; \alpha)$$
 and  $H(X \mid \Pi_X \cup Y) < H(X \mid \Pi_X \cup Y; \alpha)$ 

as proved in Theorem 1, and

$$BDs(X \mid \Pi_X \cup Y; \alpha) = BDeu(X \mid \Pi_X \cup Y; 2\alpha) > BDeu(X \mid \Pi_X \cup Y; \alpha)$$

following Theorem 2.

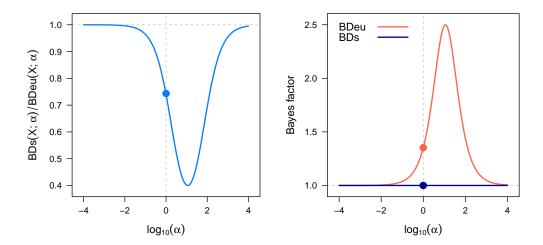


Figure 3.3: The ratio between  $BDs(X | \Pi_X \cup Y; \alpha)$  and  $BDeu(X | \Pi_X \cup Y; \alpha)$  (left panel) from Example 2; and the Bayes factors for  $\mathcal{G}^+$  versus  $\mathcal{G}^-$  computed using BDeu and BDs (right panel; in orange and dark blue, respectively). The bullet points correspond to the values observed for  $\alpha = 1$ .

Example 2 (Continued) Consider again the data set  $\mathcal{D}_2$ . BDs yields

$$BDs(X | \Pi_X; 1) = BDs(X | \Pi_X \cup Y; 1) = 0.0326,$$

which leads to  $\mathcal{G}^+$  being discarded in favour of  $\mathcal{G}^-$  since its score is not strictly greater. Similarly,

$$\tilde{H}(X \mid \Pi_X; 1) = \tilde{H}(X \mid \Pi_X \cup Y; 1) = 0.652.$$

We can also verify that the limit results in Theorems 3 and 4 hold for  $\mathcal{G}^+$  (BDeu and BDs are identical for  $\mathcal{G}^-$ ):

$$\lim_{\alpha_i^* \to 0} \frac{\operatorname{BDs}(X \,|\, \Pi_X \cup Y; \alpha)}{\operatorname{BDeu}(X \,|\, \Pi_X \cup Y; \alpha)} = \left(\frac{4}{4}\right)^{d_{\operatorname{EP}}^{(X, \mathcal{G}^+)}} = 1 \qquad \lim_{\alpha_i^* \to \infty} \frac{\operatorname{BDs}(X \,|\, \Pi_X \cup Y; \alpha)}{\operatorname{BDeu}(X \,|\, \Pi_X \cup Y; \alpha)} = 1,$$

where  $d_{EP}^{(X,\mathcal{G}^+)} = 4 - 4 = 0$ . This is illustrated in the left panel of Figure 3.3.

If the positivity assumption holds, we will eventually observe all parents configurations in the data and thus  $\mathrm{BDs}(X_i \mid \Pi_{X_i}; \alpha) \to \mathrm{BDeu}(X_i \mid \Pi_{X_i}; \alpha)$  as  $n \to \infty$ . Note, however, that BDs is not score equivalent for finite n unless all  $n_{ij} > 0$ . A numeric example is given below.

**Example 3** Consider two binary variables X and Y with data  $\mathcal{D}_3$  as follows:

$$\begin{array}{c|cccc} & & Y \\ & & 0 & 1 \\ \hline X & 0 & 0 & 2 \\ & 1 & 0 & 5 \end{array}$$

If 
$$\alpha = 1$$
,  $\mathcal{G}_1 = \{Y \to X\}$  and  $\mathcal{G}_2 = \{X \to Y\}$ , then

$$BDs(\mathcal{G}_{1}, \mathcal{D}_{3}; 1) = \left[\frac{\Gamma(1)}{\Gamma(1+7)} \frac{\Gamma(1/2+\theta)}{\Gamma(1/2)} \frac{\Gamma(1/2+7)}{\Gamma(1/2)}\right] \left[\frac{\Gamma(1)}{\Gamma(1+7)} \frac{\Gamma(1/2+2)}{\Gamma(1/2)} \frac{\Gamma(1/2+5)}{\Gamma(1/2)}\right] = 0.0009,$$

$$\begin{split} \mathrm{BDs}(\mathcal{G}_2,\mathcal{D}_3;1) &= \left[ \frac{\Gamma(1)}{\Gamma(1+7)} \frac{\Gamma(1/2+2)}{\Gamma(1/2)} \frac{\Gamma(1/2+5)}{\Gamma(1/2)} \right] \cdot \\ &\cdot \left[ \frac{\Gamma(1/2)}{\Gamma(1/2+2)} \frac{\Gamma(1/2)}{\Gamma(1/2+5)} \frac{\Gamma(1/4+0)}{\Gamma(1/4)} \frac{\Gamma(1/4+2)}{\Gamma(1/4)} \frac{\Gamma(1/4+5)}{\Gamma(1/4)} \right] = 0.0006; \end{split}$$

as a term of comparison the empty DAG  $\mathcal{G}_0$  has BDs( $\mathcal{G}_0, \mathcal{D}_3$ ) = 0.0009.

In the general case, BDs breaks the score equivalence condition in Heckerman et al. (1995) because it potentially associates a different imaginary sample size to each node as shown in (13).

Since Steck and Jaakkola (2003) showed that BDeu favours the inclusion of spurious arcs for sparse  $X_i \mid \Pi_{X_i}$ , BDs should lead to sparser DAGs and reduce overfitting; we have seen some evidence of that in Example 2. The difference in their model selection choices can be characterised by the Bayes factor computed using BDs with that computed using BDeu. If we apply Theorem 3 to (7) we obtain:

$$\underbrace{\frac{\operatorname{BDs}(X_i \mid \Pi_{X_i} \cup X_l; \alpha)}{\operatorname{BDs}(X_i \mid \Pi_{X_i}; \alpha)}}_{\operatorname{Bayes factor from BDs}} = \underbrace{\frac{(q_i/\tilde{q}_i)^{d_{\operatorname{EP}}^{(X_i, \mathcal{G}^+)}}}{(q_i'/\tilde{q}_i')^{d_{\operatorname{EP}}^{(X_i, \mathcal{G}^-)}}}_{\operatorname{implicit prior}} \cdot \underbrace{\frac{\operatorname{BDeu}(X_i \mid \Pi_{X_i} \cup X_l; \alpha)}{\operatorname{BDeu}(X_i \mid \Pi_{X_i}; \alpha)}}_{\operatorname{Bayes factor from BDeu}}.$$
(14)

The first term on the right-hand side can be interpreted as a ratio of empirical prior probabilities implied by BDs, which are a function of the sparsity of  $\mathcal{G}^+$  and  $\mathcal{G}^-$  in the parameter space. If all parents configurations are observed in both models  $(q_i = \tilde{q}_i \text{ and } q'_i = \tilde{q}'_i)$ , then the prior ratio term vanishes for small  $\alpha$ . If at least one of  $\mathcal{G}^+$  and  $\mathcal{G}^-$  contains unobserved configurations of  $\Pi_{X_i}$ , then BDs leads to different choices than BDeu as shown below.

**Theorem 5** Let  $\mathcal{G}^+$  and  $\mathcal{G}^-$  be two DAGs differing from a single arc  $X_l \to X_i$ , and let  $\alpha_i^* \to 0$ . Then the Bayes factor computed using BDs corresponds to the Bayes factor computed using BDeu weighted by the following implicit prior ratio:

$$\frac{\mathrm{P}(\mathcal{G}^+)}{\mathrm{P}(\mathcal{G}^-)} = \frac{(q_i/\tilde{q}_i)^{d_{\mathrm{EP}}^{(X_i,\mathcal{G}^+)}}}{(q_i'/\tilde{q}_i')^{d_{\mathrm{EP}}^{(X_i,\mathcal{G}^-)}}}.$$

and from (6) and (7) can be written as

$$\frac{\operatorname{BDs}(X_i \mid \Pi_{X_i} \cup X_l; \alpha)}{\operatorname{BDs}(X_i \mid \Pi_{X_i}; \alpha)} = \frac{(q_i / \tilde{q}_i)^{d_{\operatorname{EP}}^{(X_i, \mathcal{G}^+)}} \alpha^{d_{\operatorname{EP}}^{(\mathcal{G}^+)}}}{(q_i' / \tilde{q}_i')^{d_{\operatorname{EP}}^{(X_i, \mathcal{G}^-)}} \alpha^{d_{\operatorname{EP}}^{(\mathcal{G}^-)}}} \\
\rightarrow \begin{cases} 0 & \text{if } d_{\operatorname{EDF}} > -\log_{\alpha}(\operatorname{P}(\mathcal{G}^+) / \operatorname{P}(\mathcal{G}^-)) \\ +\infty & \text{if } d_{\operatorname{EDF}} < -\log_{\alpha}(\operatorname{P}(\mathcal{G}^+) / \operatorname{P}(\mathcal{G}^-)) \end{cases}.$$

As we can see in the right panels of Figures 3.2 and 3.3, the Bayes factor constructed from BDeu can assume very different values for the  $\mathcal{G}^+$  and  $\mathcal{G}^-$  in Examples 1 and 2 depending on the value of  $\alpha$ , which is not the case for the Bayes factor constructed from BDs. Considering that in a Bayesian setting we rely on the ordering Bayes factors to choose the best candidate DAG in each step of structure learning, and that Bayes factors constructed from BDeu will vary in different ways for different pairs of DAGs even for the same  $\alpha$ , this is highly problematic for BDeu and a strong point in favour of BDs.

# 3.2 The Marginal Uniform (MU) Graph Prior

We now propose a modified prior over for  $\mathcal{G}$  with the same aims. We again start from the consideration that score-based structure learning algorithms typically generate new candidate DAGs by a single arc addition, deletion or reversal. So, for example

$$P(\mathcal{G}^+ | \mathcal{D}) > P(\mathcal{G}^- | \mathcal{D}) \Rightarrow \text{accept } \mathcal{G}^+ \text{ and discard } \mathcal{G}^-.$$
 (15)

When using the U prior we can rewrite the left-hand of (15) as

$$\frac{P(\mathcal{G}^{+} \mid \mathcal{D})}{P(\mathcal{G}^{-} \mid \mathcal{D})} = \frac{P(\mathcal{G}^{+})}{P(\mathcal{G}^{-})} \frac{P(\mathcal{D} \mid \mathcal{G}^{+})}{P(\mathcal{D} \mid \mathcal{G}^{-})} > 1.$$
(16)

The fact that U always simplifies is equivalent to assigning equal probabilities to all possible states of an arc (subject to the acyclicity constraint), say  $\overrightarrow{p_{ij}} = \overleftarrow{p_{ij}} = p_{ij}^* = 1/3$  using the notation in (8). The probabilities in (16) are different from the marginal probabilities in (9) because they represent the conditional inclusion probabilities for an arc  $X_l \to X_i$  given the rest of  $\mathcal{G}^+$ , which is kept fixed as the "baseline"  $\mathcal{G}^-$  DAG. As a result, U favours the inclusion of new arcs as  $\overrightarrow{p_{ij}} + \overleftarrow{p_{ij}} = 2/3$ . (The same is true for the completed prior from Castelo and Siebes (2000), at least for the pairs of nodes for which we do not elicitate prior probabilities.) Since in Scutari (2013) we also showed that arcs incident on a common node are correlated and may favour each other's inclusion, U may then contribute to overfitting.

Therefore, we introduce the  $marginal\ uniform\ (MU)\ prior$ , in which we assume an independent prior for each arc as in Castelo and Siebes (2000), with probabilities

$$\overrightarrow{p_{ij}} = \overleftarrow{p_{ij}} = \frac{\beta}{2}$$
 and  $\overrightarrow{p_{ij}} = 1 - \beta$ ,  $\beta \in (0, 1)$ 

for all arcs. For  $\beta = 1/2$  we obtain

$$\overrightarrow{p_{ij}} = \overleftarrow{p_{ij}} = \frac{1}{4}$$
 and  $\overrightarrow{p_{ij}} = \frac{1}{2}$  for all  $i \neq j$ 

as in Scutari (2013), which is essentially the median-probability prior described in Barbieri and Berger (2004). These assumptions make MU computationally trivial to use: the ratio of the prior probabilities is  $^{1}/_{2}$  for arc addition, 2 for arc deletion and 1 for arc reversal, for all arcs. Furthermore, arc inclusion now has the same prior probability as arc exclusion  $(\overrightarrow{p_{ij}} + \overleftarrow{p_{ij}} = p_{ij}^{\circ} = ^{1}/_{2})$  and arcs incident on a common node are no longer correlated, thus limiting overfitting and preventing the inclusion of spurious arcs to propagate. However, the marginal distribution for each arc is the same as in (9) for large N, hence the name "marginal uniform".

While the median-probability prior has been shown to result in better predictive power than the uniform prior (Barbieri and Berger, 2004; Scott and Berger, 2010), we note that its expected number of arcs is

$$E(|A|) = \frac{N(N-1)}{2}\beta = O(N^2\beta)$$

which at least in principle would encourage the selection of dense DAGs, leaving it to the marginal likelihood to penalise overly complex BNs. Therefore, we may want to consider

$$\beta = cN \cdot \frac{2}{N(N-1)} = \frac{2c}{N-1}$$
 (17)

for some small positive constant c, so that  $\mathrm{E}(|A|) = O(N)$ . That constant should be greater or equal to 1, since we need more arcs than nodes to have a fully connected DAG; c=1 implies that expected DAG in the prior is a tree. In practice, we may want to consider only values smaller than 5 as in our experience real-world BNs typically have fewer than 5N arcs.

#### 4. Simulation Study

We assessed BDs and MU on a set of 10 reference BNs (Table 4.1) covering a wide range of N (20 to 442),  $p = |\Theta|$  (230 to 77K) and number of arcs |A| (25 to 602). For each BN:

1. We generated 20 training samples of size n/p = 0.1, 0.2, 0.5, 1.0, 2.0, and 5.0 (to allow for meaningful comparisons between BNs with such different N and p).

network	N	A	p
ALARM	37	46	509
ANDES	223	338	1157
CHILD	20	25	230
DIABETES	413	602	429409
HAILFINDER	56	66	2656

network	N	A	p
HEPAR 2	70	123	1453
INSURANCE	27	52	984
PATHFINDER	135	200	77155
PIGS	442	592	5618
WATER	32	66	10083

Table 4.1: Reference BNs from the BN repository (Scutari, 2012) with the respective numbers of nodes (N), numbers of arcs (|A|) and numbers of parameters  $(p = |\Theta|)$ .

- 2. We learned  $\mathcal{G}$  using U+BDeu, U+BDs, MU+BDeu and MU+BDs with  $\alpha=1,5,10$  and  $\beta=1/2$ ,  $\beta=2c/(N-1)$  for c=1,2,5 on each sample. For U + BDeu we also considered the optimal  $\alpha$  from Steck (2008), denoted  $\alpha_S$ . In addition, we considered BIC as a term of comparison, since BIC  $\rightarrow$  log BDeu as  $n\rightarrow\infty$ .
- 3. We measured the performance of different scoring strategies in terms of:
  - the quality of the learned DAG using the SHD distance (Tsamardinos et al., 2006) from the  $\mathcal{G}_{REF}$  of the reference BN;
  - the number of arcs compared to  $|A_{REF}|$  in  $\mathcal{G}_{REF}$ ;
  - predictive accuracy, computing the log-likelihood on a test set of size 10k as an approximation of the corresponding Kullback-Leibler distance.

The significance of the difference between different scoring strategies for these quantities was assessed using paired t-tests (Wasserman, 2007) with a p-value threshold of 0.01, accompanied by the number of combinations of BNs and n/p (out of 60) in which the scoring strategy of interest is better.

For parameter learning, we used Dirichlet posterior estimates and  $\alpha=1$  as suggested in Koller and Friedman (2009). All simulations were performed using the hill-climbing implementation in the *bnlearn* R package (Scutari, 2010), which provides several options for structure learning, parameter learning and inference on BNs (including the proposed MU and BDs). Since  $\alpha=5$  produced performance measures that are always in between those for  $\alpha=1$  and  $\alpha=10$ , we omit its discussion for brevity.

### 4.1 Comparing U+BDeu with MU+BDs

Firstly, we compare U+BDeu, U+BDs, MU+BDeu and MU+BDs for  $\beta=1/2$ , that is, taking the median-probability prior for MU. SHD distances are reported in Table B.1, from which we observe the following.

- MU+BDs outperforms U+BDeu in terms of SHD (p-value:  $1.8 \times 10^{-4}$  for  $\alpha = 1$ ,  $4.5 \times 10^{-9}$  for  $\alpha = 10$ ; 59/60 and 58/60 simulations respectively), and it is the best score overall in 40/60 simulations.
- BIC also outperforms U+BDeu for  $\alpha = 10$  (p-value:  $2 \times 10^{-4}$ ; 54/60); but it does not significantly outperform U+BDeu for  $\alpha = 1$  (p-value: 0.11; 40/60). Furthermore, BIC does not outperform MU+BDs for either  $\alpha = 1$  (p-value: 0.97; 17/60) or  $\alpha = 10$  (p-value: 0.11, 34/60). BIC is the best score overall in only 13/60 simulations.
- The improvement in SHD given by using BDs instead of BDeu and by using MU instead of U appears to be somewhat non-additive; MU+BDs in most cases has the same or nearly the same SHD as the best between U+BDs and MU+BDeu. MU+BDs does not significantly outperform either MU+BDeu for for  $\alpha = 1$  (p-value: 0.043; 4/60) or U+BDs (p-value: 0.058 for  $\alpha = 1$ , 0.029 for  $\alpha = 10$ ; 17/60, 4/60). However, it does significantly outperform MU+BDeu for  $\alpha = 10$  (p-value:  $3.7 \times 10^{-6}$ ; 53/60).

Overall, MU+BDs outperforms the best between MU+BDeu and U+BDs for both  $\alpha = 1$  (p-value: 0.009) and  $\alpha = 10$  (p-value: 8.2 × 10<sup>-5</sup>); so we recommend it over other combinations of graph priors and marginal likelihoods.

Finally, we note that MU+BDeu is tied with MU+BDs for the best SHD more often than U+BDs (25/27 vs 2/13) which suggests improvements in SHD can be attributed more to the use of MU than that of BDs.

- For U+BDeu,  $\alpha = 1$  very often results in a lower SHD than  $\alpha_s$  (p-value:  $7.4 \times 10^{-6}$ ; 53/60) and  $\alpha = 10$  (p-value:  $1 \times 10^{-5}$ ; 60/60), which is in agreement with Ueno (2010).
- For all scoring strategies we observe a strong (≤ −0.85) negative correlation between SHD and log(n/p) for 7 out of 10 BNs, which suggests that the SHD distance from G<sub>REF</sub> decreases linearly as log(n/p) increases. This observation complements the results on the decay of the probability of single-step structural learning error presented in Zuk et al. (2006). Interestingly, correlation is positive for two BNs − DIABETES and PIGS − as we can see that SHD is increasing in log n/p in Table B.1. We have no explanation for this phenomenon, which represents an interesting direction for future research.

The higher SHD for U+BDeu seems to be a consequence of the higher number of arcs present in the learned DAGs, shown in Table B.2.

- MU+BDs learns significantly fewer arcs than U+BDeu for both  $\alpha=1$  (p-value:  $2.4\times 10^{-8};\ 57/60$ ) and  $\alpha=10$  (p-value:  $3.5\times 10^{-13};\ 60/60$ ). MU+BDs learns too many arcs (that is, the ratio with  $|A_{\rm REF}|$  is greater than 1) in 23/60 and 30/60 simulations, as opposed to 32/60 and 56/60 for U+BDeu.
- The same is true for BIC, which learns fewer arcs than U+BDeu (p-value:  $1.4 \times 10^{-10}$  for  $\alpha = 1$ ,  $6.8 \times 10^{-14}$  for  $\alpha = 10$ ; 59/60 and 60/60) and learns too many arcs in only 18/60 simulations. If we compare BIC with an oracle learner which always learns the correct number of arcs, we find that BIC learns networks that are too sparse (p-value:  $3.7 \times 10^{-9}$ ). Only for n/p = 5 the underfitting stops being significant (p-value: 0.09).
- As we argued in Section 3, replacing U with MU results in DAGs with fewer arcs for all 60/60 simulations. Replacing BDeu with BDs results in fewer arcs in 32/60 simulations for  $\alpha = 1$  and in 59/60 for  $\alpha = 10$ , which suggests that the overfitting observed for U+BDeu can be attributed to both U and BDeu.

The rescaled predictive log-likelihoods in Table B.3 show that U+BDeu never outperforms MU+BDs for n/p < 1.0 for the same  $\alpha$ ; for larger n/p all scores are tied, and are not reported for brevity. Even so, the difference between MU+BDs and U+BDeu is too small to be significant (p-value: 0.040 for  $\alpha = 1$ , 0.0027 for  $\alpha = 10$ ). The same is true for BIC (p-value: 0.15; 22/30). U+BDeu for  $\alpha_s$  is at best tied with the corresponding score for  $\alpha = 1$  or  $\alpha = 10$ . The overall best score is MU+BDs for 7/10 BNs and BIC for the remaining 3/10.

### 4.2 Comparing Different Sparsity Levels for MU

We now discuss the effect of the choice of the  $\beta$  parameter of MU on both BDeu and BDs. The results for BDeu are reported in Tables B.4 (SHD), B.6 (number of arcs) and B.8 (predictive log-likelihood). We observe the following:

- MU with  $\beta = 1/2$  does not significantly outperform any of c = 1, 2, 5 in terms of SHD for  $\alpha = 1$  (p-value: 0.99, 0.66, 0.99; 12/60, 34/60, 18/60) or  $\alpha = 10$  (p-value: 0.99, 0.99, 0.99; 7/60, 8/60, 17/60). On the other hand, c = 1 significantly outperforms  $\beta = 1/2$  (p-value:  $2.5 \times 10^{-4}$ ; 53/60). This suggests that enforcing sparsity with c = 1 is beneficial and results in more accurate structure learning than the median-probability prior.
- MU with c=1,5 outperform c=2 in terms of SHD for  $\alpha=1$  (p-value:  $3.6 \times 10^{-8}$ ,  $1.3 \times 10^{-7}$ ; 50/60, 47/60), but for  $\alpha=10, c=1$  outperforms c=2 (p-value:  $5.4 \times 10^{-8}$ ; 51/60) which in turn outperforms c=5 (p-value:  $2.2 \times 10^{-8}$ ; 54/60). This suggests that enforcing increasing levels of sparsity in the prior does not monotonically reduce SHD for  $\alpha=1$ , but it does that for  $\alpha=10$ .
  - It does, however, reduce the number of arcs as expected. For  $\alpha=1,\,c=1$  produces sparser DAGs than c=2 (p-value:  $8.3\times 10^{-8};\,49/60$ ), c=2 produces sparser DAGs than c=5 (p-value:  $3.1\times 10^{-5};\,48/60$ ), and c=5 produces sparser DAGs than  $\beta=1/2$  (p-value:  $8.7\times 10^{-5};\,43/60$ ). The situation is similar for  $\alpha=10$  (p-value:  $3.8\times 10^{-10},\,4.2\times 10^{-7},\,1.4\times 10^{-4};\,52/60,\,54/60,\,45/60$ ).
- There is no correspondence between the number of arcs expected in the prior and the number of arcs present in the learned DAGs, which is roughly the same for all c=1,2,5. Even  $\beta=1/2$  results in only 1.26 as many arcs as c=1. Furthermore, there is no apparent relationship between the value of c that gives the best SHD and  $|A_{\rm REF}|$ : for instance, WATER has  $|A_{\rm REF}|/N=2.06$  but c=1 results in lower SHDs than c=2, while ANDES has  $|A_{\rm REF}|/N=1.51$  but c=5 has the lowest SHD.
- We can still recommend the use  $\alpha=1$  over  $\alpha=10$  for BDeu when using MU since the former produces significantly smaller SHDs than the latter for  $\beta=1/2$  (p-value:  $6.7 \times 10^{-6}$ ; 53/60), c=1 (p-value:  $9.8 \times 10^{-7}$ ; 43/60), c=5 (p-value:  $3.8 \times 10^{-10}$ ; 51/60), but not for c=2 (p-value: 0.89; 0/60) since almost all SHDs are tied in that case.
- Even though SHD improves when moving away from the median-probability prior, additional sparsity does not improve predictive log-likelihood for either  $\alpha=1$  or  $\alpha=10$  (p-values: 0.06, 0.07, 0.09, for c=1,2,5 for both).

The results for BDs are reported in Tables B.5 (SHD), B.7 (number of arcs) and B.9 (predictive log-likelihood), and lead to similar considerations as the above.

• All of c = 1, 2, 5 produce significantly lower SHD values than  $\beta = 1/2$  for  $\alpha = 1$  (p-values:  $2.0 \times 10^{-4}$ ,  $2.3 \times 10^{-4}$ ,  $3.9 \times 10^{-4}$ ; 46/60, 45/60, 40/60) and for  $\alpha = 10$  (p-values:  $1.2 \times 10^{-3}$ ,  $1.6 \times 10^{-3}$ ,  $2.9 \times 10^{-3}$ ; 52/60, 51/60, 45/60). For  $\alpha = 1$ , SHD for c = 1 is not significantly better than for c = 2 (p-value: 0.71; 28/60), but it is for

c=2 compared to c=5 (p-value:  $8.4\times 10^{-4}$ ; 38/60). For  $\alpha=10$ , SHD for c=1 is better than for c=2 (p-value:  $3.1\times 10^{-7}$ ; 49/60) which is better than c=5 (p-value:  $3.6\times 10^{-7}$ ; 50/60). This again suggests enforcing sparsity improves the accuracy of BN structure learning.

- For BDs,  $\alpha=1$  does not significantly outperform  $\alpha=10$  in terms of SHD for  $\beta=1/2$  (p-value: 0.012, 42/60) nor for any of c=1,2,5 (p-values: 0.85, 0.49, 0.049; 30/60, 36/60, 40/60). In all cases we  $\alpha=1$  produces smaller SHDs than  $\alpha=10$  in more than half of the simulations, but the difference is small enough that it does not reach statistical significance.
- As was the case for BDeu, there is no correspondence between the number of arcs expected in the prior and the number of arcs present in the learned DAGs, and there is no apparent relationship between the value of c that gives the best SHD and  $|A_{\rm REF}|$ .
- There is no improvement in the predictive log-likelihood for any of c = 1, 2, 5 over  $\beta = 1/2$  for either  $\alpha = 1$  or  $\alpha = 0.10$  (all *p*-values are greater than 0.99).

#### 5. Conclusions and Discussion

In this paper we proposed a new posterior score for discrete BN structure learning. We defined it as the combination of a new prior over the space of DAGs, the "marginal uniform" (MU) prior, and of a new empirical Bayes marginal likelihood, which we call "Bayesian Dirichlet sparse" (BDs). Both have been designed to address the inconsistent behaviour of the classic uniform (U) prior and of BDeu, without requiring any prior information on the probabilistic structure of the data.

Issues arising from the use of BDeu have been explored by Silander et al. (2007), Steck and Jaakkola (2003), Ueno (2010) and Suzuki (2016) among others. In particular, our aim was to prevent the inclusion of spurious arcs, particularly in the common case of small, sparse data and small imaginary sample sizes. We complemented the results presented in the papers above, and in particular in Suzuki (2016), by investigating how BDeu model selection is inconsistent and can assign different scores to DAGs that encode exactly the same information from the data. From an information theoretic perspective, we find that the reason of this inconsistency is that the prior distribution assumed in BDeu lead to a biased estimation of the entropy of BNs learned from sparse data. From a more probabilistic perspective, we can equivalently say that in such cases part of the prior probability mass is lost for models with unobserved parent configurations for at least one node, and this makes Bayesian model selection inconsistent. These new results motivated the construction of BDs and the assumption of a piecewise uniform prior on the parameter space.

We also used results from our previous work (Scutari, 2013) on the properties of U to motivate the introduction of MU. Firstly, score-based structure learning explored the space of DAGs with single-arc moves, and this leads to a probability of inclusion  $\overrightarrow{p_{ij}} + \overleftarrow{p_{ij}} = 2/3$  for each arc and in turn to dense DAGs. Secondly, arcs incident on a common node are correlated in U, which means that the inclusion of each false positive leads to an increased probability of more false positive, making errors in structure learning cascade and multiply. To address these problems we propose MU and assume independent priors for each arc with

 $\overrightarrow{p_{ij}} + \overleftarrow{p_{ij}} \leqslant 1/2$ . In this context we investigate both the median-probability prior and sparsity inducing priors with O(N) expected arcs.

In an extensive simulation study based on 10 reference BNs we find that MU+BDs (assuming  $\beta=1/2$ ) outperforms U+BDeu for all combinations of BN and sample sizes in the quality of the learned DAGs. Predictive accuracy is not significantly different between the two scores. We confirm that  $\alpha=1$  is a good default as suggested by Ueno (2010), for both BDeu and BDs. As for MU, the median-probability prior with  $\beta=1/2$  is outperformed in terms of SHD by the  $\beta$  corresponding to c=1. Clearly, this result only generalises to data whose underlying DAGs are sparse, as is the case for the reference BNs.

This is achieved without increasing the computational complexity of the posterior score, since MU+BDs can be computed in the same time as U+BDeu. In this respect, the posterior score we propose is preferable to similar proposals in the literature. For instance, the NIP-BIC score from Ueno (2011) and the NIP-BDe/Expected log-BDe scores from Ueno and Uto (2012) outperform BDeu but at a significant computational cost. The same is true for the optimal  $\alpha$  proposed by Steck (2008) for BDeu, whose estimation requires multiple runs of the structure learning algorithm to converge. The Max-BDe and Min-BDe scores in Scanagatta et al. (2014) overcome in part the limitations of BDeu by optimising for either goodness of fit at the expense of predictive accuracy, or vice versa. As a further term of comparison, we also included BIC in the simulation; while it outperforms U+BDeu in some circumstances and it is computationally efficient, MU+BDs is better overall in the DAGs it learns and competitive in predictive accuracy.

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# Appendix A. Proofs

**Proof of Theorem 1.** The posterior probabilities  $p_{ijk}^{(\alpha)}$  can be rewritten as

$$p_{ij\,|\,k}^{(\alpha_i^*)} = \frac{\alpha_i^* + n_{ijk}}{r_i \alpha_i^* + n_{ij}} = \frac{\alpha_i^*}{r_i \alpha_i^* + n_{ij}} \cdot \frac{\alpha_i^*}{r_i \alpha_i^*} + \frac{n_{ij}}{r_i \alpha_i^*} \cdot \frac{n_{ijk}}{n_{ij}} \cdot \frac{1}{n_{ijk}} = \lambda \frac{1}{r_i} + (1 - \lambda_{ij}) p_{ijk}$$

with

$$\lambda_{ij} = \frac{r_i \alpha_i^*}{r_i \alpha_i^* + n_{ij}},$$

which is a weighted average between the uniform prior  $(1/r_i)$  and the observed empirical frequencies  $(p_{ijk})$ . We can decompose the posterior entropy along the same lines, and use the concavity of entropy (Cover and Thomas, 2006):

$$\begin{split} \mathrm{H}(X_{i} \,|\, \Pi_{X_{i}}; \alpha) &= \sum_{j=1}^{q_{i}} \mathrm{H}(X_{i} \,|\, \Pi_{X_{i}} = j; \alpha) = \sum_{j=1}^{q_{i}} \mathrm{H}\left((1 - \lambda_{ij})(X_{i} \,|\, \Pi_{X_{i}} = j) + \lambda_{ij} U\right) \geqslant \\ &\geqslant \sum_{j=1}^{q_{i}} (1 - \lambda_{ij}) \,\mathrm{H}(X_{i} \,|\, \Pi_{X_{i}} = j) + \lambda_{ij} \,\mathrm{H}(U). \end{split}$$

First, we note that this implies  $H(X_i | \Pi_{X_i}; \alpha) \ge H(X_i | \Pi_{X_i})$  for any  $\alpha > 0$ :

$$\begin{split} \sum_{j=1}^{q_{i}} (1 - \lambda_{ij}) \, \mathrm{H}(X_{i} \, | \, \Pi_{X_{i}} = j) + \lambda_{ij} \, \mathrm{H}(U) \geqslant \\ \geqslant \sum_{j=1}^{q_{i}} (1 - \lambda_{ij}) \, \mathrm{H}(X_{i} \, | \, \Pi_{X_{i}} = j) + \lambda_{ij} \, \mathrm{H}(X_{i} \, | \, \Pi_{X_{i}} = j) \\ = \sum_{j=1}^{q_{i}} \mathrm{H}(X_{i} \, | \, \Pi_{X_{i}} = j) = \mathrm{H}(X_{i} \, | \, \Pi_{X_{i}}), \end{split}$$

with the equality holding iff  $H(U) = H(X_i | \Pi_{X_i} = j)$ . Furthermore, we can compose weighted averages and write

$$p_{ijk}^{(\beta)} = \delta_{ij} \frac{1}{r_i} + (1 - \delta_{ij}) p_{ij|k}^{(\alpha)} = \delta_{ij} \lambda_{ij} \frac{1}{r_i} + (1 - \delta_{ij} \lambda_{ij}) p_{ij|k}$$

and since  $\beta > \alpha > 0$  we have

$$\delta_{ij}\lambda_{ij} = \frac{\beta_{ij}}{\beta_{ij} + n_{ij}} > \frac{r_i\alpha_i^*}{r_i\alpha_i^* + n_{ij}} > 0.$$

Proceeding along the same lines as above we obtain

$$H(X_i | \Pi_{X_i}; \beta) \ge \sum_{j=1}^{q_i} (1 - \delta_{ij}) H(X_i | \Pi_{X_i} = j; \alpha) + \delta_{ij} H(U) \ge H(X_i | \Pi_{X_i}; \alpha)$$

with equality iff  $H(U) = H(X_i | \Pi_{X_i} = j; \alpha)$  as required.

**Proof of Theorem 2.** A Laurent series expansion for  $\beta_i^* = \beta/(r_i q_i)$ ,  $\beta_i^* \to 0$  for fixed  $r_i$  gives

$$\frac{\Gamma(r_i \beta_i^*)}{\Gamma(r_i \beta_i^* + n_{ij})} \approx \frac{1}{r_i \beta_i^* \Gamma(n_{ij})} \quad \text{and} \quad \frac{\Gamma(\beta_i^* + n_{ijk})}{\Gamma(\beta_i^*)} \approx \beta_i^* \Gamma(n_{ijk}); \quad (18)$$

Since  $\beta > \alpha \to 0$ ,  $\beta_i^* > \alpha_i^* \to 0$  we have

$$\prod_{j:n_{ij}>0} \left[ \frac{1}{r_{i}\beta_{i}^{*}\Gamma(n_{ij})} \prod_{k:n_{ijk}>0} \beta_{i}^{*}\Gamma(n_{ijk}) \right] > \prod_{j:n_{ij}>0} \left[ \frac{1}{r_{i}\alpha_{i}^{*}\Gamma(n_{ij})} \prod_{k:n_{ijk}>0} \alpha_{i}^{*}\Gamma(n_{ijk}) \right] 
\prod_{j:n_{ij}>0} \left[ \frac{1}{\beta_{i}^{*}} \prod_{k:n_{ijk}>0} \beta_{i}^{*} \right] > \prod_{j:n_{ij}>0} \left[ \frac{1}{\alpha_{i}^{*}} \prod_{k:n_{ijk}>0} \alpha_{i}^{*} \right] 
(\beta_{i}^{*})^{-\tilde{q}_{i}} (\beta_{i}^{*})^{\sum_{k} \tilde{r}_{ij}} > (\alpha_{i}^{*})^{-\tilde{q}_{i}} (\alpha_{i}^{*})^{\sum_{k} \tilde{r}_{ij}} 
(\beta_{i}^{*})^{d_{\mathrm{EP}}^{(X_{i},\mathcal{G})}} > (\alpha_{i}^{*})^{d_{\mathrm{EP}}^{(X_{i},\mathcal{G})}}$$

as required. If  $d_{\text{EP}}^{(X_i,\mathcal{G})} = \sum_k \tilde{r}_{ij} - \tilde{q}_i = 0$ , there is only a single  $n_{ijk} > 0$  for each  $n_{ij} > 0$  so  $n_{ijk} = n_{ij}$ . Then

$$\prod_{j:n_{ij}>0} \left[ \frac{1}{r_i \alpha_i^* \Gamma(n_{ij})} \prod_{k:n_{ijk}>0} \alpha_i^* \Gamma(n_{ijk}) \right] = \prod_{j:n_{ij}>0} \left[ \frac{1}{\underline{r_i \alpha_i^* \Gamma(n_{ij})}} \underbrace{r_i \alpha_i^* \Gamma(n_{ij})}_{r_i} \right] = \left(\frac{1}{r_i}\right)^{\tilde{q}_i}$$

which proves the second case.

using the fact that  $\tilde{\alpha}_i = \alpha_i^*(q_i/\tilde{q}_i)$ .

**Proof of Theorem 3.** Substituting the approximation from (18) in (12) yields

$$BDs(X_{i} | \Pi_{X_{i}}; \alpha) \approx \prod_{j:n_{ij}>0} \left[ \frac{1}{r_{i}\tilde{\alpha}_{i}\Gamma(n_{ij})} \prod_{k:n_{ijk}>0} \tilde{\alpha}_{i}\Gamma(n_{ijk}) \right] =$$

$$= \prod_{j:n_{ij}>0} \left[ \frac{1}{r_{i}\alpha_{i}^{*}\Gamma(n_{ij})} \prod_{k:n_{ijk}>0} \alpha_{i}^{*}\Gamma(n_{ijk}) \right] \cdot \left( \frac{\tilde{q}_{i}}{q_{i}} \right)^{\tilde{q}_{i}} \left( \frac{q_{i}}{\tilde{q}_{i}} \right)^{\sum_{j} \tilde{r}_{ij}} =$$

$$= BDeu(X_{i} | \Pi_{X_{i}}; \alpha) \cdot \left( \frac{q_{i}}{\tilde{q}_{i}} \right)^{\sum_{j} \tilde{r}_{ij} - \tilde{q}_{i}} = BDeu(X_{i} | \Pi_{X_{i}}; \alpha) \cdot \left( \frac{q_{i}}{\tilde{q}_{i}} \right)^{d_{EP}^{(X_{i}, \mathcal{G})}}$$

**Proof of Theorem 4.** Under condition 1, all  $n_{ijk} > 0$  by the law of large numbers. Therefore all  $n_{ij} > 0$  and  $\tilde{q}_i = q_i$ , leading to  $\mathrm{BDs}(X_i \mid \Pi_{X_i}; \alpha) = \mathrm{BDeu}(X_i \mid \Pi_{X_i}; \alpha)$ . As for condition 2,  $\alpha \to \infty$  implies  $r_i \tilde{\alpha}_i \to \infty$  and  $\tilde{\alpha}_i \to \infty$  since  $\tilde{\alpha}_i = \alpha/(r_i \tilde{q}_i)$  and  $r_i, q_i$  are fixed

for a given network. Then by Stirling's approximation we have that

$$\frac{\Gamma(r_i\tilde{\alpha}_i)}{\Gamma(r_i\tilde{\alpha}_i + n_{ij})} \approx (r_i\tilde{\alpha}_i)^{-n_{ij}} \quad \text{and} \quad \frac{\Gamma(\tilde{\alpha}_i + n_{ijk})}{\Gamma(\tilde{\alpha}_i)} \approx (\tilde{\alpha}_i)^{n_{ijk}}$$

and by substituting the above in (12) we obtain

$$\begin{split} \operatorname{BDs}(X_i \mid \Pi_{X_i}; \alpha) &\approx \prod_{j: n_{ij} > 0} \left[ (r_i \tilde{\alpha}_i)^{-n_{ij}} \prod_{k: n_{ijk} > 0} (\tilde{\alpha}_i)^{n_{ijk}} \right] = \\ &= \prod_{j: n_{ij} > 0} \left[ (r_i \alpha_i^*)^{-n_{ij}} \prod_{k: n_{ijk} > 0} (\alpha_i^*)^{n_{ijk}} \right] \left[ \underbrace{\left( \frac{q_i}{\tilde{q}_i} \right)^{-n_{ij}}}_{k: n_{ijk} > 0} \underbrace{\left( \frac{q_i}{\tilde{q}_i} \right)^{n_{ijk}}}_{k: n_{ijk} > 0} \right] \approx \\ &\approx \prod_{j: n_{ij} > 0} \left[ \frac{\Gamma(r_i \alpha_i^*)}{\Gamma(r_i \alpha_i^* + n_{ij})} \prod_{k: n_{ijk} > 0} \frac{\Gamma(\alpha_i^* + n_{ijk})}{\Gamma(\alpha_i^*)} \right] = \operatorname{BDeu}(X_i \mid \Pi_{X_i}; \alpha). \end{split}$$

**Proof of Theorem 5.** The Bayes factor for BDs can be obtained by combining (6), (7) and (14):

$$\frac{\operatorname{BDs}(X_{i} \mid \Pi_{X_{i}} \cup X_{l}; \alpha)}{\operatorname{BDs}(X_{i} \mid \Pi_{X_{i}}; \alpha)} = \frac{(q_{i} / \tilde{q}_{i})^{d_{\operatorname{EP}}^{(X_{i}, \mathcal{G}^{+})}} \alpha^{d_{\operatorname{EP}}^{(\mathcal{G}^{+})}}}{(q_{i}' / \tilde{q}_{i}')^{d_{\operatorname{EP}}^{(X_{i}, \mathcal{G}^{-})}} \alpha^{d_{\operatorname{EP}}^{(\mathcal{G}^{-})}}} = \frac{\alpha^{d_{\operatorname{EP}}^{(\mathcal{G}^{+})} + d_{\operatorname{EP}}^{(X_{i}, \mathcal{G}^{+})} \log_{\alpha} q_{i} / \tilde{q}_{i}}}{\alpha^{d_{\operatorname{EP}}^{(\mathcal{G}^{-})} + d_{\operatorname{EP}}^{(X_{i}, \mathcal{G}^{-})} \log_{\alpha} q_{i}' / \tilde{q}_{i}'}}.$$

Following (7) we can then write

$$\frac{\operatorname{BDs}(X_i \mid \Pi_{X_i} \cup X_l; \alpha)}{\operatorname{BDs}(X_i \mid \Pi_{X_i}; \alpha)} \to \begin{cases} 0 & \text{if } d_{\text{EDF}} > 0\\ +\infty & \text{if } d_{\text{EDF}} < 0 \end{cases}$$

since we operate under the same assumptions and since the left-hand term differs from that in (7) by a constant multiplier that does not depend on  $\alpha$ . The Bayes factor then diverges if and only if

$$d_{\mathrm{EP}}^{(\mathcal{G}^+)} + d_{\mathrm{EP}}^{(X_i,\mathcal{G}^+)} \log_{\alpha} q_i/\tilde{q}_i < d_{\mathrm{EP}}^{(\mathcal{G}^-)} + d_{\mathrm{EP}}^{(X_i,\mathcal{G}^-)} \log_{\alpha} q_i'/\tilde{q}_i'$$

which is equivalent to

$$\underbrace{d_{\mathrm{EP}}^{(\mathcal{G}^{+})} - d_{\mathrm{EP}}^{(\mathcal{G}^{-})}}_{d_{\mathrm{EDF}}} < \underbrace{d_{\mathrm{EP}}^{(X_{i},\mathcal{G}^{-})} \log_{\alpha} q_{i}' / \tilde{q}_{i}' - d_{\mathrm{EP}}^{(X_{i},\mathcal{G}^{+})} \log_{\alpha} q_{i} / \tilde{q}_{i}}_{-\log_{\alpha}(\mathrm{P}(\mathcal{G}^{+}) / \mathrm{P}(\mathcal{G}^{-}))}$$

and it converges to zero otherwise.

## Appendix B. Additional Simulation Results

In this appendix we report the detailed results of the simulations described in Section 4, organised in tables as follows.

- Table B.1: average SHD from  $\mathcal{G}_{REF}$ , discussed in Section 4.1. This table compares U+BDeu, U+BDs, MU+BDeu, MU+BDs and BIC. For MU,  $\beta$  is fixed to  $^{1}/_{2}$  to give the median-probability model.
- Table B.2: average number of arcs relative to  $\mathcal{G}_{REF}$ , discussed in Section 4.1. This table compares U+BDeu, U+BDs, MU+BDeu, MU+BDs and BIC like Table B.1.
- Table B.3: average predictive log-likelihood values from Section 4.1. This table compares U+BDeu, U+BDs, MU+BDeu, MU+BDs and BIC like Tables B.1 and B.2.
- Table B.4: average SHD for BDeu and different MU priors, discussed in Section 4.2. Results for U from Table B.1 are included as well for ease of reference.
- Table B.5: average SHD for BDs and different MU priors, discussed in Section 4.2. Results for U from Table B.2 are included as well for ease of reference.
- Table B.6: average number of arcs for BDeu and different MU priors, discussed in Section 4.2. Results for U from Table B.2 are included as well for ease of reference.
- Table B.7: average number of arcs for BDs and different MU priors, discussed in Section 4.2. Results for U from Table B.2 are included as well for ease of reference.
- Table B.8: average predictive log-likelihood values for BDeu and different MU priors, discussed in Section 4.2. Results for U from Table B.3 are included as well for ease of reference.
- Table B.9: average predictive log-likelihood values for BDs and different MU priors, discussed in Section 4.2. Results for U from Table B.3 are included as well for ease of reference.

NETWORK	m /m	BIC		U + BDe	eu	U +	BDs	MU +	BDeu	MU -	+ BDs
NETWORK	n/p		1	$\alpha_S$	10	1	10	1	10	1	10
	0.1	55.5	78.0	80.5	112.7	64.2	87.3	53.0	83.5	53.0	65.5
	0.2	50.8	49.2	56.1	92.8	49.5	75.2	39.6	68.3	39.6	56.2
	0.5	40.8	35.5	41.9	72.0	34.9	61.5	31.3	53.5	31.3	46.1
ALARM	1.0	33.7	31.9	37.6	62.6	29.1	51.8	27.1	49.8	27.1	42.1
	2.0	28.1	26.3	31.9	53.1	23.1	44.5	22.9	41.0	22.9	36.5
	5.0	22.6	24.4	30.1	41.6	20.9	35.0	20.4	31.6	20.4	28.9
	0.1	367.6	642.1	997.6	1071.0	786.5	1367.8	439.9	765.9	439.9	829.9
	0.2	278.3	450.1	686.9	773.4	522.8	957.0	313.0	560.4	313.0	572.4
ANDEG	0.5	197.4	264.9	445.3	576.0	278.4	590.7	197.1	409.1	197.1	386.2
ANDES	1.0	147.3	196.3	320.7	467.1	196.3	434.3	143.3	331.4	143.3	299.4
	2.0	116.2	142.6	246.6	388.3	139.4 100.8	345.5	109.9	280.2	$109.9 \\ 78.2$	243.9 $176.5$
	5.0	78.3	103.5	172.2	289.2		253.6	78.2	206.5		
	$0.1 \\ 0.2$	28.4 25.2	39.6	44.8	51.5	38.6	46.5	31.6 <b>24.6</b>	36.5	31.6 <b>24.6</b>	33.6
	$0.2 \\ 0.5$	25.2 $21.0$	26.9	$33.0 \\ 23.6$	$36.0 \\ 25.0$	29.9	$38.1 \\ 24.6$	18.9	27.5	18.9	$27.8 \\ 20.7$
CHILD	1.0	18.5	21.1 18.1	$\frac{23.0}{20.0}$	$\frac{25.0}{19.9}$	21.4 18.1	$\frac{24.0}{20.0}$	17.7	$21.1 \\ 18.0$	17.7	20.7 17.8
CHILD	2.0	1	17.0	15.6		17.0		15.8			13.4
	$\frac{2.0}{5.0}$	16.1 14.4	14.7	15.6 $12.4$	$15.4 \\ 12.3$	14.7	15.4 $12.3$	12.8	13.4 <b>9.4</b>	15.8 12.8	9.4
	0.1	484.3	399.9	522.6	444.8	387.8	378.8	400.4	429.5	400.4	$\frac{9.4}{378.6}$
	$0.1 \\ 0.2$	549.4	399.9	522.0 $533.2$	444.8 $435.0$	377.5	383.2	381.0	$\frac{429.5}{385.6}$	381.0	$378.6 \\ 377.3$
	$0.2 \\ 0.5$	416.8	399.6	533.2 531.2	435.0 $440.0$	387.9	373.9	392.2	430.0	392.2	373.9
DIABETES	1.0	412.3	373.0	530.9	420.3	375.0	372.2	368.5	430.0 $415.8$	368.5	373.9
DIADETES	2.0	384.8	380.9	551.6	435.3	<b>365.6</b>	395.7	375.7	432.8	375.7	395.0
	5.0	402.1	413.6	599.0	465.0	408.0	427.0	412.6	465.8	412.6	426.7
	0.1	63.1	66.4	49.6	50.4	62.0	46.1	63.0	48.0	63.0	48.1
	0.1	48.9	54.7	49.0 $44.1$	40.8	50.6	36.3	51.7	38.4	51.7	45.1 $45.3$
	0.5	31.9	40.0	46.9	35.1	34.7	29.9	36.8	32.1	36.8	38.5
HAILFINDER	1.0	34.5	33.8	48.4	40.5	31.1	35.3	30.7	39.2	30.7	35.2
III III II I	2.0	36.4	42.0	38.8	38.4	36.0	33.3	39.0	37.1	39.0	33.1
	5.0	16.9	24.4	27.9	21.1	18.4	15.1	21.4	19.0	21.4	15.0
	0.1	143.0	183.7	226.7	269.9	192.4	292.2	149.1	209.8	149.1	210.2
	0.2	126.6	153.7	183.8	220.2	157.4	231.1	134.3	175.6	134.3	171.9
	0.5	101.5	115.1	138.6	166.6	116.8	167.3	105.3	138.2	105.3	134.2
HEPAR2	1.0	85.0	93.0	108.5	132.8	94.2	128.1	88.0	109.8	88.0	105.8
	2.0	73.9	76.5	89.3	106.6	77.5	102.3	75.0	89.0	75.0	87.0
	5.0	58.6	60.1	63.0	73.0	60.5	69.5	58.7	62.2	58.6	59.5
	0.1	49.5	50.6	57.1	67.8	53.0	63.0	48.5	59.7	48.5	56.9
	0.2	46.3	47.5	55.5	63.8	49.4	60.1	45.9	58.5	45.9	53.7
	0.5	46.9	45.9	52.5	59.0	45.9	52.2	43.6	55.5	43.6	49.1
INSURANCE	1.0	49.8	42.3	48.0	53.6	43.7	50.2	42.3	51.0	42.2	46.3
	2.0	46.4	42.9	48.0	53.9	42.8	49.0	43.0	51.6	42.6	46.2
	5.0	47.1	39.5	44.3	48.8	39.1	46.2	39.5	47.2	39.1	44.6
	0.1	278.2	269.2	398.1	345.9	250.3	292.9	237.8	309.0	237.8	257.9
	0.2	261.0	256.2	382.7	336.2	221.1	251.2	234.2	304.6	234.2	246.8
	0.5	259.6	255.0	351.6	299.4	189.2	203.2	234.2	277.4	234.2	193.7
PATHFINDER	1.0	240.2	242.8	342.0	289.4	171.3	182.6	220.5	264.9	220.5	173.8
	2.0	225.9	232.3	333.9	277.8	156.9	169.7	218.2	253.2	218.2	177.8
	5.0	218.5	208.1	320.5	263.4	124.7	130.2	189.8	239.2	189.8	119.5
	0.1	130.7	114.8	155.4	203.3	116.2	163.0	106.3	166.7	106.3	146.7
	0.2	118.0	137.1	142.3	165.6	136.7	127.5	127.5	143.2	127.5	111.5
	0.5	131.1	132.9	134.8	142.4	131.3	110.5	122.6	126.5	122.6	$\bf 95.4$
PIGS	1.0	133.8	135.2	136.2	138.9	132.5	104.8	122.0	124.5	122.0	91.2
	2.0	138.7	142.8	143.6	144.8	137.2	109.0	128.2	128.8	128.2	89.0
	5.0	149.8	155.5	155.1	156.6	150.2	116.9	140.6	140.7	140.6	99.2
	0.1	61.3	70.0	74.80	97.1	62.2	84.2	61.1	87.9	61.1	78.6
		010	62.7	68.45	89.4	57.9	78.7	55.6	80.9	55.6	74.0
	0.2	61.2									
	0.5	57.8	60.2	63.95	84.0	54.3	73.3	53.8	79.0	53.8	70.9
WATER	$0.5 \\ 1.0$	57.8 <b>53.7</b>	60.2 60.9	63.95 $64.20$	84.0 79.0	54.3 55.0	$73.3 \\ 71.7$	54.9	74.3	<b>53.8</b> 54.9	69.6
WATER	0.5	57.8	60.2	63.95	84.0	54.3	73.3			53.8	

Table B.1: Average SHD from  $\mathcal{G}_{\text{REF}}$  (lower is better, best in bold).

	,	BIC	1	U + BDeı	1	U +	BDs	MU +	BDeu	MU -	- BDs
NETWORK	n/p	D10	1	$\alpha_S$	10	1	10	1	10	1	10
	0.1	0.596	1.635	1.697	2.550	1.329	1.875	1.040	1.854	1.040	1.351
	0.2	0.662	1.272	1.448	2.278	1.321	1.874	1.049	1.730	1.049	1.436
	0.5	0.746	1.174	1.290	1.993	1.213	1.775	1.060	1.605	1.060	1.436
ALARM	1.0	0.859	1.165	1.302	1.830	1.180	1.667	1.071	1.553	1.071	1.426
	2.0	0.972	1.117	1.236	1.664	1.098	1.528	1.064	1.445	1.064	1.377
	5.0	1.092	1.098	1.208	1.457	1.086	1.386	1.061	1.286	1.061	1.252
	0.1	1.069	1.910	3.020	3.248	2.339	4.121	1.294	2.329	1.294	2.510
	0.2	1.032	1.550	2.303	2.570	1.764	3.115	1.129	1.926	1.129	1.963
	0.5	1.018	1.224	1.794	2.195	1.258	2.236	1.011	1.694	1.011	1.622
ANDES	1.0	1.011	1.156	1.556	1.999	1.154	1.898	0.991	1.593	0.991	1.496
	2.0	1.007	1.073	1.399	1.829	1.063	1.702	0.996	1.507	0.996	1.399
	5.0	0.999	1.056	1.275	1.642	1.046	1.541	0.970	1.394	0.970	1.309
	0.1	0.442	1.150	1.470	1.802	1.114	1.564	0.788	1.098	0.788	0.956
	0.2	0.588	0.894	1.250	1.366	1.014	1.444	0.744	0.992	0.744	0.998
	0.5	0.642	0.730	1.080	1.134	0.744	1.132	0.658	0.942	0.658	0.950
CHILD	1.0	0.730	0.774	1.006	1.020	0.772	1.016	0.736	0.912	0.736	0.920
	2.0	0.808	0.842	1.000	0.994	0.842	0.994	0.820	0.962	0.820	0.962
	5.0	0.914	0.908	1.046	1.034	0.908	1.034	0.898	1.012	0.898	1.012
	0.1	1.023	1.107	1.419	1.252	1.122	1.158	1.107	1.229	1.107	1.157
	0.2	1.065	1.115	1.447	1.237	1.136	1.169	1.115	1.200	1.115	1.168
	0.5	1.051	1.150	1.442	1.224	1.158	1.189	1.138	1.205	1.138	1.189
DIABETES	1.0	1.048	1.156	1.499	1.236	1.164	1.193	1.149	1.228	1.149	1.193
	2.0	1.083	1.176	1.539	1.281	1.192	1.264	1.167	1.276	1.167	1.262
	5.0	1.158	1.260	1.619	1.349	1.281	1.322	1.261	1.350	1.260	1.321
	0.1	0.699	0.774	1.077	0.972	0.707	0.880	0.714	0.928	0.714	0.862
	0.2	0.782	0.901	1.098	0.977	0.839	0.880	0.852	0.942	0.852	0.873
	0.5	0.843	0.933	1.117	0.995	0.854	0.886	0.886	0.970	0.886	0.892
HAILFINDER	1.0	0.892	0.967	1.145	1.014	0.884	0.904	0.919	0.992	0.919	0.901
	2.0	0.898	0.989	1.189	1.049	0.898	0.942	0.943	1.027	0.943	0.936
	5.0	0.986	1.059	1.231	1.099	0.968	0.978	1.013	1.067	1.013	0.977
	0.1	0.451	0.886	1.338	1.723	0.972	1.944	0.527	1.198	0.527	1.202
	0.2	0.433	0.739 $0.654$	$1.121 \\ 0.962$	1.472 $1.250$	$0.786 \\ 0.680$	1.576	0.491 0.498	1.063	$0.491 \\ 0.498$	1.039 0.922
HEPAR2	$0.5 \\ 1.0$	$0.467 \\ 0.525$	0.635	0.962 $0.885$	1.230 $1.140$	0.653	1.252 $1.111$	0.498 $0.551$	$\begin{array}{c} 0.967 \\ 0.908 \end{array}$	0.498	0.922 $0.875$
HEFAR2	2.0	0.525	0.660	0.885	1.140 $1.069$	0.668	1.041	0.598	0.890	0.598	0.873
	5.0	0.681	0.726	0.883	1.009	0.729	0.992	0.598	0.830	0.697	0.887
	0.1	0.405	0.626	0.829	1.042	0.663	0.937	0.549	0.870	0.549	0.779
	0.1	0.447	0.647	0.825	1.042 $1.010$	0.674	0.927	0.603	0.901	0.603	0.819
	0.5	0.535	0.689	0.859	1.048	0.700	0.906	0.662	0.962	0.662	0.830
INSURANCE	1.0	0.638	0.760	0.906	1.054	0.776	0.941	0.746	0.989	0.746	0.870
11.0010111.012	2.0	0.723	0.806	0.942	1.103	0.811	1.012	0.799	1.058	0.799	0.941
	5.0	0.797	0.880	1.011	1.096	0.887	1.040	0.870	1.057	0.870	0.994
-	0.1	0.815	1.154	1.862	1.591	1.062	1.337	0.961	1.391	0.961	1.112
	0.2	0.805	1.096	1.852	1.538	0.992	1.190	0.941	1.376	0.941	1.044
	0.5	0.871	1.096	1.846	1.438	0.985	1.102	0.963	1.320	0.963	1.014
PATHFINDER	1.0	0.864	1.081	1.871	1.477	0.965	1.068	0.951	1.343	0.951	0.999
	2.0	0.859	1.095	1.907	1.470	0.966	1.014	1.004	1.346	1.004	0.958
	5.0	0.864	1.071	1.945	1.467	0.919	0.974	0.985	1.347	0.985	0.946
	0.1	1.047	1.050	1.098	1.176	1.049	1.156	1.044	1.122	1.044	1.112
	0.2	1.059	1.063	1.071	1.112	1.062	1.091	1.052	1.082	1.052	1.065
	0.5	1.062	1.065	1.067	1.079	1.063	1.060	1.059	1.066	1.059	1.048
PIGS	1.0	1.064	1.067	1.069	1.073	1.064	1.051	1.058	1.062	1.058	1.044
	2.0	1.073	1.075	1.076	1.079	1.069	1.074	1.062	1.066	1.062	1.044
	5.0	1.078	1.085	1.085	1.086	1.079	1.061	1.074	1.074	1.074	1.052
	0.1	0.302	0.721	0.795	1.141	0.517	0.882	0.552	0.966	0.552	0.788
	0.2	0.329	0.760	0.836	1.156	0.566	0.903	0.631	0.996	0.631	0.816
	0.5	0.389	0.791	0.876	1.172	0.610	0.932	0.672	1.059	0.672	0.882
WATER	1.0	0.423	0.812	0.909	1.199	0.627	0.939	0.717	1.093	0.717	0.899
	2.0	0.470	0.846	1.012	1.230	0.672	0.942	0.751	1.141	0.751	0.907
	5.0	0.527	0.931	1.119	1.274	0.736	0.956	0.826	1.192	0.826	0.927

Table B.2: Average number of arcs (rescaled by  $|A_{\rm REF}|$ ; closer to 1 is better, best in bold).

NETHODI		BIC	J	J + BDeu	1	U+	BDs	MU +	BDeu	MU +	- BDs
NETWORK	n/p		1	$\alpha_S$	10	1	10	1	10	1	10
-	0.1	1.54	1.67	1.68	1.85	1.67	1.80	1.51	1.69	1.51	1.60
ALARM	0.2	1.33	1.32	1.34	1.44	1.35	1.43	1.29	1.36	1.29	1.34
	0.5	1.21	1.17	1.17	1.21	1.17	1.20	1.16	1.18	1.16	1.17
	0.1	11.12	13.14	17.56	18.59	14.75	24.40	11.90	15.77	11.90	17.77
ANDES	0.2	10.00	10.56	11.53	11.96	10.88	13.30	10.16	11.13	10.16	11.47
	0.5	9.50	9.60	9.80	9.96	9.63	10.07	9.53	9.73	9.53	9.74
	0.1	1.82	2.03	2.19	2.30	2.07	2.31	1.91	2.04	1.91	2.00
CHILD	0.2	1.58	1.66	1.77	1.82	1.71	1.88	1.62	1.68	1.62	1.69
	0.5	1.39	1.40	1.44	1.46	1.40	1.46	1.39	1.42	1.39	1.42
	0.1	20.54	19.40	19.26	19.27	19.34	19.26	19.40	19.26	19.40	19.26
DIABETES	0.2	19.87	19.14	19.13	19.13	19.20	19.13	19.14	19.10	19.14	19.13
	0.5	19.24	19.05	19.03	19.04	19.10	19.00	19.05	19.04	19.05	19.00
	0.1	5.31	5.31	5.24	5.23	5.30	5.23	5.31	5.22	5.31	5.22
HAILFINDER	0.2	5.13	5.13	5.09	5.09	5.12	5.08	5.13	5.08	5.13	5.08
	0.5	5.01	5.01	5.00	5.01	5.01	4.99	5.01	4.99	5.01	4.99
	0.1	3.49	3.73	3.98	4.24	3.81	4.68	3.58	3.90	3.58	4.04
HEPAR2	0.2	3.37	3.45	3.54	3.63	3.47	3.74	3.40	3.51	3.40	3.53
	0.5	3.30	3.32	3.34	3.36	3.32	3.37	3.31	3.33	3.31	3.33
	0.1	1.61	1.59	1.60	1.64	1.59	1.66	1.58	1.61	1.58	1.62
INSURANCE	0.2	1.52	1.46	1.46	1.47	1.46	1.49	1.46	1.47	1.46	1.47
	0.5	1.43	1.38	1.37	1.37	1.38	1.38	1.38	1.37	1.38	1.37
	0.1	2.65	2.51	2.49	2.49	2.50	2.49	2.51	2.49	2.51	2.49
PATHFINDER	0.2	2.54	2.43	2.43	2.43	2.43	2.43	2.43	2.43	2.43	2.43
	0.5	2.45	2.39	2.38	2.39	2.39	2.38	2.39	2.39	2.39	2.38
	0.1	33.49	33.25	33.29	33.36	33.24	33.36	33.24	33.31	33.24	33.31
PIGS	0.2	33.15	33.13	33.14	33.16	33.13	33.15	33.13	33.14	33.13	33.14
	0.5	33.05	33.05	33.04	33.05	33.04	33.04	33.04	33.04	33.04	33.04
	0.1	1.30	1.29	1.29	1.30	1.29	1.30	1.29	1.29	1.29	1.30
WATER	0.2	1.30	1.29	1.29	1.29	1.29	1.29	1.29	1.29	1.29	1.29
	0.5	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28

Table B.3: Average predictive log-likelihood (rescaled by -10000; lower is better, best in bold).  $^{n}/_{p}=1.0, 2.0, 5.0$  showed the same value for all scores and are omitted for brevity.

NETWORK	n/p	U		MU (A	S = 1/2	MU (	c = 1		c=2)	MU (d	
		1	10	1	10	1	10	1	10	1	10
	0.1	78.0	112.7	53.0	83.5	42.9	47.1	53.1	53.1	46.8	68.8
	$0.2 \\ 0.5$	49.2 35.5	$92.8 \\ 72.0$	39.6 31.3	$68.3 \\ 53.5$	33.8 27.2	$40.7 \\ 33.1$	46.3 37.9	$46.3 \\ 37.9$	36.6 29.2	$59.3 \\ 48.2$
ALARM	1.0	31.9	62.6	27.1	49.8	25.6	32.1	35.8	35.8	27.1	45.2
711111111	2.0	26.3	53.1	22.9	41.0	22.5	28.9	31.7	31.7	23.6	37.0
	5.0	24.4	41.6	20.4	31.6	21.9	26.9	28.1	28.1	22.3	31.3
	0.1	642.1	1071.0	439.9	765.9	229.0	224.1	238.3	238.3	223.6	268.3
	0.2	450.1	773.4	313.0	560.4	168.9	176.5	190.2	190.2	167.2	222.5
	0.5	264.9	576.0	197.1	409.1	121.2	132.0	141.7	141.7	118.3	165.9
ANDES	1.0	196.3	467.1	143.3	331.4	89.7	100.2	112.7	112.7	86.8	132.0
	2.0	142.6	388.3	109.9	280.2	71.1	89.6	94.6	94.6	70.3	112.8
	5.0	103.5	289.2	78.2	206.5	56.9	77.9	82.6	82.6	55.1	97.0
	0.1	39.6	51.5	31.6	36.5	23.9	22.6	25.7	25.7	32.3	40.8
	0.2	26.9	36.0	24.6	27.5	19.9	19.9	21.4	21.4	24.8	30.7
CHILD	$0.5 \\ 1.0$	21.1 18.1	$25.0 \\ 19.9$	18.9 17.7	$21.1 \\ 18.0$	18.6 17.2	18.6 $16.9$	19.3 17.3	$19.3 \\ 17.3$	19.7 17.8	$\frac{22.0}{18.7}$
CHILD	2.0	17.0	15.4	15.8	13.4	17.2	15.3	15.4	17.3 $15.4$	17.0	15.5
	5.0	14.7	12.3	12.8	9.4	14.8	12.4	12.5	12.5	14.8	12.5
	0.1	399.9	444.8	400.4	429.5	390.6	411.9	413.5	413.5	391.5	415.2
	0.2	381.0	435.0	381.0	385.6	359.4	409.1	409.3	409.3	359.6	409.6
	0.5	399.6	440.0	392.2	430.0	375.8	418.1	418.1	418.1	375.8	418.1
DIABETES	1.0	373.0	420.3	368.5	415.8	346.5	393.6	393.6	393.6	346.5	393.6
	2.0	380.9	435.3	375.7	432.8	357.1	421.6	421.8	421.7	357.1	422.0
	5.0	413.6	465.0	412.6	465.8	406.4	461.2	461.2	461.2	406.4	461.2
	0.1	66.4	50.4	63.0	48.0	59.9	46.0	45.6	45.6	62.2	45.7
	0.2	54.7	40.8	51.7	38.4	48.3	37.0	37.1	37.1	50.4	38.0
II A II DINDED	0.5	40.0	35.1	36.8	32.1	33.5	28.9	28.9	28.9	36.6	29.6
HAILFINDER	1.0	33.8	40.5	30.7	39.2	29.0	37.1	37.3	37.3	30.2	38.2
	$\frac{2.0}{5.0}$	42.0 24.4	$38.4 \\ 21.1$	39.0 21.4	37.1 $19.0$	37.0 19.1	35.3 <b>16.9</b>	<b>35.2</b> 17.0	<b>35.2</b> 17.0	37.9 20.3	$36.1 \\ 18.0$
	0.1	183.7	269.9	149.1	209.8	119.1 119.4	121.6	127.2	127.2	122.2	141.1
	0.1	153.7	220.2	134.3	175.6	115.4	114.0	117.7	127.2 $117.7$	115.2	129.0
	0.5	115.1	166.6	105.3	138.2	98.2	97.7	99.7	99.7	96.4	106.4
HEPAR2	1.0	93.0	132.8	88.0	109.8	85.7	84.3	84.9	84.9	84.6	89.0
	2.0	76.5	106.6	75.0	89.0	74.9	69.4	71.0	71.0	74.9	73.4
	5.0	60.1	73.0	58.7	62.2	60.3	48.5	48.7	48.7	58.8	50.9
	0.1	50.6	67.8	48.5	59.7	47.2	52.9	54.4	54.4	48.2	59.8
	0.2	47.5	63.8	45.9	58.5	44.5	52.4	53.8	53.8	45.7	59.1
	0.5	45.9	59.0	43.6	55.5	43.0	50.6	52.5	52.5	44.2	55.0
INSURANCE	1.0	42.3	53.6	42.3	51.0	42.0	47.3	48.2	48.2	41.3	51.1
	2.0	42.9	53.9	43.0	51.6	42.4	49.2	50.6	50.6	41.8	52.0
	5.0	39.5 269.2	48.8 345.9	39.5 237.8	47.2 309.0	41.8 238.1	47.1 258.2	47.5 263.9	47.5 263.9	<b>41.7</b> 241.1	$\frac{48.7}{281.6}$
	$0.1 \\ 0.2$	256.2	336.2	234.2	304.6	177.8	236.2 $222.0$	233.0	203.9 $233.0$	179.8	243.0
	0.5	255.0	299.4	234.2	277.4	150.7		209.5		151.9	243.0 $218.4$
PATHFINDER	1.0	242.8	289.4	220.5	264.9	136.0	196.0	200.6	200.6	137.1	205.5
1111111111111	2.0	232.3	277.8	218.2	253.2	122.9	185.7	188.0	188.0	123.4	195.5
	5.0	208.1	263.4	189.8	239.2	103.1	173.0	173.9	173.9	103.3	181.4
	0.1	114.8	203.3	106.3	166.7	109.8	136.9	137.9	137.9	110.0	139.5
	0.2	137.1	165.6	127.5	143.2	132.8	140.9	141.1	141.1	133.4	141.4
	0.5	132.9	142.4	122.6	126.5	129.5	133.5	133.7	133.7	129.6	134.4
PIGS	1.0	135.2	138.9	122.0	124.5	133.5	134.6	134.6	134.6	133.6	134.3
	2.0	142.8	144.8	128.2	128.8	139.5	142.8	142.8	142.8	139.6	143.1
	5.0	155.5	156.6	140.6	140.7	154.6	156.5	156.5	156.5	154.7	156.5
	0.1	70.0	97.1	61.1	87.9	56.7	80.0	81.7	81.7	59.5	88.1
	$0.2 \\ 0.5$	62.7 60.2	89.4 84.0	55.6 53.8	$80.9 \\ 79.0$	52.3 49.9	$73.2 \\ 72.0$	76.4 75.7	$76.4 \\ 75.7$	53.2 50.5	$80.3 \\ 77.0$
WATER	1.0	60.2	79.0	54.9	79.0 $74.3$	49.9	68.1	71.4	71.4	49.2	77.0 $73.5$
WATEH	$\frac{1.0}{2.0}$	58.1	79.0 75.6	51.7	69.9	45.1	64.1	66.8	66.8	49.2	69.4
	5.0	61.6	76.7	55.1	72.3	48.0	65.8	69.0	69.0	52.9	70.2
	5.0	01.0	10.1	55.1	14.0	1 40.0	00.0	03.0	03.0	02.9	10.2

Table B.4: Average SHD for BDeu and different MU priors (lower is better, best in bold).

NETWORK	n/p	J	J	MU (β		MU (	c = 1)	MU (		MU (	c = 5)
		1	10	1	10	1	10	1	10	1	10
	0.1	64.2	87.3	53.0	65.5	43.6	45.6	44.2	48.8	48.9	56.6
	0.2	49.5	75.2	39.6	56.2	34.2	37.3	34.2	40.0	37.2	47.4
AT ADM	0.5	34.9	61.5	31.3	46.1	24.5	29.7	24.8	33.0	26.8	40.3
ALARM	1.0	29.1	51.8	27.1	42.1	21.8	25.7	21.9	28.8	23.4	36.7
	2.0	23.1	44.5	22.9	36.5	16.6	23.3	16.6	25.7	17.1	31.2
	5.0	20.9	35.0	20.4	28.9	18.5	21.5	18.7	22.5	18.9	25.6
	$0.1 \\ 0.2$	$786.5 \\ 522.8$	1367.8 $957.0$	439.9 313.0	$829.9 \\ 572.4$	228.8 168.2	223.8 $166.1$	224.8 <b>164.2</b>	225.3 $173.9$	<b>223.8</b> 166.8	$247.7 \\ 202.6$
	0.2	278.4	590.7	197.1	386.2	119.9	122.0	117.9	175.9 $135.1$	117.4	155.0
ANDES	1.0	196.3	434.3	143.3	299.4	89.1	95.6	86.9	103.1	86.1	124.1
ANDES	2.0	139.4	345.5	109.9	243.9	70.3	81.3	69.5	86.6	69.4	102.1
	5.0	100.8	253.6	78.2	176.5	56.8	66.2	55.7	68.9	55.0	77.4
	0.1	38.6	46.5	31.6	33.6	24.1	23.0	25.6	25.3	34.2	37.9
	0.2	29.9	38.1	24.6	27.8	20.5	20.4	21.0	21.8	26.9	30.7
	0.5	21.4	24.6	18.9	20.7	18.6	18.6	18.6	19.5	20.0	21.9
CHILD	1.0	18.1	20.0	17.7	17.8	17.2	16.8	17.4	17.3	17.8	18.8
·	2.0	17.0	15.4	15.8	13.4	17.1	15.3	16.8	15.4	17.0	15.5
	5.0	14.7	12.3	12.8	9.4	14.7	12.3	14.6	12.5	14.8	12.4
	0.1	387.8	378.8	400.4	378.6	376.0	350.6	375.7	350.5	374.4	350.5
	0.2	377.5	383.2	381.0	377.3	353.3	344.4	353.2	344.4	353.0	344.3
	0.5	387.9	373.9	392.2	373.9	363.4	335.7	363.4	335.6	363.4	335.5
DIABETES	1.0	375.0	372.2	368.5	372.1	339.5	329.2	339.5	329.2	339.5	329.2
	2.0	365.6	395.7	375.7	395.0	349.4	360.7	349.5	361.1	349.5	361.6
	5.0	408.0	427.0	412.6	426.7	403.5	398.2	403.5	398.3	403.5	398.4
	0.1	62.0	46.1	63.0	48.1	60.7	43.3	61.0	43.3	61.0	43.5
	0.2	50.6	36.3	51.7	45.3	49.8	34.3	49.7	34.3	50.0	34.4
	0.5	34.7	29.9	36.8	38.5	34.1	26.1	34.1	26.3	34.3	26.5
HAILFINDER	1.0	31.1	35.3	30.7	35.2	27.3	34.3	27.4	34.3	27.6	34.2
	2.0	36.0	33.3	39.0	33.1	35.0	32.1	34.9	32.2	34.9	32.2
	5.0	18.4	15.1	21.4	15.0	17.1	13.9	17.1	13.9	17.3	14.0
	0.1	192.4	292.2	149.1	210.2	119.5	120.6	120.5	126.0	122.6	136.9
	0.2	157.4	231.1	134.3	171.9	115.1	113.0	115.1	115.7	115.1	124.7
******	0.5	116.8	167.3	105.3	134.2	98.2	97.0	97.1	99.6	96.3	104.8
HEPAR2	1.0	94.2	128.1	88.0	105.8	85.7	83.5	84.5	83.9	84.7	86.6
	2.0	77.5	102.3	75.0	87.0	74.9	68.6	74.9	69.7	75.0	71.7
	5.0	60.5	69.5	58.6	59.5	60.2	48.4	59.3	48.5	58.7	50.2
	0.1	53.0	63.0	48.5	56.9	48.5	51.3	49.2	51.6	49.8	55.3
	0.2	49.4	60.1	45.9	53.7	45.5	50.8	46.0	51.9	47.6	55.0
INSURANCE	0.5	45.9	52.2	$43.6 \\ 42.2$	49.1	44.1	46.5	44.4	47.4	45.0	48.7
INSURANCE	$\frac{1.0}{2.0}$	43.7 $42.8$	$50.2 \\ 49.0$	42.2	$46.3 \\ 46.2$	43.2 42.2	$44.2 \\ 42.4$	42.7 <b>42.1</b>	$44.6 \\ 43.4$	42.9 42.3	$45.9 \\ 45.5$
	5.0	39.1	46.2	39.1	44.6	41.9	43.8	41.9	44.9	41.9	46.4
	0.1	250.3	292.9	237.8	257.9	252.0	250.3	253.7	253.2	256.5	258.3
	0.1	250.5 $221.1$	251.2	234.2	246.8	202.0	230.3 $219.2$	203.8	233.2 $221.3$	204.8	236.5 $224.7$
	0.5	189.2	203.2	234.2	193.7	195.8	196.4	196.4	198.0	198.4	200.6
PATHFINDER	1.0	171.3	182.6	220.5	173.8	169.7	176.3	170.3	178.5	171.6	181.2
	2.0	156.9	169.7	218.2	177.8	135.7	141.7	136.4	143.9	137.1	145.4
	5.0	124.7	130.2	189.8	119.5	102.4	106.4	102.4	106.6	102.7	107.2
	0.1	116.2	163.0	106.3	146.7	110.2	96.6	111.3	96.7	110.6	97.6
	0.2	136.7	127.5	127.5	111.5	132.4	99.9	132.6	100.7	132.6	101.5
	0.5	131.3	110.5	122.6	95.4	128.0	101.9	127.6	102.3	128.8	102.9
PIGS	1.0	132.5	104.8	122.0	91.2	130.7	100.6	131.2	100.6	131.3	100.6
	2.0	137.2	109.0	128.2	89.0	134.2	108.3	134.9	108.3	134.9	108.1
	5.0	150.2	116.9	140.6	99.2	148.6	116.2	148.6	116.2	148.6	116.2
	0.1	62.2	84.2	61.1	78.6	53.3	70.7	53.4	72.9	53.8	77.8
	0.2	57.9	78.7	55.6	74.0	48.6	65.5	48.9	67.4	48.7	72.1
					70.0	4 7 0	COF	47.9	64.8	48.0	69.6
	0.5	54.3	73.3	53.8	70.9	47.8	62.5	41.9			
WATER	1.0	55.0	71.7	54.9	69.6	49.0	63.8	49.2	66.1	49.4	69.2
WATER											

Table B.5: Average SHD for BDs and different MU priors (lower is better, best in bold).

NETWORK	,	Ţ	J	MU (£	B = 1/2	MU (	c = 1	MU (	c=2	MU (d	c = 5
NETWORK	n/p	1	10	1	10	1 `	10	1	10	1`	10
	0.1	1.635	2.550	1.040	1.854	0.638	0.876	0.698	1.073	0.841	1.497
	0.2	1.272	2.278	1.038	1.730	0.766	1.049	0.821	1.201	0.947	1.510
	0.5	1.174	1.993	1.060	1.605	0.876	1.121	0.911	1.235	0.979	1.463
ALARM	1.0	1.165	1.830	1.071	1.553	0.995	1.164	0.975	1.253	1.040	1.457
	2.0	1.117	1.664	1.064	1.445	1.039	1.151	1.047	1.209	1.063	1.336
	5.0	1.098	1.457	1.061	1.286	1.053	1.129	1.055	1.158	1.061	1.226
	0.1	1.910	3.248	1.294	2.329	0.407	0.464	0.445	0.563	0.516	0.701
	0.2	1.550	2.570	1.129	1.926	0.559	0.658	0.581	0.720	0.620	0.849
ANDES	0.5	1.224 1.156	2.195 $1.999$	$1.011 \\ 0.991$	1.694	$0.676 \\ 0.763$	$0.782 \\ 0.863$	$0.690 \\ 0.774$	$0.836 \\ 0.907$	$0.721 \\ 0.793$	0.932
ANDES	$\frac{1.0}{2.0}$	1.130	1.829	0.991	1.593 $1.507$	0.703	0.803 $0.897$	0.774	0.907 $0.923$	0.793	$0.972 \\ 0.986$
	5.0	1.056	1.642	0.977	1.394	0.859	0.953	0.813	0.923 $0.977$	0.873	1.026
	0.1	1.150	1.802	0.788	1.098	0.388	0.392	0.472	0.556	0.836	1.288
	0.1	0.894	1.366	0.744	0.992	0.500	0.632	0.560	0.718	0.786	1.136
	0.5	0.730	1.134	0.658	0.998	0.580	0.724	0.614	0.824	0.674	0.942
CHILD	1.0	0.774	1.020	0.736	0.912	0.678	0.822	0.710	0.850	0.750	0.942
OIII D	2.0	0.842	0.994	0.820	0.962	0.796	0.910	0.804	0.934	0.830	0.972
	5.0	0.908	1.034	0.898	1.002	0.886	0.988	0.894	1.002	0.906	1.022
	0.1	1.107	1.252	1.107	1.229	1.099	1.219	1.100	1.224	1.101	1.231
	0.2	1.115	1.237	1.115	1.200	1.114	1.207	1.115	1.208	1.114	1.210
	0.5	1.150	1.224	1.138	1.205	1.150	1.217	1.150	1.217	1.150	1.217
DIABETES	1.0	1.156	1.236	1.149	1.228	1.156	1.234	1.156	1.234	1.156	1.234
	2.0	1.176	1.281	1.167	1.276	1.176	1.278	1.176	1.278	1.176	1.278
	5.0	1.260	1.349	1.261	1.350	1.258	1.348	1.258	1.348	1.258	1.348
	0.1	0.774	0.972	0.714	0.928	0.620	0.823	0.630	0.838	0.679	0.855
	0.2	0.901	0.977	0.852	0.942	0.777	0.877	0.792	0.883	0.823	0.905
	0.5	0.933	0.995	0.886	0.970	0.836	0.914	0.866	0.920	0.883	0.946
HAILFINDER	1.0	0.967	1.001	0.919	0.992	0.895	0.948	0.897	0.974	0.916	0.991
	2.0	0.989	1.049	0.943	1.027	0.927	1.005	0.928	1.006	0.943	1.023
-	5.0	1.059	1.099	1.013	1.067	0.993	1.047	1.009	1.048	1.012	1.065
	0.1	0.886	1.723	0.527	1.198	0.147	0.289	0.173	0.375	0.226	0.541
	0.2	0.739	1.472	0.491	1.063	0.204	0.367	0.224	0.440	0.268	0.587
HEDADO	0.5	0.654	1.250	0.498	0.967	0.315	0.459	0.333	0.507	0.367	0.628
HEPAR2	1.0	0.635	1.140	0.551	0.908	0.420	0.554	0.438	0.596	0.465	0.677
	$\frac{2.0}{5.0}$	$0.660 \\ 0.726$	$1.069 \\ 1.020$	0.598 $0.697$	$0.890 \\ 0.913$	0.517 0.643	$0.619 \\ 0.730$	$0.532 \\ 0.652$	$0.652 \\ 0.751$	$0.550 \\ 0.669$	$0.719 \\ 0.793$
		0.726			0.913		0.750		0.731		$\frac{0.793}{0.857}$
	$0.1 \\ 0.2$	0.626 $0.647$	$1.042 \\ 1.010$	0.549 0.603	0.870	$0.464 \\ 0.544$	0.634 $0.742$	$0.490 \\ 0.560$	0.721 $0.784$	0.534 $0.589$	0.898
	$0.2 \\ 0.5$	0.689	1.010 $1.048$	0.662	0.961	0.632	0.142	0.638	0.764	0.657	0.962
INSURANCE	1.0	0.760	1.054	0.746	0.989	0.723	0.889	0.729	0.919	0.741	0.988
11.0010111.02	2.0	0.806	1.103	0.799	1.058	0.783	0.971	0.785	1.002	0.792	1.056
	5.0	0.880	1.096	0.870	1.057	0.858	0.990	0.862	1.008	0.868	1.051
	0.1	1.154	1.591	0.961	1.391	0.853	1.080	0.862	1.111	0.875	1.205
	0.2	1.099	1.538	0.941	1.376	0.861	1.096	0.867	1.150	0.872	1.207
	0.5	1.096	1.438	0.963	1.320	0.880	1.089	0.883	1.133	0.886	1.170
PATHFINDER	1.0	1.081	1.477	0.951	1.343	0.875	1.147	0.877	1.166	0.881	1.191
	2.0	1.095	1.470	1.004	1.346	0.894	1.158	0.895	1.168	0.898	1.208
	5.0	1.071	1.467	0.985	1.347	0.884	1.157	0.885	1.164	0.885	1.205
	0.1	1.050	1.176	1.044	1.122	1.046	1.066	1.046	1.067	1.047	1.069
	0.2	1.063	1.112	1.052	1.082	1.060	1.068	1.060	1.068	1.060	1.069
	0.5	1.065	1.079	1.059	1.066	1.062	1.068	1.062	1.068	1.062	1.069
PIGS	1.0	1.067	1.073	1.058	1.062	1.066	1.068	1.066	1.068	1.066	1.069
	2.0	1.075	1.079	1.062	1.066	1.073	1.077	1.073	1.078	1.073	1.077
	5.0	1.085	1.086	1.074	1.074	1.084	1.086	1.084	1.086	1.084	1.086
	0.1	0.721	1.141	0.552	0.966	0.425	0.842	0.461	0.867	0.502	0.965
	0.2	0.760	1.156	0.631	0.996	0.510	0.864	0.513	0.921	0.563	0.987
MATTER	0.5	0.791	1.172	0.672	1.059	0.560	0.922	0.561	0.982	0.607	1.026
WATER	1.0	0.812	1.199	0.717	1.093	0.591	0.961	0.609	1.015	0.632	1.062
	2.0	0.846	1.230	0.751	1.141	0.633	1.014	0.665	1.056	0.681	1.118
	5.0	0.931	1.274	0.826	1.192	0.701	1.051	0.734	1.101	0.709	1.159

Table B.6: Average number of arcs for BDeu and different MU priors (closer to 1 is better, best in bold).

NETWORK	n/p	Ţ			S = 1/2		c = 1		c=2	MU (	,
		1	10	1	10	1	10	1	10	1	10
	0.1	1.329	1.875	1.040	1.351	0.649	0.736	0.723	0.862	0.911	1.121
	0.2	1.321	1.874	1.049	1.436	0.797	0.909	0.847	1.016	0.974	1.236
ATADM	0.5	1.213	1.775	1.060	1.436	0.885	1.053	0.911	1.140	0.988	1.302
ALARM	1.0	1.180	1.667	1.071	1.426	0.962	1.107	0.983	1.182	1.018	1.337
	2.0	1.098	1.528	1.064	1.377	1.017	1.107	1.023	1.153	1.033	1.266
	5.0	1.086	1.386	1.061	1.252	1.045	1.096	1.048	1.117	1.051	1.182
	0.1	2.339	4.121	1.294	2.510	0.408	0.461	0.445	0.520	0.518	0.659
	0.2	1.764	3.115	1.129	1.963	0.559	0.627	0.582	0.674	0.622	0.789
ANDEC	0.5	1.258	2.236	1.011	1.622	0.676	0.753	0.690	0.814	0.722	0.898
ANDES	1.0	1.154	1.898	0.991	1.496	0.763	0.846	0.774	0.882	0.793	0.947
	2.0	1.063	1.702	0.996	1.399	0.814	0.875	0.819	0.901	0.830	0.956
	5.0	1.046	1.541	<b>0.970</b> 0.788	1.309 <b>0.956</b>	0.859	0.923	0.863 $0.492$	0.942 $0.510$	0.872 $0.914$	$\frac{0.959}{1.122}$
	0.1	1.014	1.304 $1.444$	0.744	0.998	0.528	0.622	0.492 $0.582$	0.708	0.914	1.122 $1.126$
	$0.2 \\ 0.5$	0.744	1.444 $1.132$	0.744	0.950	0.528	0.022 $0.730$	0.582	0.708	0.682	1.120 $1.004$
CHILD	1.0	0.744	1.016	0.736	0.920	0.676	0.730	0.706	0.848	0.032	0.938
CHILD	2.0	0.772	0.994	0.730	0.920 $0.962$	0.796	0.818 $0.912$	0.700	0.934	0.740	0.938 $0.972$
	5.0	0.908	1.034	0.820	1.012	0.130	0.912	0.894	1.012	0.906	1.022
	0.1	1.122	1.158	1.107	1.157	1.115	1.116	1.116	1.116	1.117	1.116
	0.1	1.136	1.169	1.115	1.168	1.115	1.110	1.135	1.110	1.135	1.110 $1.129$
	0.5	1.158	1.189	1.138	1.189	1.158	1.148	1.158	1.148	1.158	1.149
DIABETES	1.0	1.164	1.193	1.149	1.193	1.164	1.152	1.164	1.140 $1.152$	1.164	1.153
DIMBLIES	2.0	1.192	1.264	1.143	1.262	1.191	1.217	1.191	1.218	1.191	1.219
	5.0	1.132	1.322	1.260	1.321	1.281	1.217	1.281	1.210	1.281	1.213
	0.1	0.707	0.880	0.714	0.862	0.633	0.785	0.643	0.802	0.661	0.815
	0.2	0.839	0.880	0.852	0.873	0.800	0.836	0.810	0.840	0.818	0.846
	0.5	0.854	0.886	0.886	0.892	0.845	0.870	0.845	0.873	0.848	0.876
HAILFINDER	1.0	0.884	0.904	0.919	0.901	0.869	0.898	0.872	0.898	0.877	0.900
IIIIIII II III	2.0	0.898	0.942	0.943	0.936	0.897	0.930	0.898	0.930	0.898	0.933
	5.0	0.968	0.978	1.013	0.977	0.964	0.971	0.964	0.972	0.967	0.973
-	0.1	0.972	1.944	0.527	1.202	0.148	0.278	0.174	0.361	0.230	0.502
	0.2	0.786	1.576	0.491	1.039	0.205	0.357	0.224	0.422	0.269	0.552
	0.5	0.680	1.252	0.498	0.922	0.315	0.452	0.333	0.496	0.367	0.603
HEPAR2	1.0	0.653	1.111	0.551	0.875	0.420	0.550	0.438	0.584	0.465	0.655
	2.0	0.668	1.041	0.598	0.873	0.517	0.617	0.533	0.647	0.550	0.708
	5.0	0.729	0.992	0.697	0.887	0.643	0.729	0.652	0.749	0.669	0.783
	0.1	0.663	0.937	0.549	0.779	0.476	0.589	0.508	0.649	0.564	0.761
	0.2	0.674	0.927	0.603	0.819	0.556	0.700	0.575	0.735	0.615	0.820
	0.5	0.700	0.906	0.662	0.830	0.645	0.774	0.651	0.797	0.669	0.830
INSURANCE	1.0	0.776	0.941	0.746	0.870	0.741	0.823	0.746	0.834	0.754	0.863
	2.0	0.811	1.012	0.799	0.941	0.788	0.869	0.789	0.887	0.799	0.931
	5.0	0.887	1.040	0.870	0.994	0.862	0.934	0.867	0.948	0.881	0.947
	0.1	1.062	1.337	0.961	1.112	0.910	0.965	0.921	0.982	0.936	1.016
	0.2	0.992	1.190	0.941	1.044	0.892	0.943	0.899	0.955	0.910	0.974
	0.5	0.985	1.102	0.963	1.014	0.906	0.937	0.912	0.946	0.921	0.960
PATHFINDER	1.0	0.965	1.068	0.951	0.999	0.902	0.940	0.906	0.950	0.912	0.963
	2.0	0.966	1.014	1.004	0.958	0.918	0.919	0.921	0.927	0.925	0.934
	5.0	0.919	0.974	0.985	0.946	0.891	0.918	0.891	0.921	0.893	0.923
	0.1	1.049	1.156	1.044	1.112	1.044	1.039	1.045	1.039	1.045	1.041
	0.2	1.062	1.091	1.052	1.065	1.059	1.043	1.060	1.043	1.060	1.045
	0.5	1.063	1.060	1.059	1.048	1.060	1.048	1.060	1.048	1.061	1.049
PIGS	1.0	1.064	1.051	1.058	1.044	1.063	1.047	1.064	1.047	1.064	1.047
	2.0	1.069	1.074	1.062	1.044	1.068	1.053	1.068	1.053	1.068	1.053
	5.0	1.079	1.061	1.074	1.052	1.079	1.060	1.079	1.060	1.079	1.060
	0.1	0.517	0.882	0.552	0.788	0.384	0.614	0.388	0.654	0.405	0.757
	0.2	0.566	0.903	0.631	0.816	0.442	0.642	0.447	0.683	0.452	0.777
****	0.5	0.610	0.932	0.672	0.882	0.498	0.706	0.502	0.751	0.508	0.856
WATER	1.0	0.627	0.939	0.717	0.899	0.520	0.774	0.502	0.818	0.525	0.895
	2.0	0.672	0.942	0.751	0.907	0.572	0.816	0.573	0.845	0.578	0.884
	5.0	0.736	0.956	0.826	0.927	0.635	0.866	0.635	0.882	0.637	0.906

Table B.7: Average number of arcs for BDs and different MU priors (closer to 1 is better, best in bold).

NEWWORK		U		MU (β	l = 1/2	MU (	c=1)	MU (	c=2	MU (c = 5)	
NETWORK	n/p	1	10	1	10	1	10	1	10	1	10
	0.1	1.67	1.85	1.51	1.69	1.42	1.44	1.43	1.48	1.47	1.58
ALARM	0.2	1.32	1.44	1.29	1.36	1.26	1.28	1.26	1.29	1.28	1.33
	0.5	1.17	1.21	1.16	1.18	1.15	1.15	1.15	1.16	1.15	1.17
	0.1	13.14	18.59	11.90	15.77	10.26	10.19	10.24	10.22	10.26	10.39
ANDES	0.2	10.56	11.96	10.16	11.13	9.72	9.69	9.70	9.72	9.71	9.81
	0.5	9.60	9.96	9.53	9.73	9.47	9.45	9.47	9.45	9.46	9.46
	0.1	2.03	2.30	1.91	2.04	1.73	1.71	1.77	1.77	1.93	2.12
CHILD	0.2	1.66	1.82	1.62	1.68	1.56	1.54	1.57	1.58	1.64	1.75
	0.5	1.40	1.46	1.39	1.42	1.38	1.39	1.39	1.40	1.39	1.43
	0.1	19.40	19.27	19.40	19.26	19.35	19.21	19.35	19.21	19.35	19.21
DIABETES	0.2	19.14	19.13	19.14	19.10	19.16	19.16	19.16	19.16	19.16	19.16
	0.5	19.05	19.04	19.05	19.04	19.07	19.06	19.07	19.06	19.07	19.06
	0.1	5.31	5.23	5.31	5.22	5.33	5.22	5.33	5.22	5.32	5.22
HAILFINDER	0.2	5.13	5.09	5.13	5.08	5.14	5.08	5.14	5.08	5.14	5.08
	0.5	5.01	5.01	5.01	4.99	5.01	4.99	5.01	4.99	5.01	4.99
	0.1	3.73	4.24	3.58	3.90	3.41	3.41	3.41	3.44	3.43	3.50
HEPAR2	0.2	3.45	3.63	3.40	3.51	3.36	3.35	3.36	3.36	3.36	3.39
	0.5	3.32	3.36	3.31	3.33	3.30	3.30	3.30	3.30	3.30	3.31
	0.1	1.59	1.64	1.58	1.61	1.56	1.57	1.56	1.58	1.56	1.60
INSURANCE	0.2	1.46	1.47	1.46	1.47	1.47	1.47	1.46	1.47	1.46	1.47
	0.5	1.38	1.37	1.38	1.37	1.39	1.38	1.39	1.38	1.38	1.38
	0.1	2.51	2.49	2.51	2.49	2.52	2.49	2.51	2.49	2.51	2.49
PATHFINDER	0.2	2.43	2.43	2.43	2.43	2.44	2.43	2.44	2.43	2.44	2.43
	0.5	2.39	2.39	2.39	2.39	2.39	2.39	2.39	2.39	2.39	2.39
	0.1	33.25	33.36	33.24	33.31	33.25	33.25	33.25	33.25	33.25	33.25
PIGS	0.2	33.13	33.16	33.13	33.14	33.16	33.16	33.16	33.16	33.16	33.16
	0.5	33.05	33.05	33.04	33.04	33.07	33.07	33.07	33.07	33.07	33.07
	0.1	1.29	1.30	1.29	1.29	1.29	1.29	1.29	1.29	1.29	1.29
WATER	0.2	1.29	1.29	1.29	1.29	1.29	1.29	1.29	1.29	1.29	1.29
	0.5	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28

Table B.8: Average predictive log-likelihood for BDeu and different MU priors (rescaled by -10000; lower is better, best in bold). n/p = 1.0, 2.0, 5.0 showed the same value for all scores and are omitted for brevity.

NETWORK	/	J	J	MU (β	l = 1/2	MU (	(c=1)	MU (	(c=2)	MU (	(c=5)
NEIWORK	n/p	1	10	1	10	1	10	1	10	1	10
	0.1	1.67	1.80	1.51	1.60	1.42	1.42	1.43	1.44	1.50	1.52
ALARM	0.2	1.35	1.43	1.29	1.34	1.27	1.27	1.27	1.28	1.29	1.31
	0.5	1.17	1.20	1.16	1.17	1.14	1.15	1.14	1.15	1.15	1.16
	0.1	14.75	24.40	11.90	17.77	10.25	10.19	10.24	10.19	10.26	10.34
ANDES	0.2	10.88	13.30	10.16	11.47	9.71	9.68	9.70	9.70	9.71	9.72
	0.5	9.63	10.07	9.53	9.74	9.47	9.45	9.47	9.45	9.46	9.46
	0.1	2.07	2.31	1.91	2.00	1.72	1.71	1.77	1.76	1.97	2.10
CHILD	0.2	1.71	1.88	1.62	1.69	1.57	1.55	1.59	1.58	1.69	1.76
	0.5	1.40	1.46	1.39	1.42	1.39	1.39	1.39	1.40	1.39	1.44
	0.1	19.34	19.26	19.40	19.26	19.29	19.21	19.29	19.21	19.29	19.21
DIABETES	0.2	19.20	19.13	19.14	19.13	19.22	19.15	19.22	19.15	19.22	19.15
	0.5	19.10	19.00	19.05	19.00	19.12	19.02	19.12	19.01	19.12	19.01
	0.1	5.30	5.23	5.31	5.22	5.33	5.22	5.32	5.22	5.31	5.22
HAILFINDER	0.2	5.12	5.08	5.13	5.08	5.14	5.08	5.13	5.08	5.13	5.08
	0.5	5.01	4.99	5.01	4.99	5.01	4.99	5.01	4.99	5.01	4.99
	0.1	3.81	4.68	3.58	4.04	3.41	3.41	3.41	3.43	3.43	3.49
HEPAR2	0.2	3.47	3.74	3.40	3.53	3.36	3.35	3.36	3.36	3.36	3.39
	0.5	3.32	3.37	3.31	3.33	3.30	3.30	3.30	3.30	3.30	3.31
	0.1	1.59	1.66	1.58	1.62	1.56	1.56	1.56	1.56	1.56	1.60
INSURANCE	0.2	1.46	1.49	1.46	1.47	1.46	1.46	1.46	1.47	1.46	1.48
	0.5	1.38	1.38	1.38	1.37	1.39	1.37	1.38	1.38	1.38	1.38
	0.1	2.50	2.49	2.51	2.49	2.51	2.49	2.51	2.49	2.51	2.49
PATHFINDER	0.2	2.43	2.43	2.43	2.43	2.44	2.43	2.44	2.43	2.44	2.43
	0.5	2.39	2.38	2.39	2.38	2.39	2.39	2.39	2.39	2.39	2.39
	0.1	33.24	33.36	33.24	33.31	33.24	33.23	33.24	33.23	33.24	33.23
PIGS	0.2	33.13	33.15	33.13	33.14	33.16	33.15	33.16	33.15	33.16	33.15
	0.5	33.04	33.04	33.04	33.04	33.07	33.07	33.07	33.07	33.07	33.07
	0.1	1.29	1.30	1.29	1.29	1.29	1.30	1.29	1.30	1.29	1.30
WATER	0.2	1.29	1.29	1.29	1.29	1.29	1.29	1.29	1.29	1.29	1.29
	0.5	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28	1.28

Table B.9: Average predictive log-likelihood for BDs and different MU priors (rescaled by -10000; lower is better, best in bold). n/p = 1.0, 2.0, 5.0 showed the same value for all scores and are omitted for brevity.

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