Is a single unique Bayesian network enough to accurately represent your data?

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Abstract—Bayesian network (BN) modelling is extensively used in systems epidemiology. Usually it consists in selecting and reporting the best-fitting structure conditional to the data. A major practical concern is avoiding overfitting, on account of its extreme flexibility and its modelling richness. Many approaches have been proposed to control for overfitting. Unfortunately, they essentially all rely on very crude decisions that result in too simplistic approaches for such complex systems. In practice, with limited data sampled from complex systems, this approach seems too simplistic. An alternative would be to use the Monte Carlo Markov chain model choice ((MC)3), which samples overall possible structures and moves from structure to structure according to its support by the data. Indeed, the posterior probability of any structural feature could be obtained from a Markov chain sample computed from graph structures by

$$E[f|D] \approx \frac{1}{S} \sum_{s=1}^{S} f(G^s), \text{ where } G^s \sim p(G|D)$$  \hspace{1cm} (1)

where $f$ is any structural query, $D$ is the data, $S$ is the set of visited structures $G$, and $p(G|D)$ is the posterior distribution of the structures.

I. INTRODUCTION

Bayesian Networks modelling is becoming more and more popular in systems epidemiology [1], [2]. It is highly suitable for epidemiological datasets that are messy and highly correlated or when it is not clear which variable would be the outcome. It is also well-adapted to contexts where no prior model exists or when experts want a data-driven approach for selecting optimal models. However, in highly interdisciplinary research fields, some concerns have been raised against BN modelling. A fully data-driven approach could select a model that is statistically supported by the data but that does not have plausible epidemiological interpretation. To overcome this limitation, there exists a popular workaround: one can either ban or retain some parts of the structure to account for those biological constrains. This modelling approach thus ends up in a semi-supervised approach. Once this first guiding step is performed, all other arcs are either present or absent in the model.

From practice and modelling perspectives, a major concern of BN modelling is the tendency to overfit the data and to select overly complicated models that generalise poorly. To compensate, parametric or non-parametric approaches prune the selected structure. Usually, a unique and theory-compatible structure is reported. Albeit being popular and accepted, this process makes very crude choices regarding the possible connections in the model and diminishes the range of possible interpretation. Indeed, an arc is either present or absent. This is exceptionally rudimentary considering the massive number of a priori networks.

Classically in statistics, any relationship between variables is given with an estimate of the relationship based on data. A possible counterpart in BN modelling could be the Monte Carlo Markov chain model choice ((MC)3), which samples overall possible structures and moves from structure to structure according to its support by the data. Indeed, the posterior probability of any structural feature could be obtained from a Markov chain sample computed from graph structures by

$$E[f|D] \approx \frac{1}{S} \sum_{s=1}^{S} f(G^s), \text{ where } G^s \sim p(G|D)$$  \hspace{1cm} (1)

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II. OUTLINE OF THE APPROACH

Sampling BN using MCMC algorithms is a complicated task. The classical structural approach makes single-edge operations (addition, deletion and reversal of an edge). It is known that naive structural approaches will fail to efficiently sample BN landscapes in large problems. Indeed, sampling algorithms mix slowly and hardly converge for large problem. A popular solution is to sample from the space of node ordering using order MCMC sampling schemes [3]. But it is not possible to explicitly express priors on graph structures in this context. This is of particular importance in systems epidemiology where the data are usually scarce and, as a result, the posterior depends heavily on the prior choice. Again, from a data analysis point of view, this would weaken the analysis and render it not fully adapted.

Two structurally transparent workarounds have been proposed: the new edge reversal move [4] and Markov blanket resampling [5]. The former advocates to make a reversal move in resampling the parent set. Indeed, the classical reversal move depends on the global configuration of the parents and children, but then fails to propose MCMC jumps that produce valid but very different DAGs in a unique move. The latter workaround applies the same idea but to the entire Markov blanket of a randomly chosen node. Single edge and both structural methods were implemented in MCMCABN.
III. SIMULATION STUDY

To illustrate the usability of the approach for a typical systems epidemiology dataset, we simulate a sparse BN of five nodes and five arcs (Fig. 3). 250, 500, 1000, 10,000 binomial observations were simulated from the DAG. A cache of scores for each possible set of parents was computed for each simulated dataset. The synthetic data was generated using the R package ABN [6]. Afterwards, $10^5$ sampling steps were performed for each dataset. For computational reasons, the starting point of the MCMC chain is the true model and no burn-in phase nor thinning has been considered. All computations were performed using R.

![Fig. 1. Normalized maximal score in functions of the sorted simulated DAGs on a logarithmic scale for different sample sizes.](image1)

Figure 1 illustrates the variability of the scores over the MCMC steps. For visual clarity, the scores are normalized and the MCMC samples have been reordered (by increasing score). As dataset size increases, less variability in term of structure is generated during the MCMC exploration. Because we started at the true model, we observe genuine sampling variability and not burn-in effects.

![Fig. 2. Frequency of MCMC-generated DAGs for different sample sizes.](image2)

Figure 2 shows the frequencies of sampled DAGs ordered by decreasing score of the largest dataset. For this, the posterior consists almost exclusively of four DAGs of relatively similar scores. The truth is captured in 1/3 of the cases. However, 250 observations are not enough to accurately sample the space of DAGs. 1000 observations lead to a substantial improvement of having high frequencies of the dominant DAGs.

IV. DISCUSSION

The proposed approach makes it possible to find the optimal network by MCMC over DAG structures. However, much more efficient algorithms have been proposed and are already implemented in the R package ABN [6]. Thus, the most desirable feature of the presented approach is to enrich the analysis by computing structural queries over the DAG landscape. Examples of such queries are shown in Fig. 3 where, not surprisingly, more observations lead to better structural estimates. Here, the relationships between nodes are not directed.

![Fig. 3. Five-node DAG (left) and summaries of associated structural queries (%)(right). Green indicates where the link is expected and red where it is not.](image3)

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