Approximate learning of high dimensional Bayesian network structures via pruning of Candidate Parent Sets

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Abstract
Score-based algorithms that learn Bayesian Network (BN) structures provide solutions ranging from different levels of approximate learning to exact learning. Approximate solutions exist because exact learning is generally not applicable to networks of moderate or higher complexity. In general, approximate solutions tend to sacrifice accuracy for speed, where the aim is to minimise the loss in accuracy and maximise the gain in speed. While some approximate algorithms are optimised to handle thousands of variables, these algorithms may still be unable to learn such high dimensional structures. Some of the most efficient score-based algorithms cast the structure learning problem as a combinatorial optimisation of candidate parent sets. This paper explores a strategy towards pruning the size of candidate parent sets, aimed at high dimensionality problems. The results illustrate how different levels of pruning affect the learning speed in conjunction to the loss in accuracy in terms of model fitting, and show that aggressive pruning may be required to produce approximate solutions for high complexity problems.

Keywords: structure learning; probabilistic graphical models; pruning.

1. Introduction
A Bayesian Network (BN) (Pearl, 1988) is a probabilistic graphical model represented by a Directed Acyclic Graph (DAG). The structure of a BN captures the relationships between nodes, whereas the conditional parameters between nodes, often specified as a conditional probability distribution, capture the type and magnitude of the relationship between nodes. A BN differs from other graphical models, such as neural networks, in that it offers a transparent solution where the relationships between variables (i.e., arcs) can be interpreted causally. Moreover, the uncertain conditional distributions in BNs can be used for both predictive and diagnostic (i.e., inverse) inference, providing the potential for a higher level of artificial intelligence.

Formally, a BN model represents a factorisation of the joint distribution of random variables
\[ X = (X_1, X_2, \ldots, X_n) \]. Each BN has two elements, structure \( G \) and parameters \( \theta \). Constructing a BN involves both structure learning and parameter learning, and both learning approaches may involve combination of data with knowledge (Amirkhani et al., 2017; Guo et al., 2017). Given observational data \( D \), a complete BN \( \{G, \theta\} \) can be learnt by maximising the likelihood:

\[
P(G, \theta|D) = P(G|D)P(\theta|G, D). \tag{1}
\]
and the parameters of the network can be learnt by maximising

\[ P(\theta|G, D). \]
\[ P(\theta|G, D) = \prod_{i=1}^{n} P(\theta_i|\Pi_i, D) \]  

where, \( \Pi_i \) denotes the parents of node \( X_i \) indicated by structure \( G \). Depending on the prior assumption, the parameter learning process of each node can be solved using Maximum Likelihood estimation given data \( D \), or Maximum A Posteriori estimation given data \( D \) and a subjective prior.

On the other hand, the BN structure learning (BNSL) problem represents a more challenging task in that it cannot be solved by simply maximising the fitting of the local networks to the data. The structure learning process must take into consideration the dimensionality of the model in order to avoid overfitting. In fact, the problem of BNSL is NP-hard, which means that it is generally not possible to perform exhaustive search in the search space of possible graphs, and this is because the number of possible structures grows super-exponentially with the number of nodes. Algorithms that learn BN structures are typically classified into three categories: a) score-based learning that searches over the space of possible graphs and returns the graph that maximises a scoring function, b) constraint-based learning that prunes and orientates edges using conditional independence tests, and c) hybrid learning that combines the above two strategies. In this paper, we focus on the problem of score-based learning.

A score-based algorithm is generally composed of two parts: a) a search strategy that transverses the search space, and b) a scoring function that evaluates a given graph with respect to the observed data. Well-known search strategies in the field of BNSL include the greedy hill-climbing search, tabu search, simulated annealing, genetic algorithms, dynamic programming, A* algorithm, and branch-and-bound strategies. The objective functions are typically based on either the Bayesian score or other model selection scores. Bayesian scores evaluate the posterior probability of the candidate structures and include variations of the Bayesian Dirichlet score, such as the Bayesian Dirichlet with equivalence and uniform priors (BDeu) (Buntine, 1991; Heckerman et al., 1995), and the Bayesian Dirichlet sparse (BDs) (Scutari, 2016). Well-established scores for model selection include the Akaike Information Criterion (AIC) (Akaike, 1973) and the Bayesian Informatic Criterion (BIC), often also referred to as the Minimum Description Length (MDL) (Suzuki, 1993). Other less popular model selection scores include the Mutual Information Test (MIT) (de Campos, 2006), the factorized Normalized Maximum Likelihood (fNML) (Silander et al., 2008), and the quotient Normalized Maximum Likelihood (qNML) (Silander et al., 2018).

Score-based approaches further operate in two different ways. The first approach involves scoring a graph only when the graph is visited by the search method, which typically involves exploring neighbouring graphs and following the search path that maximises the fitting score via arc reversals, additions and removals. The second approach involves generating scores for local networks (i.e., a node and its parents) in advance, and searching over combinations of local networks given the pre-generated scores, thereby formulating a combinatorial optimisation problem. The algorithms that fall in the former category are generally based on efficient heuristics such as hill-climbing, but tend to stuck in local maximum solutions; thereby offering an approximate solution to the problem of BNSL. While algorithms of the latter category are also generally approximate, they can be more easily adjusted to offer exact learning solutions that guarantee to return a graph with score not lower than the global maximum score. This paper focuses on this latter subcategory of score-based learning.

Algorithms such as the Integer Linear Programming (ILP) (Jaakkola et al., 2010; Bartlett and Cussens, 2015) explore local networks in the form of the Candidate Parent Sets (CPSs), usually up to a
bounded maximum in-degree, and offer an exact learning solution. Other exact learning algorithms which cast the BNSL problem as a combinatorial optimisation problem include the Dynamic Programming (DP) (Koivisto and Sood, 2004; Silander and Myllymäki, 2006), the A* algorithm (Yuan and Malone, 2013) and the Branch-and-Bound (B&B) (de Campos and Ji, 2011; van Beek and Hoffmann, 2015). However, exact learning is generally restricted to problems of low complexity. Evidently, the efficiency of these algorithms is determined by the number of CPSs. For example, the ILP algorithm is restricted to CPSs of size up to one million. Moreover, order-based algorithms such as OBS (Teyssier and Koller, 2005), ASOBS (Scanagatta et al., 2015, 2018) and MINOBS (Lee and van Beek, 2017), which are more efficient due to pruning the search space of possible graphs, can still spend hours searching for an approximate solution in problems that involve hundreds of variables.

In this paper we focus on score-based algorithms that learn BN graphs via local learning of CPTs. Specifically, we investigate the dependency between different levels of pruning on CPSs and the loss in accuracy in terms of model fitting. The remainder of this paper is organised as follows: Section 2 provides the problem statement and methodology, Section 3 provides the results, and we provide our concluding remarks and directions for future research in Section 4.

2. Problem Statement and Methodology

Different pruning rules have been proposed to improve the scalability and the efficiency of score-based algorithms that operate on CPSs. Pruning approaches in this context generally aim to reduce the number of CPSs (de Campos and Ji, 2010, 2011; Cussens, 2012; Suzuki, 2017; Correia et al., 2019). The efficacy of a pruning strategy can be significant in the reduction of structure learning runtime, and this depends on both the number of the variables and the number of observations in the data. For example, Table 1 presents a sample of the CPSs of node “0” in the Audio-train data set, which consists of 100 variables and 15,000 observations. If we assume maximum in-degree of 3, this generates \( (C_0^{99} + C_1^{99} + C_2^{99} + C_3^{99}) = 16,180,000 \) possible CPSs. Pruning rules can be used to determine the number of legal CPSs, which for this case is 7,343,077 using the GOBNILP software.

Legal CPSs refer to the CPSs that incorporate only the most probable, in terms of dependency, parents of the child node. The link between a legal CPS and the sample size comes from assessing dependencies between variables. In general, the combinatorial optimisation problem of CPSs remains unsolvable for data sets that are large both in terms of the number of the variables and the sample size of the data.

In this paper, we investigate the effect of different levels of pruning on legal CPSs. The effect is investigated both in terms of the gain in speed and the loss in accuracy, where the loss in accuracy is measured as a discrepancy \( \Delta \) between the fitting scores of two learnt graphs defined as

\[
\Delta = \frac{(S^* - S)}{S^*}
\]

where, \( S \) denotes the BDeu score of a graph generated from pruning and \( S^* \) denotes the BDeu score of the baseline graph generated without pruning. This approach is based on the B&B algorithm proposed by Cassio de Campos (de Campos and Ji, 2011), where the construction of the graph iterates over possible CPSs and starts from the most likely CPS per node. Specifically, we explore the CPSs

1. https://github.com/arranger1044/awesome-spn#dataset
2. https://www.cs.york.ac.uk/aig/sw/gobnilp/
expressed in the format shown in Table 1, where legal CPSs for each node are sorted in a descending order as determined by the local BDeu score. Different levels of pruning are explored by pruning different percentages of legal CPSs for each node, starting from the bottom-ranked CPSs of each node. This means that the search in the space of possible DAGs starts from the most promising parent sets of each node. A valid DAG is ensured by skipping CPSs that lead to cycles. To ensure that a valid DAG can always be produced, the legal CPSs of a node must always include the case of “no parent”.

Pruning is investigated using both exact and approximate learning, depending on the complexity of the experiment. The pruned result is compared to the unpruned result which serves as the baseline outcome. Three different levels of complexity are investigated, which we define as follows:

a) moderate complexity, which assumes less than 1 million legal CPSs per network,
b) high complexity, which assumes more than 1 million and less than 10 million legal CPSs per network, and
c) very high complexity, which assumes more than 10 million legal CPSs per network.

We generate BDeu scores using the GOBNILP software and search for the optimal CPSs using different algorithms. All the experiments in this study were carried on an Intel Core i7-8750H CPU at 2.2 GHz with 16 GB of RAM, where each optimisation is assigned a maximum 9.2 GB of memory. All experiments are restricted to 24 hours of structure learning runtime.

3. Results

3.1 Pruning legal CPSs of moderate complexity

We start the investigation by focusing on BNSL problems of moderate complexity, which we define as CPSs that consists of up to 1 million legal CPSs. This set of experiments is based on six relevant networks taken from the GOBNILP website. Table 2 lists the six networks along with the number of legal CPSs that correspond to setting specified, under the assumption that maximum in-degree is 3.

Tables 3 and 4 present the loss in accuracy from different levels of CPSs pruning. The effect is measured by the discrepancy $\Delta$ as defined in Section 2. For example, in Table 3, 90% pruning of the CPSs on Asia with sample size 100 leads to a graph that deviates 6.7‰, or 0.67%, in terms
Table 2: Moderate complexity case studies (nodes|max in-degree in true networks), with the total number of legal CPSs per network and the average number of legal CPSs per node in the network, for each sample size. The number of CPSs assume a maximum in-degree of 3.

| Pruning | Asia (100) | Asia (1000) | Asia (10000) | Insurance (100) | Insurance (1000) | Insurance (10000) | Water (100) | Water (1000) | Water (10000) |
|---------|------------|-------------|--------------|-----------------|------------------|-------------------|-------------|--------------|--------------|
| 90%     | -6.70‰    | -1.26‰     | -1.33‰      | -30.74‰        | -62.92‰         | -35.26‰          | -11.84‰    | -28.11‰     | -15.50‰     |
| 80%     | -6.70‰    | -1.26‰     | -1.06‰      | -30.74‰        | -37.77‰         | -7.99‰           | -11.15‰    | -19.37‰     | -8.12‰      |
| 70%     | -6.70‰    | -1.26‰     | -1.06‰      | -10.50‰        | -13.80‰         | -7.13‰           | -8.21‰     | -2.99‰      | -0.68‰      |
| 60%     | -6.70‰    | -1.26‰     | -0.72‰      | -8.32‰         | -6.73‰          | -5.32‰           | -6.70‰     | -2.81‰      | -0.44‰      |
| 50%     | -6.68‰    | -1.26‰     | -0.72‰      | -7.94‰         | -4.14‰          | -2.83‰           | -1.24‰     | -1.02‰      | -0.27‰      |
| 40%     | -0.04‰   | -1.26‰     | -0.72‰      | -2.33‰         | -1.28‰          | -2.07‰           | -0.64‰     | 0‰          | 0‰          |
| 30%     | 0‰        | -0.9‰      | -0.25‰      | -2.23‰         | 0‰              | -1.22‰           | -0.32‰     | 0‰          | 0‰          |
| 20%     | 0‰        | 0‰         | 0‰          | 0‰             | 0‰              | 0‰               | 0‰         | 0‰          | 0‰          |
| 10%     | 0‰        | 0‰         | 0‰          | 0‰             | 0‰              | 0‰               | 0‰         | 0‰          | 0‰          |
| 0%      | 0‰        | 0‰         | 0‰          | 0‰             | 0‰              | 0‰               | 0‰         | 0‰          | 0‰          |

Table 3: Results from different levels of pruning as a discrepancy \(\Delta\) from the unpruned score, based on different sample sizes of the Asia, Insurance and Water data sets.

| Pruning | Alarm (100) | Alarm (1000) | Alarm (10000) | Hailfinder (100) | Hailfinder (1000) | Hailfinder (10000) | Carpo (100) | Carpo (1000) | Carpo (10000) |
|---------|-------------|-------------|---------------|-----------------|------------------|-------------------|-------------|-------------|---------------|
| 90%     | -78.39‰    | -46.86‰    | -23.13‰      | -34.15‰        | -8.21‰          | -8.82‰           | -7.88‰     | -3.84‰      | -2.90‰       |
| 80%     | -30.04‰    | -38.71‰    | -14.44‰      | -25.02‰        | -4.17‰          | -6.05‰           | -5.29‰     | -3.13‰      | -1.99‰       |
| 70%     | -18.87‰    | -22.93‰    | -3.88‰       | -10.03‰        | -4.17‰          | -4.23‰           | -4.33‰     | -2.02‰      | -1.94‰       |
| 60%     | -13.55‰    | -14.33‰    | -1.99‰       | -2.23‰         | -2.16‰          | -2.33‰           | -4.33‰     | -1.78‰      | -1.85‰       |
| 50%     | -4.27‰     | -5.23‰     | -1.79‰       | -1.57‰         | -1.60‰          | -0.57‰           | -3.97‰     | -1.73‰      | -1.10‰       |
| 40%     | -3.60‰     | -1.82‰     | -0.20‰       | -1.57‰         | -1.03‰          | -0.57‰           | -2.33‰     | -1.54‰      | -1.06‰       |
| 30%     | -1.06‰     | -0.30‰     | 0‰           | -1.27‰         | -0.20‰          | -0.06‰           | -1.51‰     | -1.17‰      | -0.93‰       |
| 20%     | -1.06‰     | -0.30‰     | 0‰           | -0.07‰         | -0.19‰          | -0.06‰           | -1.01‰     | -0.25‰      | -0.35‰       |
| 10%     | 0‰         | -0.15‰     | 0‰           | 0‰             | 0‰              | 0‰               | 0‰         | 0‰          | 0‰           |
| 0%      | 0‰         | 0‰         | 0‰           | 0‰             | 0‰              | 0‰               | 0‰         | 0‰          | 0‰           |

Table 4: Results from different levels of pruning as a discrepancy \(\Delta\) from the unpruned score, based on different sample sizes of the Alarm, Hailfinder and Carpo data sets.

Overall, the results suggest that higher sample sizes encourage more aggressive pruning. This is reasonable because a higher sample size implies that the ordering of legal CPSs is more accurate and hence, the pruning also becomes more accurate in terms of pruning the least relevant CPSs.
The results show that, in most cases, the loss in accuracy increases faster when pruning exceeds the level of 30%. However, the results from the Hailfinder and Carpo networks suggest that even minor levels of pruning can have a negative impact on the fitting score, however small this impact may be. All the moderate complexity experiments completed search within four minutes, except the case of Carpo-10000 which took approximately twelve minutes to complete. From this, we can conclude that unless the intention is to save seconds or minutes of structure learning runtime, pruning of legal CPSs is less desirable in problems of moderate complexity.

### 3.2 Pruning legal CPSs of high complexity

This subsection reports the results from pruning based on high complexity case studies, which involve problems where the total number of legal CPSs ranges between 1 million and 10 million. For this scenario, we used the real-world data set called Audio-train which consists of 100 variables and 15,000 observations, and which is also retrieved from the GOBNILP website. We used GOBNILP to generate the BDeu scores for CPSs. This process took 90 seconds to complete and GOBNILP returned 7,343,077 legal CPSs.

Because GOBNILP’s ILP algorithm is restricted to CPSs of size less than 1 million, we replaced ILP with an approximate algorithm called MINOBS3. The change from exact to approximate learning was inevitable since exact solutions are only applicable to problems of relatively low complexity. In fact, the results show that even an approximate algorithm such as MINOBS did not manage to complete search (without pruning) within the 24-hour runtime limit. When this happens, we stop the search and obtain the highest scoring graph discovered up to that point in time.

Table 5 presents the results from this set of experiments, which suggest that problems of high complexity may benefit considerably more from pruning compared to problems of moderate complexity. In fact, the results show that it may be safe to perform aggressive pruning on legal CPSs without, or with limited, loss in accuracy, in exchange for a significant reduction in runtime. For example, 90% pruning on the CPSs of the Audio-train data set are found to reduce the optimisation runtime by approximately 21 folds in exchange for a trivial reduction in the BDeu score of the overall graph. Note that the somewhat abnormal runtime result at 60% pruning could be explained by the search initialisation in MINOBS, which is random and will sometimes influence the total runtime.

The increased benefit from pruning observed in the case of the Audio-train dataset can be explained by the higher number of variables in the network. This is because when working with hundreds of variables and a low bounded maximum in-degree (in this case, 3), even 90% pruning of legal CPSs makes it likely that the top three most relevant variables, out of hundreds of variables, will make it into the top 10% of the unpruned CPSs. While these results encourage aggressive pruning of CPSs in cases similar to the Audio-train data set, more experiments are needed to derive confident conclusions.

### 3.3 Pruning legal CPSs of very high complexity

Lastly, we investigate the effect of pruning on a case study with more than 10 million legal CPSs. For this purpose, we used the Reuters-52-train data set taken from the same repository. Reuters-52-train consists of 889 variables and 6,532 observations. As with the high complexity case study, we

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3. https://github.com/kkourin/mobs
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| Pruning (%) | Legal CPSs (graph) | Legal CPSs (per node) | ∆ (%) | Time (secs) |
|-------------|--------------------|-----------------------|-------|-------------|
| 90%         | 734,414            | 7,344                 | -0.002% | 1.035       |
| 80%         | 1,468,717          | 14,687                | 0%    | 2.952       |
| 70%         | 2,203,033          | 22,030                | 0%    | 3.908       |
| 60%         | 2,937,329          | 29,373                | 0%    | 5.344       |
| 50%         | 3,671,663          | 36,717                | 0%    | 4,334       |
| 40%         | 4,405,948          | 44,059                | 0%    | 4,587       |
| 30%         | 5,140,257          | 51,403                | 0%    | 10,028      |
| 20%         | 5,874,560          | 58,746                | 0%    | 10,442      |
| 10%         | 6,608,876          | 66,089                | 0%    | 11,385      |
| 0%          | 7,343,077          | 73,431                | 0%    | 21,643      |

Table 5: Results from different levels of pruning as a discrepancy ∆ from the unpruned score, based on the Audio-train data set, where Time is the number of seconds the algorithm needed to first discover the highest scoring graph over 24 hours of search.

As shown in Table 6, MINOBS did not produce any results in experiments with pruning less than 60% due to running out of memory. This outcome was rather unexpected, considering that MINOBS was proposed for structure learning with thousands of variables. While it is acknowledged that MINOBS is intended for problems with sparse data (Lee and van Beek [2017]), this case study involves hundreds of variables with relatively few observations, and with the maximum in-degree restricted to 2. As a result, the discrepancy ∆ is measured with respect to the result obtained at 60% pruning, which serves as the benchmark score for this case study. While the results show that pruning has had a relatively minor impact on accuracy, the limited number of results do not enable us to derive meaningful conclusions about the effectiveness of this type of pruning in problems of very high complexity. Moreover, the impact on the BDeu score is not entirely consistent across all the experiments, and this may be due to the high dimensionality of this case study. It may be the case that 24 hours of search is not sufficient to explore a reasonably large portion of the search space. This would increase the risk that many high scoring graphs will remain unexplored, thereby leading to inconsistencies in the effect of pruning. Still, the impact on time complexity is more convincing since 90% pruning provided a reduction in runtime of more than 12 hours, in terms of the point in time in which the highest scoring graph was discovered within the 24-hour limit, and with respect to the benchmark result at 60%. These results are useful because they highlight the need for aggressive pruning in problems of very high complexity and invite further investigation.

4. Conclusions

This study investigated the effect of pruning legal CPSs that associate with each node in a BN. The experiments involved different levels of pruning applied to varying degrees of model complexity. The results suggest that it is generally not beneficial to perform pruning of legal CPSs on problems of moderate or lower complexity. This is because low complexity case studies increase the risk to prune relevant parent-sets in exchange for minor improvements in speed. On the other hand, the results from problems of higher complexity show potential for major benefit from this type of prun-
Pruning Legal CPSs (graph) Legal CPSs (per node) ∆ Time (secs)
90% 3,748,921 4,217 -0.046‰ 8,707
80% 7,496,843 8,433 0‰ 40,059
70% 11,244,877 12,649 -0.020‰ 53,047
60% 14,992,798 16,865 0‰ 52,620
50% 18,741,002 21,081 N/A N/A
40% 22,488,769 25,297 N/A N/A
30% 26,236,772 29,513 N/A N/A
20% 29,984,724 33,729 N/A N/A
10% 33,732,728 37,945 N/A N/A
0% 37,479,789 42,159 N/A N/A

Table 6: Results from different levels of pruning as a discrepancy ∆ from the baseline score (in this case, the score obtained at 60% pruning), based on the Reuters-52-train data set, where Time is the number of seconds the algorithm needed to first discover the highest scoring graph over 24 hours of search.

Fitting. This is because these problems tend to incorporate hundreds or thousands of variables which makes it easier to determine and prune irrelevant parent-sets, thereby minorly impacting accuracy in exchange for considerable gains in speed. Importantly, problems of very high complexity are often unsolvable and could benefit enormously from any form of effective pruning. The pruning strategy investigated in this paper applies to any type of score-based learning, including the traditional greedy hill-climbing heuristics where pruned legal CPSs could be used to restrict the path of arc additions.

Future work can be extended in various relevant directions. First, more experiments are be needed to derive stronger conclusions about the effect of this type of pruning, which could be investigated in conjunction with different settings of bounded maximum in-degree, data variables and data observations. Extensive results from experiments that account all these different combinations of settings would potentially enable us to determine optimal levels of pruning that minimise the loss in accuracy and maximise the gain in speed, depending on the complexity of the problem at hand. Other research directions include investigating this type of pruning on ordered-based algorithms, where pruned legal CPSs could potentially be used to restrict the space of possible ordered-based searches. Lastly, other studies have shown that maximising model fitting does not necessarily imply a more accurate causal graph, especially when the data incorporate noise (Constantinou et al., 2020). Thus, this reduces the importance of exact learning, and invites future work where the effect of pruning is judged both in terms of its impact on the fitting score as well as in terms of its impact on the graphical structure.

Acknowledgments

This research was supported by the ERSRC Fellowship project EP/S001646/1 on Bayesian Artificial Intelligence for Decision Making under Uncertainty (Constantinou, 2018), and by The Alan Turing Institute in the UK under the EPSRC grant EP/N510129/1.
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