Data	n	N	T_k (s)	k	T_{EC} (s)	$\lvert\mathcal{G}_k\rvert$	T_{20} (s)	$\lvert\mathcal{G}_{20}\rvert$	$\lvert\mathcal{M}_{20}\rvert$
			0.2	10	0.5	67			
tic tac toe	10	958	2.8	100	6.0	673	0.6	152	24
			70.7	1,000	78.5	7,604			
			3.4	10	12.0	60			
wine	14	178	85.0	100	168.4	448	35.9	8,734	6,262
			3,420.4	1,000	3,064.4	4,142			
			3.3	10	633.5	68			
adult	14	32,561	73.6	100	63,328.9	1,340	9.3	792	19
			2,122.8	1,000	OT	—			
			11.8	10	47,338.4	552			
nltcs	16	3,236	406.6	100	OT	—	125.5	652	326
			13,224.6	1,000	OT	—			
msnbc	17	58,265	ES	—	ES	—	4,018.9	24	24
			26.0	10	18,788.0	200			
letter	17	20,000	909.8	100	OT	—	56,344.8	20	10
			41,503.9	1,000	OT	—			
			34.1	10	101.9	30			
voting	17	435	1,125.7	100	1,829.2	3,392	6.0	621	207
			38,516.2	1,000	42,415.3	3,665			
			33.5	10	99.8	52			
zoo	17	101	1,041.7	100	1,843.4	100	8,418.8	29,073	6,761
			41,412.1	1,000	OT	—			
			351.2	10	872.3	89			
hepatitis	20	155	13,560.3	100	20,244.7	842	441.4	28,024	3,534
			OT	1,000	OT	—			
			3,908.2	10	OT	—			
parkinsons	23	195	OT	100	OT	—	1,515.9	150,000	42,448
			OT	1,000	OT	—			
autos	26	159	OM	1	OM	—	OT	—	—
insurance	27	1,000	OM	1	OM	—	8.3	1,081	133

Table 2: The search time T and the number of collected networks k, $\lvert\mathcal{G}_k\rvert$ and $\lvert\mathcal{G}_{20}\rvert$ for KBest, KbestEC and GOBNILP_dev (BF = 20) using BDeu, where n is the number of random variables in the dataset, N is the number of instances in the dataset, OM = Out of Memory, OT = Out of Time and ES = Error in Scoring. Note that $\lvert\mathcal{G}_k\rvert$ is the number of DAGs covered by the k-best MECs in KBestEC and $\lvert\mathcal{M}_{20}\rvert$ is the number of MECs in the networks collected by GOBNILP_dev.

lar posterior probabilities to the best network. Although the desired level of BF for a study, like the p-value, is often determined with domain knowledge, the proposed approach, given sufficient samples, will produce meaningful results that can be used for further analysis.

Bayes Factor vs. k-Best

In this section, we compare our approach with published solvers that are able to find a subset of top-scoring networks with the given parameter k. The solvers under consideration are KBest_12b[5] from (**?**), KBestEC[6] from (**?**), and GOBNILP 1.6.3 (**?**), referred to as KBest, KBestEC and GOBNILP below. The first two solvers are based on the dynamic programming approach introduced in (**?**). Due to the lack of support for BIC in KBest and KBestEC, only BDeu with a equivalent sample size of one is used in corresponding experiments.

The most recent stable version of GOBNILP is 1.6.3 that works with SCIP 3.2.1. The default configuration is used and experiments are conducted for both BIC and BDeu scoring functions. However, the k-best results are omitted here due to its poor performance. Despite that GOBNILP can iteratively find the k-best networks in descending order by adding linear constraints, the pruning rules designed to find the best network are turned off to preserve sub-optimal networks. In fact, the memory usage often exceeded 64 GB during the initial ILP formulation, indicating that the lack of pruning rules posed serious challenge for GOBNILP. GOBNILP_dev, on the other hand, can take advantage of the pruning rules presented above in the proposed BF approach and its results compare favorably to KBest and KBestEC.

The experimental results of KBest, KBestEC and GOBNILP_dev are reported in Table 2, where n is the number of random variables in the dataset, N is the number of instances in the dataset, and k is the number of top scoring networks. The search time T is reported for KBest, KBestEC and GOBNILP_dev (BF = 20). The number of DAGs covered by the k MECs $\lvert\mathcal{G}_k\rvert$ is reported for KBestEC. In comparison, the last two columns are the number of found networks $\lvert\mathcal{G}_{20}\rvert$ and the number of MECs $\lvert\mathcal{M}_{20}\rvert$ using the BF approach with a given BF of 20 and BDeu scoring function.

As the number of requested networks k increases, the

[5] http://web.cs.iastate.edu/~jtian/Software/UAI-10/KBest.htm

[6] http://web.cs.iastate.edu/~jtian/Software/AAAI-14-yetian/KBestEC.htm

search time for both KBest and KBestEC grows exponentially. The KBest and KBestEC are designed to solve problems of size fewer than 20[7], and so they have some difficulty with larger datasets. They also fail to generate correct scoring files for msnbc. KBestEC seems to successfully expand the coverage of DAGs with some overhead for checking equivalence classes. However, KBestEC took much longer than KBest for some instances, e.g., nltcs and letter, and the number of DAGs covered by the found MECs is inconsistent for nltcs, letter and zoo. The search time for the BF approach is improved over the k-best approach except for datasets with very large sample sizes. The generalized pruning rules are very effective in reducing the search space, which then allows GOBNILP_dev to solve the ILP problem subsequently. Comparing to the improved results in (**?**, **?**; **?**), our approach can scale to larger networks if the scoring file can be generated.[8]

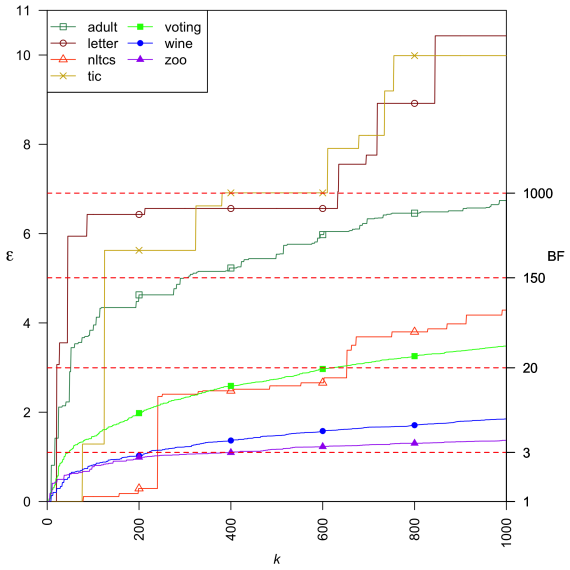

Figure 2: The deviation ϵ from the optimal BDeu score by k using results from KBest. The corresponding values of the BF ($\epsilon = \log(BF)$, see Equation 3) are presented on the right. For example, if the desired BF value is 20, then all networks falling below the dash line at 20 are credible.

Now we show that different datasets have distinct score patterns in the top scoring networks. The scores of the 1,000-best networks for some datasets in the KBest experiment are plotted in Figure 2. A specific line for a dataset indicates the deviation ϵ from the optimal BDeu score by the kth-best network. For reference, the red dash lines represent different levels of BFs calculated by $\epsilon = \log BF$ (See Equation 3). The figure shows that it is difficult to pick a value for k *a priori* to capture the appropriate set of top scoring networks. For a few datasets such as adult and letter, it only takes fewer than 50 networks to reach a BF of 20, whereas zoo needs more than 10,000 networks. The sample size has a significant effect on the number of networks at a given BF since the lack of data leads to many BNs with similar probabilities. It would be reasonable to choose a large value for k in model averaging when data is scarce and vice versa, but only the BF approach is able to automatically find the appropriate and credible set of networks for further analysis.

[7]Obtained through correspondence with the author.

[8]We are unable to generate BDeu score files for datasets with over 30 variables.

Conclusion

Existing approaches for model averaging for Bayesian network structure learning either severely restrict the structure of the Bayesian network or have only been shown to scale to networks with fewer than 30 random variables. In this paper, we proposed a novel approach to model averaging inspired by performance guarantees in approximation algorithms that considers all networks within a factor of optimal. Our approach has two primary advantages. First, our approach only considers *credible* models in that they are optimal or near-optimal in score. Second, our approach is significantly more efficient and scales to much larger Bayesian networks than existing approaches. We modified GOBNILP (**?**), a state-of-the-art method for finding an optimal Bayesian network, to implement our generalized pruning rules and to find all *near*-optimal networks. Our experimental results demonstrate that the modified GOBNILP scales to significantly larger networks without resorting to restricting the structure of the Bayesian networks that are learned.

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