

# Predicting the Hardness of Learning Bayesian Networks

Brandon Malone and Kustaa Kangas and Matti Järvisalo and Mikko Koivisto and Petri Myllymäki  
Helsinki Institute for Information Technology & Department of Computer Science, University of Helsinki, Finland  
{brandon.malone, juho-kustaa.kangas, matti.jarvisalo, mikko.koivisto, petri.myllymaki}@helsinki.fi

## Abstract

There are various algorithms for finding a Bayesian network structure (BNS) that is optimal with respect to a given scoring function. No single algorithm dominates the others in speed, and, given a problem instance, it is *a priori* unclear which algorithm will perform best and how fast it will solve the problem. Estimating the runtimes directly is extremely difficult as they are complicated functions of the instance. The main contribution of this paper is characterization of the empirical hardness of an instance for a given algorithm based on a novel collection of non-trivial, yet efficiently computable features. Our empirical results, based on the largest evaluation of state-of-the-art BNS learning algorithms to date, demonstrate that we can predict the runtimes to a reasonable degree of accuracy, and effectively select algorithms that perform well on a particular instance. Moreover, we also show how the results can be utilized in building a portfolio algorithm that combines several individual algorithms in an almost optimal manner.

## 1 Introduction

Since the formalization and popularization of Bayesian networks (Pearl 1988), much research has been devoted to learning them from data. Cast as a problem of optimizing a score function for given data, the structure learning problem is notoriously (NP-)hard, chiefly due to the acyclicity (DAG) constraint imposed on the graph structure to be learned (Chickering 1996). Consequently, early work has focused on local search algorithms which unfortunately are unable to provide guarantees on the quality of the produced network; this uncertainty hampers the use of the network in probabilistic inference or causal discovery.

The last decade has, however, raised hopes of solving larger instances to optimum. The first *solvers* of this kind adopted a dynamic programming (DP) approach (Ott, Imoto, and Miyano 2004; Koivisto and Sood 2004; Singh and Moore 2005; Silander and Myllymäki 2006) to avoid exhaustive search in the space of DAGs. Later algorithms have expedited the DP algorithms using admissible best-first heuristics ( $A^*$ ) (Yuan and Malone 2013) or employed branch and bound (BB) (de Campos and Ji 2011) and integer linear programming (ILP) (Jaakkola et al. 2010; Cussens 2011; Bartlett and Cussens 2013).

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Due to the intrinsic differences between the algorithmic approaches underlying the solvers, it is not surprising that their relative efficiency varies on a per-instance basis. To exemplify this, a comparison of the runtimes of two current state-of-the-art solvers, GOBNILP (ILP-based) and URLearning ( $A^*$ -based), is illustrated in Fig. 1 using typical benchmark datasets. Evidently, neither of these two solvers dominates the other, as there clearly are instances on which one solver is much more efficient than the other.

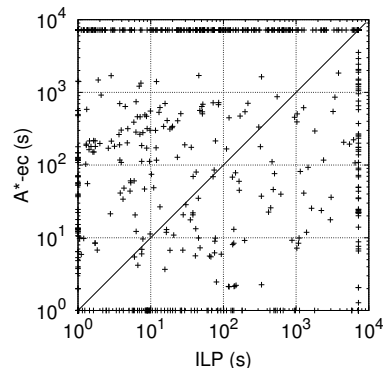


Figure 1: Comparison of two state-of-the-art algorithms for finding an optimal Bayesian network. Runtimes below 1 or above 7200 seconds are rounded to 1 and 7200, respectively. See Sect. 5 for descriptions of the solvers and the datasets.

Fig. 1 suggests that, to improve over the state of the art, an alternative to developing yet another solver is to design *hybrid* algorithms, or *algorithm portfolios*, which would ideally combine the best-case performance of both of the ILP- and  $A^*$ -based solvers. Indeed, in this work we do not focus on developing or improving an individual algorithmic approach. Instead, we aim to predict the relative and absolute performance of different types of algorithmic approaches.

To explain the observed orthogonal performance characteristics shown in Fig. 1, it has been suggested, roughly, that typical instances can be solved to optimum by  $A^*$ , if the *number of variables*  $n$  is at most 40, and by ILP if the number of so-called *candidate parent sets*  $m$  is not very large.

Unfortunately, beyond this rough characterization, the practical time complexity of the fastest algorithms is currently poorly understood. The gap between the analytic worst-case and best-case bounds is very large, and typical in-

stances fall somewhere in between. Moreover, the sophisticated search heuristics employed by the algorithms are quite sensitive to small variations in the instances, which results in somewhat chaotic looking behavior of runtimes. Even the following basic questions are open:

- Q1** Are the simple features, the number of variables  $n$  and the number of candidate parent sets  $m$ , sufficient for determining which of the available solvers is fastest for a given instance?
- Q2** Are there other efficiently computable features that capture the hardness of the problem significantly more accurately than  $n$  and  $m$  alone?

In this paper, we answer both these questions in the affirmative. Our results are empirical in that they rely on training and testing a model with a large set of problem instances collected from various sources. We answer Q1 by learning a simple, yet nontrivial, model that accurately predicts the fastest solver for a given instance based on  $n$  and  $m$  only. We show how this yields an algorithm portfolio that almost always runs as fast as the fastest algorithm, thus significantly outperforming any fixed algorithm on a large collection of instances. However, a closer inspection reveals that the predicted runtimes often differ from the actual runtimes by one to two orders of magnitude. To address this issue and answer Q2, we introduce and study several additional features that potentially capture the hardness of the problem more accurately for a given solver. We focus on two specific solvers, an A\* implementation (Yuan and Malone 2013) and ILP implementation (Bartlett and Cussens 2013), as these turn out to dominate the other solvers in our empirical study. In particular, we show that learning models with a much wider variety of features yields significant improvement in the prediction accuracy: by an order of magnitude for A\* and close to that for ILP. Significant in its own right, the empirical work associated with this paper also provides the most elaborate empirical evaluation of state-of-the-art solvers to date.

**Related Work** The idea of learning to predict an algorithm’s runtime from empirical data is not new. Rice (1976) proposed feature-based modeling to facilitate the selection of the best-performing algorithm for a given problem instance, considering various example problems. Later works (Carbonell et al. 1991; Fink 1998; Lobjois and Lemaître 1998) demonstrated the efficacy of applying machine learning techniques to learn models from empirical performance data. A Bayesian approach was proposed by Horvitz et al. (2001). More recently, empirical hardness models (Leyton-Brown, Nudelman, and Shoham 2002) have been used in solver portfolios for various NP-hard problems, such as Boolean satisfiability (SAT) (Xu et al. 2008), constraint programming (Gebroers et al. 2005), and Quantified Boolean formulas (Pulina and Tacchella 2008). To the best of our knowledge, for the problem of learning Bayesian networks, the present work is the first to adopt the approach.

## 2 Learning Bayesian Networks

A Bayesian network  $(G, P)$  consists of a directed acyclic graph (DAG)  $G$  on a set of random variables  $X_1, \dots, X_n$

and a joint distribution  $P$  over the  $X_i$ s that factorizes into a product of the conditional distributions  $P(X_i|G_i)$ . Here  $G_i$  is the set of parents of  $X_i$ ; a variable  $X_j$  is a *parent* of  $X_i$ , and  $X_i$  a *child* of  $X_j$ , if  $G$  contains an arc from  $X_j$  to  $X_i$ .

Structure learning in Bayesian networks concerns finding a DAG  $G$  that best fits some observed data on the variables. A good fit can be specified by a real-valued scoring function  $s(G)$ . Frequently used scoring functions, such as those based on (penalized) likelihood, MDL, Bayesian principles (e.g., BDeu and other forms of marginal likelihood), decompose into a sum of local scores  $s_i(G_i)$  for each variable and its parents (Heckerman, Geiger, and Chickering 1995). For each  $i$  the local scores are defined for all the  $2^{n-1}$  possible parent sets. This number is greatly reduced by enforcing a small upper bound for the size of the parent sets  $G_i$  or by pruning (de Campos and Ji 2011), as preprocessing, parent sets that provably cannot belong to an optimal DAG, resulting in a collection of *candidate parent sets* denoted by  $\mathcal{G}_i$ .

This motivates the following formulation of the *Bayesian network structure learning* problem (BNSL): given local scores  $s_i(G_i)$  for a collection of candidate parent sets  $G_i \in \mathcal{G}_i$ , for  $i = 1, \dots, n$ , find a DAG  $G$  that minimizes the score  $s(G) = \sum_i s_i(G_i)$ . Along with the number of variables  $n$ , another key parameter describing the size of the input is the total number of candidate parent sets  $m = |\mathcal{G}_1| + \dots + |\mathcal{G}_n|$ .

## 3 Capturing Hardness

The *hardness* of a BNSL instance, relative to a given solver, is the runtime of the solver on the instance. This extends to a set of solvers by taking the minimum of the solvers’ runtimes. As long as we consider only deterministic solvers, the hardness is hereby a well-defined mapping from BNSL instances to real numbers (extended with  $\infty$ ), even if presumably computationally hard to evaluate.

We aim to find a *model* that approximates the hardness function and is efficient to evaluate for any given instance. To this end, we work with the hypothesis that an accurate model can be built based on a small set of efficiently computable *features* of BNSL instances. We can then learn the model by computing the feature values and collecting empirical runtime data from a set of BNSL instances. In what follows, we will first introduce several candidate features that are potentially informative about the hardness of BNSL instances for one or more solvers. A vast majority of these features have not been previously considered for characterizing the difficulty of BNSL. We then explain how we learn a hardness model and estimate its prediction accuracy.

### Features for BNSL

We consider several features which naturally fall into four categories, explained next, based on the strategy used to compute them: **Basic**, **Basic extended**, **Lower bounding**, and **Probing**. Table 1 lists the features in each category.

The **Basic** features include the number of variables  $n$  and the mean number of candidate parent sets per variable,  $m/n$ , that can be viewed as a natural definition of the “density” of an instance. The features in **Basic extended** are other simple features that summarize the size distribution of the collections  $\mathcal{G}_i$  and the parent sets  $G_i$  in each  $\mathcal{G}_i$ . In the **Lower**

**bounding** category, the features reflect statistics from a directed graph that is an optimal solution to a relaxation of the original BNSL problem. In the **Simple LB** subcategory, a graph is obtained by letting each variable select its best parent set according to the scores. Note that the resulting graph may contain cycles and that the associated score is a lower bound on the score of an optimal DAG. Many of the reviewed state-of-the-art solvers use this lower bounding technique; however, they have not used this information to estimate the difficulty of a given instance. The features summarize structural properties of the graph: in- and out-degree distribution over the variables, and the number and size of non-trivial strongly connected components (SCCs). In the **Pattern database LB** subcategory, the features are the same but the graph is obtained by solving a more sophisticated relaxation of the BNSL problem using the *pattern databases* technique (Yuan and Malone 2012).

Probing refers to running a solver for several seconds and collecting statistics about its behavior during the run. We consider three probing strategies: greedy hill climbing with a TABU list and random restarts, an anytime variant of A\* (Malone and Yuan 2013), and the default version of ILP (Bartlett and Cussens 2013). All of these algorithms have anytime characteristics, so they can be stopped at any time

and output the best DAG found so far. Furthermore, the A\* and ILP implementations give guaranteed error bounds on the quality of the found DAGs; an error bound can also be calculated for the DAG found using greedy hill climbing by using the lower bounding techniques discussed above. Probing is implemented in practice by running each algorithm for 5 seconds and then collecting several features, including in- and out-degree statistics and error bound. We refer to these feature subcategories of **Probing** as **Greedy probing**, **A\* probing**, and **ILP probing**, respectively.

## Model Training and Evaluation

Based on the features discussed in the previous section, we trained models to predict the runtime of an instance of BNSL for a particular solver. As the models, we considered both reduced error pruning trees (REP trees) (Quinlan 1987) and M5' trees (Wang and Witten 1997). Briefly, REP trees are decision trees which contain a single value in each leaf; that value is predicted for all instances which reach that leaf. M5' trees are also decision trees; however, each leaf in these trees contains a linear equation which is used to calculate predictions for instances which reach that leaf. We chose these decision tree models because of their interpretability, compared to techniques such as neural networks or support vector machines, and because of their flexibility, compared to linear regression and less expressive model classes.

We evaluated the portfolios using the standard 10-fold cross-validation technique. That is, the data is partitioned into 10 non-overlapping subsets. In each fold, 9 of the subsets are used to train the model, and the remaining set is used for testing; each subset is used as the testing set once. For the instances in the testing set, we predicted the runtime of each solver using the model learned with the training set. We then either selected the solver with the lowest predicted runtime (and examined its actual runtime against the runtime of the fastest solver) or compared the predicted runtimes to the actual runtimes. The overall performance of the portfolio is the union of its performance on each test subset.

## 4 Experiment Setup

### Solvers

Our focus is on *complete* BNSL solvers that are capable of producing guaranteed-optimal solutions. Specifically, we evaluate three complete approaches: Integer-Linear Programming (ILP), A\*-based state-space search (A\*), and branch-and-bound (BB). The non-default parameterizations of the solvers were suggested to us by the solver developers.

**ILP.** We use the GOBNILP solver, version 1.4.1 (<http://www.cs.york.ac.uk/aig/sw/gobnilp/>) as a representative for ILP. GOBNILP uses the SCIP framework (<http://scip.zib.de/>) and an external linear program solver; we used SCIP 3.0.1 and SoPlex 1.7.1 (<http://soplex.zib.de/>). In the experiments reported in this paper, we consider two options for GOBNILP. First, in addition to using nested integer programs, it can either search for BNSL-specific cutting planes using graph-based cycle finding algorithms (ILP) or not (ILP-nc). Second, it can either

Table 1: BNSL features

<b>Basic</b>
1. <b>Number of variables</b>
2. <b>Mean number of CPSs</b> (candidate parent sets)
<b>Basic extended</b>
3–5. <b>Number of CPSs</b> max, sum, sd (standard deviation)
6–8. <b>CPS cardinalities</b> max, mean, sd
<b>Lower bounding</b>
<i>Simple LB</i>
9–11. <b>Node in-degree</b> max, mean, sd
12–14. <b>Node out-degree</b> max, mean, sd
15–17. <b>Node degree</b> max, mean, sd
18. <b>Number of root nodes</b> (no parents)
19. <b>Number of leaf nodes</b> (no children)
20. <b>Number of non-trivial SCCs</b> (strongly connected components)
21–23. <b>Size of non-trivial SCCs</b> max, mean, sd
<i>Pattern database LB</i>
24–38. The same features as for <i>Simple LB</i> but calculated on the graph derived from the pattern databases
<b>Probing</b>
<i>Greedy probing</i>
39–41. <b>Node in-degree</b> max, mean, sd
42–44. <b>Node out-degree</b> max, mean, sd
45–47. <b>Node degree</b> max, mean, sd
48. <b>Number of root nodes</b>
49. <b>Number of leave nodes</b>
50. <b>Error bound</b> , derived from the score of the graph and the pattern database lower bound
<i>A* probing</i>
51–62. The same features as for <i>Greedy probing</i> but calculated on the graph learned with A* probing
<i>ILP probing</i>
63–74. The same features as for <i>A* probing</i> but calculated on the graph learned with ILP probing

enforce a total ordering on the variables (-to) or not. In total, we evaluated four parameterizations of the GOBNILP implementation (ILP, ILP-nc, ILP-to, ILP-nc-to).

**A\*.** We use the URLearning solver (<http://url.cs.gc.cuny.edu/software/URLearning.html>) as a representative for A\*. The URLearning implementation of A\* includes several options which affect its performance on different instances: it can use either a list (A\*) or a tree (A\*-tree) for internal computations; it can use either static pattern databases, dynamic pattern databases (-ed3) or a combination of the two (-ec); pruning behavior is controlled by using an anytime variant (-atw) or not. In total, we considered six parameterizations of the URLearning implementation (A\*, A\*-ed3, A\*-ec, A\*-tree, A\*-atw, A\*-atw-tree).

**BB.** We use the sl solver (<http://www.ecse.rpi.edu/~cvrl/structlearning.html>) as a representative of BB. The sl implementation does not expose any parameters to control its behavior.

## Benchmark Datasets

Our training data includes 48 distinct datasets:

- Datasets sampled from benchmark Bayesian networks, downloaded from <http://www.cs.york.ac.uk/aig/sw/gobnilp/>. 19 datasets.
- Datasets originating from the UCI repository (Bache and Lichman 2013). 19 datasets.
- Datasets sampled from synthetic Bayesian networks. We generated random networks of varying number of nodes (20–60) and edges (80–150), and sampled 2000 data points from each. 7 datasets.
- Datasets we compiled by collecting letter and word occurrences in log files. 3 datasets.

We preprocessed each dataset by removing all continuous variables, variables with very large domains (e.g. unique identifiers), and variables that take on only one value. We considered 5 different scoring functions<sup>1</sup>: BDeu with the Equivalent Sample Size parameter selected from {0.1, 1, 10, 100} and the BIC scores. For each dataset and scoring function, we generated scores with parent limits ranging from 2 to up to 6. Due to score pruning, some parent limits for some datasets result in the same set of local scores; we removed these duplicates. In total, we obtained 713 distinct instances. The size of the datasets ranged from about 100 records to over 60,000 records. For portfolio construction we removed very easy instances (solved within 5 seconds by all solvers) as uninteresting, and instances on which all solvers failed, leaving 586 instances<sup>2</sup>.

For running the experiments we used a cluster of Dell PowerEdge M610 computing nodes equipped with two 2.53-GHz Intel Xeon E5540 CPUs and 32-GB RAM. For each individual run, we used a timeout of 2 hours and a 28-GB memory limit. We treat the runtime of any instance as 2 hours if a solver exceeds either the time or memory limit.

<sup>1</sup>In our experiments, the results were not very sensitive to the scoring function, except its effect on the number of CPSs, so our results can generalize to other decomposable scores as well.

<sup>2</sup>This is in line with related work on portfolio construction in other domains such as SAT (Hutter et al. 2014).

## 5 Portfolios for BNSL

This section focuses on the construction of practical BNSL solver portfolios in order to address question Q1. Optimal portfolio behavior is to always select the best-performing solver for a given instance. As the main results, we will show that, perhaps somewhat surprisingly, it is possible to construct a practical BNSL solver portfolio that is close-to-optimal using only the **Basic** features.

As the basis of this work, we ran all the solvers and their parameterizations on all the benchmark instances. Fig. 2 shows the number of instances for which each solver was the fastest. Here we note that, among the ILP parameterizations, the default version performs the best. For A\*, the A\*-ec parameterization outperforms the other variants; more details are available in an online supplement at <http://bnportfolio.cs.helsinki.fi/>. The performance of BB is in general inferior to the other solvers; in the following we will focus on ILP and A\*-ec. However, recall Fig. 1: while ILP is clearly best measured in the number of instances solved the fastest, the performance of ILP on a per-instance basis is very much orthogonal to that of A\*. We now show that a simple BNSL solver portfolio can capture the best-case performance of *both* of these approaches.

### A Very Simple Solver Portfolio

We found that using only the **Basic** features (number of variables and mean number of candidate parent sets) are enough to construct a highly efficient BNSL solver portfolio. We emphasize that, while on an intuitive level the importance of these two features may be to some extent unsurprising, such intuition does not directly translate into an actual predictor that would close-to-optimally predict the best-performing solver. Moreover, only *two solver parameterizations*, ILP and A\*-ec are enough for reaching close-to-optimal performance when compared to *all* the solvers and their parameterizations we considered.

Fig. 3 shows the performance of each individual solver parameterization, as well as the Virtual Best Solver (VBS), which is the theoretically optimal portfolio which always selects the best algorithm, constructed by selecting *a posteriori* the fastest solver for each input instance. “portfolio” is our simple portfolio which uses only the **Basic** features and the ILP and A\*-ec solvers, constructed and evaluated as described in Sect. 3. REP trees were the base model in this

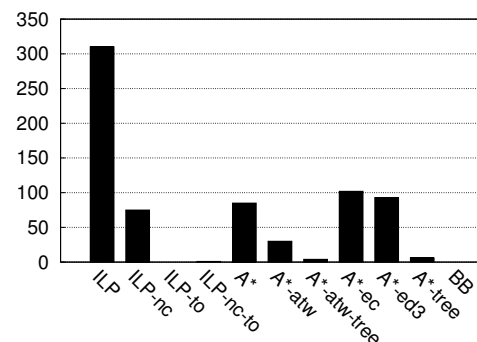


Figure 2: VBS contributions of each solver, i.e., the number of instances for which a solver was fastest.

Table 2: The cumulative runtimes of each solving strategy on all instances. Instances which failed count as 7200s.

Algorithm	Cumulative runtime (s)
VBS	140, 213
portfolio	212, 237
ILP	661, 539
A*-ec	1, 917, 293
BB	4, 149, 928

portfolio (M5' trees are discussed in Sect. 6). As Table 2 shows, the performance of our simple portfolio is very close to the theoretically optimal performance of VBS and greatly outperforms the individual solvers.

For more in-depth understanding, Fig. 4 gives more insight into the effect of the **Basic** features on the solver runtimes. We observe that the runtimes of A\*-ec and ILP correlate well with the number of variables (Fig. 4, left) and the mean number of candidate parent sets (Fig. 4, center).

## 6 Predicting Runtimes

To address Q2, i.e. the harder task of predicting per-instance runtimes of individual solvers, and investigate the effect of the feature sets (cf. Sect. 3) on runtime prediction accuracy.

As just shown, the **Basic** features can effectively distinguish between solvers to use on a particular instance of BNSL. However, notable improvements in runtime prediction accuracy are gained by employing a much wider range of features. In the following we present prediction results for the REP tree models; see the online supplement for results using M5' trees. Fig. 5 (left) compares the actual runtimes for A\*-ec to the predictions made by the REP tree model trained using only the **Basic** features. The model clearly splits the instances into only a few bins and predicts the same runtime for all instances in the bin. The actual runtime ranges are quite wide within each bin. For example, for the bin with predictions near 80 seconds, the actual runtimes span from around 5 seconds to about an hour. Even though these predictions allow for good portfolio behavior, they are not useful to estimate actual runtime.

On the other hand, Fig. 5 (right) shows the same comparison for models learned using **A\* probing** features (1–38, 51–62). Many more of the predictions fall along or near the main diagonal. That is, the larger, more sophisticated feature set results in more accurate runtime predictions. We ob-

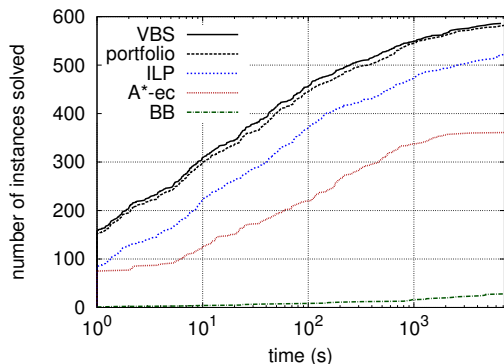


Figure 3: Solver performance: VBS, our simple portfolio, ILP, A\*-ec, and BB.

served similar, though less pronounced, trends for ILP (see the online supplement for details).

We also evaluated the impact of incrementally adding sets of features. Fig. 6 shows how the prediction error changes as we incrementally add **Basic** (features 1–2), **Basic extended** (1–23), **Lower bounding** (1–38), and the relevant probing features for both A\*-ec (1–38, 51–62) and ILP (1–38, 63–74); results for **Greedy probing** and *all* features fall in-between these; see the online supplement for details. The figure clearly shows that some features help more than others for the different algorithms. For example, the **Basic extended** features do not improve the A\*-ec predictions compared to the **Basic** features. On the other hand, the extra information about CPSs significantly improves the ILP predictions. The size and difficulty of the linear programs solved by ILP are directly affected by the CPSs, so the performance of our predictor agrees with our intuition about how the algorithm behaves. Similarly, the addition of the **Lower bounding** features greatly improves the predictions of A\*-ec compared to the **Basic** and **Basic extended** features. The efficacy of the lower bound heuristics directly impacts the performance of A\*-ec. Our predictor again effectively exploits features we intuitively expect to characterize runtime behavior. Probing offers a glimpse at the true runtime behavior of the algorithms, and the predictor leverages this information to further improve prediction accuracy. The results clearly show that predictions using the **Basic** features are much worse than those incorporating the other features. As in Fig. 5, we see that the more expressive features are necessary for accurate predictions.

Following (Xu et al. 2008), we also trained models which used multiplicative pairs of features (for all combinations of feature sets). We observed similar trends regardless of whether the pairs were included; see the online supplement for details. We also evaluated the prediction accuracy using all subsets of features mentioned in Sect. 3. We observed similar and expected results. For example, ILP probing features did not improve A\*-ec predictions, and supersets of the above features yielded similar prediction results.

### REP Tree Characteristics

For additional insight, we look at the complexity of the learned REP trees to predict the runtimes for A\*-ec and ILP. As Table 3 shows, for A\*-ec, given the simple features, the trees are rather simple, but they become somewhat more

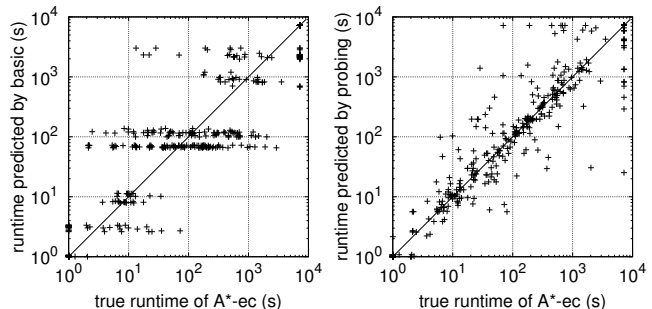


Figure 5: Predicted v actual runtimes for A\*-ec using **Basic** features only (left) and all features up to A\* probing (right).

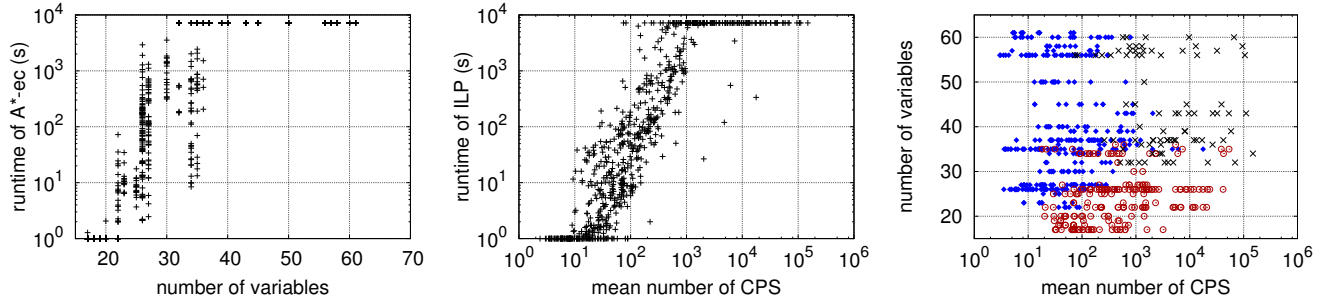


Figure 4: Correlation between the **Basic** features and the runtimes of A\*-ec (left) and ILP (center). On the right, the two features plotted against each other and marked depending on whether A\* is faster ( $\odot$ ), ILP is faster ( $\blacklozenge$ ), or both solvers fail ( $\times$ ).

Table 3: The size of the REP trees learned for A\*-ec and ILP.

Algorithm	Features	Depth	Size (nodes)
A*-ec	<b>Basic</b>	$3.70 \pm 0.48$	$11.90 \pm 1.20$
A*-ec	<b>A* probing</b> (1–38, 51–62)	$12.60 \pm 1.07$	$156.40 \pm 17.69$
ILP	<b>Basic</b>	$12.60 \pm 2.80$	$157.20 \pm 16.23$
ILP	<b>ILP probing</b> (1–38, 63–74)	$11.90 \pm 1.20$	$206.40 \pm 24.68$

complex as new features are added. On the other hand, for ILP, the trees using the additional features do not grow in depth much. The sizes of the trees show similar behavior<sup>3</sup>.

Table 4 shows how often specific features were selected. A feature is rarely selected for predicting both solvers. This further confirms that the solver runtimes are influenced by different structural properties of instances. Nevertheless, **Simple LB** features were helpful for both algorithms. Somewhat surprisingly, the **Pattern database LB** features were more useful for ILP, even though A\*-ec directly uses the pattern database in its search. As shown in Fig. 6, though, those features do not significantly improve upon the ILP predictions using **Basic extended** features. For all of the graph-based features (node degree and non-trivial SCCs), the standard deviation was always selected over the maximum and mean. This suggests that systematic variations between nodes are important for determining the hardness of an instance. The table also shows that a small number

<sup>3</sup>The size of the tree can be larger than the number of features because features can be used at multiple nodes in the tree.

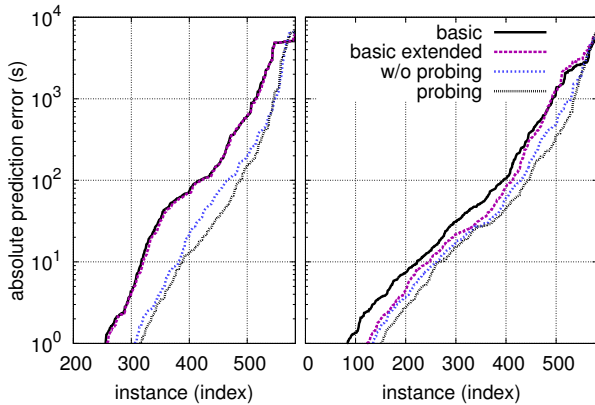


Figure 6: Prediction errors using different sets of features: A\* (left) and ILP (right). Instances are sorted according to absolute prediction error, defined as the absolute difference between the actual and predicted runtimes.

of features were consistently selected for most of the cross-validation folds for any particular solver. Qualitatively, this implies that most of the trees were based on the same small set of features. Developing a more in-depth understanding of these instance characteristics in light of solver performance is an important aspect of future work.

## 7 Concluding Remarks

It is possible to construct a surprisingly simple yet highly-efficient BNSL solver portfolio based on a small set of state-of-the-art BNSL solvers, by using machine learning techniques to learn accurate empirical hardness models. Thus the answer to question Q1 is ‘yes’: a simple model yields a very efficient algorithm portfolio. Even though the solvers’ runtimes are extremely complicated functions of the instances, the runtime on a given instance can be relatively accurately predicted from an extended set of non-trivial but fast-to-compute features. Thus the answer to question Q2 is also ‘yes’: easily computable, more informative features than the simple  $m$  and  $n$  are needed in order to improve prediction accuracy for the solver runtimes. Further improvements to the predictions are plausible by searching for yet more informative features of BNSL and using other statistical models.

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Table 4: Features used for A\*-ec and ILP in more than 5 of the 10 cross-validation folds. For each solver, the set of possible features consisted of non-probing features (1–38) and the relevant probing features.

Feature	A*-ec	ILP
(1) Number of variables, $n$	10	0
(2) Number of CPS, mean	0	7
(3) Number of CPS, sum, $m$	2	10
(4) Number of CPS, max	0	7
(8) CPS cardinalities, $sd$	0	8
(11) Simple LB, Node in-degree, $sd$	0	7
(14) Simple LB, Node out-degree, $sd$	8	0
(17) Simple LB, Node degree, $sd$	10	0
(26) Pd LB, Node in-degree, $sd$	1	9
(38) Pd LB, Size of non-trivial SCCs, $sd$	0	8
(62) A* probing, Error bound	10	0
(68) ILP probing, Node out-degree, $sd$	0	10
(74) ILP probing, Error bound	0	10

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