



HAL
open science

Structured Set Variable Domains in Bayesian Network Structure Learning

Fulya Trösser, Simon De Givry, George Katsirelos

► **To cite this version:**

Fulya Trösser, Simon De Givry, George Katsirelos. Structured Set Variable Domains in Bayesian Network Structure Learning. The 28th International Conference on Principles and Practice of Constraint Programming, Jul 2022, Haifa, Israel. 10.4230/LIPIcs.CP.2022.40 . hal-03674105

HAL Id: hal-03674105

<https://hal.science/hal-03674105v1>

Submitted on 20 May 2022

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

1 Structured Set Variable Domains in Bayesian 2 Network Structure Learning

3 Fulya Trösser ✉

4 Université Fédérale de Toulouse, ANITI, INRAE, UR 875, 31326 Toulouse, France

5 Simon de Givry ✉ 

6 Université Fédérale de Toulouse, ANITI, INRAE, UR 875, 31326 Toulouse, France

7 George Katsirelos ✉ 

8 Université Fédérale de Toulouse, ANITI, INRAE, MIA Paris, AgroParisTech, 75231 Paris, France

9 — Abstract —

10 Constraint programming is a state of the art technique for learning the structure of Bayesian
11 Networks from data (Bayesian Network Structure Learning – BNSL). However, scalability both for
12 CP and other combinatorial optimization techniques for this problem is limited by the fact that the
13 basic decision variables are set variables with domain sizes that may grow super polynomially with
14 the number of random variables. Usual techniques for handling set variables in CP are not useful,
15 as they lead to poor bounds. In this paper, we propose using decision trees as a data structure for
16 storing sets of sets to represent set variable domains. We show that relatively simple operations are
17 sufficient to implement all propagation and bounding algorithms, and that the use of these data
18 structures improves scalability of a state of the art CP-based solver for BNSL.

19 **2012 ACM Subject Classification** Computing methodologies → Learning in probabilistic graphical
20 models; Theory of computation → Discrete optimization

21 **Keywords and phrases** Combinatorial Optimization, Bayesian Networks, Decision Trees

22 **Digital Object Identifier** 10.4230/LIPIcs.CP.2022.40

23 **Supplementary Material** *Software (Source Code):* <https://gkatsi.github.io/elsa-cp22.tar.gz>

24 **Funding** This work has been partly funded by the “Agence nationale de la Recherche” (ANR-16-
25 CE40-0028 Demograph project and ANR-19-PIA3-0004 ANTI-DIL chair of Thomas Schiex).

26 **Acknowledgements** Thanks to the GenoToul (Toulouse, France) Bioinformatics platform for com-
27 putational support.

28 **1** Introduction

29 Bayesian Networks (BNs) are directed probabilistic graphical models, which can describe a
30 normalized joint probability distribution over a potentially large set of random variables, by
31 exploiting conditional independence to decompose the function. Learning the structure of
32 BNs from data (the Bayesian Network Structure Learning problem, BNSL) is a challenging
33 combinatorial optimization problem. There exist constraint-based approaches to learn BNs,
34 which use local conditional independence tests, and score-based approaches, which use a
35 decomposable score function to score each potential structure and aim to find the structure
36 that minimizes this score. The former are known to be efficient, but have trouble with noisy
37 data. The latter yield a known to be NP-hard problem [4], which additionally has proved
38 very challenging in practice.

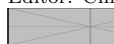
39 There exist complete methods for score-based BNSL based on dynamic programming [20],
40 heuristic search [24, 8], maximum satisfiability [2], branch-and-cut [1] and constraint pro-
41 gramming [22, 21]. Branch-and-cut and constraint programming have proven to be the most
42 successful of these methods. However, scaling them up remains challenging. One challenge



© Fulya Trösser, Simon de Givry, and George Katsirelos;
licensed under Creative Commons License CC-BY 4.0

28th International Conference on Principles and Practice of Constraint Programming (CP 2022).

Editor: Christine Solnon; Article No. 40; pp. 40:1–40:10



Leibniz International Proceedings in Informatics

Schloss Dagstuhl – Leibniz-Zentrum für Informatik, Dagstuhl Publishing, Germany

43 has to do with the decomposition of the scoring functions: these assign a score to each
 44 potential set of parents of each vertex and the score of a specific structure is the sum of the
 45 scores of each parent set. This means that the objective function must have a term for each
 46 potential parent set, a potentially exponential number of terms. There are various methods
 47 by which this number is made manageable, but it is still among the greatest obstacles to
 48 scalability. Moreover, the best solvers, ILP-based GOBNILP [1], and CP-based ELSA [21]
 49 also explicitly have this set of parent sets in other parts of the model as well, in the case of
 50 ELSA as domains of variables.

51 Here, we propose exploiting the fact that these domains are structured, i.e., that each
 52 value is a set. Specifically, we show that we can represent potential parent sets as paths on
 53 decision trees and that using these decision trees we can answer queries more efficiently than
 54 by traversing a list of domain values. This feature has not been exploited in BNSL in the
 55 past and allows us to solve large instances more efficiently.

56 2 Background

57 2.1 Bayesian Networks

58 A Bayesian Network is a directed graphical model $B = \langle G, P \rangle$ where $G = \langle V, E \rangle$ is a directed
 59 acyclic graph (DAG) called the structure of B and P are its parameters. A BN describes
 60 a normalized joint probability distribution. Each vertex of the graph corresponds to a
 61 random variable and presence of an edge between two vertices denotes direct conditional
 62 dependence. Each vertex v_i is also associated with a Conditional Probability Distribution
 63 $P(v_i | \text{parents}(v_i))$. The CPDs are the parameters of B .

64 Learning a BN from a set of multivariate discrete data using the score based method uses
 65 a decomposable scoring function (such as BIC [19, 14] or BDeu [3, 12]) which assigns, based
 66 on the data, a score to each potential parent set of each vertex. The BNSL problem is the
 67 problem of finding the structure G which minimizes this scoring function.

68 The number of candidate parent sets can in principle be exponentially large, but it is
 69 typically kept in check. For one, the BIC scoring function [19, 14] guarantees that the number
 70 of candidate parent sets grows only logarithmically with the size of the data set. Second,
 71 there exist dedicated pruning rules [7, 6] which reduce the set further. As a last resort, an
 72 upper bound can be placed on the cardinality of parent sets. This is necessary especially in
 73 larger instances, where it is necessary to limit cardinality to as low as 3 in some cases.

74 2.2 CP-based BNSL

75 ELSA [21] is a CP-based solver for the BNSL, based on the CPBayes solver [22]. The
 76 constraint model used in ELSA has several features that we do not discuss here. Instead,
 77 we focus on the part that is relevant to our contribution. For each random variable X ,
 78 there exists a corresponding CSP variable P_X whose domain is the set of candidate parent
 79 sets of X . These are unsurprisingly called parent set variables. There exists an acyclicity
 80 constraint over these which requires that their instantiation yields an acyclic graph. ELSA
 81 enforces GAC on this constraint. The central part of the GAC algorithm is algorithm 1,
 82 `acycChecker`. `acycChecker` determines in time $O(n^2d)$ whether the current set of domains
 83 admits an acyclic solution, based on the property that in any acyclic graph, for any subset
 84 of vertices C , at least one of the vertices $v \in C$ has a parent set that does not intersect C .

85 In addition, ELSA computes lower bounds by approximately solving the linear relaxation

Algorithm 1 Acyclicity checker

```

1 acycChecker ( $\mathbf{P}$ ,  $D$ )
2  $order \leftarrow \{\}$ 
3  $changes \leftarrow true$ 
4 while  $changes$  do
5    $changes \leftarrow false$ 
6   foreach  $v \in \mathbf{P} \setminus order$  do
7     if  $\exists S \in D(v)$  s.t.  $S \subseteq order$  then
8        $order \leftarrow order + v$ 
9        $changes \leftarrow true$ 
10
11 return  $order$ 

```

86 of the ILP (1), which was proposed by Bartlett and Cussens [1] for the GOBNILP solver.

$$87 \quad \min \sum_{v \in \mathbf{P}, S \subseteq V \setminus \{v\}} \sigma^v(S) x_{v,S} \quad (1a)$$

$$88 \quad s.t. \sum_{S \in PS(v)} x_{v,S} = 1 \quad \forall v \in \mathbf{P} \quad (1b)$$

$$89 \quad \sum_{v \in C, S \in PS^{-C}(v)} x_{v,S} \geq 1 \quad \forall C \subseteq \mathbf{P} \quad (1c)$$

$$90 \quad x_{v,S} \in \{0, 1\} \quad \forall v \in \mathbf{P}, S \in PS(v) \quad (1d)$$

92
 93 This is an exponentially large ILP, but on the flip side, the constraints (1c), called *cluster*
 94 *constraints* are facets of the polytope [5]. Hence, following GOBNILP, ELSA starts with none
 95 of the cluster constraints in the linear relaxation and then adds only those that can improve
 96 the dual bound. This is an NP-hard problem. GOBNILP solves this NP-hard problem to find
 97 violated cluster constraints, while ELSA uses a polynomial time algorithm which can identify
 98 a strict subset of all improving cluster constraints. The central element of the algorithm used
 99 in ELSA to find cluster constraints uses algorithm 1 on the domains restricted only to values
 100 which have reduced cost 0 in the current dual solution of the linear relaxation.

101 Both in finding improving cluster constraints and in enforcing GAC on the acyclicity
 102 constraint, the main bottleneck is line 8 of algorithm 1, which tests whether there exists in
 103 $D(v)$ a value which is a subset of a given set. As domain sizes grow drastically faster than
 104 the number of random variables, it is crucial to optimize this step. In practical terms, even
 105 given the mitigations mentioned earlier, the average domain size can be in the thousands for
 106 larger instances.

107 3 Related work

108 A typical approach to dealing with large domain sizes in constraint programming is to enclose
 109 the set of domain values with an underestimation and an overestimation and reason with
 110 those instead. Sometimes, this can even be achieved without any loss in strength of inference.
 111 This is the case, for example, when representing only the bounds of a variables that are only
 112 used in linear inequalities. In the case where the values of a domain are sets, the variable is
 113 called a set variable. Its domain can be represented with the subset bound scheme [9], which

114 underestimates by a set indicating all elements which appear in all remaining domain values
 115 and overestimates by a set indicating all elements which appear in any remaining domain
 116 value. The length-lex scheme uses lexicographic and cardinality information to get a tighter
 117 under- and over-estimation [10]. However, detecting infeasibility of the acyclicity constraint
 118 is crucial for the performance of CPBayes and even more for ELSA. Hence, over-estimating
 119 the actual domain in our case would lead to poor performance.

120 Hawkins et al. [11] followed an approach which is closer to our own, by using ROBDDs
 121 (reduced ordered binary decision diagrams) to represent domains. ROBDDs are diagrams
 122 like decision trees, but they require the same variable ordering in each branch and isomorphic
 123 subgraphs are merged, so that the underlying graph is a DAG rather than a tree. They can
 124 be significantly more compact than decision trees. However, Hawkins et al. used them in a
 125 setting where all constraints can be expressed as operations on ROBDDs. They do not deal
 126 with costs of the domain values, and in particular with reduced cost filtering.

127 **4** Decision Trees as domain store

128 The set of sets that are in a domain can be seen as the set of solutions of a propositional
 129 formula, in which we have a propositional variable for each element of the universe. Therefore,
 130 knowledge compilation languages such as ROBDDs can be used to represent a domain.

131 There exist several queries and operations performed on the domains in ELSA, but not
 132 all are critical to optimize, as they are not performed often enough to dominate the runtime.
 133 In particular, we want to address the test in line 8, which asks whether the domain contains
 134 a set which is a subset of another given set. Therefore, the main queries that need to be
 135 supported efficiently by a domain store for our purposes are:

- 136 1. Does there exist a domain value S such that $S \subseteq T$ for some T ?
- 137 2. Does there exist a domain value S with reduced cost 0 such that $S \subseteq T$ for some T ?

138 And the main operations, which also have to support backtracking, are:

- 139 1. Pruning a single value S
- 140 2. Updating the reduced cost of a value

141 The main issue that disqualifies ROBDDs and other reduced representations for us is
 142 that operation 1, reduced cost filtering, may remove arbitrary values, shattering the shared
 143 suffixes that an ROBDD exploits, which means that pruning may result in increasing the
 144 size of the representation and is not even guaranteed to be in linear time. Instead, we use
 145 decision trees here, in particular binary decision trees with implied literals, inspired by a
 146 similar technique in BDDs [13]. The main use of decision trees is in machine learning for
 147 classification, but their use as a data structure for representing sets of sets (or, equivalently,
 148 a knowledge compilation language) is straightforward.

149 We give below definitions for the specific case of binary decision trees and binary classifi-
 150 cation, as that is all we need.

151 ► **Definition 1** (Binary decision tree). *Let A be a set of features $\{a_1, \dots, a_n\}$ with Boolean
 152 domains and C_1, C_2 be two classes. A binary decision tree \mathcal{T} over the features A is a directed
 153 rooted binary tree. Each internal node n of \mathcal{T} is labeled with a feature $l(n) \in A$ and each
 154 arc e (of the at most two outgoing arcs) from n is labeled with $l(e) \in \{\text{true}, \text{false}\}$ and are
 155 mutually exclusive. Each leaf node t is labeled with $l(t) \in \{C_1, C_2\}$. Given an instantiation I
 156 of the features, there is a unique path from the root to a leaf t so that for each arc $e = (n, c)$*

157 along that path, it holds that $I(l(n)) = l(e)$. We say that \mathcal{T} classifies I as $l(n)$ and that I
 158 and the path from the root to n are consistent with each other, or simply that I and n are
 159 consistent with each other.

160 To see how we can use binary decision trees as a data structure for a set of sets, observe
 161 that we can set the features to be the variables of the indicator function of the sets in the
 162 domain and the classes as *in-set* and *not-in-set*.

163 This allows us to further optimize the representation. Since we only care about the *in-set*
 164 class, from now on we assume that all nodes and arcs that do not appear on a path from the
 165 root to a leaf n with $l(n) = \textit{in-set}$ are removed from the decision tree.

166 Additionally, we can eliminate some nodes by adding *implied literals* in each node of the
 167 tree.

168 ► **Definition 2** (Binary decision tree with implied literals). *A binary decision tree with implied*
 169 *literals is a decision tree in which each node n (internal or leaf) is additionally labeled with a*
 170 *set of literals $\textit{lit}(n, C_i) \subseteq \{a = v \mid a \in A, v \in \{\textit{true}, \textit{false}\}\}$ for $i \in \{1, 2\}$. An instantiation*
 171 *I is consistent with a path to a leaf t with $l(t) = C_i$ if it is consistent with all the arcs it*
 172 *follows and all implied literal labels $\textit{lit}(n, C_i)$ for each node n on the path from the root to t .*

173 In our case, we abbreviate $\textit{lit}(n, \textit{in-set})$ to $\textit{lit}(n)$, as we ignore the class *not-in-set*.
 174 Decision trees with implied literals allow us to collapse chains, i.e., paths along which every
 175 node has outdegree 1, into a single node. Hence, they are not more compact than those
 176 without implied literals by more than a linear factor, but they have almost no overhead and,
 177 in preliminary experiments, we found them to provide some performance improvement.

178 In machine learning, the objective is not only to construct models that perform well on
 179 the training set, but that also generalize. Hence, it is not only acceptable, but also desirable
 180 to misclassify some samples in training sets, if that means a smaller and hence more general
 181 decision tree. In our setting, however, where we use decision trees to model a Boolean
 182 function, we accept no error. So no two sets that belong to different classes, i.e., one in *in-set*
 183 and one in *not-in-set*, are allowed to both be consistent with the same leaf node.

184 We place an additional constraint on the decision trees we construct, which is that each
 185 leaf node must be consistent with exactly one positive instantiation. This ensures that
 186 there exists a bijection between leaves of the tree and values in the domain. This is not
 187 as significant a constraint as it might seem at first. A leaf node n that is consistent only
 188 with positive instantiations but more than one of them is expanded into a full binary tree
 189 of depth k , where k is the number of variables (features) which have not appeared on the
 190 path from the root to n . However, for the queries that we care about, this means only that
 191 the corresponding algorithm will have to traverse an additional k nodes before answering,
 192 and, crucially, will only arrive at this point when it is guaranteed that it will give a positive
 193 answer. Even that overhead can be eliminated with some care. Indeed, while traversing
 194 the decision tree, we can determine that we have reached such a node n if the number of
 195 possible instantiations that are consistent with n is equal to the number of leaves reachable
 196 from n . The former is 2^{n-lvl} , where lvl is the distance from the root to n . The latter can be
 197 computed on construction and updated as values are removed. If these are equal, we know
 198 that the subtree contains all possible subsets and we can answer our query without more
 199 search. We give more detail later.

200 Constructing decision trees.

201 Constructing a minimum decision tree is NP-hard with respect to several metrics [15]. We
 202 use the *information gain* heuristic [17] to choose which variable to branch on in each node.

203 It is a natural side effect of computing the information gain that we learn how many of the
 204 sets that are consistent with a node n contain the literals $a = true$ and $a = false$ for all
 205 $a \in A$. If either of these is 0, then its negation is added to the implied literal label for n and
 206 a is not considered as a candidate for branching. We also experimented with optimizing the
 207 in-memory layout for better cache behavior. Compared to the van-Emde Boas layout [23], a
 208 depth-first, false-child first layout performed better.

209 Maintaining a decision tree during search

210 It is fairly straightforward to update a decision tree for a pruning. In order to prune a value,
 211 we remove the unique leaf node that corresponds to it. Once we remove a leaf, its parent
 212 may no longer be able to reach any more leaves, hence we propagate this removal upwards.
 213 We associate each removed node with the decision level in which it was removed, so on
 214 backtracking we add them back to restore the tree to its correct state.

215 This guarantees that the tree representation of a domain only shrinks down a branch of
 216 the branch and bound tree. Hence, the tree can remain static and we only mask nodes that
 217 do not lead to any leaves that correspond to unpruned values, which is simple to implement.

218 Reduced costs

219 ELSA solves the linear relaxation (1) from scratch at every node, and then strengthens it by
 220 discovering new violated cluster inequalities using the acyclicity checker (algorithm 1). Both
 221 these algorithms require an efficient implementation of the subset query on the subset of
 222 values which have reduced cost 0. In contrast to the domain itself, however, this set is reset
 223 to the empty set at the beginning of every node and grows monotonically until it admits an
 224 acyclic solution. Here again, the fact that there exists a bijection between values and leaves
 225 of the tree allows us to represent the set of 0-cost values as a subset of the full decision tree.
 226 Every time the reduced cost of a value reaches 0, the unique leaf it corresponds to, as well as
 227 all its parents, are added to the set of visible nodes for these queries. This is implemented as
 228 an additional mask on top of that which hides pruned values.

229 Subset queries

230 To answer the query “does the domain contain a value S such that $S \subseteq T$?”, we perform a
 231 depth first traversal of the tree. At each node n , we check $l(n)$. If $l(n) \notin T$, we only allow
 232 DFS to follow the outgoing arc labeled with false. If $l(n) \in T$, we allow DFS to follow both
 233 outgoing arcs. If the label $lit(n)$ contains a literal $p \notin T$, we backtrack. If we reach a leaf, we
 234 stop and report success. If we exhaust the search without reaching a leaf, we report failure.

235 When this procedure reaches a node which is the root of a complete subtree of depth k ,
 236 with no additional implied literal labels, it is guaranteed to terminate after visiting exactly k
 237 nodes and report success. Indeed, since this is a complete subtree, one of the outgoing arcs
 238 is always available to the depth first search, and it will reach a leaf after k more steps.

239 This procedure can be used to answer subset queries either on the entire domain, masking
 240 away only pruned values, or on those values which have reduced cost 0, masking away both
 241 pruned values and those whose reduced cost is greater than 0.

242 5 Experimental Results

243 We implemented decision trees as the domain representation on top of ELSA. The default
 244 implementation of a subset query in ELSA iterates over all domain values and returns if

245 it finds one that is a subset of T . We replaced this by the depth-first traversal described
 246 in section 4 and denote this solver ¹ ELSA^{IG}. We compare against the previous version of
 247 ELSA², GOBNILP³, and CPBayes⁴.

248 The datasets come from the UCI Machine Learning Repository⁵, the Bayesian Network
 249 Repository⁶, and the Bayesian Network Learning and Inference Package⁷. We have 51
 250 medium datasets with $|V| < 64$, and 18 large datasets with $64 \leq |V| < 128$.

251 Local scores were computed from the datasets using B. Malone’s code⁸. BDeu and BIC
 252 scores were used for medium datasets (less than 64 variables) and only BIC score for large
 253 datasets (above 64 variables). The maximum number of parents was limited to 5 for large
 254 datasets (except for `accidents.test` with maximum of 8), a high value that allows learning
 255 even complex structures [18]. For example, `jester.test` has 100 random variables, a sample
 256 size of 4, 116 and 770, 950 parent set values. For medium datasets, no restriction was applied
 257 except for some BDeu scores, where we limit sets to 6 or 8 to complete the computation of
 258 the local scores within 24 hours of CPU-time [16].

259 For the experiments, we modified the C++ source of CPBayes v1.1 just to allow us to
 260 run it with datasets having more than 64 variables. All computations were performed on
 261 a single core of Intel(R) Xeon(R) Gold 6248R CPU @ 3.00GHz and 1 TB of RAM with
 262 a 1-hour CPU time limit for the 51 medium datasets, as well as 3 of the large datasets:
 263 `kdd.ts`, `kdd.test`, and `kdd.valid`. For the remaining 15 large datasets, we had a 10-hour
 264 CPU time limit. For the preprocessing phase, we used two different settings depending
 265 on problem size $n = |V|$: $l_{min} = 20, l_{max} = 26, r_{min} = 50, r_{max} = 500$ if $n \leq 64$, else
 266 $l_{min} = 20, l_{max} = 20, r_{min} = 15, r_{max} = 30$, where l_{min}, l_{max} are partition lower bound sizes
 267 and r_{min}, r_{max} are the number of restarts for the local search.

268 In Table 1, we show the time needed to find the optimal solution and prove optimality for
 269 all these solvers. We see that, while the use of decision trees has little effect, either positive
 270 or negative, for the smaller instances, it makes a great difference in the larger instances.
 271 In particular, ELSA^{IG} is the only solver that can prove optimality for the `baudio.test`
 272 and `jester.valid` datasets. For the only instances where ELSA is significantly worse
 273 than CPBayes, `bnetflix.ts`, `bnetflix.test`, and `bnetflix.valid`, ELSA^{IG} either closes
 274 the gap back down (`bnetflix.valid`) or is faster yet than CPBayes (`bnetflix.ts` and
 275 `bnetflix.test`). However, ELSA^{IG} regresses with respect to ELSA in the `accidents`
 276 dataset and in `plants.test`. Part of the reason for this is that the benefit of the decision
 277 trees in terms of the reduction of the cost in answering the subset queries is comparatively
 278 reduced, hence the other overheads of decision trees dominate. For example, in `bnetflix.ts`,
 279 where ELSA^{IG} significantly outperforms ELSA, ELSA looks at an average of 3315 values to
 280 answer each subset test, while ELSA^{IG} visits just 90 nodes of the decision tree. On the other
 281 hand, in `accidents.test`, ELSA looks at an average of 80 values to answer each subset test,
 282 while ELSA^{IG} visits 20 nodes of the decision tree. This difference is not enough to overcome
 283 other overheads.

284 With respect to GOBNILP, ELSA^{IG} mostly outperforms it, but there are some instances

¹ Available at <https://gkatsi.github.io/elsa-cp22.tar.gz>

² Available at <https://gkatsi.github.io/elsa-ijcai21.tar.gz>

³ Version 1.6.3 with CPLEX 12.7.1

⁴ Retrieved from <http://cs.uwaterloo.ca/~vanbeek/Publications/CPBayes.zip>

⁵ <http://archive.ics.uci.edu/ml>

⁶ <http://www.bnlearn.com/bnrepository>

⁷ <https://ipg.idsia.ch/software.php?id=132>

⁸ <http://urlearning.org>

	n	sum D	GOBNILP	CPBayes	ELSA	ELSA ^{IG}
carpo100_BIC	60	423	0.5	76.7 (27.5)	52.6 (0.1)	52.5 (0.0)
insurance1000_BIC	27	506	0.6	31.6 (0.0)	32.8 (0.0)	37.2 (0.0)
spectf_BIC	45	610	1.4	4.2 (3.5)	0.8 (0.0)	1.0 (0.1)
sponge_BIC	45	618	1.6	5.1 (3.3)	1.8 (0.0)	2.1 (0.0)
insurance1000_BDe	27	792	0.6	34.8 (0.0)	34.3 (0.0)	39.2 (0.0)
alarm1000_BIC	37	1002	1.3	191.1 (159.1)	34.4 (1.0)	37.9 (1.9)
flag_BDe	29	1324	4.0	16.6 (15.6)	1.0 (0.2)	1.3 (0.2)
autos_BIC	26	2391	11.9	18.4 (0.0)	19.2 (0.0)	19.9 (0.1)
soybean_BIC	36	5926	48.9	51.9 (1.7)	50.8 (3)	49.6 (0.0)
wdbc_BIC	31	14613	86.3	459.4 (398.0)	56.0 (2.4)	61.7 (1.7)
autos_BDe	26	25238	1005.2	239.5 (0.1)	145.8 (0.8)	177.1 (0.3)
kdd.ts	64	43584	508.8	†	1452.3 (274.6)	1355.2 (141.3)
steel_BIC	28	93026	†	1265.6 (1196.1)	124.2 (71.8)	100.6 (45.7)
kdd.test	64	152873	3178.0	†	1594.3 (224.4)	1519.6 (48.9)
mushroom_BDe	23	438185	†	167.0 (4.9)	182.6 (58.9)	150.1 (16.7)
bnetflix.ts	100	446406	†	1086.9 (876.3)	2103.1 (1900.9)	557.9 (358.4)
plants.test	111	520148	†	†	28049.6 (26312.9)	35961.7 (33712.7)
jester.ts	100	531961	†	†	21550.5 (21003.7)	7951.4 (7301.6)
accidents.ts	100	568160	1932.2	†	2302.2 (930.0)	†
plants.valid	111	684141	†	†	17801.6 (14080.2)	19819.2 (14547.9)
jester.test	100	770950	†	†	30186.8 (29455.0)	9644.5 (8742.8)
baudio.test	100	1016403	†	†	†	31077.1 (29028.1)
bnetflix.test	100	1103968	†	5794.5 (5486.2)	10333.1 (10096.5)	1448.8 (1137.7)
bnetflix.valid	111	1325818	†	998.1 (451.0)	10871.7 (10527.7)	1476.5 (1041.5)
accidents.test	100	1425966	14453.1	†	3641.7 (680.7)	8434.1 (4723.0)
jester.valid	100	1463335	†	†	†	31949.5 (30624.2)
accidents.valid	100	1617862	27730.5	†	†	†

■ **Table 1** Comparison of GOBNILP, CPBayes, ELSA, and ELSA^{IG} in terms of total running (and search) time in seconds. Time limit for the datasets above the line is 1 hour, and for the rest it is 10 hours. Datasets are sorted by increasing total domain size for each time limit category. For CPBayes as well as all variants of ELSA we report in parentheses time spent in search, after preprocessing finishes. † indicates a timeout.

285 where neither ELSA nor ELSA^{IG} can match it. It seems, however, that ELSA^{IG} is overall
286 the best performer.

287 6 Conclusion

288 We have shown that, in the BNSL problem, we can exploit the structure of domains to get
289 a significant speedup in learning the structure of BNs of larger datasets. Specifically, we
290 have shown that by treating domains as sets of sets instead of sets of values, and using
291 decision trees to represent these sets, we can answer subset queries significantly faster. This
292 is unlike the typical approach to handling large domains in CP, which uses over- and under-
293 approximations. Although the current implementation shows some significant improvements,
294 answering subset queries is still the most time consuming operation performed by the solver.
295 Moreover, the fact remains that decision trees as a knowledge compilation language are fairly
296 weak in terms of conciseness. It remains an open question whether we can overcome the
297 issues with ROBDDs or even DNNFs to achieve even more significant speedups.

298 — References —

- 299 1 Mark Bartlett and James Cussens. Integer linear programming for the bayesian network
300 structure learning problem. *Artificial Intelligence*, pages 258–271, 2017.

- 301 **2** Jeremias Berg, Matti Järvisalo, and Brandon Malone. Learning optimal bounded treewidth
302 bayesian networks via maximum satisfiability. In *Artificial Intelligence and Statistics*, pages
303 86–95. PMLR, 2014.
- 304 **3** Wray Buntine. Theory refinement on bayesian networks. In *Proc. of UAI*, pages 52–60.
305 Elsevier, 1991.
- 306 **4** David Maxwell Chickering. Learning bayesian networks is NP-Complete. In *Proc. of Fifth
307 Int. Workshop on Artificial Intelligence and Statistics (AISTATS)*, pages 121–130, Key West,
308 Florida, USA, 1995. doi:10.1007/978-1-4612-2404-4_12.
- 309 **5** James Cussens, Matti Järvisalo, Janne H Korhonen, and Mark Bartlett. Bayesian network
310 structure learning with integer programming: Polytopes, facets and complexity. *Journal of
311 Artificial Intelligence Research*, 58:185–229, 2017.
- 312 **6** Cassio P de Campos, Mauro Scanagatta, Giorgio Corani, and Marco Zaffalon. Entropy-based
313 pruning for learning bayesian networks using BIC. *Artificial Intelligence*, 260:42–50, 2018.
- 314 **7** Cassio Polpo de Campos and Qiang Ji. Properties of bayesian dirichlet scores to learn bayesian
315 network structures. In *Proc. of AAAI-10*, Atlanta, Georgia, USA, 2010.
- 316 **8** Xiannian Fan and Changhe Yuan. An improved lower bound for bayesian network structure
317 learning. In *Proc. of AAAI-15*, Austin, Texas, 2015.
- 318 **9** Carmen Gervet. Conjunto: Constraint logic programming with finite set domains. In Maurice
319 Bruynooghe, editor, *Logic Programming, Proceedings of the 1994 International Symposium,
320 Ithaca, New York, USA, November 13-17, 1994*, pages 339–358. MIT Press, 1994.
- 321 **10** Carmen Gervet and Pascal Van Hentenryck. Length-lex ordering for set CSPs. In *Proceedings
322 of AAAI*, 2006.
- 323 **11** Peter Hawkins, Vitaly L. Lagoon, and Peter J. Stuckey. Solving set constraint satisfaction
324 problems using ROBDDs. *Journal of Artificial Intelligence Research*, 24:109–156, 2005.
- 325 **12** David Heckerman, Dan Geiger, and David M Chickering. Learning bayesian networks: The
326 combination of knowledge and statistical data. *Machine learning*, 20(3):197–243, 1995.
- 327 **13** Y. Lai, D. Liu, and S. Wang. Reduced ordered binary decision diagram with implied literals:
328 A new knowledge compilation approach. *Knowledge and Information Systems*, 35(3):665–712,
329 2013.
- 330 **14** Wai Lam and Fahiem Bacchus. Using new data to refine a bayesian network. In *Proc. of UAI*,
331 pages 383–390, 1994.
- 332 **15** Hyafil Laurent and Ronald L Rivest. Constructing optimal binary decision trees is NP-complete.
333 *Information processing letters*, 5(1):15–17, 1976.
- 334 **16** Colin Lee and Peter van Beek. An experimental analysis of anytime algorithms for bayesian
335 network structure learning. In *Advanced Methodologies for Bayesian Networks*, pages 69–80,
336 2017.
- 337 **17** J.R. Quinlan. Induction of decision trees. *Machine Learning*, 1:81–107, 1986.
- 338 **18** Mauro Scanagatta, Cassio P de Campos, Giorgio Corani, and Marco Zaffalon. Learning
339 bayesian networks with thousands of variables. *Proc. of NeurIPS*, 28:1864–1872, 2015.
- 340 **19** Gideon Schwarz. Estimating the dimension of a model. *The Annals of Statistics*, 6(2):461–464,
341 1978.
- 342 **20** Tomi Silander and Petri Myllymäki. A simple approach for finding the globally optimal
343 bayesian network structure. In *Proc. of UAI’06*, Cambridge, MA, USA, 2006.
- 344 **21** Fulya Trösser, Simon de Givry, and George Katsirelos. Improved acyclicity reasoning for
345 bayesian network structure learning with constraint programming. In *Proceedings of IJCAI*,
346 pages 4250–4257, 2021.

40:10 Structured Set Variable Domains in Bayesian Network Structure Learning

- 347 **22** Peter van Beek and Hella-Franziska Hoffmann. Machine learning of bayesian networks using
348 constraint programming. In *Proc. of International Conference on Principles and Practice of*
349 *Constraint Programming*, pages 429–445, Cork, Ireland, 2015.
- 350 **23** Peter van Emde Boas. Preserving order in a forest in less than logarithmic time. In *Proceedings*
351 *of the 16th Annual Symposium on Foundations of Computer Science*, pages 75–84, 1975.
- 352 **24** Changhe Yuan and Brandon Malone. Learning optimal bayesian networks: A shortest path
353 perspective. *J. of Artificial Intelligence Research*, 48:23–65, 2013.