Probabilistic Inference in Graphical and Relational Models

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1 Introduction

This document has four sections and four appendices:

- Section 2 contains background information on various representations of probability distributions, their applications, and inference algorithms.
- Section 3 describes the research progress made this academic year.
- Section 4 provides a plan for the rest of my degree.
- Appendices A to C contain papers either published or submitted since last year's review.
- And last year's review itself is included in Appendix D.

2 Background

2.1 Representations

- RDDL [42],
- ProbLog [40] (ILP [32], PILP [38])
- Bayesian networks [36]
- relational Bayesian networks [21]
- Markov random fields [44]
- Markov logic networks [41]
- ICL [37]
- PRISM [43]
- CP-logic [45]
- BLOG [30]
- Church [20]

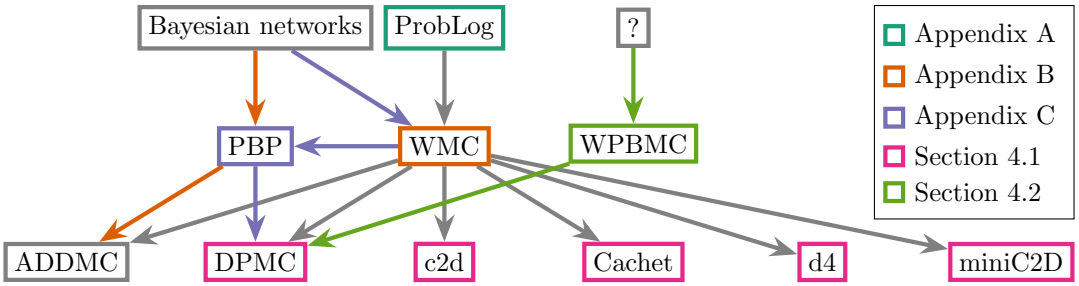

Figure 1: Outline of concepts relevant to my past and future work. The first row contains representations of probability distributions that are and have been relevant to my work. The second row contains encodings, i.e., computational problems that encode probabilistic inference. The third row contains WMC algorithms. The question mark denotes a representation that is yet to be identified. Gray arrows and boxes denote connections and concepts that are already known from previous work. A coloured arrow or box indicates that my work relates to that concept or interaction of concepts, and the colour coding describes which past or future paper the concept is related to.

2.2 Applications

- mining electronic health records [33]
- extracting value from dark data [34, 46]
- language modelling [22], NLP [15]
- planning under uncertainty [6]
- robotics [2, 31]
- cancer diagnosis [9]
- genetic data analysis [27]
- many more examples here [39]

2.3 Inference

- WMC [8]
- WMI [4]
- WFOMC [14, 19]
- generalisations [5, 1, 23]
- knowledge compilation stuff:
  - d-DNNF [10]
  - SDDs [12]
  - PSDDs [24]
  - (RO)BDDs [7]
- variable elimination [13]
- recursive conditioning [11]

- join tree [26]
- belief propagation [35]

3 Progress To Date

In this section, the progress made throughout this academic year is described with respect to the work plan from my first year review.[1]

WP 1 ('On the Equivalence of Constants in Relational Knowledge Bases') was abandoned. While trying to take reviewer feedback into consideration as well as update and strengthen the paper, I found an important ambiguity: when defining what constants are 'captured' and 'transferred' by a clause, I fail to specify whether each relevant 'spot' is occupied by a constant or a variable. In the former case, that makes the main theorem of the paper completely trivial. While in the latter case, the theorem becomes incorrect. I spent a couple of weeks looking for ways to transform the paper into something both correct and valuable. The best idea I could find was to use the perspective from this paper in the context of inductive logic programming; however, I did not want to explore this direction further.

WP 2 ('Generating Random Logic Programs Using Constraint Programming') was revised to include an experimental comparison of ProbLog inference algorithms and published and presented in CP 2020 (see Appendix A for the camera-ready version). I also gave three more talks about it:

- at the local AIAI seminar,
- for the Formal Analysis, Theory and Algorithms research section at the University of Glasgow,
- and at the FMAI 2021 workshop.

WP 3 was completed in full, although the emphasis shifted more towards experimental results than theory. It was first (unsuccessfully) submitted to AAAI 2021. Based on reviewer feedback, I updated the experimental section to compare not just various encodings with the same algorithm but also all of the encodings with the algorithms used in the original papers. The updated version can be found in Appendix B and was submitted to UAI 2021. I was also invited to the program committee for this conference.

WP 4 was abandoned due to lack of contributions that could be made. Indeed, any contribution would have to be theoretical, empirical, or interpretability-related. Significant theoretical contributions are unlikely because the theory of abstractions has already been explored before without leaving behind any big unanswered questions [3]. While previous work could be rephrased in a simpler way and extended with more detail, the contributions would still be marginal.

Furthermore, considering abstractions at their full level of generality is unlikely to be a viable method for improving inference speed because any abstraction is likely to be more computationally expensive than inference. Moreover, previous work on preprocessing for WMC left the field in an uncomfortable situation: preprocessing techniques for WMC were identified and described in a paper [25] whose main focus is on model counting; and the closed-source implementation of those techniques is unsuitable for WMC.

Finally, a substantial issue with considering abstraction as a tool for interpretability—especially in the context of probabilistic relational models—is that the low-level building blocks such as predicate and constant names are usually semantically meaningful. Thus, replacing such a model with a simpler alternative that instead uses high-level concepts that are unlikely to correspond to words in any natural language is unlikely to improve interpretability despite the potential simplicity of this type of abstraction.

[1] The first year review (with its own appendices) is included as Appendix D.

Furthermore, a new paper (not covered in the previous annual report) was written and submitted to SAT 2021 (see Appendix C). It originated as an attempt to improve **WP 3**: while the experimental results were impressive in the initial version of the paper, adding other algorithms revealed that instead of improving the state of the art by two orders of magnitude as originally thought, the suggested encoding was only fixing an underperforming algorithm and making its performance in line with other algorithms. The algorithm used for these experiments (ADDMC) was published only last year [17] and its experimental study includes some of the data used in my experiments as well as some new instances—one has to wonder whether the latter were added to improve the algorithm's comparative performance.

First, my new paper replaces the previously used algorithm with its even newer version DPMC [18]. The main improvement over ADDMC comes from the use of approximately-minimal-treewidth tree decompositions instead of heuristics for planning the order of multiplication and projection operations. After checking that DPMC performs very similarly with all encodings (including my own) and similarly to other WMC algorithms, the need to shift the contribution of my paper elsewhere became apparent.

The main advantage of the encoding I proposed earlier was that it avoided parameter variables—something I claimed is completely unnecessary at least in WMC algorithms based on algebraic decision diagrams (ADDs) (i.e., a representation of pseudo-Boolean functions). However, the encoding was particularly rigid in that it always compiled each conditional probability table (CPT) in a Bayesian network into an ADD before doing anything else. Although this resulted in great inference speed improvements on some instances, e.g., when most of the probabilities in a CPT are equal, there is no reason to believe that such an approach is always optimal. Being unable to suggest a new encoding that clearly outperforms others, I decided to investigate how parameter variables could be removed from already-existing encodings. This led to a generalisation of WMC based on pseudo-Boolean functions that I named pseudo-Boolean projection (PBP). I then show how any WMC instance can be transformed into a PBP instance and identify conditions under which such a transformation can remove parameter variables. This transformation is applicable to four out of the five WMC encodings for Bayesian networks. Finally, experiments showed that (at least for some encodings) parameter variable removal can significantly improve inference speed and supersede the previous state of the art.

4 Future Goals

4.1 Parameterized Complexity of WMC in Theory and Practice

The experiments in my papers in Appendices B and C as well as in previous work by others [17, 18] demonstrate that the differences amongst WMC algorithms are poorly understood, i.e., the algorithms perform very similarly overall, but with significant differences on subsets of benchmark data. In other words, which algorithm is the best depends entirely on who provides the data, and we have no idea what properties of a WMC instance make it more suitable for a search-based, a compilation-based, or an ADD-based approach. Therefore, the paper I am working on now aims to:

- Establish the parameterized complexity of DPMC, showing that it scales worse (than other algorithms) with respect to the treewidth of the primal graph of the input propositional formula in conjunctive normal form (CNF) (we call this *primal treewidth*).
- Propose a new random model for CNF formulas that allows us to generate instances of varying primal treewidth and use it to experimentally show how the performance of WMC algorithms depends on various properties of the instance such as density, primal treewidth, and the proportion of literal weights that are particularly 'simplifying', e.g., zero, one, and perhaps a half.

Risks and contingencies. One risk that I have already encountered is that having all of the following can lead to an infeasible amount of computation time:

- a time limit that is both similar to the time limits used in other experimental studies and provides enough 'space' for a growth curve to express itself,
- enough different parameter values so that the plots look more like the beautiful and barely-pixelated plots of today (e.g., [28, 29]) and less like my tiny experimental setup in Appendix A,
- enough different random instances for each combination of parameter values so that a reliable median can be observed despite high variance.

This risk has been addressed in two ways:

- The time limit was reduced to 100 s and could be reduced further (e.g., a similar paper uses only a 10 s time limit [16]).
- Instead of iterating over the values of all parameters in one big experiment, I split it into two smaller experiments where some variables are held constant and others are allowed to vary.

Another risk is that the experimental results may be unclear and/or not easily explainable. However, as random WMC instance generation is a completely unexplored area, even weird or imperfect results still count as valuable and interesting. Moreover, any unexpected differences in the way the algorithms perform on random and real data can always be likened to the equivalent situation with SAT algorithms.

4.2 Weighted Pseudo-Boolean Model Counting

Appendix B and partially Appendix C address one issue with the traditional definition of WMC, i.e., that restricting weights to literals leads to most measures being unrepresentable without the addition of more variables and clauses. It would be thematic to end the thesis by addressing the other issue: at least for solvers such as ADDMC [17] and DPMC [18], there is no reason for a clause to be just a clause, i.e., a disjunction of literals. Instead, it can be an arbitrary pseudo-Boolean function. In Appendix C, I suggested that two-valued pseudo-Boolean function are particularly convenient because they can be defined with a formal equivalent of the statement 'if formula ϕ is satisfied, then the value is p, otherwise the value is q'. Moreover, there is no reason for the formula to be propositional! Instead, we can consider *pseudo-Boolean constraints*, i.e., an intermediary between SAT and constraint satisfaction problems that supports linear and multilinear inequality constraints on logical variables that are interpreted as ones and zeros. Perhaps one can even use these constraints to encode almost arbitrary arithmetic constraints on integers.

Extending DPMC to support such constraints is unlikely to be difficult. The challenge is in finding at least one suitable application. The kind of Bayesian network encodings that I investigated in Appendices B and C *can* benefit from this (as they have counting constraints) but only marginally since each counting constraint is usually only applied to two or three variables. There must be some domain where probabilistic (or some other kind of weighted) inference is needed in the context of integer arithmetic, counting, or knapsack-style constraints, but so far I was not able to find one.

Risks and contingencies. If I am unable to find a good application,...

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A Published Paper (CP 2020)

Generating Random Logic Programs Using Constraint Programming

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Abstract. Testing algorithms across a wide range of problem instances is crucial to ensure the validity of any claim about one algorithm's superiority over another. However, when it comes to inference algorithms for probabilistic logic programs, experimental evaluations are limited to only a few programs. Existing methods to generate random logic programs are limited to propositional programs and often impose stringent syntactic restrictions. We present a novel approach to generating random logic programs and random probabilistic logic programs using constraint programming, introducing a new constraint to control the independence structure of the underlying probability distribution. We also provide a combinatorial argument for the correctness of the model, show how the model scales with parameter values, and use the model to compare probabilistic inference algorithms across a range of synthetic problems. Our model allows inference algorithm developers to evaluate and compare the algorithms across a wide range of instances, providing a detailed picture of their (comparative) strengths and weaknesses.

Keywords: Constraint programming · Probabilistic logic programming · Statistical relational learning

1 Introduction

Unifying logic and probability is a long-standing challenge in artificial intelligence [24], and, in that regard, statistical relational learning (SRL) has developed into an exciting area that mixes machine learning and symbolic (logical and relational) structures. In particular, probabilistic logic programs—including languages such as PRISM [25], ICL [22], and ProbLog [11]—are promising frameworks for codifying complex SRL models. With the enhanced structure, however, inference becomes more challenging. At the moment, we have no precise way of evaluating and comparing inference algorithms. Incidentally, if one were to survey the literature, one often finds that an inference algorithm is only tested on a small number (1–4) of data sets [5, 16, 28], originating from areas such as social networks, citation patterns, and biological data. But how confident can we be that an algorithm works well if it is only tested on a few problems?

About thirty years ago, SAT solving technology was dealing with a similar lack of clarity [26]. This changed with the study of generating random SAT

instances against different input parameters (e.g., clause length and the total number of variables) to better understand the behaviour of algorithms and their ability to solve random synthetic problems. Unfortunately, when it comes to generating random logic programs, all approaches so far focused exclusively on propositional programs [1, 2, 30, 32], often with severely limiting conditions such as two-literal clauses [20, 21] or clauses of the form $a \leftarrow \neg b$ [31].

In this work (Sects. 3 to 5), we introduce a constraint-based representation for logic programs based on simple parameters that describe the program's size, what predicates and constants it uses, etc. This representation takes the form of a *constraint satisfaction problem* (CSP), i.e., a set of discrete variables and restrictions on what values they can take. Every solution to this problem (as output by a constraint solver) directly translates into a logic program. One can either output all (sufficiently small) programs that satisfy the given conditions or use random value-ordering heuristics and restarts to generate random programs. For sampling from a uniform distribution, the CSP can be transformed into a belief network [12]. In fact, the same model can generate both probabilistic programs in the syntax of ProbLog [11] and non-probabilistic Prolog programs. To the best of our knowledge, this is the first work that (a) addresses the problem of generating random logic programs in its full generality (i.e., including first-order clauses with variables), and (b) compares and evaluates inference algorithms for probabilistic logic programs on more than a handful of instances.

A major advantage of a constraint-based approach is the ability to add additional constraints as needed, and to do that efficiently (compared to generate-and-test approaches). As an example of this, in Sect. 7 we develop a custom constraint that, given two predicates P and Q, ensures that any ground atom with predicate P is independent of any ground atom with predicate Q. In this way, we can easily regulate the independence structure of the underlying probability distribution. In Sect. 6 we also present a combinatorial argument for correctness that counts the number of programs that the model produces for various parameter values. We end the paper with two experimental results in Sect. 8: one investigating how the constraint model scales when tasked with producing more complex programs, and one showing how the model can be used to evaluate and compare probabilistic inference algorithms.

Overall, our main contributions are concerned with logic programming-based languages and frameworks, which capture a major fragment of SRL [9]. However, since probabilistic logic programming languages are closely related to other areas of machine learning, including (imperative) probabilistic programming [10], our results can lay the foundations for exploring broader questions on generating models and testing algorithms in machine learning.

2 Preliminaries

The basic primitives of logic programs are *constants*, *(logic) variables*, and *predicates* with their *arities*. A *term* is either a variable or a constant, and an *atom* is a predicate of arity n applied to n terms. A *formula* is any well-formed ex-

pression that connects atoms using conjunction $\wedge$, disjunction $\vee$, and negation $\neg$. A *clause* is a pair of a *head* (which is an atom) and a *body* (which is a formula[3]). A *(logic) program* is a set of clauses, and a ProbLog *program* is a set of clause-probability pairs [14].

In the world of CSPs, we also have *(constraint) variables*, each with a *domain*, whose values are restricted using *constraints*. All constraint variables in the model are integer or set variables, however, if an integer refers to a logical construct (e.g., a logical variable or a constant), we will make no distinction between the two. We say that a constraint variable is *(fully) determined* if its domain (at the time) has exactly one value. We let $\square$ denote the absent/disabled value of an optional variable [19]. We write $\texttt{a}[b] \in c$ to mean that $\texttt{a}$ is an array of variables of length b such that each element of $\texttt{a}$ has domain c. Similarly, we write $\texttt{c} : \texttt{a}[b]$ to denote an array $\texttt{a}$ of length b such that each element of $\texttt{a}$ has type $\texttt{c}$. Finally, we assume that all arrays start with index zero.

Parameters of the model. We begin by defining sets and lists of the primitives used in constructing logic programs: a list of predicates $\mathcal{P}$, a list of their corresponding arities $\mathcal{A}$ (so $|\mathcal{A}| = |\mathcal{P}|$), a set of variables $\mathcal{V}$, and a set of constants $\mathcal{C}$. Either $\mathcal{V}$ or $\mathcal{C}$ can be empty, but we assume that $|\mathcal{C}| + |\mathcal{V}| > 0$. Similarly, the model supports zero-arity predicates but requires at least one predicate to have non-zero arity. For notational convenience, we also set $\mathcal{M}_\mathcal{A} = \max \mathcal{A}$. Next, we need a measure of how complex a body of a clause can be. As we represent each body by a tree (see Sect. 4), we set $\mathcal{M}_\mathcal{N} \geq 1$ to be the maximum number of nodes in the tree representation of any clause. We also set $\mathcal{M}_\mathcal{C}$ to be the maximum number of clauses in a program. We must have that $\mathcal{M}_\mathcal{C} \geq |\mathcal{P}|$ because we require each predicate to have at least one clause that defines it. The model supports enforcing predicate independence (see Sect. 7), so a set of independent pairs of predicates is another parameter. Since this model can generate probabilistic as well as non-probabilistic programs, each clause is paired with a probability which is randomly selected from a given list—our last parameter. For generating non-probabilistic programs, one can set this list to [1]. Finally, we define $\mathcal{T} = \{\neg, \wedge, \vee, \top\}$ as the set of tokens that (together with atoms) form a clause. All decision variables of the model can now be divided into $2 \times \mathcal{M}_\mathcal{C}$ separate groups, treating the body and the head of each clause separately. We say that the variables are contained in two arrays: $\texttt{Body} : \texttt{bodies}[\mathcal{M}_\mathcal{C}]$ and $\texttt{Head} : \texttt{heads}[\mathcal{M}_\mathcal{C}]$.

3 Heads of Clauses

We define the *head* of a clause as a $\texttt{predicate} \in \mathcal{P} \cup \{\square\}$ and $\texttt{arguments}[\mathcal{M}_\mathcal{A}] \in \mathcal{C} \cup \mathcal{V} \cup \{\square\}$. Here, we use $\square$ to denote either a disabled clause that we choose

[3] Our model supports arbitrarily complex bodies of clauses (e.g., $\neg\mathsf{P}(X) \vee (\mathsf{Q}(X) \wedge \mathsf{P}(X))$) because ProbLog does too. However, one can easily restrict our representation of a body to a single conjunction of literals (e.g., $\mathsf{Q}(X) \wedge \neg\mathsf{P}(X)$)) by adding a couple of additional constraints.

not to use or disabled arguments if the arity of the `predicate` is less than $\mathcal{M}_\mathcal{A}$. The reason why we need a separate value for the latter (i.e., why it is not enough to fix disabled arguments to a single already-existing value) will become clear in Sect. 5. This `predicate` variable has a corresponding arity that depends on the `predicate`. We can define $\texttt{arity} \in [0, \mathcal{M}_\mathcal{A}]$ as the arity of the `predicate` if $\texttt{predicate} \in \mathcal{P}$ and zero otherwise using the table constraint [17]. This constraint uses a set of pairs of the form (p, a), where p ranges over all possible values of the `predicate`, and a is either the arity of predicate p or zero. Having defined arity, we can now fix the superfluous arguments.

Constraint 1. *For* $i = 0, \ldots, \mathcal{M}_\mathcal{A} - 1$, $\texttt{arguments}[i] = \square \iff i \geq \texttt{arity}$.

We also add a constraint that each predicate should get at least one clause.

Constraint 2. *Let* $P = \{h.\texttt{predicate} \mid h \in \texttt{heads}\}$ *be a multiset. Then*

$$\texttt{nValues}(P) = \begin{cases} |\mathcal{P}| & \text{if } \texttt{count}(\square, P) = 0 \\ |\mathcal{P}| + 1 & \text{otherwise,} \end{cases}$$

where $\texttt{nValues}(P)$ *counts the number of unique values in* P*, and* $\texttt{count}(\square, P)$ *counts how many times* $\square$ *appears in* P*.*

Finally, we want to disable duplicate clauses but with one exception: there may be more than one disabled clause, i.e., a clause with head $\texttt{predicate} = \square$. Assuming a lexicographic order over entire clauses such that $\square > \mathsf{P}$ for all $\mathsf{P} \in \mathcal{P}$ and the head predicate is the 'first digit' of this representation, the following constraint disables duplicates as well as orders the clauses.

Constraint 3. *For* $i = 1, \ldots, \mathcal{M}_\mathcal{C} - 1$, *if* $\texttt{heads}[i].\texttt{predicate} \neq \square$, *then*

$$(\texttt{heads}[i-1], \texttt{bodies}[i-1]) < (\texttt{heads}[i], \texttt{bodies}[i]).$$

4 Bodies of Clauses

As was briefly mentioned before, the *body* of a clause is represented by a tree. It has two parts. First, there is the $\texttt{structure}[\mathcal{M}_\mathcal{N}] \in [0, \mathcal{M}_\mathcal{N} - 1]$ array that encodes the structure of the tree using the following two rules: $\texttt{structure}[i] = i$ means that the ith node is a root, and $\texttt{structure}[i] = j$ (for $j \neq i$) means that the ith node's parent is node j. The second part is the array $\texttt{Node} : \texttt{values}[\mathcal{M}_\mathcal{N}]$ such that $\texttt{values}[i]$ holds the value of the ith node, i.e., a representation of the atom or logical operator.

We can use the `tree` constraint [13] to forbid cycles in the `structure` array and simultaneously define $\texttt{numTrees} \in \{1, \ldots, \mathcal{M}_\mathcal{N}\}$ to count the number of trees. We will view the tree rooted at the zeroth node as the main tree and restrict all other trees to single nodes. For this to work, we need to make sure that the zeroth node is indeed a root, i.e., fix $\texttt{structure}[0] = 0$. For convenience, we also define $\texttt{numNodes} \in \{1, \ldots, \mathcal{M}_\mathcal{N}\}$ to count the number of nodes in the main tree. We define it as $\texttt{numNodes} = \mathcal{M}_\mathcal{N} - \texttt{numTrees} + 1$.

Example 1. Let $\mathcal{M}_\mathcal{N} = 8$. Then $\neg\mathsf{P}(X) \vee (\mathsf{Q}(X) \wedge \mathsf{P}(X))$ can be encoded as:

$$\texttt{structure} = [0, 0, 0, \quad 1, \quad 2, \quad 2, \quad 6, 7], \quad \texttt{numNodes} = 6,$$
$$\texttt{values} = [\vee, \neg, \wedge, \mathsf{P}(X), \mathsf{Q}(X), \mathsf{P}(X), \top, \top], \quad \texttt{numTrees} = 3.$$

Here, $\top$ is the value we use for the remaining one-node trees. The elements of the `values` array are nodes. A *node* has a $\texttt{name} \in \mathcal{T} \cup \mathcal{P}$ and $\texttt{arguments}[\mathcal{M}_\mathcal{A}] \in \mathcal{V} \cup \mathcal{C} \cup \{\square\}$. The node's `arity` can then be defined in the same way as in Sect. 3. Furthermore, we can use Constraint 1 to again disable the extra arguments.

Example 2. Let $\mathcal{M}_\mathcal{A} = 2$, $X \in \mathcal{V}$, and let P be a predicate with arity 1. Then the node representing atom $\mathsf{P}(X)$ has: $\texttt{name} = \mathsf{P}$, $\texttt{arguments} = [X, \square]$, $\texttt{arity} = 1$.

We need to constrain the forest represented by the `structure` array together with its `values` to eliminate symmetries and adhere to our desired format. First, we can recognise that the order of the elements in the `structure` array does not matter, i.e., the structure is only defined by how the elements link to each other, so we can add a constraint for sorting the `structure` array. Next, since we already have a variable that counts the number of nodes in the main tree, we can fix the structure and the values of the remaining trees to some constant values.

Constraint 4. *For* $i = 1, \ldots, \mathcal{M}_\mathcal{N} - 1$*, if* $i < \texttt{numNodes}$*, then*

$$\texttt{structure}[i] = i, \quad \textit{and} \quad \texttt{values}[i].\texttt{name} = \top,$$

else $\texttt{structure}[i] < i$.

The second part of this constraint states that every node in the main tree except the zeroth node cannot be a root and must have its parent located to the left of itself. Next, we classify all nodes into three classes: predicate (or empty) nodes, negation nodes, and conjunction/disjunction nodes based on the number of children (zero, one, and two, respectively).

Constraint 5. *For* $i = 0, \ldots, \mathcal{M}_\mathcal{N} - 1$*, let* C_i *be the number of times* i *appears in the* `structure` *array with index greater than* i*. Then*

$$C_i = 0 \iff \texttt{values}[i].\texttt{name} \in \mathcal{P} \cup \{\top\},$$
$$C_i = 1 \iff \texttt{values}[i].\texttt{name} = \neg,$$
$$C_i > 1 \iff \texttt{values}[i].\texttt{name} \in \{\wedge, \vee\}.$$

The value $\top$ serves a twofold purpose: it is used as the fixed value for nodes outside the main tree, and, when located at the zeroth node, it can represent a clause with an empty body. Thus, we can say that only root nodes can have $\top$ as the value.

Constraint 6. *For* $i = 0, \ldots, \mathcal{M}_\mathcal{N} - 1$*,*

$$\texttt{structure}[i] \neq i \implies \texttt{values}[i].\texttt{name} \neq \top.$$

Finally, we add a way to disable a clause by setting its head predicate to $\square$.

Constraint 7. *For* $i = 0, \ldots, \mathcal{M}_\mathcal{C} - 1$*, if* $\texttt{heads}[i].\texttt{predicate} = \square$*, then*

$$\texttt{bodies}[i].\texttt{numNodes} = 1, \quad \textit{and} \quad \texttt{bodies}[i].\texttt{values}[0].\texttt{name} = \top.$$

5 Variable Symmetry Breaking

Ideally, we want to avoid generating programs that are equivalent in the sense that they produce the same answers to all queries. Even more importantly, we want to avoid generating multiple internal representations that ultimately result in the same program. This is the purpose of *symmetry-breaking constraints*, another important benefit of which is that the constraint solving task becomes easier [29]. Given any clause, we can permute the variables in that clause without changing the meaning of the clause or the entire program. Thus, we want to fix the order of variables. Informally, we can say that variable X goes before variable Y if the first occurrence of X in either the head or the body of the clause is before the first occurrence of Y. Note that the constraints described in this section only make sense if $|\mathcal{V}| > 1$ and that all definitions and constraints here are on a per-clause basis.

Definition 1. *Let* $N = \mathcal{M}_\mathcal{A} \times (\mathcal{M}_\mathcal{N} + 1)$*, and let* $\texttt{terms}[N] \in \mathcal{C} \cup \mathcal{V} \cup \{\square\}$ *be a flattened array of all arguments in a particular clause. Then we can use a channeling constraint to define* $\texttt{occ}[|\mathcal{C}| + |\mathcal{V}| + 1]$ *as an array of subsets of* $\{0, \ldots, N-1\}$ *such that for all* $i = 0, \ldots, N-1$*, and* $t \in \mathcal{C} \cup \mathcal{V} \cup \{\square\}$*,*

$$i \in \texttt{occ}[t] \quad \iff \quad \texttt{terms}[i] = t.$$

Next, we introduce an array that holds the first occurrence of each variable.

Definition 2. *Let* $\texttt{intros}[|\mathcal{V}|] \in \{0, \ldots, N\}$ *be such that for* $v \in \mathcal{V}$*,*

$$\texttt{intros}[v] = \begin{cases} 1 + \min \texttt{occ}[v] & \text{if } \texttt{occ}[v] \neq \emptyset \\ 0 & \text{otherwise.} \end{cases}$$

Here, a value of zero means that the variable does not occur in the clause (this choice is motivated by subsequent constraints). As a consequence, all other indices are shifted by one. Having set this up, we can now eliminate variable symmetries simply by sorting `intros`. In other words, we constrain the model so that the variable listed first (in whatever order $\mathcal{V}$ is presented in) has to occur first in our representation of a clause.

Example 3. Let $\mathcal{C} = \emptyset$, $\mathcal{V} = \{X, Y, Z\}$, $\mathcal{M}_\mathcal{A} = 2$, $\mathcal{M}_\mathcal{N} = 3$, and consider the clause $\mathsf{sibling}(X, Y) \leftarrow \mathsf{parent}(X, Z) \wedge \mathsf{parent}(Y, Z)$. Then

$$\begin{aligned} \texttt{terms} &= [X, Y, \square, \square, X, Z, Y, Z], \\ \texttt{occ} &= [\{0, 4\}, \{1, 6\}, \{5, 7\}, \{2, 3\}], \\ \texttt{intros} &= [0, 1, 5], \end{aligned}$$

where the $\square$'s correspond to the conjunction node.

We end the section with several redundant constraints that make the CSP easier to solve. First, we can state that the positions occupied by different terms must be different.

Constraint 8. *For* $u \neq v \in \mathcal{C} \cup \mathcal{V} \cup \{\square\}$, $\texttt{occ}[u] \cap \texttt{occ}[v] = \emptyset$.

The reason why we use zero to represent an unused variable is so that we could now use the 'all different except zero' constraint for the `intros` array. We can also add another link between `intros` and `occ` that essentially says that the smallest element of a set is an element of the set.

Constraint 9. *For* $v \in \mathcal{V}$, $\texttt{intros}[v] \neq 0 \iff \texttt{intros}[v] - 1 \in \texttt{occ}[v]$.

Finally, we define an auxiliary set variable to act as a set of possible values that `intros` can take. Let $\texttt{potentials} \subseteq \{0, \ldots, N\}$ be such that for $v \in \mathcal{V}$, $\texttt{intros}[v] \in \texttt{potentials}$. Using this new variable, we can add a constraint saying that non-predicate nodes in the tree representation of a clause cannot have variables as arguments.

Constraint 10. *For* $i = 0, \ldots, \mathcal{M}_\mathcal{N} - 1$, *let*

$$S = \{\mathcal{M}_\mathcal{A} \times (i+1) + j + 1 \mid j = 0, \ldots, \mathcal{M}_\mathcal{A} - 1\}.$$

If $\texttt{values}[i].\texttt{name} \notin \mathcal{P}$, *then* $\texttt{potentials} \cap S = \emptyset$.

6 Counting Programs

To demonstrate the correctness of the model, this section derives combinatorial expressions for counting the number of programs with up to $\mathcal{M}_\mathcal{C}$ clauses and up to $\mathcal{M}_\mathcal{N}$ nodes per clause, and arbitrary $\mathcal{P}$, $\mathcal{A}$, $\mathcal{V}$, and $\mathcal{C}$. Being able to establish two ways to generate the same sequence of numbers (i.e., numbers of programs with certain properties and parameters) allows us to gain confidence that the constraint model accurately matches our intentions. For this section, we introduce the term *total arity* of a body of a clause to refer to the sum total of arities of all predicates in the body.

We will first consider clauses with *gaps*, i.e., without taking variables and constants into account. Let $T(n, a)$ denote the number of possible clause bodies with n nodes and total arity a. Then $T(1, a)$ is the number of predicates in $\mathcal{P}$ with arity a, and the following recursive definition can be applied for $n > 1$:

$$T(n,a) = T(n-1,a) + 2 \sum_{\substack{c_1+\cdots+c_k=n-1,\\ 2\leq k\leq \frac{a}{\min \mathcal{A}},\\ c_i\geq 1 \text{ for all } i}} \sum_{\substack{d_1+\cdots+d_k=a,\\ d_i\geq \min \mathcal{A} \text{ for all } i}} \prod_{i=1}^{k} T(c_i, d_i).$$

The first term here represents negation, i.e., negating a formula consumes one node but otherwise leaves the task unchanged. If the first operation is not a negation, then it must be either conjunction or disjunction (hence the coefficient '2'). In the first sum, k represents the number of children of the root node, and each c_i is the number of nodes dedicated to child i. Thus, the first sum iterates over all possible ways to partition the remaining $n - 1$ nodes. Similarly, the second sum considers every possible way to partition the total arity a across the

k children nodes. We can then count the number of possible clause bodies with total arity a (and any number of nodes) as

$$C(a) = \begin{cases} 1 & \text{if } a = 0 \\ \sum_{n=1}^{\mathcal{M}_\mathcal{N}} T(n, a) & \text{otherwise.} \end{cases}$$

The number of ways to select n terms is

$$P(n) = |\mathcal{C}|^n + \sum_{\substack{1 \leq k \leq |\mathcal{V}|, \\ 0 = s_0 < s_1 < \cdots < s_k < s_{k+1} = n+1}} \prod_{i=0}^{k} (|\mathcal{C}| + i)^{s_{i+1} - s_i - 1}.$$

The first term is the number of ways to select n constants. The parameter k is the number of variables used in the clause, and $s_1, \ldots, s_k$ mark the first occurrence of each variable. For each gap between any two introductions (or before the first introduction, or after the last introduction), we have $s_{i+1} - s_i - 1$ spaces to be filled with any of the $|\mathcal{C}|$ constants or any of the i already-introduced variables.

Let us order the elements of $\mathcal{P}$, and let a_i be the arity of the ith predicate. The number of programs is then:

$$\sum_{\substack{\sum_{i=1}^{|\mathcal{P}|} h_i = n, \\ |\mathcal{P}| \leq n \leq \mathcal{M}_\mathcal{C}, \\ h_i \geq 1 \text{ for all } i}} \prod_{i=1}^{|\mathcal{P}|} \binom{\sum_{a=0}^{\mathcal{M}_\mathcal{A} \times \mathcal{M}_\mathcal{N}} C(a) P(a + a_i)}{h_i}, \tag{1}$$

Here, we sum over all ways to distribute $|\mathcal{P}| \leq n \leq \mathcal{M}_\mathcal{C}$ clauses among $|\mathcal{P}|$ predicates so that each predicate gets at least one clause. For each predicate, we can then count the number of ways to select its clauses out of all possible clauses. The number of possible clauses can be computed by considering each possible arity a, and multiplying the number of 'unfinished' clauses $C(a)$ by the number of ways to select the required $a + a_i$ terms in the body and the head of the clause. Finally, we compare the numbers produced by (1) with the numbers of programs generated by our model in 1032 different scenarios, thus showing that the combinatorial description developed in this section matches the model's behaviour.

7 Stratification and Independence

Stratification is a condition necessary for probabilistic logic programs [18] and often enforced on logic programs [4] that helps to ensure a unique answer to every query. This is achieved by restricting the use of negation so that any program $\mathscr{P}$ can be partitioned into a sequence of programs $\mathscr{P} = \bigsqcup_{i=1}^{n} \mathscr{P}_i$ such that, for all i, the negative literals in $\mathscr{P}_i$ can only refer to predicates defined in $\mathscr{P}_j$ for $j \leq i$ [4].

Independence, on the other hand, is defined on a pair of predicates (say, $\mathsf{P}, \mathsf{Q} \in \mathcal{P}$) and can be interpreted in two ways. First, if P and Q are independent,

then any ground atom of P is independent of any ground atom of Q in the underlying probability distribution of the probabilistic program. Second, the part of the program needed to fully define P is disjoint from the part of the program needed to define Q.

These two seemingly disparate concepts can be defined using the same building block, i.e., a predicate dependency graph. Let $\mathscr{P}$ be a probabilistic logic program with its set of predicates $\mathcal{P}$. Its *(predicate) dependency graph* is a directed graph $G_{\mathscr{P}}$ with elements of $\mathcal{P}$ as nodes and an edge between $\mathsf{P}, \mathsf{Q} \in \mathcal{P}$ if there is a clause in $\mathscr{P}$ with Q as the head and P mentioned in the body. We say that the edge is *negative* if there exists a clause with Q as the head and at least one instance of P at the body such that the path from the root to the P node in the tree representation of the clause passes through at least one negation node; otherwise, it is *positive*. We say that $\mathscr{P}$ (or $G_{\mathscr{P}}$) has a *negative cycle* if $G_{\mathscr{P}}$ has a cycle with at least one negative edge. A program $\mathscr{P}$ is *stratified* if $G_{\mathscr{P}}$ has no negative cycles.[4] Thus a simple entailment algorithm for stratification can be constructed by selecting all clauses, all predicates of which are fully determined, and looking for negative cycles in the dependency graph constructed based on those clauses using an algorithm such as Bellman-Ford.

For any predicate $\mathsf{P} \in \mathcal{P}$, the set of *dependencies* of P is the smallest set D_{P} such that $\mathsf{P} \in D_{\mathsf{P}}$, and, for every $\mathsf{Q} \in D_{\mathsf{P}}$, all direct predecessors of Q in $G_{\mathscr{P}}$ are in D_{P}. Two predicates P and Q are *independent* if $D_{\mathsf{P}} \cap D_{\mathsf{Q}} = \emptyset$.

Example 4. Consider the following (fragment of a) program:

$$\begin{aligned} \mathsf{sibling}(X, Y) &\leftarrow \mathsf{parent}(X, Z) \wedge \mathsf{parent}(Y, Z), \\ \mathsf{father}(X, Y) &\leftarrow \mathsf{parent}(X, Y) \wedge \neg\mathsf{mother}(X, Y). \end{aligned} \tag{2}$$

Its predicate dependency graph is in Fig. 1. Because of the negation in (2), the edge from mother to father is negative, while the other two edges are positive. The dependencies of each predicate are:

$$\begin{aligned} D_{\mathsf{parent}} &= \{\mathsf{parent}\}, & D_{\mathsf{sibling}} &= \{\mathsf{sibling}, \mathsf{parent}\}, \\ D_{\mathsf{mother}} &= \{\mathsf{mother}\}, & D_{\mathsf{father}} &= \{\mathsf{father}, \mathsf{mother}, \mathsf{parent}\}. \end{aligned}$$

Hence, we have two pairs of independent predicates, i.e., mother is independent of parent and sibling.

Since the definition of independence relies on the dependency graph, we can represent this graph as an adjacency matrix constructed as part of the model. Let $\mathbf{A}$ be a $|\mathcal{P}| \times |\mathcal{P}|$ binary matrix defined element-wise by stating that $\mathbf{A}[i][j] = 0$ if and only if, for all $k = 0, \ldots, \mathcal{M}_{\mathcal{C}} - 1$, either $\texttt{heads}[k].\texttt{predicate} \neq j$ or $i \notin \{a.\texttt{name} \mid a \in \texttt{bodies}[k].\texttt{values}\}$.

Given a partially-solved model with its predicate dependency graph, let us pick an arbitrary path from Q to P (for some $\mathsf{P}, \mathsf{Q} \in \mathcal{P}$) that consists of determined edges that are denoted by 1 in $\mathbf{A}$ and potential/undetermined edges that

[4] This definition is an extension of a well-known result for logic programs [3] to probabilistic logic programs with arbitrary complex clause bodies.

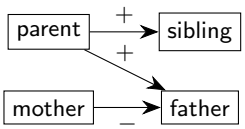


Fig. 1. The predicate dependency graph of the program from Example 4. Positive edges are labelled with '+', and negative edges with '−'.

Table 1. Types of (potential) dependencies of a predicate P based on the number of undetermined edges on the path from the dependency to P

Edges	Name	Notation
0	Determined	$\Delta(p)$
1	Almost determined	$\Gamma(p, s, t)$
> 1	Undetermined	$\Upsilon(p)$

Algorithm 1: Entailment for independence

Data: predicates p_1, p_2
$D \leftarrow \{(d_1, d_2) \in \texttt{deps}(p_1,\ 1) \times \texttt{deps}(p_2,\ 1) \mid d_1.\mathsf{predicate} = d_2.\mathsf{predicate}\}$;
if $D = \emptyset$ **then return** TRUE;
if $\exists(\Delta\ \_, \Delta\ \_) \in D$ **then return** FALSE **else return** UNDEFINED;

are denoted by $\{0, 1\}$. Each such path characterises a *(potential) dependency* Q for P. We classify all such dependencies into three classes depending on the number of undetermined edges on the path. These classes are outlined in Table 1, where p represents the dependency predicate Q, and, in the case of Γ, $(s, t) \in \mathcal{P}^2$ is the one undetermined edge on the path. For a dependency d—regardless of its exact type—we will refer to its predicate p as $d.\mathsf{predicate}$. In describing the algorithms, we will use '_' to replace any of p, s, t in situations where the name is unimportant.

Each entailment algorithm returns one out of three values: TRUE if the constraint is guaranteed to hold, FALSE if the constraint is violated, and UNDEFINED if whether the constraint will be satisfied or not depends on the future decisions made by the solver. Algorithm 1 outlines a simple entailment algorithm for the independence of two predicates p_1 and p_2. First, we separately calculate all dependencies of p_1 and p_2 and look at the set D of dependencies that p_1 and p_2 have in common. If there are none, then the predicates are clearly independent. If they have a dependency in common that is already fully determined (Δ) for both predicates, then they cannot be independent. Otherwise, we return UNDEFINED.

Propagation algorithms have two goals: causing a contradiction (failing) in situations where the corresponding entailment algorithm would return FALSE, and eliminating values from domains of variables that are guaranteed to cause a contradiction. Algorithm 2 does the former on Line 2. Furthermore, for any dependency shared between predicates p_1 and p_2, if it is determined (Δ) for one predicate and almost determined (Γ) for another, then the edge that prevents the Γ from becoming a Δ cannot exist—Line 3 handles this possibility.

The function `deps` in Algorithm 3 calculates D_p for any predicate p. It has two versions: $\texttt{deps}(p, 1)$ returns all dependencies, while $\texttt{deps}(p, 0)$ returns only determined and almost-determined dependencies. It starts by establishing the predicate p itself as a dependency and continues to add dependencies of depen-

Algorithm 2: Propagation for independence

```
Data: predicates p_1, p_2; adjacency matrix A
for (d_1, d_2) ∈ deps(p_1, 0) × deps(p_2, 0) s.t. d_1.predicate = d_2.predicate do
    if d_1 is Δ(_) and d_2 is Δ(_) then fail();
    if {d_1, d_2} = {Δ(_), Γ(_, s, t)} then A[s][t].removeValue(1);
```

Algorithm 3: Dependencies of a predicate

```
Data: adjacency matrix A
Function deps(p, allDeps):
    D ← {Δ(p)};
    while true do
        D' ← ∅;
        for d ∈ D and q ∈ 𝒫 do
            edge ← A[q][d.predicate] = {1};
            if edge and d is Δ(_) then D' ← D' ∪ {Δ(q)};
            else if edge and d is Γ(_, s, t) then D' ← D' ∪ {Γ(q, s, t)};
            else if |A[q][d.predicate]| > 1 and d is Δ(r) then
                D' ← D' ∪ {Γ(q, q, r)};
            else if |A[q][d.predicate]| > 1 and allDeps then D' ← D' ∪ {ϒ(q)};
        if D' = D then return D else D ← D';
```

dencies until the set D stabilises. For each dependency $d \in D$, we look at the in-links of d in the predicate dependency graph. If the edge from some predicate q to $d.\mathsf{predicate}$ is fully determined and d is determined, then q is another determined dependency of p. If the edge is determined but d is almost determined, then q is an almost-determined dependency. The same outcome applies if d is fully determined but the edge is undetermined. Finally, if we are interested in collecting all dependencies regardless of their status, then q is a dependency of p as long as the edge from q to $d.\mathsf{predicate}$ is possible. Note that if there are multiple paths in the dependency graph from q to p, Algorithm 3 could include q once for each possible type (Δ, Υ, and Γ), but Algorithms 1 and 2 would still work as intended.

Example 5. Consider this partially determined (fragment of a) program:

$$\square(X, Y) \leftarrow \mathsf{parent}(X, Z) \wedge \mathsf{parent}(Y, Z),$$
$$\mathsf{father}(X, Y) \leftarrow \mathsf{parent}(X, Y) \wedge \neg\mathsf{mother}(X, Y),$$

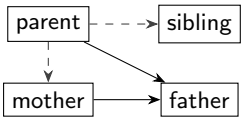
where $\square$ indicates an unknown predicate with domain

$$D_\square = \{\mathsf{father}, \mathsf{mother}, \mathsf{parent}, \mathsf{sibling}\}.$$

The predicate dependency graph is pictured in Fig. 2. Suppose we have a constraint that mother and parent must be independent. The lists of potential de-

$$\begin{array}{l} \mathsf{father} \\ \mathsf{mother} \\ \mathsf{parent} \\ \mathsf{sibling} \end{array} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & \boxed{\{\ 0,\ 1\ \}} & \{0,1\} & \{0,1\} \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

(a) The adjacency matrix of the graph. The boxed value is the decision variable that will be propagated by Algorithm 2.



(b) A drawing of the graph. Dashed edges are undetermined—they may or may not exist.

Fig. 2. The predicate dependency graph of Example 5

pendencies for both predicates are:

$$D_{\mathsf{mother}} = \{\Delta(\mathsf{mother}), \Gamma(\mathsf{parent}, \mathsf{parent}, \mathsf{mother})\},$$
$$D_{\mathsf{parent}} = \{\Delta(\mathsf{parent})\}.$$

An entailment check at this stage would produce UNDEFINED, but propagation replaces the boxed value in Fig. 2a with zero, eliminating the potential edge from parent to mother. This also eliminates mother from $D_{\square}$, and this is enough to make Algorithm 1 return TRUE.

8 Experimental Results

We now present the results of two experiments: in Sect. 8.1 we examine the scalability of our constraint model with respect to its parameters and in Sect. 8.2 we demonstrate how the model can be used to compare inference algorithms and describe their behaviour across a wide range of programs. The experiments were run on a system with Intel Core i5-8250U processor and 8 GB of RAM. The constraint model was implemented in Java 8 with Choco 4.10.2 [23]. All inference algorithms are implemented in ProbLog 2.1.0.39 and were run using Python 3.8.2 with PySDD 0.2.10 and PyEDA 0.28.0. For both sets of experiments, we generate programs without negative cycles and use a 60 s timeout.

8.1 Empirical Performance of the Model

Along with constraints, variables, and their domains, two more design decisions are needed to complete the model: heuristics and restarts. By trial and error, the variable ordering heuristic was devised to eliminate sources of *thrashing*, i.e., situations where a contradiction is being 'fixed' by making changes that have no hope of fixing the contradiction. Thus, we partition all decision variables into an ordered list of groups and require the values of all variables from one group to be determined before moving to the next group. Within each group, we use the 'fail first' variable ordering heuristic. The first group consists of all head predicates. Afterwards, we handle all remaining decision variables from the

first clause before proceeding to the next. The decision variables within each clause are divided into (a) the `structure` array, (b) body predicates, (c) head arguments, (d) (if $|\mathcal{V}| > 1$) the `intros` array, (e) body arguments. For instance, in the clause from Example 3, all visible parts of the clause would be decided in this order:

$$\overset{1}{\mathsf{sibling}}(\overset{3}{X}, \overset{3}{Y}) \leftarrow \overset{2}{\mathsf{parent}}(\overset{4}{X}, \overset{4}{Z}) \overset{2}{\wedge} \overset{2}{\mathsf{parent}}(\overset{4}{Y}, \overset{4}{Z}).$$

We also employ a geometric restart policy, restarting after $10, 10 \times 1.1, 10 \times 1.1^2, \ldots$ contradictions.[5] We ran 399 360 experiments, investigating the model's efficiency and gaining insight into what parameter values make the CSP harder. For $|\mathcal{P}|$, $|\mathcal{V}|$, $|\mathcal{C}|$, $\mathcal{M}_\mathcal{N}$, and $\mathcal{M}_\mathcal{C} - |\mathcal{P}|$ (i.e., the number of clauses in addition to the mandatory $|\mathcal{P}|$ clauses), we assign all combinations of 1, 2, 4, 8. $\mathcal{M}_\mathcal{A}$ is assigned to values 1–4. For each $|\mathcal{P}|$, we also iterate over all possible numbers of independent pairs of predicates, ranging from 0 up to $\binom{|\mathcal{P}|}{2}$. For each combination of the above-mentioned parameters, we pick ten random ways to assign arities to predicates (such that $\mathcal{M}_\mathcal{A}$ occurs at least once) and ten random combinations of independent pairs.

The majority (97.7 %) of runs finished in under 1 s, while four instances timed out: all with $|\mathcal{P}| = \mathcal{M}_\mathcal{C} - |\mathcal{P}| = \mathcal{M}_\mathcal{N} = 8$ and the remaining parameters all different. This suggests that—regardless of parameter values—most of the time a solution can be identified instantaneously while occasionally a series of wrong decisions can lead the solver into a part of the search space with no solutions.

In Fig. 3, we plot how the mean number of nodes in the binary search tree grows as a function of each parameter (the plot for the median is very similar). The growth of each curve suggests how the model scales with higher values of the parameter. From this plot, it is clear that $\mathcal{M}_\mathcal{N}$ is the limiting factor. This is because some tree structures can be impossible to fill with predicates without creating either a negative cycle or a forbidden dependency, and such trees become more common as the number of nodes increases. Likewise, a higher number of predicates complicates the situation as well.

8.2 Experimental Comparison of Inference Algorithms

For this experiment, we consider clauses of two types: *rules* are clauses such that the head atom has at least one variable, and *facts* are clauses with empty bodies and no variables. We use our constraint model to generate the rules according to the following parameter values: $|\mathcal{P}|, |\mathcal{V}|, \mathcal{M}_\mathcal{N} \in \{2, 4, 8\}$, $\mathcal{M}_\mathcal{A} \in \{1, 2, 3\}$, $\mathcal{M}_\mathcal{C} = |\mathcal{P}|$, $\mathcal{C} = \emptyset$. These values are (approximately) representative of many standard benchmarking instances which often have 2–8 predicates of arity one or two, 0–8 rules, and a larger database of facts [14]. Just like before, we explore all possible numbers of independent predicate pairs. We also add a constraint that forbids empty bodies. For both rules and facts, probabilities are uniformly sampled

[5] Restarts help overcome early mistakes in the search process but can be disabled if one wants to find all solutions, in which case search is complete regardless of the variable ordering heuristic.

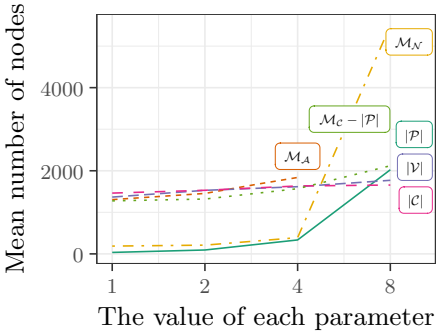


Fig. 3. The mean number of nodes in the binary search tree for each value of each experimental parameter. Note that the horizontal axis is on a $\log_2$ scale.

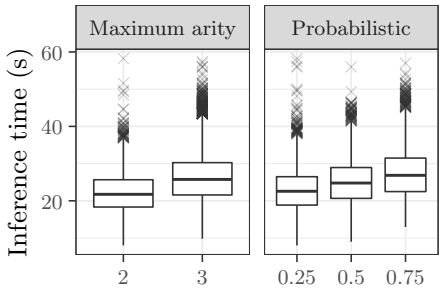


Fig. 4. Inference time for different values of $\mathcal{M}_{\mathcal{A}}$ and proportions of probabilistic facts that are probabilistic. The total number of facts is fixed at 10^5.

from $\{0.1, 0.2, \ldots, 0.9\}$. Furthermore, all rules are probabilistic, while we vary the proportion of probabilistic facts among 25 %, 50 %, and 75 %. For generating facts, we consider $|\mathcal{C}| \in \{100, 200, 400\}$ and vary the number of facts among 10^3, 10^4, and 10^5 but with one exception: the number of facts is not allowed to exceed 75 % of all possible facts with the given values of $\mathcal{P}$, $\mathcal{A}$, and $\mathcal{C}$. Facts are generated using a simple procedure that randomly selects a predicate, combines it with the right number of constants, and checks whether the generated atom is already included or not. We randomly select configurations from the description above and generate ten programs with a complete restart of the constraint solver before the generation of each program, including choosing different arities and independent pairs. Finally, we set the query of each program to a random fact not explicitly included in the program and consider six natively supported algorithms and knowledge compilation techniques: binary decision diagrams (BDDs) [6], negation normal form (NNF), deterministic decomposable NNF (d-DNNF) [8], K-Best [11], and two encodings based on sentential decision diagrams [7], one of which encodes the entire program (SDDX), while the other one encodes only the part of the program relevant to the query (SDD).[6]

Out of 11 310 generated problem instances, about 35 % were discarded because one or more algorithms were not able to ground the instance unambiguously. The first observation (pictured in Fig. 5) is that the algorithms are remarkably similar, i.e., the differences in performance are small and consistent across all parameter values (including parameters not shown in the figure). Unsurprisingly, the most important predictor of inference time is the number of facts. However, after fixing the number of facts to a constant value, we can still observe that inference becomes harder with higher arity predicates as well as

[6] Forward SDDs (FSDDs) and forward BDDs (FBDDs) [27, 28] are omitted because the former uses too much memory and the implementation of the latter seems to be broken at the time of writing.

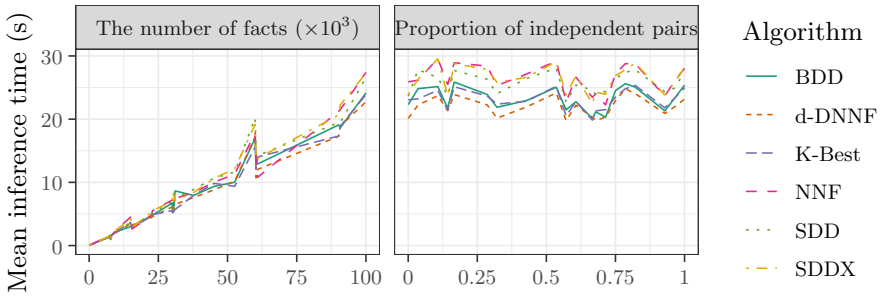


Fig. 5. Mean inference time for a range of ProbLog inference algorithms as a function of the total number of facts in the program and the proportion of independent pairs of predicates. For the second plot, the number of facts is fixed at 10^5.

when facts are mostly probabilistic (see Fig. 4). Finally, according to Fig. 5, the independence structure of a program does not affect inference time, i.e., state-of-the-art inference algorithms—although they are supposed to [15]—do not exploit situations where separate parts of a program can be handled independently.

9 Conclusion

We described a constraint model for generating both logic programs and probabilistic logic programs. The model avoids unnecessary symmetries, is reasonably efficient and supports additional constraints such as predicate independence. Our experimental results provide the first comparison of inference algorithms for probabilistic logic programming languages that generalises over programs, i.e., is not restricted to just a few programs and data sets. While the results did not reveal any significant differences among the algorithms, they did reveal a shared weakness, i.e., the inability to ignore the part of a program that is easily seen to be irrelevant to the given query.

Nonetheless, we would like to outline two directions for future work. First, the experimental evaluation in Sect. 8.1 revealed scalability issues, particularly concerning the length/complexity of clauses. However, this particular issue is likely to resolve itself if the format of a clause is restricted to a conjunction of literals. Second, random instance generation typically focuses on either realistic instances or sampling from a simple and well-defined probability distribution. Our approach can be used to achieve the former, but it is an open question how it could accommodate the latter.

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A Example Programs

In this appendix, we provide examples of probabilistic logic programs generated by various combinations of parameters. In all cases, we use

$$\{0.1, 0.2, \ldots, 0.9, 1, 1, 1, 1, 1\}$$

as the multiset of probabilities. Each clause is written on a separate line and ends with a full stop. The head and the body of each clause are separated with `:-` (instead of $\leftarrow$). The probability of each clause is prepended to the clause, using `::` as a separator. Probabilities equal to one and empty bodies of clauses can be omitted. Conjunction, disjunction, and negation are denoted by commas, semicolons, and '`\+`', respectively. Parentheses are used to demonstrate precedence, although many of them are redundant.

By setting $\mathcal{P} = [\mathtt{p}]$, $\mathcal{A} = [1]$, $\mathcal{V} = \{\mathtt{X}\}$, $\mathcal{C} = \emptyset$, $\mathcal{M}_{\mathcal{N}} = 4$, and $\mathcal{M}_{\mathcal{C}} = 1$, we get fifteen one-line programs, six of which are without negative cycles (as highlighted below). Only the last program has no cycles at all.

```
 1. 0.5 :: p(X) :- (\+(p(X))), (p(X)).
 2. 0.8 :: p(X) :- (\+(p(X))); (p(X)).
 3. 0.8 :: p(X) :- (p(X)); (p(X)).
 4. 0.7 :: p(X) :- (p(X)), (p(X)).
 5. 0.6 :: p(X) :- (p(X)), (\+(p(X))).
 6. p(X) :- (p(X)); (\+(p(X))).
 7. 0.1 :: p(X) :- (p(X)); (p(X)); (p(X)).
 8. 0.8 :: p(X) :- (p(X)), (p(X)), (p(X)).
 9. p(X) :- \+(p(X)).
10. 0.1 :: p(X) :- \+(\+(p(X))).
11. p(X) :- \+((p(X)); (p(X))).
12. 0.4 :: p(X) :- \+((p(X)), (p(X))).
13. 0.4 :: p(X) :- \+(\+(\+(p(X)))).
14. 0.7 :: p(X) :- p(X).
15. p(X).
```

Note that:

- A program such as Program 14, because of its cyclic definition, defines a predicate that has probability zero across all constants. This can more easily be seen as solving equation $0.7x = x$.
- Programs 10 and 14 are not equivalent (i.e., double negation does not cancel out) because Program 10 has a negative cycle and is thus considered to be ill-defined.

To demonstrate variable symmetry reduction in action, we set $\mathcal{P} = [\mathtt{p}]$, $\mathcal{A} = [3]$, $\mathcal{V} = \{\mathtt{X}, \mathtt{Y}, \mathtt{Z}\}$, $\mathcal{C} = \emptyset$, $\mathcal{M}_{\mathcal{N}} = 1$, $\mathcal{M}_{\mathcal{C}} = 1$, and forbid all cycles. This gives us the following five programs:

- `0.8 :: p(Z, Z, Z).`

- `p(Y, Y, Z).`
- `p(Y, Z, Z).`
- `p(Y, Z, Y).`
- `0.1 :: p(X, Y, Z).`

This is one of many possible programs with $\mathcal{P} = [\mathtt{p}, \mathtt{q}, \mathtt{r}]$, $\mathcal{A} = [1, 2, 3]$, $\mathcal{V} = \{\mathtt{X}, \mathtt{Y}, \mathtt{Z}\}$, $\mathcal{C} = \{\mathtt{a}, \mathtt{b}, \mathtt{c}\}$, $\mathcal{M}_{\mathcal{N}} = 5$, $\mathcal{M}_{\mathcal{C}} = 5$, and without negative cycles:

```
p(b) :- \+((q(a, b)), (q(X, Y)), (q(Z, X))).
0.4 :: q(X, X) :- \+(r(Y, Z, a)).
q(X, a) :- r(Y, Y, Z).
q(X, a) :- r(Y, b, Z).
r(Y, b, Z).
```

Finally, we set $\mathcal{P} = [\mathtt{p}, \mathtt{q}, \mathtt{r}]$, $\mathcal{A} = [1, 1, 1]$, $\mathcal{V} = \emptyset$, $\mathcal{C} = \{\mathtt{a}\}$, $\mathcal{M}_{\mathcal{N}} = 3$, $\mathcal{M}_{\mathcal{C}} = 3$, forbid negative cycles, and constrain predicates `p` and `q` to be independent. The resulting search space contains thousands of programs such as:

- ```
  0.5 :: p(a) :- (p(a)); (p(a)).
  0.2 :: q(a) :- (q(a)), (q(a)).
  0.4 :: r(a) :- \+(q(a)).
  ```
- ```
  p(a) :- p(a).
  0.5 :: q(a) :- (r(a)); (q(a)).
  r(a) :- (r(a)); (r(a)).
  ```
- ```
  p(a) :- (p(a)); (p(a)).
  0.6 :: q(a) :- q(a).
  0.7 :: r(a) :- \+(q(a)).
  ```
  ```

B Submitted Paper (AAAI 2021 and UAI 2021)

Weighted Model Counting with Conditional Weights for Bayesian Networks

Abstract

Weighted model counting (WMC) has emerged as the unifying inference mechanism across many (probabilistic) domains. Encoding an inference problem as an instance of WMC typically necessitates adding extra literals and clauses. This is partly so because the predominant definition of WMC assigns weights to models based on weights on literals, and this severely restricts what probability distributions can be represented. We develop a measure-theoretic perspective on WMC and propose a way to encode conditional weights on literals analogously to conditional probabilities. This representation can be as succinct as standard WMC with weights on literals but can also expand as needed to represent probability distributions with less structure. To demonstrate the performance benefits of conditional weights over the addition of extra literals, we develop a new WMC encoding for Bayesian networks and adapt a state-of-the-art WMC algorithm ADDMC to the new format. Our experiments show that the new encoding significantly improves the performance of the algorithm on most benchmark instances. Furthermore, the same idea can be adapted to other WMC algorithms and other problem domains.

1 INTRODUCTION

Weighted model counting (WMC), i.e., an extension of model counting (#SAT) that assigns a weight to every model [Sang et al., 2005], has emerged as one of the most dominant and competitive approaches for handling inference tasks in a wide range of formalisms including Bayesian networks [Sang et al., 2005, Darwiche, 2009], probabilistic graphical models more generally [Choi et al., 2013], and probabilistic programs [Fierens et al., 2015, Holtzen et al., 2020]. Over the last fifteen years, WMC has been extended and generalised in many ways, e.g., to handle continuous probability distributions [Belle et al., 2015], first-order probabilistic theories [Van den Broeck et al., 2011, Gogate and Domingos, 2016], and infinite domains [Belle, 2017]. Furthermore, by generalising the notion of weights to an arbitrary semiring, a range of other problems are also captured [Kimmig et al., 2017]. Exact WMC solvers typically rely on either knowledge compilation [Oztok and Darwiche, 2015, Lagniez and Marquis, 2017] or exhaustive DPLL search [Sang et al., 2005], whereas approximate solvers work by sampling [Chakraborty et al., 2014] and performing local search [Wei and Selman, 2005].

The most well-known version of WMC assigns weights to models based on weights on literals, i.e., the weight of a model is the product of the weights of all literals in it. This simplification is motivated by the fact that the number of models scales exponentially with the number of atoms, so listing the weight of every model is intractable. However, this also severely restricts what probability distributions can be represented. A common way to overcome this limitation is by adding more literals. While we show that this is always possible, we demonstrate that it can be significantly more efficient to encode weights in a more flexible format instead.

After briefly reviewing the background in Section 2, in Section 3 we describe three equivalent perspectives on the subject based on logic, set theory, and Boolean algebras. Furthermore, we describe the space of functions on Boolean algebras and various operations on those functions. Section 4 introduces WMC as the problem of computing the value of a measure on a Boolean algebra. We show that not all measures can be represented using literal-based WMC, but all Boolean algebras can be extended to make any measure representable in such a manner.

This new perspective allows us to not only encode any discrete probability distribution but also improve inference speed. In Section 5 we demonstrate this by developing a new WMC encoding for Bayesian networks that uses *conditional*

weights on literals (in the spirit of conditional probabilities) that have literal-based WMC as a special case. We prove the correctness of the encoding and show how a state-of-the-art WMC solver ADDMC [Dudek et al., 2020a] can be adapted to the new format. ADDMC is a recently-proposed algorithm for WMC based on manipulating functions on Boolean algebras using an efficient representation for such functions known as algebraic decision diagrams (ADDs) [Bahar et al., 1997]. ADDMC was already shown to be capable of solving instances other solvers fail at and being the fastest solver on the largest number of instances [Dudek et al., 2020a]. Our experiments in Section 6 focus on further improving the performance of ADDMC on instances that originate from Bayesian networks. We show how our new encoding improves inference on the vast majority of benchmark instances, often by one or two orders of magnitude. We explain the performance benefits by showing how our encoding has asymptotically fewer variables and ADDs.

2 RELATED WORK

Performing inference on Bayesian networks by encoding them into instances of WMC is a well-established idea with a history of almost twenty years. Five encodings have been proposed so far (we will identify them based on the initials of authors as well as publications years): `d02` [Darwiche, 2002], `sbk05` [Sang et al., 2005], `cd05` [Chavira and Darwiche, 2005], `cd06` [Chavira and Darwiche, 2006], and `bklm16` [Bart et al., 2016][1]. Below we summarise the observed performance differences among them.

Sang et al. [2005] claim that `sbk05` is a smaller encoding than `d02` with respect to both the number of clauses and the number of variables but provide no experimental comparison. Chavira and Darwiche [2005] compare `cd05` with `d02` by measuring the time it takes to compile either encoding into an arithmetic circuit. They show that `cd05` always compiles faster and results in a smaller arithmetic circuit (as measured by the number of edges). In their subsequent paper, the same authors perform two sets of experiments (that are relevant to this summary) [Chavira and Darwiche, 2006]. First, they compile `cd05` and `cd06` encodings into d-DNNF (i.e., deterministic decomposable negation normal form [Darwiche, 2001]), measuring both compilation time and numbers of edges in the d-DNNF diagram. The results are mostly in favour of `cd06`. Second, they compare the inference time of `sbk05` run with Cachet [Sang et al., 2004] with the compile times of `cd05` and `cd06`, but only on five (types of) instances. In these experiments, `cd06` is always faster than `cd05`, while the comparison with `sbk05` is mixed. The performance difference between `sbk05` and `cd05` is even harder to judge: `sbk05` is better on three out of five instances and worse on the remaining two. Finally, Bart et al. [2016] introduce `bklm16` and show that it has both fewer variables and fewer clauses than `cd06`. Their experiments show `bklm16` to be superior to `cd06` with respect to both compilation time and encoding size when both are compiled using c2d[2] [Darwiche, 2004] but inferior to `cd06` when `cd06` is compiled using Ace[3] (which still uses c2d but considers the structure of the Bayesian network along with its encoding). Our experiments in Section 6 confirm some of the findings outlined in this section while also showing that the performance of each encoding depends on the WMC algorithm in use, and smaller encodings are not necessarily faster.

[1] Vomlel and Tichavský [2013] also propose an encoding, but only for networks of a particular bipartite structure and without any evaluation.

3 BOOLEAN ALGEBRAS, POWER SETS, AND PROPOSITIONAL LOGIC

In this section, we give a brief introduction to two alternative ways to think about logical constructs such as models and formulas. Let us consider a simple example of a propositional logic $\mathscr{L}$ with only two atoms a and b, and let $U = \{a, b\}$. Then 2^U, the power set of U, is the set of all models of $\mathscr{L}$, and 2^{2^U} is the set of all formulas. These sets can also be represented as Boolean algebras (e.g., using the syntax $(2^{2^U}, \wedge, \vee, \neg, \bot, \top)$) with a partial order $\leq$ that corresponds to set inclusion $\subseteq$—see Table 1 for examples of how various elements can be represented in both notations. Most importantly, note that the word *atom* has completely different meanings in logic and Boolean algebras. An atom in $\mathscr{L}$ is an atomic formula, i.e., an element of U, whereas an atom in a Boolean algebra is (in set-theoretic terms) a singleton set. For instance, an atom in 2^{2^U} corresponds to a model of $\mathscr{L}$, i.e., an element of 2^U. Unless referring specifically to a logic, we will use the algebraic definition of an atom and refer to logical atoms as *variables*. In the rest of the paper, for any set U, we will use set-theoretic notation for 2^U and Boolean-algebraic notation for 2^{2^U}, except for (Boolean) atoms in 2^{2^U} that are denoted as $\{x\}$ for some model $x \in 2^U$.

3.1 FUNCTIONS ON BOOLEAN ALGEBRAS

We also consider the space of all functions from any Boolean algebra to $\mathbb{R}_{\geq 0}$ together with some operations on those functions. They will be instrumental in defining WMC as a measure in Section 4 and can be efficiently represented using ADDs. Furthermore, all of the operations are supported by CUDD [Somenzi, 2015]—a package used by ADDMC for ADD manipulation [Dudek et al., 2020a]. The definitions of multiplication and projection are as defined by Dudek et al. [2020a], while others are new.

[2] `http://reasoning.cs.ucla.edu/c2d/`
[3] `http://reasoning.cs.ucla.edu/ace/`

Table 1: Notation for a logic with two atoms. The elements in both columns are listed in the same order.

Name in logic	Boolean-algebraic notation	Set-theoretic notation
Atoms (elements of U)	a, b	a, b
Models (elements of 2^U)	$\neg a \wedge \neg b, a \wedge \neg b, \neg a \wedge b, a \wedge b$	$\emptyset, \{a\}, \{b\}, \{a,b\}$
Formulas (elements of 2^{2^U})	$\top$	$\{\emptyset, \{a\}, \{b\}, \{a,b\}\}$
	$\neg a \vee \neg b, a \rightarrow b$	$\{\emptyset, \{a\}, \{b\}\}, \{\emptyset, \{a\}, \{a,b\}\}$
	$b \rightarrow a, a \vee b$	$\{\emptyset, \{b\}, \{a,b\}\}, \{\{a\}, \{b\}, \{a,b\}\}$
	$\neg b, \neg a, a \leftrightarrow b$	$\{\emptyset, \{a\}\}, \{\emptyset, \{b\}\}, \{\emptyset, \{a,b\}\}$
	$(a \wedge \neg b) \vee (b \wedge \neg a), a, b$	$\{\{a\}, \{b\}\}, \{\{a\}, \{a,b\}\}, \{\{b\}, \{a,b\}\}$
	$\neg a \wedge \neg b, a \wedge \neg b, \neg a \wedge b, a \wedge b$	$\{\emptyset\}, \{\{a\}\}, \{\{b\}\}, \{\{a,b\}\}$
	$\bot$	$\emptyset$

Definition 1 (Operations on functions)**.** Let $\alpha\colon 2^X \to \mathbb{R}_{\geq 0}$ and $\beta\colon 2^Y \to \mathbb{R}_{\geq 0}$ be functions, $p \in \mathbb{R}_{\geq 0}$, and $x \in X$. We define the following operations:

Addition: $\alpha + \beta\colon 2^{X \cup Y} \to \mathbb{R}_{\geq 0}$ is such that $(\alpha + \beta)(T) = \alpha(T \cap X) + \beta(T \cap Y)$ for all $T \in 2^{X \cup Y}$.

Multiplication: $\alpha \cdot \beta\colon 2^{X \cup Y} \to \mathbb{R}_{\geq 0}$ is such that $(\alpha \cdot \beta)(T) = \alpha(T \cap X) \cdot \beta(T \cap Y)$ for all $T \in 2^{X \cup Y}$.

Scalar multiplication: $p\alpha\colon 2^X \to \mathbb{R}_{\geq 0}$ is such that $(p\alpha)(T) = p \cdot \alpha(T)$ for all $T \in 2^X$.

Complement: $\overline{\alpha}\colon 2^X \to \mathbb{R}_{\geq 0}$ is such that $\overline{\alpha}(T) = 1 - \alpha(T)$ for all $T \in 2^X$.

Projection: $\exists_x \alpha\colon 2^{X \setminus \{x\}} \to \mathbb{R}_{\geq 0}$ is such that $(\exists_x \alpha)(T) = \alpha(T) + \alpha(T \cup \{x\})$ for all $T \in 2^{X \setminus \{x\}}$. For any $Z = \{z_1, \ldots, z_n\} \subseteq X$, we write $\exists_Z$ to mean $\exists_{z_1} \ldots \exists_{z_n}$.

In summary, addition, multiplication, and scalar multiplication are defined pointwise, while complement and projection interact with the algebraic structure of the domains 2^X and 2^Y. Specifically, note that both addition and multiplication are both associative and commutative. We end the discussion on function spaces by defining several special functions: unit $1\colon 2^\emptyset \to \mathbb{R}_{\geq 0}$ defined as $1(\emptyset) = 1$, zero $0\colon 2^\emptyset \to \mathbb{R}_{\geq 0}$ defined as $0(\emptyset) = 0$, and function $[a]\colon 2^{\{a\}} \to \mathbb{R}_{\geq 0}$ defined as $[a](\emptyset) = 0$, $[a](\{a\}) = 1$ for any a. Henceforth, for any function $\alpha\colon 2^X \to \mathbb{R}_{\geq 0}$ and any set T, we will write $\alpha(T)$ to mean $\alpha(T \cap X)$.

4 WMC AS A MEASURE ON A BOOLEAN ALGEBRA

In this section, we introduce an alternative definition of WMC and demonstrate how it relates to the standard one. Let U be a set. A *measure* is a function $\mu\colon 2^{2^U} \to \mathbb{R}_{\geq 0}$ such that $\mu(\bot) = 0$, and $\mu(a \vee b) = \mu(a) + \mu(b)$ for all $a, b \in 2^{2^U}$ whenever $a \wedge b = \bot$ [Gaifman, 1964, Jech, 1997]. A *weight function* is a function $\nu\colon 2^U \to \mathbb{R}_{\geq 0}$. A weight function is *factored* if $\nu = \prod_{x \in U} \nu_x$ for some functions $\nu_x\colon 2^{\{x\}} \to \mathbb{R}_{\geq 0}$, $x \in U$. We say that a weight function $\nu\colon 2^U \to \mathbb{R}_{\geq 0}$ *induces* a measure $\mu_\nu\colon 2^{2^U} \to \mathbb{R}_{\geq 0}$ if $\mu_\nu(x) = \sum_{\{u\} \leq x} \nu(u)$.

Theorem 1. *The function μ_ν is a measure.*

Finally, a measure $\mu\colon 2^{2^U} \to \mathbb{R}_{\geq 0}$ is *factorable* if there exists a factored weight function $\nu\colon 2^U \to \mathbb{R}_{\geq 0}$ that induces μ. In this formulation, WMC corresponds to the process of calculating the value of $\mu_\nu(x)$ for some $x \in 2^{2^U}$ with a given definition of ν.

Relation to the classical (logic-based) view of WMC. Let $\mathscr{L}$ be a propositional logic with two atoms a and b as in Section 3 and $w\colon \{a, b, \neg a, \neg b\} \to \mathbb{R}_{\geq 0}$ a weight function defined as $w(a) = 0.3$, $w(\neg a) = 0.7$, $w(b) = 0.2$, $w(\neg b) = 0.8$. Furthermore, let Δ be a theory in $\mathscr{L}$ with a sole axiom a. Then Δ has two models: $\{a, b\}$ and $\{a, \neg b\}$ and its WMC [Chavira and Darwiche, 2008] is

$$\begin{aligned} \mathrm{WMC}(\Delta) &= \sum_{\omega \models \Delta} \prod_{\omega \models l} w(l) \\ &= w(a)w(b) + w(a)w(\neg b) = 0.3. \end{aligned} \tag{1}$$

Alternatively, we can define $\nu_a\colon 2^{\{a\}} \to \mathbb{R}_{\geq 0}$ as $\nu_a(\{a\}) = 0.3$, $\nu_a(\emptyset) = 0.7$ and $\nu_b\colon 2^{\{b\}} \to \mathbb{R}_{\geq 0}$ as $\nu_b(\{b\}) = 0.2$, $\nu_b(\emptyset) = 0.8$. Let μ be the measure on 2^{2^U} induced by $\nu = \nu_a \cdot \nu_b$. Then, equivalently to Eq. (1), we can write

$$\begin{aligned} \mu(a) &= \nu(\{a, b\}) + \nu(\{a\}) \\ &= \nu_a(\{a\})\nu_b(\{b\}) + \nu_a(\{a\})\nu_b(\emptyset) = 0.3. \end{aligned}$$

Thus, one can equivalently think of WMC as summing over models of a theory or over atoms below an element of a Boolean algebra.

4.1 NOT ALL MEASURES ARE FACTORABLE

Using this new definition of WMC, we can show that WMC with weights defined on literals is only able to capture a subset of all possible measures on a Boolean algebra. This can be demonstrated with a simple example.

Example 1. Let $U = \{a, b\}$ be a set of atoms and $\mu\colon 2^{2^U} \to \mathbb{R}_{\geq 0}$ a measure defined as $\mu(a \wedge b) = 0.72$, $\mu(a \wedge \neg b) = 0.18$, $\mu(\neg a \wedge b) = 0.07$, $\mu(\neg a \wedge \neg b) = 0.03$.[4] If μ could be represented using literal-weight (factored) WMC, we would have to find two weight functions $\nu_a\colon 2^{\{a\}} \to \mathbb{R}_{\geq 0}$ and $\nu_b\colon 2^{\{b\}} \to \mathbb{R}_{\geq 0}$ such that $\nu = \nu_a \cdot \nu_b$ induces μ, i.e., ν_a and ν_b would have to satisfy this system of equations:

$$\begin{aligned} \nu_a(\{a\}) \cdot \nu_b(\{b\}) &= 0.72 \\ \nu_a(\{a\}) \cdot \nu_b(\emptyset) &= 0.18 \\ \nu_a(\emptyset) \cdot \nu_b(\{b\}) &= 0.07 \\ \nu_a(\emptyset) \cdot \nu_b(\emptyset) &= 0.03, \end{aligned}$$

which has no solutions.

Alternatively, we can let b depend on a and consider weight functions $\nu_a\colon 2^{\{a\}} \to \mathbb{R}_{\geq 0}$ and $\nu_b\colon 2^{\{a,b\}} \to \mathbb{R}_{\geq 0}$ defined as $\nu_a(\{a\}) = 0.9$, $\nu_a(\emptyset) = 0.1$, and $\nu_b(\{a, b\}) = 0.8$, $\nu_b(\{a\}) = 0.2$, $\nu_b(\{b\}) = 0.7$, $\nu_b(\emptyset) = 0.3$. One can easily check that with these definitions ν indeed induces μ.

Note that in this case, we chose to interpret ν_b as $\Pr(b \mid a)$ while—with a different definition of ν_b that represents the joint probability distribution $\Pr(a, b)$—ν_b by itself could induce μ. In general, however, factorising the full weight function into several smaller functions often results in weight functions with smaller domains which leads to increased efficiency and decreased memory usage [Dudek et al., 2020a]. We can easily generalise this example further.

Theorem 2. *For any set U such that $|U| \geq 2$, there exists a non-factorable measure $2^{2^U} \to \mathbb{R}_{\geq 0}$.*

Since many measures of interest may not be factorable, a well-known way to encode them into instances of WMC is by adding more literals [Chavira and Darwiche, 2008]. We can use the measure-theoretic perspective on WMC to show that this is always possible, however, as ensuing sections will demonstrate, it can make the inference task much harder in practice.[5]

Theorem 3. *For any set U and measure $\mu\colon 2^{2^U} \to \mathbb{R}_{\geq 0}$, there exists a set $V \supseteq U$, a factorable measure $\mu'\colon 2^{2^V} \to \mathbb{R}_{\geq 0}$, and a formula $f \in 2^{2^V}$ such that $\mu(x) = \mu'(x \wedge f)$ for all formulas $x \in 2^{2^U}$.*

5 ENCODING BAYESIAN NETWORKS USING CONDITIONAL WEIGHTS

In this section, we describe a way to encode Bayesian networks into WMC without restricting oneself to factorable measures and thus having to add extra variables. We will refer to it as `cw`. A Bayesian network is a directed acyclic graph with random variables as vertices that defines a probability distribution over them. Let $\mathcal{V}$ denote this set of random variables. For any random variable $X \in \mathcal{V}$, let $\operatorname{im} X$ denote its set of values and $\operatorname{pa}(X)$ its set of parents. The full probability distribution is then equal to $\prod_{X \in \mathcal{V}} \Pr(X \mid \operatorname{pa}(X))$. For discrete Bayesian networks (and we only consider discrete networks in this paper), each factor of this product can be represented by a CPT. See Fig. 1 for an example Bayesian network that we will refer to throughout this section. For this network, $\mathcal{V} = \{W, F, T\}$, $\operatorname{pa}(W) = \emptyset$, $\operatorname{pa}(F) = \operatorname{pa}(T) = \{W\}$, $\operatorname{im} W = \operatorname{im} F = \{0, 1\}$, and $\operatorname{im} T = \{l, m, h\}$.

Definition 2 (Indicator variables)**.** Let $X \in \mathcal{V}$ be a random variable. If X is binary (i.e., $|\operatorname{im} X| = 2$), we can arbitrary identify one of the values as 1 and the other one as 0 (i.e, $\operatorname{im} X \cong \{0, 1\}$). Then X can be represented by a single *indicator variable* $\lambda_{X=1}$. For notational simplicity, for any set S, we write $\lambda_{X=0} \in S$ or $S = \{\lambda_{X=0}, \dots\}$ to mean $\lambda_{X=1} \notin S$.

On the other hand, if X is not binary, we represent X with $|\operatorname{im} X|$ indicator variables, one for each value. We let

$$\mathscr{E}(X) = \begin{cases} \{\lambda_{X=1}\} & \text{if } |\operatorname{im} X| = 2 \\ \{\lambda_{X=x} \mid x \in \operatorname{im} X\} & \text{otherwise.} \end{cases}$$

denote the set of indicator variables for X and $\mathscr{E}^*(X) = \mathscr{E}(X) \cup \bigcup_{Y \in \operatorname{pa}(X)} \mathscr{E}(Y)$ denote the set of indicator variables for X and its parents in the Bayesian network. Finally, let $U = \bigcup_{X \in \mathcal{V}} \mathscr{E}(X)$ denote the set of all indicator variables for all random variables in the Bayesian network. For example, in the Bayesian network from Fig. 1, $\mathscr{E}^*(T) = \{\lambda_{T=l}, \lambda_{T=m}, \lambda_{T=h}, \lambda_{W=1}\}$.

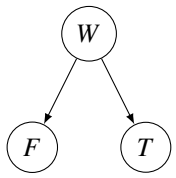
Algorithm 1 shows how a Bayesian network with vertices $\mathcal{V}$ can be represented as a weight function $\phi\colon 2^U \to \mathbb{R}_{\geq 0}$. The algorithm begins with the unit function and multiplies it by $\mathrm{CPT}_X\colon 2^{\mathscr{E}^*(X)} \to \mathbb{R}_{\geq 0}$ for each random variable $X \in \mathcal{V}$. We call each such function a *conditional weight function* as it represents a conditional probability distribution. However, the distinction is primarily a semantic one: a function $2^{\{a,b\}} \to \mathbb{R}_{\geq 0}$ can represent $\Pr(a \mid b)$, $\Pr(b \mid a)$, or something else entirely, e.g., $\Pr(a \wedge b)$, $\Pr(a \vee b)$, etc.

For a binary random variable X, CPT_X is simply a sum of smaller functions, one for each row of the CPT. If X has more than two values, we also multiply CPT_X by 'clause' functions that restrict the value of $\phi(T)$ to zero whenever $|\mathscr{E}(X) \cap T| \neq 1$. For the Bayesian network in Fig. 1, we get:

$$\begin{aligned} \mathrm{CPT}_\mathrm{F} &= 0.6[\lambda_{F=1}] \cdot [\lambda_{W=1}] + 0.4[\lambda_{F=0}] \cdot [\lambda_{W=1}] \\ &\quad + 0.1[\lambda_{F=1}] \cdot [\lambda_{W=0}] + 0.9[\lambda_{F=0}] \cdot [\lambda_{W=0}], \\ \mathrm{CPT}_\mathrm{T} &= ([\lambda_{T=l}] + [\lambda_{T=m}] + [\lambda_{T=h}]) \\ &\quad \cdot (\overline{[\lambda_{T=l}] + \overline{[\lambda_{T=m}]}}) \cdot (\overline{[\lambda_{T=l}] + \overline{[\lambda_{T=h}]}}) \\ &\quad \cdot (\overline{[\lambda_{T=m}] + \overline{[\lambda_{T=h}]}}) \cdot \dots. \end{aligned}$$

[4] The value of μ on any other element of 2^{2^U} can be deduced from the definition of a measure.

[5] The proofs of this and other theoretical results can be found in the appendix.



w	$\Pr(W=w)$
1	0.5
0	0.5

w	f	$\Pr(F=f \mid W=w)$
1	1	0.6
1	0	0.4
0	1	0.1
0	0	0.9

w	t	$\Pr(T=t \mid W=w)$
1	l	0.2
1	m	0.4
1	h	0.4
0	l	0.6
0	m	0.3
0	h	0.1

Figure 1: An example Bayesian network with its CPTs.

Algorithm 1: Encoding a Bayesian network.

Data: vertices $\mathscr{V}$, probability distribution Pr
Result: $\phi\colon 2^U \to \mathbb{R}_{\geq 0}$
$\phi \leftarrow 1$;
for $X \in \mathscr{V}$ **do**
  let $\mathrm{pa}(X) = \{Y_1, \ldots, Y_n\}$;
  $\mathrm{CPT}_X \leftarrow 0$;
  if $|\operatorname{im} X| = 2$ **then**
    for $(y_i)_{i=1}^n \in \prod_{i=1}^n \operatorname{im} Y_i$ **do**
      $p_1 \leftarrow \Pr(X = 1 \mid y_1, \ldots, y_n)$;
      $p_0 \leftarrow \Pr(X \neq 1 \mid y_1, \ldots, y_n)$;
      $\mathrm{CPT}_X \leftarrow \mathrm{CPT}_X$
        $+ p_1[\lambda_{X=1}] \cdot \prod_{i=1}^n [\lambda_{Y_i=y_i}]$
        $+ p_0[\overline{\lambda_{X=1}}] \cdot \prod_{i=1}^n [\lambda_{Y_i=y_i}]$;
  else
    let $\operatorname{im} X = \{x_1, \ldots, x_m\}$;
    for $x \in \operatorname{im} X$ **and** $(y_i)_{i=1}^n \in \prod_{i=1}^n \operatorname{im} Y_i$ **do**
      $p_x \leftarrow \Pr(X = x \mid y_1, \ldots, y_n)$;
      $\mathrm{CPT}_X \leftarrow \mathrm{CPT}_X$
        $+ p_x[\lambda_{X=x}] \cdot \prod_{i=1}^n [\lambda_{Y_i=y_i}]$
        $+ [\overline{\lambda_{X=x}}] \cdot \prod_{i=1}^n [\lambda_{Y_i=y_i}]$;
    $\mathrm{CPT}_X \leftarrow \mathrm{CPT}_X \cdot (\sum_{i=1}^m [\lambda_{X=x_i}])$
      $\cdot \prod_{i=1}^m \prod_{j=i+1}^m (\overline{[\lambda_{X=x_i}]} + \overline{[\lambda_{X=x_j}]})$;
  $\phi \leftarrow \phi \cdot \mathrm{CPT}_X$;
return ϕ;

5.1 CORRECTNESS

Algorithm 1 produces a function with a Boolean algebra as its domain. This function can be represented by an ADD [Bahar et al., 1997]. ADDMC takes an ADD $\psi\colon 2^U \to \mathbb{R}_{\geq 0}$ (expressed as a product of smaller ADDs) and returns $(\exists_U \psi)(\emptyset)$ [Dudek et al., 2020a]. In this section, we prove that the function ϕ produced by Algorithm 1 can be used by ADDMC to correctly compute any marginal probability of the Bayesian network that was encoded as ϕ.[6] We begin with Lemma 1 which shows that any conditional weight function produces the right answer when given a valid encoding of variable-value assignments relevant to the CPT.

Lemma 1. *Let $X \in \mathscr{V}$ be a random variable with parents $\mathrm{pa}(X) = \{Y_1, \ldots, Y_n\}$. Then $\mathrm{CPT}_X\colon 2^{\mathscr{E}^*(X)} \to \mathbb{R}_{\geq 0}$ is such that for any $x \in \operatorname{im} X$ and $(y_1, \ldots, y_n) \in \prod_{i=1}^n \operatorname{im} Y_i$,*

$$\mathrm{CPT}_X(T) = \Pr(X = x \mid Y_1 = y_1, \ldots, Y_n = y_n),$$

where $T = \{\lambda_{X=x}\} \cup \{\lambda_{Y_i=y_i} \mid i = 1, \ldots, n\}$.

Now, Lemma 2 shows that ϕ represents the full probability distribution of the Bayesian network, i.e., it gives the right probabilities for the right inputs and zero otherwise.

Lemma 2. *Let $\mathscr{V} = \{X_1, \ldots, X_n\}$. Then*

$$\phi(T) = \begin{cases} \Pr(x_1, \ldots, x_n) & \text{if } T = \{\lambda_{X_i=x_i}\}_{i=1}^n \text{ for some } (x_i)_{i=1}^n \in \prod_{i=1}^n \operatorname{im} X_i \\ 0 & \text{otherwise,} \end{cases}$$

for all $T \in 2^U$.

We end with Theorem 4 that shows how ϕ can be combined with an encoding of a single variable-value assignment so that ADDMC would compute its marginal probability.

Theorem 4. *For any $X \in \mathscr{V}$ and $x \in \operatorname{im} X$,*

$$(\exists_U (\phi \cdot [\lambda_{X=x}]))(\emptyset) = \Pr(X = x).$$

5.2 TEXTUAL REPRESENTATION

Algorithm 1 encodes a Bayesian network into a function on a Boolean algebra, but how does it relate to the standard interpretation of a WMC encoding as a formula in conjunctive normal form (CNF) together with a collection of weights? The factors of ϕ that restrict the values of indicator variables for non-binary random variables are already expressed as a product of sums of 0/1-valued functions, i.e., a kind of CNF. Disregarding these functions, each conditional weight function CPT_X is represented by a sum with a term for every subset of $\mathscr{E}^*(X)$. To encode these terms, we introduce *extended weight clauses* to the WMC format used by Cachet

[6] Note that it can just as well compute *any* probability expressed using the random variables in $\mathscr{V}$.

[Sang et al., 2004]. For instance, here is a representation of the Bayesian network from Fig. 1:

$$
\begin{array}{llll}
\lambda_{T=l} & \lambda_{T=m} & \lambda_{T=h} & 0 \\
 & -\lambda_{T=l} & -\lambda_{T=m} & 0 \\
 & -\lambda_{T=l} & -\lambda_{T=h} & 0 \\
 & -\lambda_{T=m} & -\lambda_{T=h} & 0 \\
w & \lambda_{W=1} & 0.5 & 0.5 \\
w & \lambda_{F=1} & \lambda_{W=1} & 0.6 \quad 0.4 \\
w & \lambda_{F=1} & -\lambda_{W=1} & 0.1 \quad 0.9 \\
w & \lambda_{T=l} & \lambda_{W=1} & 0.2 \quad 1 \\
w & \lambda_{T=m} & \lambda_{W=1} & 0.4 \quad 1 \\
w & \lambda_{T=h} & \lambda_{W=1} & 0.4 \quad 1 \\
w & \lambda_{T=l} & -\lambda_{W=1} & 0.6 \quad 1 \\
w & \lambda_{T=m} & -\lambda_{W=1} & 0.3 \quad 1 \\
w & \lambda_{T=h} & -\lambda_{W=1} & 0.1 \quad 1
\end{array}
$$

where each indicator variable is eventually replaced with a unique positive integer. Each line prefixed with a w can be split into four parts: the 'main' variable (always not negated), conditions (possibly none), and two weights. For example, the line

$$w \quad \lambda_{T=m} \quad -\lambda_{W=1} \quad 0.3 \quad 1$$

encodes the function $0.3[\lambda_{T=m}] \cdot \overline{[\lambda_{W=1}]} + 1\overline{[\lambda_{T=m}]} \cdot \overline{[\lambda_{W=1}]}$ and can be interpreted as defining two conditional weights: $\nu(T = m \mid W = 0) = 0.3$, and $\nu(T \neq m \mid W = 0) = 1$, the former of which corresponds to a row in the CPT of T while the latter is artificially added as part of the encoding. In our encoding of Bayesian networks, it is always the case that, in each weight clause, either both weights sum to one, or the second weight is equal to one. Finally, note that the measure induced by these weights is not probabilistic (i.e., $\mu(\top) \neq 1$) by itself, but it becomes probabilistic when combined with the additional clauses that restrict what combinations of indicator variables can co-occur.

5.3 CHANGES TO ADDMC

Here we describe two changes to ADDMC[7] [Dudek et al., 2020a] needed to adapt it to the new format.

First, ADDMC constructs the *primal* (a.k.a. Gaifman) *graph* of the input CNF formula as an aid for the algorithm's heuristics. This graph has as vertices the variables of the formula, and there is an edge between two variables u and v if there is a clause in the formula that contains both u and v. We extend this definition to functions on Boolean algebras, i.e., the factors of ϕ. For any pair of distinct variables $u, v \in U$, we draw an edge between them in the primal graph if there is a function $\alpha\colon 2^X \to \mathbb{R}_{\geq 0}$ that is a factor of ϕ such that $u, v \in X$. For instance, a factor such as CPT_X will enable edges between all distinct pairs of variables in $\mathscr{E}^*(X)$. Second, even though the function ϕ produced by Algorithm 1 is constructed to have 2^U as its domain, sometimes the domain is effectively reduced to 2^V for some $V \subset U$ by the ADD manipulation algorithms that optimise the ADD representation of a function. For a simple example, consider $\alpha : 2^{\{a\}} \to \mathbb{R}_{\geq 0}$ defined as $\alpha(\{a\}) = \alpha(\emptyset) = 0.5$. Then α can be reduced to $\alpha'\colon 2^{\emptyset} \to \mathbb{R}_{\geq 0}$ defined as $\alpha'(\emptyset) = 0.5$. To compensate for these reductions, for the original WMC format with a weight function $w\colon U \cup \{\neg u \mid u \in U\} \to \mathbb{R}_{\geq 0}$, ADDMC would multiply its computed answer by $\prod_{u \in U \setminus V} w(u) + w(\neg u)$. With the new WMC format, we instead multiply the answer by $2^{|U \setminus V|}$. Each 'excluded' variable $u \in U \setminus V$ satisfies two properties: all weights associated with u are equal to 0.5 (otherwise the corresponding CPT would depend on u, and u would not be excluded), and all other CPTs are independent of u (or they may have a trivial dependence, where the probability stays the same if u is replaced with its complement). Thus, the CPT that corresponds to u still multiplies the weight of every atom in the Boolean algebra by 0.5, but the number of atoms under consideration is halved. To correct for this, we multiply the final answer by two for every $u \in U \setminus V$.

[7] https://github.com/vardigroup/ADDMC

Table 2: The numbers of instances (out of 1466) solved by each combination of algorithm and encoding (uniquely, faster than others, and in total).

Algorithm & Encoding	Unique	Fastest	Total
Ace + cd05	0	55	1169
Ace + cd06	**34**	218	**1259**
Ace + d02	0	46	993
ADDMC + bklm16	0	29	617
ADDMC + cw	14	**770**	919
ADDMC + d02	0	0	703
ADDMC + sbk05	0	0	729
c2d + bklm16	0	3	1017
Cachet + sbk05	13	229	928

6 EXPERIMENTAL COMPARISON

We compare the six WMC encodings for Bayesian networks when run with both ADDMC and the WMC algorithms used in the original papers.[8] We compare the encodings with respect to the total time it takes to encode a Bayesian network, compile it or run a WMC algorithm on it, and extract the (numerical) answer. Note that while all five papers that introduce other encodings include experimental comparisons of encoding size, that is not feasible with ADDMC as even instances that are fully solved in less than 0.1 s are too big to build the full ADD within reasonable time and memory lim-

[8] Both cd05 and cd06 cannot be run with most WMC algorithms including ADDMC because these encodings allow for additional models that the WMC algorithm is supposed to ignore [Chavira and Darwiche, 2005, 2006].

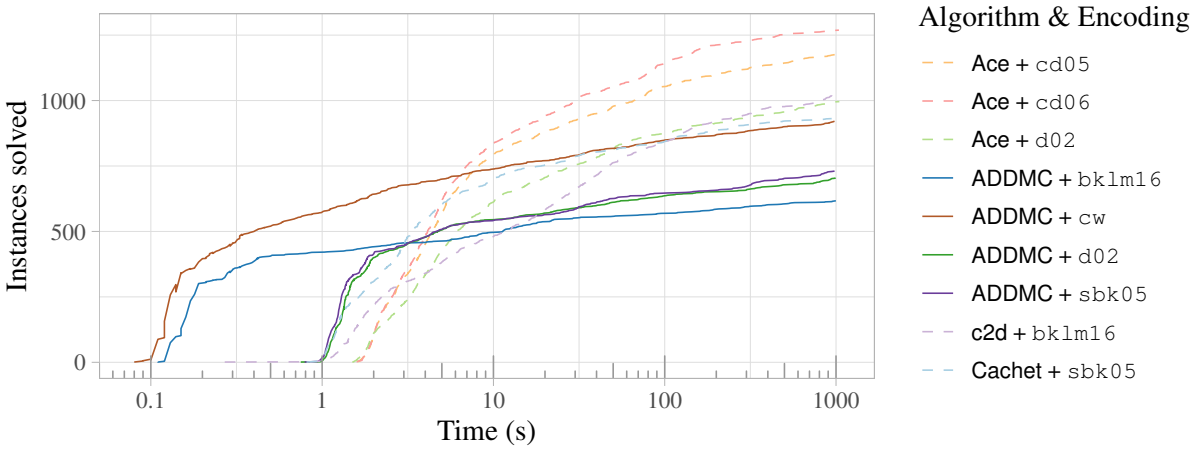


Figure 2: Cumulative numbers of instances solved by combinations of algorithms and encodings over time.

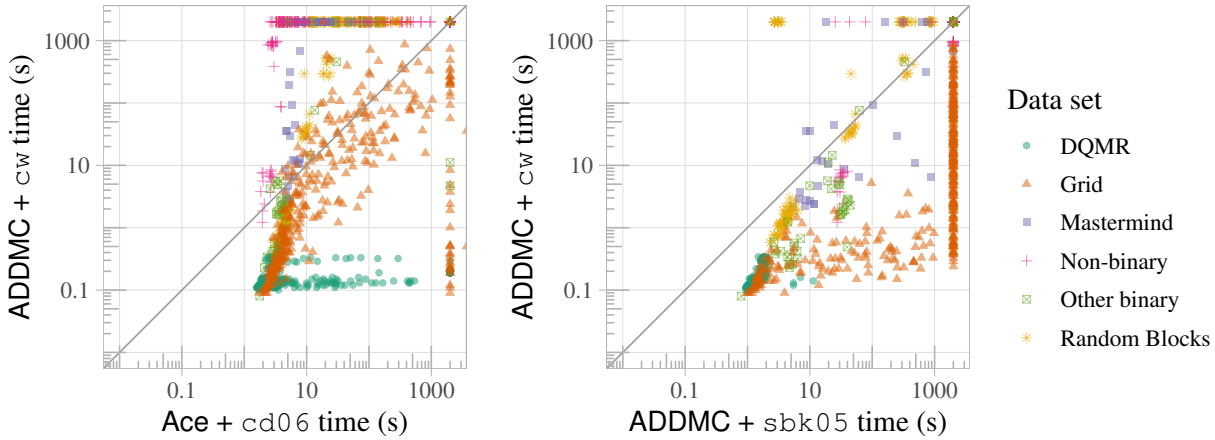


Figure 3: An instance-by-instance comparison between ADDMC + cw and the best overall combination of algorithm and encoding (Ace + cd06, on the left) as well as the second-best encoding for ADDMC (sbk05, on the right).

its. The experiments were run on a computing cluster with Intel Xeon Gold 6138 and Intel Xeon E5-2630 processors[9] running Scientific Linux 7 with a 32 GiB memory limit and a 1000 s timeout on both encoding and inference. For inference, we use Ace for cd05, cd06, and d02; Cachet[10] [Sang et al., 2004] for sbk05; and c2d [Darwiche, 2004] for compilation and query-dnnf [11] for answer computation for bklm16. For encoding, we use bn2cnf [12] for bklm16, and Ace for all other encodings (except for cw, which is implemented in Python).

Ace was not used to encode evidence, as preliminary experiments revealed that the evidence-encoding implementation contains bugs that can lead to incorrect answers or a Java exception being thrown on some instances of the data set (and the source code is not publicly available). Instead, we simply list all the evidence as additional clauses in the encoding. Furthermore, to ensure that bklm16 (whether run with ADDMC or c2d) returns correct answers on most instances, we had to disable one of the improvements that bklm16 brings over cd06, namely, the construction of a scaling factor that 'absorbs' one probability from each CDT [Bart et al., 2016]. For realistic benchmark instances, this scaling factor can easily be below 10^{-30}, and thus would require arbitrary-precision floating-point arithmetic to be usable. Even a toy Bayesian network with seven binary independent variables with probabilities 0.1 and 0.9 is enough for bn2cnf to output precisely zero as the scaling factor. We note that this issue likely remained unnoticed because Bart et al. [2016] did not attempt to compute numerical answers in their experiments.

For each Bayesian network, we need to choose a probability

[9] Each instance is run on the same processor for all encodings.

[10] https://cs.rochester.edu/u/kautz/Cachet/

[11] http://www.cril.univ-artois.fr/kc/d-DNNF-reasoner.html

[12] http://www.cril.univ-artois.fr/KC/bn2cnf.html

Table 3: Asymptotic upper bounds on the numbers of variables and clauses/ADDs for each encoding.

Encoding(s)	Variables	Clauses/ADDs
`bklm16`, `cd05`, `cd06`, `sbk05`	$O(nv^{d+1})$	$O(nv^{d+1})$
`cw`	$O(nv)$	$O(nv^2)$
`d02`	$O(nv^{d+1})$	$O(ndv^{d+1})$

to compute. Whenever a Bayesian network comes with an evidence file, we compute the probability of evidence. Otherwise, let X denote the last-mentioned vertex in the Bayesian network. If $\mathsf{true} \in \mathrm{im}X$, then we compute the marginal probability of $X = \mathsf{true}$. Otherwise, we pick the value of X which is listed first and calculate its marginal probability.

For experimental data, we use the Bayesian networks available with Ace and Cachet, most of which happen to be binary. We classify them into the following seven categories: • DQMR and • Grid networks as described by Sang et al. [2005], • Mastermind, and • Random Blocks from the work of Chavira et al. [2006], • remaining binary Bayesian networks that include Plan Recognition [Sang et al., 2005], Friends and Smokers, Students and Professors [Chavira et al., 2006], and `tcc4f`, and • non-binary classic Bayesian networks (`alarm`, `diabetes`, `hailfinder`, `mildew`, `munin1–4`, `pathfinder`, `pigs`, `water`). We run ADDMC with each of the five encodings once on each Bayesian network.

Figure 2 shows that `cd05` and `cd06` (when run with Ace) are in the lead, while ADDMC significantly underperforms when combined with any of the previous encodings. Our encoding `cw` significantly improves the performance of ADDMC, making ADDMC + `cw` comparable to Ace + `d02`, c2d + `bklm16`, and Cachet + `sbk05`. Furthermore, Table 2 shows that, while Ace + `cd06` managed to solve the most instances, ADDMC + `cw` was the best-performing algorithm-encoding combination on the largest number of instances. The scatter plot on the left-hand side of Fig. 3 add to this by showing that `cw` is particularly promising on Grid networks and tackles all DQMR instances in less than a second. The scatter plot on the right-hand side of Fig. 3 shows that `cw` is better than `sbk05` (i.e., the second-best encoding for ADDMC) on the majority of instances. Seeing how, e.g., DQMR instances are trivial for ADDMC + `cw` but hard for Ace + `cd06`, and vice versa for Mastermind instances, we conclude that the best-performing algorithm-encoding combination depends significantly on (as-of-yet unknown) properties of the Bayesian networks.

We can explain what makes ADDMC run significantly faster with `cw` than with any other encoding by considering asymptotic upper bounds on the numbers of variables and ADDs based on the size and structure of the Bayesian network. Let $n = |\mathscr{V}|$ be the number of vertices in the Bayesian network, $d = \max_{X \in \mathscr{V}} |\mathrm{pa}(X)|$ the maximum in-degree (i.e., the number of parents), and $v = \max_{X \in \mathscr{V}} |\mathrm{im}X|$ the maximum number of values per variable. Table 3 shows how `cw` has fewer variables and fewer ADDs than any other encoding. We conjecture that it is primarily the reduced number of variables that makes the ADDMC variable ordering heuristics much more effective. Note that these are upper bounds and most encodings (including `cw`) can be smaller in certain situations (e.g., with binary random variables or when a CPT has repeating probabilities). We equate clauses and ADDs (more specifically, factors of the function ϕ from Algorithm 1) here because ADDMC interprets each clause of any WMC encoding as a multiplicative factor of the ADD that represents the entire WMC instance [Dudek et al., 2020a]. For literal-weight encodings, each weight is also a factor, but that does not affect our asymptotic bounds.

7 CONCLUSIONS AND FUTURE WORK

WMC was originally motivated by an appeal to the success of SAT solvers in efficiently tackling an NP-complete problem [Sang et al., 2005]. ADDMC does not rely on SAT-based algorithmic techniques [Dudek et al., 2020a], and our proposed format diverges even more from the DIMACS CNF format for Boolean formulas. To what extent are SAT-based methods still applicable? The answer depends significantly on the problem domain. For Bayesian networks, the rules describing that each random variable can only be associated with exactly one value were still encoded as clauses. As has been noted previously [Chavira and Darwiche, 2006], rows in CPTs with probabilities equal to zero or one can be represented as clauses as well. Therefore, our work can be seen as proposing a middle ground between #SAT and probabilistic inference.

While we chose ADDMC as the WMC algorithm and Bayesian networks as a canonical example of a probabilistic inference task, these are only examples meant to illustrate the broader idea that choosing a more expressive representation of weights can outperform increasing the size of the problem to keep the weights simple. Indeed, in this work, we have provided a new theoretical perspective on the expressive power of WMC and illustrated the empirical benefits of that perspective. The same idea can be adapted to other inference problem domains such as probabilistic programs [Fierens et al., 2015, Holtzen et al., 2020] as well as to search-based solvers such as Cachet [Sang et al., 2004] and DPMC —an extension to ADDMC that adds support for computations based on tensors (rather than ADDs) and planning based on tree decompositions Dudek et al. [2020b]. Another important direction for future work is to develop a better understanding of what properties of Bayesian networks make an instance easy for some algorithm-encoding combinations more than others.

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A PROOFS

Theorem 1. *The function μ_ν is a measure.*

Proof. Note that $\mu_\nu(\bot) = 0$ since there are no atoms below $\bot$. Let $a, b \in 2^{2^U}$ be such that $a \wedge b = \bot$. By elementary properties of Boolean algebras, all atoms below $a \vee b$ are either below a or below b. Moreover, none of them can be below both a and b because then they would have to be below $a \wedge b = \bot$. Thus

$$\begin{aligned}\mu_\nu(a \vee b) &= \sum_{\{u\} \leq a \vee b} \nu(u) = \sum_{\{u\} \leq a} \nu(u) + \sum_{\{u\} \leq b} \nu(u) \\ &= \mu_\nu(a) + \mu_\nu(b)\end{aligned}$$

as required. □

Theorem 3. *For any set U and measure $\mu\colon 2^{2^U} \to \mathbb{R}_{\geq 0}$, there exists a set $V \supseteq U$, a factorable measure $\mu'\colon 2^{2^V} \to \mathbb{R}_{\geq 0}$, and a formula $f \in 2^{2^V}$ such that $\mu(x) = \mu'(x \wedge f)$ for all formulas $x \in 2^{2^U}$.*

Proof. Let $V = U \cup \{f_m \mid m \in 2^U\}$, and $f = \bigwedge_{m \in 2^U} \{m\} \leftrightarrow f_m$. We define weight function $\nu\colon 2^V \to \mathbb{R}_{\geq 0}$ as $\nu = \prod_{v \in V} \nu_v$, where $\nu_v(\{v\}) = \mu(\{m\})$ if $v = f_m$ for some $m \in 2^U$ and $\nu_v(x) = 1$ for all other $v \in V$ and $x \in 2^{\{v\}}$. Let $\mu'\colon 2^{2^V} \to \mathbb{R}_{\geq 0}$ be the measure induced by ν. It is enough to show that μ and $x \mapsto \mu'(x \wedge f)$ agree on the atoms in 2^{2^U}. For any $\{a\} \in 2^{2^U}$,

$$\begin{aligned}\mu'(\{a\} \wedge f) &= \sum_{\{x\} \leq \{a\} \wedge f} \nu(x) = \nu(a \cup \{f_a\}) \\ &= \nu_{f_a}(\{f_a\}) = \mu(\{a\})\end{aligned}$$

as required. □

Lemma 1. *Let $X \in \mathscr{V}$ be a random variable with parents $\mathrm{pa}(X) = \{Y_1, \ldots, Y_n\}$. Then $\mathrm{CPT}_X\colon 2^{\mathscr{E}^*(X)} \to \mathbb{R}_{\geq 0}$ is such that for any $x \in \mathrm{im}X$ and $(y_1, \ldots, y_n) \in \prod_{i=1}^n \mathrm{im}Y_i$,*

$$\mathrm{CPT}_X(T) = \Pr(X = x \mid Y_1 = y_1, \ldots, Y_n = y_n),$$

where $T = \{\lambda_{X=x}\} \cup \{\lambda_{Y_i=y_i} \mid i = 1, \ldots, n\}$.

Proof. If X is binary, then CPT_X is a sum of $2\prod_{i=1}^n |\mathrm{im}Y_i|$ terms, one for each possible assignment of values to variables $X, Y_1, \ldots, Y_n$. Exactly one of these terms is nonzero when applied to T, and it is equal to $\Pr(X = x \mid Y_1 = y_1, \ldots, Y_n = y_n)$ by definition.

If X is not binary, then $\left(\sum_{i=1}^m [\lambda_{X=x_i}]\right)(T) = 1$, and $\left(\prod_{i=1}^m \prod_{j=i+1}^m (\overline{[\lambda_{X=x_i}]} + \overline{[\lambda_{X=x_j}]})\right)(T) = 1$, so $\mathrm{CPT}_X(T) = \Pr(X = x \mid Y_1 = y_1, \ldots, Y_n = y_n)$ by a similar argument as before. □

Lemma 2. *Let $\mathscr{V} = \{X_1, \ldots, X_n\}$. Then*

$$\phi(T) = \begin{cases} \Pr(x_1, \ldots, x_n) & \text{if } T = \{\lambda_{X_i=x_i}\}_{i=1}^n \text{ for} \\ & \text{some } (x_i)_{i=1}^n \in \prod_{i=1}^n \mathrm{im}X_i \\ 0 & \text{otherwise,} \end{cases}$$

for all $T \in 2^U$.

Proof. If $T = \{\lambda_{X=v_X} \mid X \in \mathscr{V}\}$ for some $(v_X)_{X \in \mathscr{V}} \in \prod_{X \in \mathscr{V}} \mathrm{im}X$, then

$$\begin{aligned}\phi(T) &= \prod_{X \in \mathscr{V}} \Pr\left(X = v_X \,\middle|\, \bigwedge_{Y \in \mathrm{pa}(X)} Y = v_Y\right) \\ &= \Pr\left(\bigwedge_{X \in \mathscr{V}} X = v_X\right)\end{aligned}$$

by Lemma 1 and the definition of a Bayesian network. Otherwise there must be some non-binary random variable $X \in \mathscr{V}$ such that $|\mathscr{E}(X) \cap T| \neq 1$. If $\mathscr{E}(X) \cap T = \emptyset$, then $\left(\sum_{i=1}^m [\lambda_{X=x_i}]\right)(T) = 0$, and so $\mathrm{CPT}_X(T) = 0$, and $\phi(T) = 0$. If $|\mathscr{E}(X) \cap T| > 1$, then we must have two different values $x_1, x_2 \in \mathrm{im}X$ such that $\{\lambda_{X=x_1}, \lambda_{X=x_2}\} \subseteq T$ which means that $(\overline{[\lambda_{X=x_1}]} + \overline{[\lambda_{X=x_2}]})(T) = 0$, and so, again, $\mathrm{CPT}_X(T) = 0$, and $\phi(T) = 0$. □

Theorem 4. *For any $X \in \mathscr{V}$ and $x \in \mathrm{im}X$,*

$$(\exists_U(\phi \cdot [\lambda_{X=x}]))(\emptyset) = \Pr(X = x).$$

Proof. Let $\mathscr{V} = \{X, Y_1, \ldots, Y_n\}$. Then

$$\begin{aligned}(\exists_U(\phi \cdot [\lambda_{X=x}]))(\emptyset) &= \sum_{T \in 2^U} (\phi \cdot [\lambda_{X=x}])(T) \\ &= \sum_{\lambda_{X=x} \in T \in 2^U} \phi(T) \\ &= \sum_{\lambda_{X=x} \in T \in 2^U} \left(\prod_{Y \in \mathscr{V}} \mathrm{CPT}_Y\right)(T) \\ &= \sum_{(y_i)_{i=1}^n \in \prod_{i=1}^n \mathrm{im}Y_i} \Pr(x, y_1, \ldots, y_n) \\ &= \Pr(X = x)\end{aligned}$$

by:

- the proof of Theorem 1 by Dudek et al. [2020a];
- if $\lambda_{X=x} \notin T \in 2^U$, then $(\phi \cdot [\lambda_{X=x}])(T) = \phi(T) \cdot [\lambda_{X=x}](T \cap \{\lambda_{X=x}\}) = \phi(T) \cdot 0 = 0$;
- Lemma 2;
- marginalisation of a probability distribution.

□

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Weighted Model Counting Without Parameter Variables

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Abstract. Weighted model counting (WMC) is a powerful computational technique for a variety of problems, especially commonly used for probabilistic inference. However, the standard definition of WMC that puts weights on literals often necessitates WMC encodings to include additional variables and clauses just so each weight can be attached to a literal. This paper complements previous work by considering WMC instances in their full generality and using recent state-of-the-art WMC techniques based on pseudo-Boolean function manipulation, competitive with the more traditional WMC algorithms based on knowledge compilation and backtracking search. We present an algorithm that transforms WMC instances into a format based on pseudo-Boolean functions while eliminating around 43 % of variables on average across various Bayesian network encodings. Moreover, we identify sufficient conditions for such a variable removal to be possible. Our experiments show significant improvement in WMC-based Bayesian network inference, outperforming the current state of the art.

Keywords: Weighted model counting · Probabilistic inference · Bayesian networks.

1 Introduction

Weighted model counting (WMC), i.e., a generalisation of propositional model counting that assigns weights to literals and computes the total weight of all models of a propositional formula [12], has emerged as a powerful computational framework for problems in many domains, e.g., probabilistic graphical models such as Bayesian networks and Markov networks [4, 9, 10, 16, 34], neuro-symbolic artificial intelligence [39], probabilistic programs [27], and probabilistic logic programs [22]. It has been extended to support continuous variables [7], infinite domains [5], first-order logic [25, 38], and arbitrary semirings [6, 28]. However, as the definition of WMC puts weights on literals, additional variables often need to be added for the sole purpose of holding a weight [4, 9, 10, 16, 34]. As the parameterised complexity of model counting (and, by extension, WMC) depends on the number of variables [2, 32], this can make WMC unnecessarily slow and could be detrimental to WMC algorithms such as ADDMC [20] that depend on variable ordering heuristics.

One approach to this problem considers weighted clauses and probabilistic semantics based on Markov networks [23]. However, with a new representation comes the need to invent new encodings and inference algorithms. Our work is similar in spirit in that it introduces a new representation for computational problems but can reuse recent WMC algorithms based on pseudo-Boolean function manipulation, namely, ADDMC [20] and DPMC [21]. Furthermore, we identify sufficient conditions for transforming a WMC instance into our new format. As many WMC inference algorithms such as Ace, c2d [17], and miniC2D [30] work by compilation to tractable representations such as arithmetic circuits, deterministic, decomposable negation normal form [15], and sentential decision diagrams (SDDs) [18], another way to avoid parameter variables could be via direct compilation to a more convenient representation. Direct compilation of Bayesian networks to SDDs has been investigated [14]. However, SDDs only support weights on literals, and so are not expressive enough to avoid the issue. To the best of the authors' knowledge, neither approach [14, 23] has a publicly available implementation.

In this work, we introduce a way to transform WMC problems into a new format based on pseudo-Boolean functions—*pseudo-Boolean projection* (PBP). We formally show that every WMC problem instance has a corresponding PBP instance and identify conditions under which this transformation can remove parameter variables. Four out of the five known WMC encodings for Bayesian networks [4, 9, 10, 16, 34] can indeed be simplified in this manner. We are able to eliminate 43 % of variables on average and up to 99 % on some instances. This transformation enables two encodings that were previously incompatible with most WMC algorithms (due to using a different definition of WMC [9, 10]) to be run with ADDMC and DPMC and results in a significant performance boost for one other encoding, making it about three times faster than the state of the art. Finally, our theoretical contributions result in a convenient algebraic way of reasoning about two-valued pseudo-Boolean functions and position WMC encodings on common ground, identifying their key properties and assumptions.

2 Weighted Model Counting

We begin with an overview of some notation and terminology. Throughout the paper, we use set-theoretic notation for many concepts in logic. A *clause* is a set of literals that are part of an implicit disjunction. Similarly, a *formula* in CNF is a set of clauses that are part of an implicit conjunction. We identify a *model* with a set of variables that correspond to the positive literals in the model (and all other variables are the negative literals of the model). We can then define the *cardinality* of a model as the cardinality of this set. For example, let $\phi = (\neg a \vee b) \wedge a$ be a propositional formula over variables a and b. Then an equivalent set-theoretic representation of ϕ is $\{\{\neg a, b\}, \{a\}\}$. Any subset of $\{a, b\}$ is an interpretation of ϕ, e.g., $\{a, b\}$ is a model of ϕ (written $\{a, b\} \models \phi$) of cardinality two, while $\emptyset$ is an interpretation but not a model. We can now formally define WMC.

Definition 1 (WMC). *A* WMC instance *is a tuple* (ϕ, X_I, X_P, w)*, where* X_I *is the set of* indicator variables*,* X_P *is the set of* parameter variables *(with* $X_I \cap X_P = \emptyset$*),* ϕ *is a propositional formula in CNF over* $X_I \cup X_P$*, and* $w\colon X_I \cup X_P \cup \{\neg x \mid x \in X_I \cup X_P\} \to \mathbb{R}$ *is a* weight function *such that* $w(x) = w(\neg x) = 1$ *for all* $x \in X_I$*. The* answer *of the instance is* $\sum_{Y \models \phi} \prod_{Y \models l} w(l)$*.*

That is, the answer to a WMC instance is the sum of the weights of all models of ϕ, where the weight of a model is defined as the product of the weights of all (positive and negative) literals in it. Our definition of WMC is largely based on the standard definition [12], but explicitly partitions variables into indicator and parameter variables. In practice, we identify this partition in one of two ways. If an encoding is generated by Ace[3], then variable types are explicitly identified in a file generated alongside the encoding. Otherwise, we take X_I to be the set of all variables x such that $w(x) = w(\neg x) = 1$. Next, we formally define a variation of the WMC problem used by some of the Bayesian network encodings [9, 10].

Definition 2. *Let* ϕ *be a formula over a set of variables* X*. Then* $Y \subseteq X$ *is a* minimum-cardinality model *of* ϕ *if* $Y \models \phi$ *and* $|Y| \leq |Z|$ *for all* $Z \models \phi$*.*

Definition 3 (Minimum-Cardinality WMC). *A* minimum-cardinality WMC *instance consists of the same tuple as a WMC instance, but its* answer *is defined to be* $\sum_{Y \models \phi,\ |Y|=k} \prod_{Y \models l} w(l)$ *(where* $k = \min_{Y \models \phi} |Y|$*) if* ϕ *is satisfiable, and zero otherwise.*

Example 1. Let $\phi = (x \vee y) \wedge (\neg x \vee \neg y) \wedge (\neg x \vee p) \wedge (\neg y \vee q) \wedge x$, $X_I = \{x, y\}$, $X_P = \{p, q\}$, $w(p) = 0.2$, $w(q) = 0.8$, and $w(\neg p) = w(\neg q) = 1$. Then ϕ has two models: $\{x, p\}$ and $\{x, p, q\}$ with weights 0.2 and $0.2 \times 0.8 = 0.16$, respectively. The WMC answer is then $0.2 + 0.16 = 0.36$, and the minimum-cardinality WMC answer is 0.2.

2.1 Bayesian Network Encodings

A *Bayesian network* is a directed acyclic graph with random variables as vertices and edges as conditional dependencies. As is common in related literature [16, 34], we assume that each variable has a finite number of values. We call a Bayesian network *binary* if every variable has two values. If all variables have finite numbers of values, the probability function associated with each variable v can be represented as a *conditional probability table* (CPT), i.e., a table with a row for each combination of values that v and its parent vertices can take. Each row then also has a *probability*, i.e., a number in $[0, 1]$.

WMC is a well-established technique for Bayesian network inference, particularly effective on networks where most variables have only a few possible values [16]. Many ways of encoding a Bayesian network into a WMC instance have been proposed. We will refer to them based on the initials of the authors and

[3] Ace [12] implements most of the Bayesian network encodings and can also be used for compilation (and thus inference). It is available at http://reasoning.cs.ucla.edu/ace/.

the year of publication. Darwiche was the first to suggest the `d02` [16] encoding that, in many ways, remains the foundation behind most other encodings. He also introduced the distinction between *indicator* and *parameter variables*; the former represent variable-value pairs in the Bayesian network, while the latter are associated with probabilities in the CPTs. The encoding `sbk05` [34] is the only encoding that deviates from this arrangement: for each variable in the Bayesian network, one indicator variable acts simultaneously as a parameter variable. Chavira and Darwiche propose `cd05` [9] where they shift from WMC to minimum-cardinality WMC because that allows the encoding to have fewer variables and clauses. In particular, they propose a way to use the same parameter variable to represent all probabilities in a CPT that are equal and keep only clauses that 'imply' parameter variables (i.e., omit clauses where a parameter variable implies indicator variables).[4] In their next encoding, `cd06` [10], the same authors optimise the aforementioned implication clauses, choosing the smallest sufficient selection of indicator variables. A decade later, Bart et al. present `bklm16` [4] that improves upon `cd06` in two ways. First, they optimise the number of indicator variables used per Bayesian network variable from a linear to a logarithmic amount. Second, they introduce a scaling factor that can 'absorb' one probability per Bayesian network variable. However, for this work, we choose to disable the latter improvement since this scaling factor is often small enough to be indistinguishable from zero without the use of arbitrary precision arithmetic, making it completely unusable on realistic instances. Indeed, the reader is free to check that even a small Bayesian network with seven mutually independent binary variables, 0.1 and 0.9 probabilities each, is already big enough for the scaling factor to be exactly equal to zero (as produced by the `bklm16` encoder[5]). We suspect that this issue was not identified during the original set of experiments because they never looked at numerical answers.

Example 2. Let $\mathcal{B}$ be a Bayesian network with one variable X which has two values x_1 and x_2 with probabilities $\Pr(X = x_1) = 0.2$ and $\Pr(X = x_2) = 0.8$. Let x, y be indicator variables, and p, q be parameter variables. Then Example 1 is both the `cd05` and the `cd06` encoding of $\mathcal{B}$. The `bklm16` encoding is $(x \Rightarrow p) \wedge (\neg x \Rightarrow q) \wedge x$ with $w(p) = w(\neg q) = 0.2$, and $w(\neg p) = w(q) = 0.8$. And the `d02` encoding is $(\neg x \Rightarrow p) \wedge (p \Rightarrow \neg x) \wedge (x \Rightarrow q) \wedge (q \Rightarrow x) \wedge \neg x$ with $w(p) = 0.2$, $w(q) = 0.8$, and $w(\neg p) = w(\neg q) = 1$. Note how all other encodings have fewer clauses than `d02`. While `cd05` and `cd06` require minimum-cardinality WMC to make this work, `bklm16` achieves the same thing by adjusting weights.

3 Pseudo-Boolean Functions

In this work, we propose a more expressive representation for WMC based on pseudo-Boolean functions. A *pseudo-Boolean function* is a function of the form $\{0, 1\}^n \to \mathbb{R}$ [8]. Equivalently, let X denote a set with n elements (we will refer to

[4] Example 2 demonstrates what we mean by implication clauses.
[5] http://www.cril.univ-artois.fr/kc/bn2cnf.html

them as *variables*), and 2^X denote its powerset. Then a pseudo-Boolean function can have 2^X as its domain (then it is also known as a *set function*).

Pseudo-Boolean functions, most commonly represented as algebraic decision diagrams (ADDs) [3] (although a tensor-based approach has also been suggested [19, 21]), have seen extensive use in value iteration for Markov decision processes [26], both exact and approximate Bayesian network inference [11, 24], and sum-product network [31] to Bayesian network conversion [40]. ADDs have been extended to compactly represent additive and multiplicative structure [37], sentences in first-order logic [35], and continuous variables [36], the last of which was also applied to weighted model integration, i.e., the WMC extension for continuous variables [7, 29].

Since two-valued pseudo-Boolean functions will be used extensively henceforth, we introduce some new notation. For any propositional formula ϕ over X and $p, q \in \mathbb{R}$, let $[\phi]_q^p \colon 2^X \to \mathbb{R}$ be the pseudo-Boolean function defined as

$$[\phi]_q^p(Y) \coloneqq \begin{cases} p & \text{if } Y \models \phi \\ q & \text{otherwise} \end{cases}$$

for any $Y \subseteq X$. Next, we define some useful operations on pseudo-Boolean functions. The definitions of multiplication and projection are equivalent to those in previous work [20, 21].

Definition 4 (Operations). *Let $f, g \colon 2^X \to \mathbb{R}$ be pseudo-Boolean functions, $x, y \in X$, $Y = \{y_i\}_{i=1}^n \subseteq X$, and $r \in \mathbb{R}$. Operations such as addition and multiplication are defined pointwise, i.e., $(f+g)(Y) \coloneqq f(Y)+g(Y)$, and likewise for multiplication. Note that properties such as associativity and commutativity are inherited from $\mathbb{R}$. By regarding a real number as a constant pseudo-Boolean function, we can reuse the same definitions to define* scalar *operations as $(r + f)(Y) = r + f(Y)$, and $(r \cdot f)(Y) = r \cdot f(Y)$.*

Restrictions $f|_{x=0}, f|_{x=1} \colon 2^X \to \mathbb{R}$ *of f are defined as $f|_{x=0}(Y) \coloneqq f(Y \setminus \{x\})$, and $f|_{x=1}(Y) \coloneqq f(Y \cup \{x\})$ for all $Y \subseteq X$.*

Projection $\exists_x$ *is an endomorphism $\exists_x \colon \mathbb{R}^{2^X} \to \mathbb{R}^{2^X}$ defined as $\exists_x f \coloneqq f|_{x=1} + f|_{x=0}$. Since projection is commutative (i.e., $\exists_x \exists_y f = \exists_y \exists_x f$) [20, 21], we can define $\exists_Y \colon \mathbb{R}^{2^X} \to \mathbb{R}^{2^X}$ as $\exists_Y \coloneqq \exists_{y_1} \exists_{y_2} \dots \exists_{y_n}$. Throughout the paper, projection is assumed to have the lowest precedence (e.g., $\exists_x f g = \exists_x (f g)$).*

Below we list some properties of the operations on pseudo-Boolean functions discussed in this section that can be conveniently represented using our syntax. The proofs of all these properties follow directly from the definitions.

Proposition 1 (Basic Properties). *For any propositional formulas ϕ and ψ, and $a, b, c, d \in \mathbb{R}$,*

- $[\phi]_b^a = [\neg\phi]_a^b$;
- $c + [\phi]_b^a = [\phi]_{b+c}^{a+c}$;
- $c \cdot [\phi]_b^a = [\phi]_{bc}^{ac}$;
- $[\phi]_b^a \cdot [\phi]_d^c = [\phi]_{bd}^{ac}$;

– $[\phi]_0^1 \cdot [\psi]_0^1 = [\phi \wedge \psi]_0^1$.

And for any pair of pseudo-Boolean functions $f, g\colon 2^X \to \mathbb{R}$ *and* $x \in X$, $(fg)|_{x=i} = f|_{x=i} \cdot g|_{x=i}$ *for* $i = 0, 1$.

Remark 1. Note that our definitions of binary operations assumed equal domains. For convenience, we can assume domains to shrink whenever a function is independent of some of the variables (i.e., $f|_{x=0} = f|_{x=1}$) and expand for binary operations to make the domains of both functions equal. For instance, let $[x]_0^1, [\neg x]_0^1\colon 2^{\{x\}} \to \mathbb{R}$ and $[y]_0^1\colon 2^{\{y\}} \to \mathbb{R}$ be pseudo-Boolean functions. Then $[x]_0^1 \cdot [\neg x]_0^1$ has $2^\emptyset$ as its domain. To multiply $[x]_0^1$ and $[y]_0^1$, we expand $[x]_0^1$ into $\left([x]_0^1\right)' : 2^{\{x,y\}} \to \mathbb{R}$ which is defined as $\left([x]_0^1\right)'(Z) \coloneqq [x]_0^1(Z \cap \{x\})$ for all $Z \subseteq \{x, y\}$ (and equivalently for $[y]_0^1$).

4 Pseudo-Boolean Projection

We introduce a new type of computational problem called *pseudo-Boolean projection* based on two-valued pseudo-Boolean functions. While the same computational framework can handle any pseudo-Boolean functions, two-valued functions are particularly convenient because DPMC can be easily adapted to use them as input, and they are easily representable in both text files and using the syntax proposed in this paper.

Definition 5 (PBP Instance). *A PBP instance is a tuple* (F, X, ω)*, where* X *is the set of variables,* F *is a set of two-valued pseudo-Boolean functions* $2^X \to \mathbb{R}$*, and* $\omega \in \mathbb{R}$ *is the scaling factor.*[6] *Its* answer *is* $\omega \cdot \left(\exists_X \prod_{f \in F} f\right)(\emptyset)$.

4.1 From WMC to PBP

In this section, we describe an algorithm for transforming WMC instances to the PBP format while removing all parameter variables. The algorithm works on four out of the five Bayesian network encodings: `bklm16` [4], `cd05` [9], `cd06` [10], and `d02` [16]. There is no obvious way to adjust it to work with `sbk05` because the roles of indicator and parameter (i.e., 'chance') variables overlap [34]. The algorithm is based on several observations that will be made more precise in Section 4.2. First, all weights except for $\{w(p) \mid p \in X_P\}$ are redundant as they either duplicate an already-defined weight or are equal to one. Second, each clause has at most one parameter variable. Third, if the parameter variable is negated, we can ignore the clause (this idea first appears in the `cd05` paper [9]). Note that while we formulate our algorithm as a sequel to the WMC encoding

[6] Adding scaling factor ω to the definition allows us to remove clauses that consist entirely of a single parameter variable. The idea of extracting some of the structure of the WMC instance into an external multiplicative factor was loosely inspired by the `bklm16` encoding, where it is used to subsume the most commonly occurring probability of each CPT [4].

Algorithm 1: WMC to PBP transformation

Data: WMC (or minimum-cardinality WMC) instance (ϕ, X_I, X_P, w)
Result: PBP instance (F, X_I, ω)

$F \leftarrow \emptyset$;
$\omega \leftarrow 1$;
foreach *clause* $c \in \phi$ **do**
  if $c \cap X_P = \{p\}$ *for some* p **and** $w(p) \neq 1$ **then**
    if $|c| = 1$ **then**
      $\omega \leftarrow \omega \times w(p)$;
    else
      $F \leftarrow F \cup \left\{ \left[\bigwedge_{l \in c \setminus \{p\}} \neg l \right]_1^{w(p)} \right\}$;
  else if $\{p \mid \neg p \in c\} \cap X_P = \emptyset$ **then**
    $F \leftarrow F \cup \{[c]_0^1\}$;
foreach $v \in X_I$ *such that* $\{[v]_1^p, [\neg v]_1^q\} \subseteq F$ *for some* p *and* q **do**
  $F \leftarrow F \setminus \{[v]_1^p, [\neg v]_1^q\} \cup \{[v]_q^p\}$;

procedure primarily because the implementations of Bayesian network WMC encodings are all closed-source, as all transformations in the algorithm are local, it can be efficiently incorporated into a WMC encoding algorithm with no slowdown.

The algorithm is listed as Algorithm 1. The main part of the algorithms is the first loop that iterates over clauses. If a clause consists of a single parameter variable, we incorporate it into ω. If a clause is of the form $\alpha \Rightarrow p$, where $p \in X_P$ and α is a conjunction of literals over X_I, we transform it into a pseudo-Boolean function $[\alpha]_1^{w(p)}$. If a clause (say, $c \in \phi$) has no parameter variables, we reformulate it into a pseudo-Boolean function $[c]_0^1$. Finally, if a clause has negative parameter literals, we skip it.

As all 'weighted' pseudo-Boolean functions produced by the first loop are of the form $[\alpha]_1^p$ (for some $p \in \mathbb{R}$ and formula α), the second loop merges two functions into one whenever α is a literal. Note that taking into account the order in which clauses are typically generated by encoding algorithms allows us to do this in linear time (i.e., the two mergeable functions will be generated one after the other).

4.2 Correctness Proofs

In this section, we outline key properties that a (WMC or minimum-cardinality WMC) encoding has to satisfy for Algorithm 1 to output an equivalent PBP instance. We divide the correctness proof into two theorems: Theorem 2 for WMC encodings (i.e., `bklm16` and `d02`) and Theorem 3 for minimum-cardinality WMC encodings (i.e., `cd05` and `cd06`). We begin by listing some properties of pseudo-Boolean functions and establishing a canonical transformation from WMC to PBP.

Theorem 1 (Early Projection [20, 21]). *Let X and Y be sets of variables. For all pseudo-Boolean functions $f\colon 2^X \to \mathbb{R}$ and $g\colon 2^Y \to \mathbb{R}$, if $x \in X \setminus Y$, then $\exists_x(f \cdot g) = (\exists_x f) \cdot g$.*

Lemma 1. *For any pseudo-Boolean function $f\colon 2^X \to \mathbb{R}$, we have that $(\exists_X f)(\emptyset) = \sum_{Y \subseteq X} f(Y)$.*

Proof. If $X = \{x\}$, then

$$(\exists_x f)(\emptyset) = (f|_{x=1} + f|_{x=0})(\emptyset) = f|_{x=1}(\emptyset) + f|_{x=0}(\emptyset) = \sum_{Y \subseteq \{x\}} f(Y).$$

This easily extends to $|X| > 1$ by the definition of projection on sets of variables.

Proposition 2. *Let (ϕ, X_I, X_P, w) be a WMC instance. Then*

$$\left(\left\{[c]_0^1 \mid c \in \phi\right\} \cup \left\{[x]_{w(\neg x)}^{w(x)} \;\middle|\; x \in X_I \cup X_P\right\}, X_I \cup X_P, 1\right) \tag{1}$$

is a PBP instance with the same answer (as defined in Definitions 1 and 5).

Proof. Let $f = \prod_{c \in \phi}[c]_0^1$, and $g = \prod_{x \in X_I \cup X_P}[x]_{w(\neg x)}^{w(x)}$. Then the WMC answer is (1) is

$$(\exists_{X_I \cup X_P} fg)(\emptyset) = \sum_{Y \subseteq X_I \cup X_P} (fg)(Y) = \sum_{Y \subseteq X_I \cup X_P} f(Y)g(Y)$$

by Lemma 1. Note that

$$f(Y) = \begin{cases} 1 & \text{if } Y \models \phi, \\ 0 & \text{otherwise,} \end{cases} \quad \text{and} \quad g(Y) = \prod_{Y \models l} w(l),$$

which means that $\sum_{Y \subseteq X_I \cup X_P} f(Y)g(Y) = \sum_{Y \models \phi} \prod_{Y \models l} w(l)$ as required.

Theorem 2 (Correctness for WMC). *Algorithm 1, when given a WMC instance (ϕ, X_I, X_P, w), returns a PBP instance with the same answer (as defined in Definitions 1 and 5), provided* either *of the two conditions is satisfied:*

1. *for all $p \in X_P$, there is a non-empty family of literals $(l_i)_{i=1}^n$ such that*
   (a) *$w(\neg p) = 1$,*
   (b) *$l_i \in X_I$ or $\neg l_i \in X_I$ for all $i = 1, \ldots, n$,*
   (c) *and $\{c \in \phi \mid p \in c \text{ or } \neg p \in c\} = \{p \vee \bigvee_{i=1}^n \neg l_i\} \cup \{l_i \vee \neg p \mid i = 1, \ldots, n\}$;*

2. *or for all $p \in X_P$,*
   (a) *$w(p) + w(\neg p) = 1$,*
   (b) *for any clause $c \in \phi$, $|c \cap X_P| \leq 1$,*
   (c) *there is no clause $c \in \phi$ such that $\neg p \in c$,*
   (d) *if $\{p\} \in \phi$, then there is no clause $c \in \phi$ such that $c \neq \{p\}$ and $p \in c$,*

(e) and for any $c, d \in \phi$ such that $c \neq d$, $p \in c$ and $p \in d$, $\bigwedge_{l \in c \setminus \{p\}} \neg l \wedge \bigwedge_{l \in d \setminus \{p\}} \neg l$ is false.

Condition 1 (for `d02`) simply states that each parameter variable is equivalent to a conjunction of indicator literals. Condition 2 is for encodings that have implications rather than equivalences associated with parameter variables (which, in this case, is `bklm16`). It ensures that each clause has at most one positive parameter literal and no negative ones, and that at most one implication clause per any parameter variable $p \in X_P$ can 'force p to be positive'.

Proof. By Proposition 2,

$$\left(\left\{[c]_0^1 \mid c \in \phi\right\} \cup \left\{[x]_{w(\neg x)}^{w(x)} \;\middle|\; x \in X_I \cup X_P\right\}, X_I \cup X_P, 1\right) \tag{2}$$

is a PBP instance with the same answer as the given WMC instance. By Definition 5, its answer is $\left(\exists_{X_I \cup X_P} \left(\prod_{c \in \phi} [c]_0^1\right) \prod_{x \in X_I \cup X_P} [x]_{w(\neg x)}^{w(x)}\right)(\emptyset)$. Since both Conditions 1 and 2 ensure that each clause in ϕ has at most one parameter variable, we can partition ϕ into $\phi_* \coloneqq \{c \in \phi \mid \texttt{Vars}(c) \cap X_P = \emptyset\}$ and $\phi_p \coloneqq \{c \in \phi \mid \texttt{Vars}(c) \cap X_P = \{p\}\}$ for all $p \in X_P$. We can then use Theorem 1 to reorder the answer into $\left(\exists_{X_I} \left(\prod_{x \in X_I} [x]_{w(\neg x)}^{w(x)}\right) \left(\prod_{c \in \phi_*} [c]_0^1\right) \prod_{p \in X_P} \exists_p [p]_{w(\neg p)}^{w(p)} \prod_{c \in \phi_p} [c]_0^1\right)(\emptyset)$.

Let us first consider how the unfinished WMC instance (F, X_I, ω) after the loop on Lines 3 to 10 differs from (2). Note that Algorithm 1 leaves each $c \in \phi_*$ unchanged, i.e., adds $[c]_0^1$ to F. We can then fix an arbitrary $p \in X_P$ and let F_p be the set of functions added to F as a replacement of ϕ_p. It is sufficient to show that

$$\omega \prod_{f \in F_p} f = \exists_p [p]_{w(\neg p)}^{w(p)} \prod_{c \in \phi_p} [c]_0^1. \tag{3}$$

Note that under Condition 1, $\bigwedge_{c \in \phi_p} c \equiv p \Leftrightarrow \bigwedge_{i=1}^n l_i$ for some family of indicator variable literals $(l_i)_{i=1}^n$. Thus, $\exists_p [p]_{w(\neg p)}^{w(p)} \prod_{c \in \phi_p} [c]_0^1 = \exists_p [p]_1^{w(p)} \left[p \Leftrightarrow \bigwedge_{i=1}^n l_i\right]_0^1$. If $w(p) = 1$, then

$$\exists_p [p]_1^{w(p)} \left[p \Leftrightarrow \bigwedge_{i=1}^n l_i\right]_0^1 = \left[p \Leftrightarrow \bigwedge_{i=1}^n l_i\right]_0^1\Bigg|_{p=1} + \left[p \Leftrightarrow \bigwedge_{i=1}^n l_i\right]_0^1\Bigg|_{p=0}. \tag{4}$$

Since for any input, $\bigwedge_{i=1}^n l_i$ is either true or false, exactly one of the two summands in Eq. (4) will be equal to one, and the other will be equal to zero, and so

$$\left[p \Leftrightarrow \bigwedge_{i=1}^n l_i\right]_0^1\Bigg|_{p=1} + \left[p \Leftrightarrow \bigwedge_{i=1}^n l_i\right]_0^1\Bigg|_{p=0} = 1,$$

where 1 is a pseudo-Boolean function that always returns one. On the other side of Eq. (3), since $F_p = \emptyset$, and ω is unchanged, we get $\omega \prod_{f \in F_p} f = 1$, and so Eq. (3) is satisfied under Condition 1 when $w(p) = 1$.

If $w(p) \neq 1$, then $F_p = \left\{ \left[\bigwedge_{i=1}^n l_i\right]_1^{w(p)} \right\}$, and $\omega = 1$, and so we want to show that $\left[\bigwedge_{i=1}^n l_i\right]_1^{w(p)} = \exists_p [p]_1^{w(p)} \left[p \Leftrightarrow \bigwedge_{i=1}^n l_i\right]_0^1$, and indeed

$$\exists_p [p]_1^{w(p)} \left[p \Leftrightarrow \bigwedge_{i=1}^n l_i\right]_0^1 = w(p) \cdot \left[\bigwedge_{i=1}^n l_i\right]_0^1 + \left[\bigwedge_{i=1}^n l_i\right]_1^0 = \left[\bigwedge_{i=1}^n l_i\right]_1^{w(p)}.$$

This finishes the proof of the correctness of the first loop under Condition 1.

Now let us assume Condition 2. We still want to prove Eq. (3). If $w(p) = 1$, then $F_p = \emptyset$, and $\omega = 1$, and so the left-hand side of Eq. (3) is equal to one. Then the right-hand side is

$$\exists_p [p]_0^1 \prod_{c \in \phi_p} [c]_0^1 = \exists_p \left[p \wedge \bigwedge_{c \in \phi_p} c\right]_0^1 = \exists_p [p]_0^1 = 0 + 1 = 1$$

since $p \in c$ for every clause $c \in \phi_p$.

If $w(p) \neq 1$, and $\{p\} \in \phi_p$, then, by Condition 2d, $\phi_p = \{\{p\}\}$, and Algorithm 1 produces $F_p = \emptyset$ and $\omega = w(p)$, and so

$$\exists_p [p]_{w(\neg p)}^{w(p)} [p]_0^1 = \exists_p [p]_0^{w(p)} = w(p) = \omega \prod_{f \in F_p} f.$$

The only remaining case is when $w(p) \neq 1$ and $\{p\} \notin \phi_p$. Then $\omega = 1$, and $F_p = \left\{ \left[\bigwedge_{l \in c \setminus \{p\}} \neg l\right]_1^{w(p)} \,\middle|\, c \in \phi_p \right\}$, so we need to show that $\prod_{c \in \phi_p} \left[\bigwedge_{l \in c \setminus \{p\}} \neg l\right]_1^{w(p)} = \exists_p [p]_{1-w(p)}^{w(p)} \prod_{c \in \phi_p} [c]_0^1$. We can rearrange the right-hand side as

$$\begin{aligned}
\exists_p [p]_{1-w(p)}^{w(p)} \prod_{c \in \phi_p} [c]_0^1 &= \exists_p [p]_{1-w(p)}^{w(p)} \left[p \vee \bigwedge_{c \in \phi_p} c \setminus \{p\}\right]_0^1 \\
&= w(p) + (1 - w(p)) \left[\bigwedge_{c \in \phi_p} c \setminus \{p\}\right]_0^1 \\
&= \left[\bigwedge_{c \in \phi_p} c \setminus \{p\}\right]_{w(p)}^1 = \left[\bigvee_{c \in \phi_p} \bigwedge_{l \in c \setminus \{p\}} \neg l\right]_1^{w(p)}.
\end{aligned}$$

By Condition 2e, $\bigwedge_{l \in c \setminus \{p\}} \neg l$ can be true for at most one $c \in \phi_p$, and so $\left[\bigvee_{c \in \phi_p} \bigwedge_{l \in c \setminus \{p\}} \neg l\right]_1^{w(p)} = \prod_{c \in \phi_p} \left[\bigwedge_{l \in c \setminus \{p\}} \neg l\right]_1^{w(p)}$ which is exactly what we needed to show. This ends the proof that the first loop of Algorithm 1 preserves the answer under both Condition 1 and Condition 2. Finally, the loop on Lines 11 to 12 of Algorithm 1 replaces $[v]_1^p [\neg v]_1^q$ with $[v]_q^p$ (for some $v \in X_I$ and $p, q \in \mathbb{R}$), but, of course, $[v]_1^p [\neg v]_1^q = [v]_1^p [v]_q^1 = [v]_q^p$, i.e., the answer is unchanged.

Theorem 3 (Minimum-Cardinality Correctness). *Let (ϕ, X_I, X_P, w) be a minimum-cardinality WMC instance that satisfies Conditions 2b to 2e of Theorem 2 as well as the following:*

1. *for all parameter variables $p \in X_P$, $w(\neg p) = 1$.*
2. *all models of $\{c \in \phi \mid c \cap X_P = \emptyset\}$ (as subsets of X_I) have the same cardinality;*
3. *$\min_{Z \subseteq X_P} |Z|$ such that $Y \cup Z \models \phi$ is the same for all $Y \models \{c \in \phi \mid c \cap X_P = \emptyset\}$.*

Then Algorithm 1, when applied to (ϕ, X_I, X_P, w), outputs a PBP instance with the same answer (as defined in Definitions 3 and 5).

In this case, we have to add some assumptions about the cardinality of models. Condition 2 states that all models of the indicator-only part of the formula have the same cardinality. Bayesian network encodings such as `cd05` and `cd06` satisfy this condition by assigning an indicator variable to each possible variable-value pair and requiring each random variable to be paired with exactly one value. Condition 3 then says that the smallest number of parameter variables needed to turn an indicator-only model into a full model is the same for all indicator-only models. As some ideas duplicate between the proofs of Theorems 2 and 3, the following proof is slightly less explicit and assumes that $\omega = 1$.

Proof. Let (F, X_I, ω) be the tuple returned by Algorithm 1 and note that $F = \left\{[c]_0^1 \mid c \in \phi,\, c \cap X_P = \emptyset\right\} \cup \left\{ \left[\bigwedge_{l \in c \setminus \{p\}} \neg l\right]_1^{w(p)} \;\middle|\; p \in X_P,\, p \in c \in \phi,\, c \neq \{p\} \right\}$. We split the proof into two parts. In the first part, we show that there is a bijection between minimum-cardinality models of ϕ and $Y \subseteq X_I$ such that $\left(\prod_{f \in F} f\right)(Y) \neq 0$.[7] Let $Y \subseteq X_I$ and $Z \subseteq X_I \cup X_P$ be related via this bijection. Then in the second part we will show that

$$\prod_{Z \models l} w(l) = \left(\prod_{f \in F} f\right)(Y). \tag{5}$$

On the one hand, if $Z \subseteq X_I \cup X_P$ is a minimum-cardinality model of ϕ, then $\left(\prod_{f \in F}\right)(Z \cap X_I) \neq 0$ under the given assumptions. On the other hand, if $Y \subseteq X_I$ is such that $\left(\prod_{f \in F}\right)(Y) \neq 0$, then $Y \models \{c \in \phi \mid c \cap X_P = \emptyset\}$. Let $Y \subseteq Z \subseteq X_I \cup X_P$ be the smallest superset of Y such that $Z \models \phi$ (it exists by Condition 2c of Theorem 2). We need to show that Z has minimum cardinality. Let Y' and Z' be defined equivalently to Y and Z. We will show that $|Z| = |Z'|$. Note that $|Y| = |Y'|$ by Condition 2, and $|Z \setminus Y| = |Z' \setminus Y'|$ by Condition 3. Combining that with the general property that $|Z| = |Y| + |Z \setminus Y|$ finishes the first part of the proof.

[7] For convenience and without loss of generality we assume that $w(p) \neq 0$ for all $p \in X_P$.

For the second part, let us consider the multiplicative influence of a single parameter variable $p \in X_P$ on Eq. (5). If the left-hand side is multiplied by $w(p)$ (i.e., $p \in Z$), then there must be some clause $c \in \phi$ such that $Z \setminus \{p\} \not\models c$. But then $Y \models \bigwedge_{l \in c \setminus \{p\}} \neg l$, and so the right-hand side is multiplied by $w(p)$ as well (exactly once because of Condition 2e of Theorem 2). This argument works in the other direction as well.

5 Experimental Evaluation

We run a set of experiments, comparing all five original Bayesian network encodings (`bklm16`, `cd05`, `cd06`, `d02` `sbk05`) as well as the first four with Algorithm 1 applied afterwards.[8] For each encoding `e`, we write `e++` to denote the combination of encoding a Bayesian network as a WMC instance using `e` and transforming it into a PBP instance using Algorithm 1. Along with DPMC[9], we also include WMC algorithms used in the papers that introduce each encoding: Ace for `cd05`, `cd06`, and `d02`; Cachet[10] [33] for `sbk05`; and `c2d`[11] [17] with `query-dnnf`[12] for `bklm16`. Ace is also used to encode Bayesian networks into WMC instances for all encodings except for `bklm16` which uses another encoder mentioned previously. We focus on the following questions:

- Can parameter variable elimination improve inference speed?
- How does DPMC combined with encodings without (and with) parameter variables compare with other WMC algorithms and other encodings?
- Which instances is our approach particularly successful on (compared to other algorithms and encodings and to the same encoding before our transformation)?
- What proportion of variables is typically eliminated?
- Do some encodings benefit from this transformation more than others?

5.1 Setup

DPMC is run with tree decomposition-based planning and ADD-based execution—the best-performing combination in the original set of experiments [21]. We use a single iteration of `htd` [1] to generate approximately optimal tree decompositions—we found that this configuration is efficient enough to handle huge instances, and yet the width of the returned decomposition is unlikely to differ from optimal by more than one or two. We also enabled DPMC's greedy mode. This mode (which was not part of the original paper [21]) optimises the order in which pseudo-Boolean functions are multiplied by prioritising functions with small representations.

[8] Recall that `cd05` and `cd06` are incompatible with DPMC.
[9] https://github.com/vardigroup/DPMC
[10] https://cs.rochester.edu/u/kautz/Cachet/
[11] http://reasoning.cs.ucla.edu/c2d/
[12] http://www.cril.univ-artois.fr/kc/d-DNNF-reasoner.html

For experimental data, we use Bayesian networks available with Ace and Cachet. We split them into the following groups: – DQMR (390 instances) and – Grid networks (450 instances) as described by Sang et al. [34]; – Mastermind (144 instances) and – Random Blocks (256 instances) by Chavira et al. [13]; – other binary Bayesian networks (50 instances) including Plan Recognition [34], Friends and Smokers, Students and Professors [13], and `tcc4f`; – non-binary classic networks (176 instances): `alarm`, `diabetes`, `hailfinder`, `mildew`, `munin1`–`4`, `pathfinder`, `pigs`, and `water`.

To perform Bayesian network inference with DPMC (or with any other WMC algorithm not based on compilation such as Cachet), one needs to select a probability to compute [21, 33]. If a network comes with an evidence file, we compute the probability of this evidence. Otherwise, let X be the variable last mentioned in the Bayesian network file. If true is one of the values of X, then we compute $\Pr(X = \mathsf{true})$, otherwise we choose the first-mentioned value of X.

The experiments were run on a computing cluster with Intel Xeon E5-2630, Intel Xeon E7-4820, and Intel Xeon Gold 6138 processors with a 1000 s timeout separately on both encoding and inference, and a 32 GiB memory limit.[13]

5.2 Results

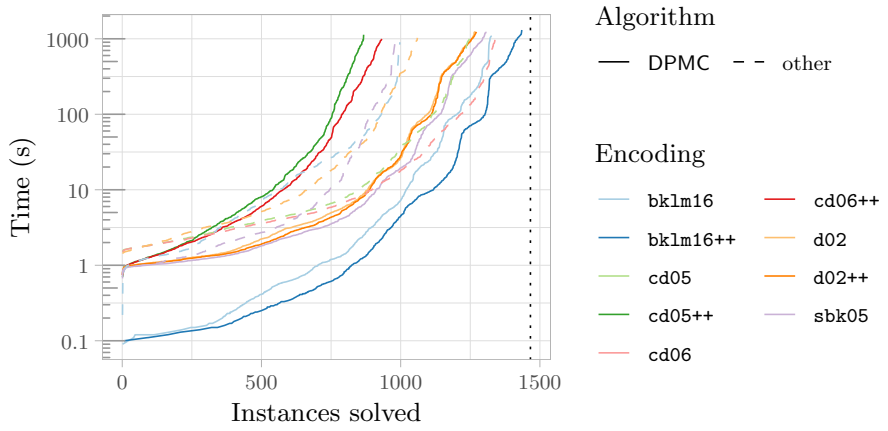

Fig. 1. Cactus plot of all algorithm-encoding pairs. The dotted line denotes the total number of instances used.

Figure 1 shows DPMC + `bklm16++` to be the best-performing combination across all time limits up to 1000 s with Ace + `cd06` and DPMC + `bklm16` not far behind. Overall, DPMC + `bklm16++` is 3.35 times faster than DPMC + `bklm16` and 2.96 times faster than Ace + `cd06`. Table 1 further shows that DPMC + `bklm16++`

[13] Each instance was run on the same processor across all algorithms and encodings.

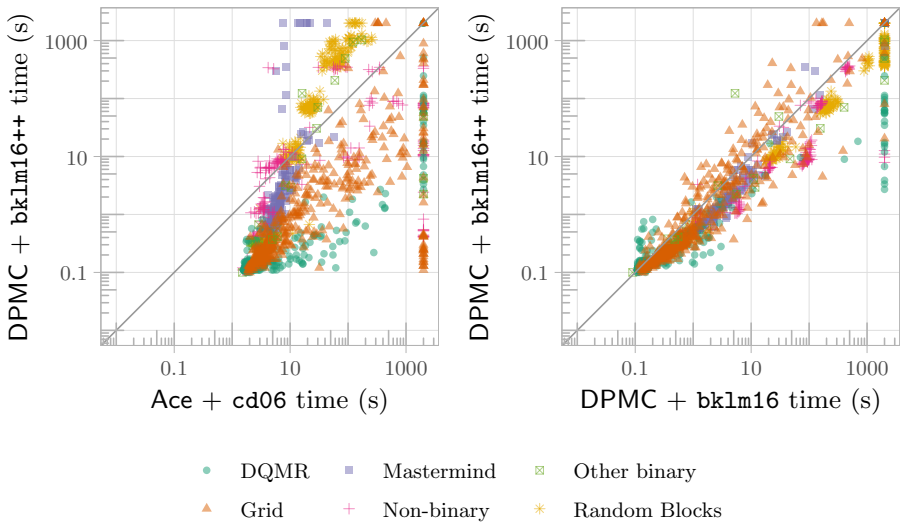

Fig. 2. An instance-by-instance comparison between DPMC + `bklm16++` (the best combination according to Fig. 1) and the second and third best-performing combinations: Ace + `cd06` and DPMC + `bklm16`.

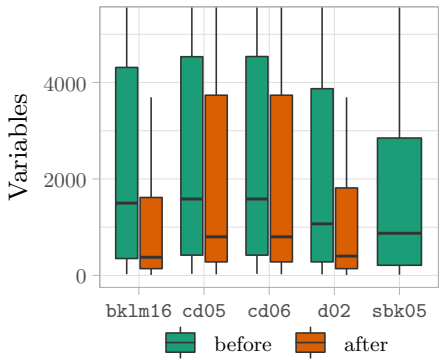

Fig. 3. Box plots of the numbers of variables in each encoding across all benchmark instances before and after applying Algorithm 1. Outliers and the top parts of some whiskers are omitted.

Table 1. The numbers of instances (out of 1466) that each algorithm and encoding combination solved faster than any other combination and in total.

Combination	Fastest	Solved
Ace + `cd05`	27	1247
Ace + `cd06`	135	1340
Ace + `d02`	56	1060
DPMC + `bklm16`	241	1327
DPMC + `bklm16++`	**992**	**1435**
DPMC + `cd05++`	0	867
DPMC + `cd06++`	0	932
DPMC + `d02`	1	1267
DPMC + `d02++`	7	1272
DPMC + `sbk05`	31	1308
c2d + `bklm16`	0	997
Cachet + `sbk05`	49	983

solves almost a hundred more instances than any other combination, and is the fastest in 69.1 % of them.

The scatter plots in Fig. 2 show that how DPMC + bklm16++ (and perhaps DPMC more generally) compares to Ace + cd06 depends significantly on the data set: the former is a clear winner on DQMR and Grid instances, while the latter performs well on Mastermind and Random Blocks. Perhaps because the underlying WMC algorithm remains the same, the difference between DPMC + bklm16 with and without applying Algorithm 1 is quite noisy, i.e, with most instances scattered around the line of equality. However, our transformation does enable DPMC to solve many instances that were previously beyond its reach.

We also record numbers of variables in each encoding before and after applying Algorithm 1. Figure 3 shows a significant reduction in the number of variables. For instance, the median number of variables in instances encoded with bklm16 was reduced four times: from 1499 to 376. While bklm16++ results in the overall lowest number of variables, the difference between bklm16++ and d02++ seems small. Indeed, the numbers of variables in these two encodings are equal for binary Bayesian networks (i.e., most of our data). Nonetheless, bklm16++ is still much faster than d02++ when run with DPMC.

Overall, transforming WMC instances to the PBP format allows us to significantly simplify each instance. This transformation is particularly effective on bklm16, allowing it to surpass cd06 and become the new state of the art. While there is a similarly significant reduction in the number of variables for d02, the performance of DPMC + d02 is virtually unaffected. Finally, while our transformation makes it possible to use cd05 and cd06 with DPMC, the two combinations remain inefficient.

6 Conclusion

In this paper, we showed how the number of variables in a WMC instance can be significantly reduced by transforming it into a representation based on two-valued pseudo-Boolean functions. In some cases, this led to significant improvements in inference speed, allowing DPMC + bklm16++ to overtake Ace + cd06 as the new state of the art WMC technique for Bayesian network inference. Moreover, we identified key properties of Bayesian network encodings that allow for parameter variable removal. However, these properties were rather different for each encoding, and so an interesting question for future work is whether they can be unified into a more abstract and coherent list of conditions.

Bayesian network inference was chosen as the example application of WMC because it is the first and the most studied one [4, 9, 10, 16, 34]. While the distinction between indicator and parameter variables is often not explicitly described in other WMC encodings [22, 27, 39], perhaps in some cases variables could still be partitioned in this way, allowing for not just faster inference with DPMC or ADDMC but also for well-established WMC encoding and inference techniques (such as in the cd05 and cd06 papers [9, 10]) to be transferred to other application domains.

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D First Year Review

Foundations for Inference in Probabilistic Relational Models

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> I am fully assured, that no *general* method for the solution of questions in the theory of probabilities can be established which does not explicitly recognize, not only the special numerical bases of the science, but also those universal laws of thought which are the basis of all reasoning, and which, whatever they may be as to their essence, are at least mathematical as to their form.
>
> George Boole [2]

1 Introduction

The quest to unify logic and probabilities dates back to George Boole [3] and is a promising contemporary area of research due to the pervasiveness of probabilistic approaches in machine learning and the expressivity of first-order logic [15, 40]. An important fundamental idea in the field was established by Nilsson [34] who recognised that, after assigning probabilities to some logical formulas, the set of probabilities that can be assigned to another formula is either a single value or an interval. Since then, many representations that can support probabilities as well as (some aspects of) logic have been suggested, and the field as a whole is most commonly known as statistical relational artificial intelligence [13]. As there is no widely-agreed general-purpose name for the assortment of representations that have been proposed, we will refer to them as *probabilistic relational models* (PRMs) and provide a formal definition shortly. Specific examples of PRMs include the independent choice logic [35] Markov logic networks [39], PRISM [44], probabilistic databases [46], and ProbLog [14]. Another way to encode complex probability distributions is with probabilistic programming languages [22], however, it falls largely outside the scope of this thesis as the support for continuous variables and Turing-complete computation brings a separate set of issues.

These models have been used in a variety of fields. The most significant area of application is knowledge extraction [36], information extraction [5], and other natural language processing tasks. Here, PRMs have been used to annotate articles [47], learn facts about the world from reading websites [6], and solve simple probability problems described in a natural language [18]. Similarly, they have been applied to stream mining [9], predicting criminal activity [16], and predicting how soon a component or a machine will have to be replaced [48]. In robotics, PRMs have been used to learn object affordances [30, 31, 32] and as an expressive knowledge representation system for robot control [25]. Finally, biological applications include the analysis of genetic [42] and breast cancer [11, 33] data. The use of PRMs in learning is primarily motivated by their

ability to learn with respect to the entire relevant structure rather than learning separate components that then have to be combined. On the other hand, the main disadvantage is usually efficiency.

Despite numerous proposed representations and many successful applications, many fundamental problems and challenges remain. My thesis establishes a unified perspective on PRMs and is broadly motivated by the following questions:

- How can we optimise the representation for efficient query handling and removal of unnecessary detail?
- How can we improve the speed of inference and learning?
- How can we identify performance weaknesses in inference algorithms?

In the remainder of this section, we introduce the basic ideas of the field from an algebraic perspective. Consider an arbitrary finite set of predicates with their arities and an arbitrary finite domain of discourse. The set of all atoms that can be constructed by combining a predicate of arity n with n elements from the domain is known as a *Herbrand base* $\mathcal{HB}$. A subset of this base is a *(relational) knowledge base*. If one assigns a non-negative real number to each possible knowledge base such that the total is equal to 1, one gets a PRM.

Furthermore, if each knowledge base $\mathcal{KB}$ is represented by a conjunction of $|\mathcal{HB}|$ literals such that all positive literals correspond to elements in $\mathcal{KB}$ and all negative literals correspond to elements in $\mathcal{HB} \setminus \mathcal{KB}$, then, treating the elements of $\mathcal{HB}$ as propositions, we can assign a probability to any propositional formula using one simple rule, i.e.,

$$\Pr(p \vee q) = \Pr(p) + \Pr(q) \quad \text{if} \quad p \wedge q = \bot$$

for any propositional formulas p and q. That is, any propositional formula can be seen as a disjunction of disjoint knowledge bases. This defines a free Boolean algebra $\mathscr{F}(\mathcal{HB})$ over $\mathcal{HB}$ with a probability measure. In a special case where we can assign a positive weight to each literal such that the probability of each knowledge base can be expressed as the product of the weights of its literals, we refer to the computation of the probability of an element in $\mathscr{F}(\mathcal{HB})$ as *weighted model counting* (WMC) [10].

2 Progress to Date

At the beginning of the academic year, discovering a general theory of PRMs was my dream goal. This goal was achieved with the help of Boolean (as well as polyadic) algebras, and the idea is briefly outlined in the introduction. Before this discovery, the research undertaken throughout the first year focused on a particular probabilistic logic programming language ProbLog. At its core, a ProbLog program is a stratified logic program with a probability attached to each clause. A program with m clauses defines a probability distribution over 2^m logic programs, and the probability of a formula f is calculated as the sum of the probabilities of logic programs that entail f. We now introduce two submitted papers related to ProbLog and logic programming more generally: one on interpreting logic programs as maps between relational knowledge bases (with applications to, e.g., knowledge base compression) and one on generating probabilistic logic programs to facilitate large-scale testing of inference algorithms.

The first project was inspired by a recent paper [19] that uses logic programs as encoders/decoders for relational data, i.e., given a (large) relational knowledge base Δ_1, a constraint solver is used to construct two programs (the encoder and the decoder) that can transform Δ_1 into a (smaller) knowledge base Δ_2 and vice versa. One can then ask 'when is that possible?' In other words, given two relational knowledge bases, under what circumstances is there a logic program that can transform one into the other? The paper answers this question in full for knowledge bases on the same domain of discourse $\mathcal{D}$. Namely, we show that a knowledge base Δ_1 can be transformed into another knowledge base Δ_2 if and only if the equivalence classes induced by Δ_1 on $\mathcal{D}$ are finer than the ones induced by Δ_2. These results have important implications for efficient inference and compressibility of PRMs and probabilistic databases [45], as logic program-based transformations can provide a computationally cheap way to significantly reduce the size of a knowledge base.

The second paper describes a way to generate random ProbLog programs using constraint programming. The idea was originally motivated by the need to test and debug predicate abstraction algorithms that perform local syntactic transformations on such programs—a project which is currently on hold in favour of better/stronger ideas. However, in the paper, the work is primarily motivated by the need for rigorous testing of inference algorithms. Indeed, many algorithms are only tested on a couple of programs [4, 27, 49]. Although some reviewers suggested that perhaps simpler methods (than constraint programming) might be just as useful, the use of constraint programming is motivated in two ways:

- With constraint programming, one can easily adjust the model and add additional constraints as needed. Specifically, we can regulate what parts of the program must be independent, require certain formulas to be included, etc.

- A simpler method such as a probabilistic context-free grammar (as suggested by one of the reviewers) would not be able to encode even such simple constraints as the fact that the order of clauses is immaterial or that each predicate should have at least one clause associated to it. A likely consequence is that the majority of generated programs would need to be discarded, and the method would be too inefficient. On the other hand, a constraint solver considers constraints much earlier in the search process, which ensures both efficiency and customisability.

Finally, we provide an overview of the results developed so far for a third paper. WMC can be interpreted as a measure over a Boolean algebra. This algebraic point of view by itself is already novel as WMC is usually studied from the perspective of logic, where one only considers the atoms of the algebra—more commonly known as models. While there have been many attempts to assign probabilities to logical formulas in a way that is consistent with (and sometimes inspired by) Boolean algebras with measures, theoretically-sound approaches often result in intractable algorithms [8, 20, 23, 28, 34]. WMC, on the other hand,—while still solving a #P-complete problem [43]—can achieve greater efficiency by building on the decades of work on efficient SAT algorithms. As WMC was motivated by efficiency and tractability more than theoretical rigour, the expressiveness and representational efficiency of WMC has never been questioned before. Moreover, an algebraic approach has already proven to be successful in establishing the main results of this paper.

First, we note that not every measure on a Boolean algebra can be defined using WMC, i.e, a measure m is WMC-definable if and only if all literals are independent according to m. The formal version of this theorem constitutes the first contribution of the upcoming paper. Given this requirement for independence, a well-known way to represent probability distributions that do not consist entirely of independent variables is by adding more literals [10]. We show that one can always extend a Boolean algebra B into a larger Boolean algebra B' such that any measure on B can be represented as a WMC measure on B'.

Furthermore, we show how the independence requirement of WMC can be seen as a consequence of constructing the Boolean algebra using coproducts. Similarly, conditional independence constraints on the measure can be constructed using pushouts. This suggests a way to relax the definition of WMC so that the independence structure of the algebra accurately represents the independence structure of the probability distribution. We conjecture that this change to the definition of WMC can come at no cost to most modern inference algorithms and result in faster inference. To summarise, a good understanding of the inherent limitations of WMC can lead to better alternatives and improvements to the method.

3 Future Goals

Along with preparing the two appended papers for resubmission and extending the third one with experimental data, the remaining time will also be spent on employing the newly gained perspective on the intersection between statistical relational artificial intelligence and algebraic logic to further the recent developments in abstraction for PRMs. Abstraction is abundant in artificial intelligence and related disciplines [41]. However, most of the previous work is focused on deterministic systems such as planning and verification [21]. Belle [1] proposed a theory of abstraction for PRMs based on defining a refinement mapping m from a high-level PRM Δ_h to a low-level PRM Δ_l, the definition of which reads:

The mapping m is assumed to extend to complex formulas $\phi \in Lang(\Delta_h)$ inductively: for atoms $\phi = p$, $m(\phi)$ is as above; $m(\neg\phi) = \neg m(\phi)$; $m(\phi \wedge \psi) = m(\phi) \wedge m(\psi)$.

This clearly describes a homomorphism, but what is the structure that is being preserved? The main claim behind this project is that these refinement mappings are Boolean homomorphisms.

Treating abstraction as a homomorphism is not a new idea. Abstractions based on homomorphisms between Markov decision processes and semi-Markov decision processes have been used extensively in the reinforcement learning and planning communities [26, 37, 38]. Abstraction homomorphisms have also been used to efficiently model concurrent systems [7, 17], solve semiring-based constraint satisfaction problems [29], and improve the efficiency of heuristic search [24]. As the approach has been successful in other fields (and since an algebraic approach towards PRMs is novel by itself), it is likely to yield valuable insights in the context of PRMs as well. Section 3.1 describes the remaining work in more detail.

3.1 Plan of Action

We divide the work into five major WPs: one for each paper as well as one for compiling the thesis itself.

3.1.1 WP 1: Logic programs as morphisms between relational knowledge bases

Before resubmitting, the paper could be improved in three ways:

- Instead of assuming that all knowledge bases are defined with respect to the same domain of discourse, the results could be extended to consider different domains.
- The paper needs to demonstrate implications for questions that the scientific community cares about (instead of just blindly claiming that those implications exist). This can be done by furthering previous work [19] on logic programs as compression schemes.
- Finally, the results could be extended to the approximate case, where the knowledge base after applying the logic program is only similar but not equal to the desired knowledge base.

For the last extension, consider two knowledge bases Δ_1 and Δ_2 and suppose that Theorem 2 of the paper shows that no logic program can transform Δ_1 into Δ_2. The paper could be extended by considering a metric between knowledge bases, establishing a theorem for the smallest possible distance between Δ_2 and everything reachable from Δ_1 via logic programs, and showing how to construct a logic program and/or a knowledge base that achieves that minimum. **Estimated duration:** 2 months.

Risks and contingencies. As the contribution of this paper is purely theoretical and not easily applied, the paper is likely to be difficult to publish. However, a sufficiently long list of potential venues, combined with adjustments according to reviewers' comments and a hint of luck should eventually yield a publication. This plan is further justified by several reviewers who were interested in and excited by the idea.

3.1.2 WP 2: Random instances of (probabilistic) logic programs and the empirical hardness of inference

Before the next submission, the paper could be improved by including an experimental comparison of ProbLog inference algorithms using the random programs generated by my model, hopefully showing interesting results about how properties of the input program affect the runtime of each inference algorithm. This involves constructing one or more scripts to generate programs and run the experiments and running them on suitable hardware. **Estimated duration:** 4 months.

Risks and contingencies. The two main risks associated with the remaining part of this project are that

- the program generation process could be too slow either for sufficiently large programs or in some specific situations (e.g., after making an incorrect decision early in the search process),
- or the number of experiments needed to properly cover a wide range of values across all relevant variables could be too large.

The former can be solved in several ways:

- by improving various aspects of the procedure even further, e.g., by adding redundant constraints, improving (or inventing new) propagation algorithms, or adjusting the variable ordering heuristic;
- by parallelising program generation task and employing more powerful hardware;
- or by settling for smaller programs (or fewer of them).

Similarly, the latter risk can also be avoided by adjusting the process to efficiently use hardware resources and by adjusting the parameter values under investigation.

3.1.3 The hidden assumptions behind WMC and how to overcome them for (algebraic) fun and (computational) profit

The work for this paper is approximately 60% complete. The main goal of the remaining work is to demonstrate how the theoretical discoveries can make inference algorithms faster.

WP 3.1 Prove that my definition of WMC allows one to encode a Bayesian network as a WMC problem with fewer variables and a shorter theory than the two encodings known in the literature [12, 43]. Modify a state-of-the-art #SAT solver to work with the new definition of WMC. **Estimated duration:** 2 months.

WP 3.2 Choose a collection of Bayesian networks, making sure to cover both fully independent and fully dependent probability distributions. Write conversion scripts to encode each Bayesian network into an instance of WMC in three different ways. Run the algorithm on the three encodings, gathering runtime and memory consumption data. **Estimated duration:** 2 months.

WP 3.3 Describe the results in a paper. **Estimated duration:** 1 month.

Risks and contingencies. The main risk of this project is that the empirical performance may not meet the expectations. Alternatively, even if my encoding successfully outperforms the other two, the contribution as a whole may be judged as too marginal by reviewers. If the empirical results are positive but weak, they should still be publishable with a sufficiently polished theoretical section. If my version of WMC yields performance on par with the traditional WMC, the theoretical part of this work can still be combined with other results.

3.1.4 Abstractions as homomorphisms

As significant contributions are yet to be made towards this project, the WPs are subject to significant adjustments.

WP 4.1 Formalise the connection between homomorphisms and refinements and map properties of abstractions such as soundness and completeness into existence/surjectivity of (restrictions of) homomorphisms. **Estimated duration:** 1 month.

WP 4.2 Many results in the previous work [1] provide *sufficient* conditions to ensure that the abstraction is 'well-behaved' with respect to the probability measure or the logical/algebraic structure. Strengthen them by identifying conditions that are both *necessary and sufficient*. **Estimated duration:** 2 months.

WP 4.3 Develop necessary conditions for constructing an abstraction from the low-level PRM itself by, e.g., clustering constants into classes or replacing multiple predicates with a single predicate [21]. More specifically, we can consider the conditions needed for refinements to preserve important properties of PRMs under this more-detailed view of abstraction construction. **Estimated duration:** 2 months.

WP 4.4 Use the algebraic structure behind the Boolean algebra (e.g., coproducts and pushouts, as described above) to develop theorems about the preservation of independence and conditional independence—properties of probabilistic models that were beyond the reach of previous logic-based frameworks. **Estimated duration:** 3 months.

WP 4.5 Describe the results in a paper. **Estimated duration:** 2 months.

Risks and contingencies. The main risk associated with the search for significant theoretical contributions is that the results may end up underwhelming. Considering the vast array of unanswered questions and the novelty of this approach, the risk is minimal although, if necessary, the work could be adjusted to focus on other issues such as infinite domains instead.

3.1.5 Summary

The last task (**WP 5**) is, of course, compiling all results into a coherent thesis. **Estimated duration:** 6 months. A picture of how the WPs could be accomplished over the next two years is in Fig. 1.

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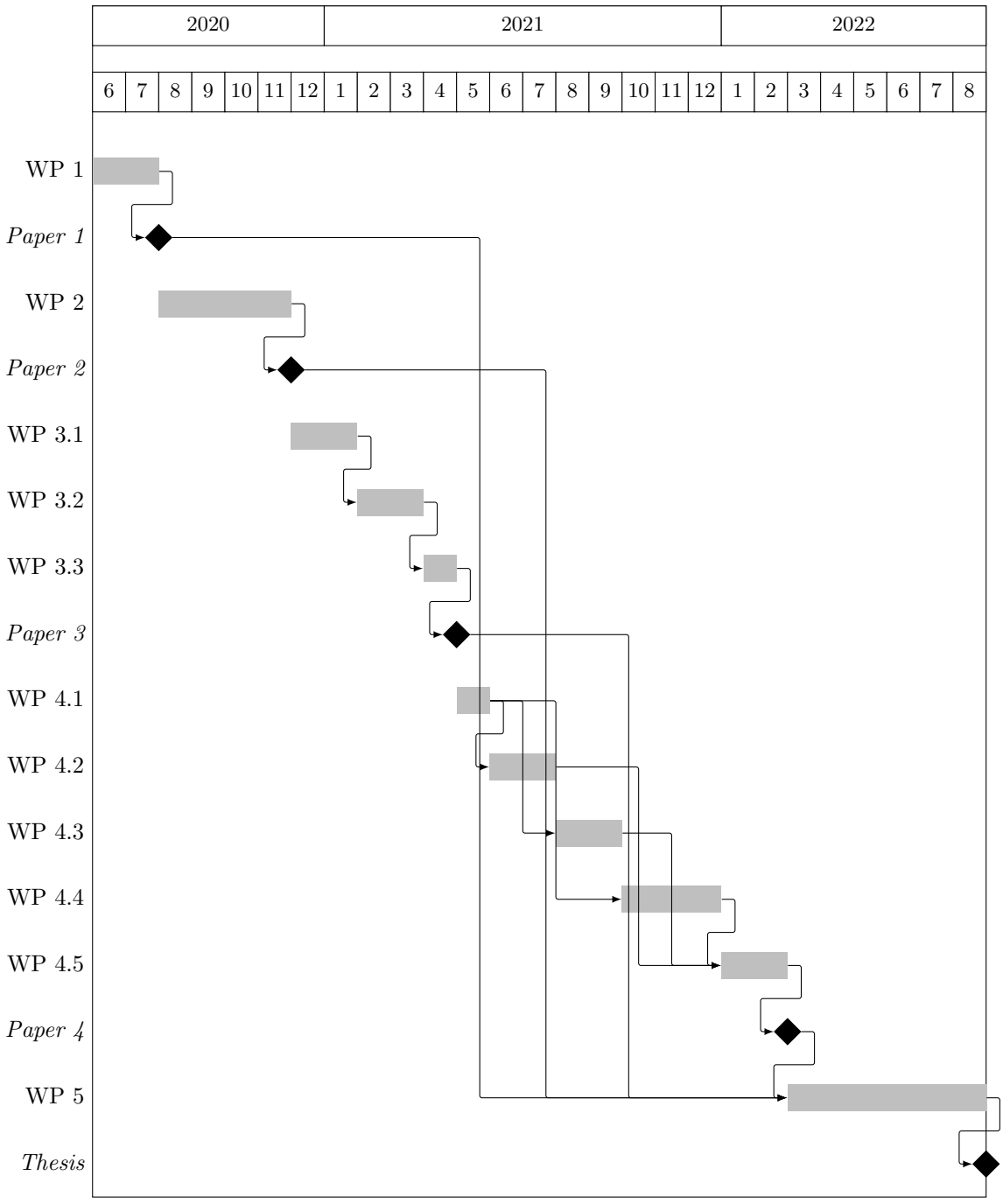

Figure 1: Gantt chart of the remaining WPs

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A Submitted Papers

On the Equivalence of Constants in Relational Knowledge Bases

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Abstract

Driven by the powerful promises of statistical relational artificial intelligence, relational structures are as important as ever. Various notions of equivalence have contributed to relational models becoming more tractable and usable. We present a fresh (function-based) perspective on relational knowledge bases and use it to formally consider equivalence of constants. We show how logic programs, acting as maps between knowledge bases, are fundamentally defined by their effects on equivalence classes. We also consider how the results can be extended to a probabilistic setting. The results unveil properties of the equivalence structure induced by knowledge bases and have important implications for lifted inference, inductive logic programming, and relational auto-encoders.

1 Introduction

Various definitions of symmetry and equivalence have demonstrated their importance in statistics [Kingman, 1978; Diaconis and Freedman, 1980], and, more recently, neural networks [Ravanbakhsh *et al.*, 2017] and statistical relational artificial intelligence [Raedt *et al.*, 2016; Bui *et al.*, 2013; Niepert and den Broeck, 2014]. These notions can enable enormous computational leverage for inference tasks, and can also lead to more robust learning of representations as entities are not treated in an i.i.d. manner.

In this paper, we consider equivalence classes of constants (and tuples of constants) in *relational knowledge bases* (KBs), defined analogously to orbits induced by renaming permutations [Bui *et al.*, 2013] in Markov logic networks [Richardson and Domingos, 2006]. Our motivation is twofold. First, we define a relation between KBs that describes whether there exists a logic program that can transform one KB to another. This provides the theoretical background to recent work in auto-encoding KBs using logic programs [Dumancic *et al.*, 2019]. The same framework can also be used to conceptualise a version of inductive logic programming [Muggleton, 1991]. Second, equivalence of constants relates to domain abstraction [Belle, 2018; Holtzen *et al.*, 2017] and exchangeability [Diaconis and Freedman, 1980], and is of great importance to efficient lifted inference [Poole, 2003; Niepert and den Broeck, 2014; Bui *et al.*, 2012; de Salvo Braz *et al.*, 2005; Kersting, 2012; Gogate and Domingos, 2010; Gogate and Domingos, 2016]. While most of this paper is dedicated to the purely logical setting, in Section 6 we briefly discuss how the work can be extended to probabilistic KBs and probabilistic logic programs. In this context, reasoning about equivalences of constants can be an efficient way to discover other types of symmetries such as symmetries of ground atoms, formulas, and assignments [Niepert, 2012].

After a review of preliminaries in Section 2, we begin with Section 3 where we present a new way to interpret logical constructs such as atoms and clauses by introducing *realisation functions*. Section 4 then defines equivalence between (tuples of) constants and outlines some key properties. Our main contribution is Theorem 2 in Section 5 that shows how the existence of a logic program that transforms one KB into another is fundamentally related to refinements of equivalence relations. We also demonstrate a concrete way of constructing such a logic program.

2 Preliminaries

In this section, we review the terminology of logic programming, introduce our notation for various constructs, and outline several key results on equivalence.

2.1 Logic and Logic Programming

The primitive building blocks of KBs and logic programs are constants (e.g., $a, b, \dots$), variables (e.g., $X, Y, \dots$), and predicates (e.g., $\mathsf{P}, \mathsf{Q}, \dots$). A *term* is either a constant or a variable. The *arity* of a predicate is the number of terms that it can be applied to (a predicate P of arity n is denoted by P/n). An *atom* is a predicate (say, of arity n) applied to n terms (e.g., $\mathsf{P}(X, a)$). A *literal* is either an atom or its negation. We define a *formula* as a conjunction of literals. An atom or a literal is *ground* if all its terms are constants. In Section 3, we will redefine some of these terms in a more rigorous way.

Definition 1. Let P and C be sets of predicates and constants, respectively. The *Herbrand base* of P and C is the set of all ground atoms that can be constructed from elements of P and C. We will use $\mathcal{KB}(P, C)$ to denote the power set of the Herbrand base. A *knowledge base* is a subset of the Herbrand

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base, containing all atoms that evaluate to true (with no additional structural restrictions), i.e., an element of $\mathcal{KB}(P, C)$. If a ground atom is in the KB, it is a *fact*.

Definition 2. A *clause* is a pair of an atom A and a formula F (written as $\mathsf{A} \leftarrow \mathsf{F}$) with an implication that for all possible ways of replacing variables in A and F with constants, if F is true, then A is also true. We say that A is the *head* of the clause, and F is the *body*.

Definition 3. Let C be a set of constants, and let P_1, P_2 be two disjoint sets of predicates. A *logic program* $\mathcal{L}$ from $\mathcal{KB}(P_1, C)$ to $\mathcal{KB}(P_2, C)$ (written $\mathcal{L} : \mathcal{KB}(P_1, C) \to \mathcal{KB}(P_2, C)$) is a set of clauses such that all head predicates are in P_2, all body predicates are in P_1, and all constants are in C.

2.2 Equivalence and Set Partitions

We briefly review some well-known results on equivalence (see, e.g., [Brualdi, 1977; Bourbaki, 2004] for more information). Let A be a non-empty set, and let $\sim$ and $\approx$ be two equivalence relations over A.

Notation. For any positive integer n, $[n] \coloneqq \{1, \ldots, n\}$ while, by abuse of notation, for any constant c, $[c]$ refers to the equivalence class of c. We let

$$A^\infty \coloneqq \bigcup_{n=1}^{\infty} A^n,$$

denote the set of all tuples of all lengths constructed from elements of A[1]. We let $A/\!\sim$ denote the *quotient set* (i.e., the set of equivalence classes) of $\sim$. Finally, let $\mathbb{B} \coloneqq \{\bot, \top\}$ be the set with two values corresponding to false and true.

Definition 4. We say that $\approx$ is *coarser* than $\sim$ (equivalently, $\sim$ is *finer* than $\approx$, or $\sim$ is a *refinement* of $\approx$) if, for any $a, b \in A$, if $a \sim b$, then $a \approx b$.

Definition 5. Let P and Q be two partitions of A. Then P is *coarser* than Q if, for every $q \in Q$, there is a $p \in P$ such that $q \subseteq p$.

Theorem 1 (Fundamental Theorem of Equivalence Relations)**.** *If $\sim$ is an equivalence relation on A, then $A/\!\sim$ is a partition of A. If P is a partition of A then there is an equivalence relation $\equiv$ on A such that $A/\!\equiv\, = P$.*

Lemma 1. *$\approx$ is coarser than $\sim$ if and only if $A/\!\approx$ is coarser than $A/\!\sim$.*

3 Variables: What Are They Made Of?

In this section, we will outline the interpretation of logical entities such as variables, atoms, and clauses that will be used throughout the paper. We will show how formulas can be characterised as compositions of functions and define a new type of functions that act as links between predicates and atoms. We will use the following as a running example:

Example 1. Let $C = \{a, b, c\}$ be a set of constants, and let $P_1 = \{\mathsf{Q}/2, \mathsf{R}/1\}$ and $P_2 = \{\mathsf{P}/2\}$ be two sets of predicates. Let $\mathcal{L} : \mathcal{KB}(P_1, C) \to \mathcal{KB}(P_2, C)$ be a logic program with

$$\mathsf{P}(X, a) \leftarrow \mathsf{Q}(X, Y) \wedge \neg \mathsf{R}(X) \tag{1}$$

as its only clause.

First, list the variables in alphabetical (or any other) order and count the number of variables. In this case, we have two variables: X and Y. Thus, our initial domain is C^2, X represents the first element of the pair, and Y the second.

Definition 6. Let A be a set, and let n, m be positive integers. Let $\{p_i\}_{i=1}^m$ be a set of projections $A^m \to A$. A function $\rho : A^n \to A^m$ is a *realisation function* if, for $i \in [m]$, $p_i \circ \rho$ is either a projection $A^n \to A$ or a constant function[2].

Definition 7. Let Δ be a KB, and let n be a positive integer. An *atom acting on n variables* in Δ is a composition

$$C^n \xrightarrow{\ \rho\ } C^m \xrightarrow{\ \mathsf{P}\ } \mathbb{B}$$

of a realisation function ρ and the evaluation function for a predicate P.

Section 3 shows how these definitions apply to the atoms in Example 1. We will now show how the same ideas can be extended to literals and formulas. To represent a literal such as $\neg\mathsf{R}(X)$, we can compose the representation of $\mathsf{R}(X)$ with $\neg$, interpreted as a function:

$$C^2 \xrightarrow{\ p_1\ } C \xrightarrow{\ \mathsf{R}\ } \mathbb{B} \xrightarrow{\ \neg\ } \mathbb{B}.$$

Keeping the number of arrows (i.e., composed functions) the same, we can formalise the literal $\mathsf{Q}(X, Y)$ as

$$C^2 \xrightarrow{\ \mathrm{id}\ } C^2 \xrightarrow{\ \mathsf{Q}\ } \mathbb{B} \xrightarrow{\ \mathrm{id}\ } \mathbb{B}.$$

Conjunction $\wedge$ then takes a product of $\mathbb{B}$'s and maps it to another $\mathbb{B}$ in the obvious way. The entire body of Clause (1) can then be visualised as[3]

$$C^2 \xrightarrow{\ \langle \mathrm{id}, p_1 \rangle\ } C^2 \times C \xrightarrow{\ \langle \mathsf{Q}, \mathsf{R} \rangle\ } \mathbb{B}^2 \xrightarrow{\ \langle \mathrm{id}, \neg \rangle\ } \mathbb{B}^2 \xrightarrow{\ \wedge\ } \mathbb{B}.$$

Applying the same reasoning to $\mathsf{P}(X, a)$ gives us two maps with the same domain and codomain:

$$\begin{array}{ccccccccc} C^2 & \xrightarrow{\langle \mathrm{id}, p_1 \rangle} & C^2 \times C & \xrightarrow{\langle \mathsf{Q}, \mathsf{R} \rangle} & \mathbb{B}^2 & \xrightarrow{\langle \mathrm{id}, \neg \rangle} & \mathbb{B}^2 & \xrightarrow{\ \wedge\ } & \mathbb{B} \\ & \searrow^{(x,y) \mapsto (x,a)} & & & & & & \nearrow_{\mathsf{P}} & \\ & & & & C^2. & & & & \end{array} \tag{2}$$

The only semantic connection between the two maps, however, is that of implication: if the top path from C^2 to $\mathbb{B}$ leads to $\top$, then so should the bottom path.

Example 1 (continued)**.** Applying the logic program $\mathcal{L}$ to the KB

$$\Delta = \{\mathsf{Q}(a, a), \mathsf{Q}(b, c), \mathsf{Q}(c, c), \mathsf{R}(b)\} \in \mathcal{KB}(P_1, C)$$

gives us

$$\mathcal{L}(\Delta) = \{\mathsf{P}(a, a), \mathsf{P}(c, a)\} \in \mathcal{KB}(P_2, C).$$

[1] While the definition implies that A^∞ is infinite, in practice, it is enough to consider a truncated (finite) version of A^∞. More generally, we implicitly assume that all sets (of constants, predicates, etc.) are finite.

[2] To make examples and computations simpler, we add an additional requirement that there must be at least one projection.

[3] Note that while $\mathsf{Q}(X, Y)$ and $\mathsf{R}(X)$ have different arities, in the context of a larger formula, they both have C^2 as the domain.

Representation of an atom			Realisation function
In a program	Diagrammatic	Algebraic	
$\mathsf{P}(X, a)$	$C^2 \xrightarrow{\rho} C^2 \xrightarrow{\mathsf{P}} \mathbb{B}$	$\mathsf{P} \circ \rho$	$\rho(x, y) = (x, a)$
$\mathsf{Q}(X, Y)$	$C^2 \xrightarrow{\mathrm{id}} C^2 \xrightarrow{\mathsf{Q}} \mathbb{B}$	$\mathsf{Q} \circ \mathrm{id}$ (or just Q)	$\mathrm{id}(x, y) = (x, y)$
$\mathsf{R}(X)$	$C^2 \xrightarrow{p_1} C \xrightarrow{\mathsf{R}} \mathbb{B}$	$\mathsf{R} \circ p_1$	$p_1(x, y) = x$

Table 1: A summary of representations of atoms from Example 1 and the associated realisation functions

However, we ought to note that there are some clauses that cannot be represented in the described manner. Assuming *negation as failure* [Clark, 1977], these are clauses that have a variable which only appears in negative literals (and not in positive literals or the head atom). For example,

$$\mathsf{S}(X) \leftarrow \neg\mathsf{T}(X, Y), \tag{3}$$

while a perfectly valid clause, cannot be represented in a manner similar to Diagram (2). However, we *can* represent a clause equivalent to Clause (3) with Y instantiated with every possible value, i.e.,

$$\mathsf{S}(X) \leftarrow \bigwedge_{y \in C} \neg\mathsf{T}(X, y).$$

The number of values y required for this clause can also be significantly reduced by only considering constants that appear as the second argument to T. We end the section by defining instantiation.

Definition 8. Let Δ be a KB with its set of constants C, and let P/n be a predicate in Δ. Let $a \in C^n$ be a tuple of constants. We say that a *instantiates* P (and write $\Delta \models \mathsf{P}(a)$ or $\mathsf{P}(a) = \top$) if the fact $\mathsf{P}(a)$ is in Δ.

Let A be an atom acting on n variables $(X_i)_{i=1}^n$. We say that $a = (a_1, \ldots, a_n) \in C^n$ *instantiates* A (and write $\Delta \models \mathsf{A}(a)$ or $\mathsf{A}(a) = \top$) if $\mathsf{A}[X_1/a_1, \ldots, X_n/a_n]$ (i.e., the atom A with variables replaced with their corresponding constants) is in Δ. This definition can be further extended to literals and formulas using the usual interpretations of negation and conjunction.

4 Equivalence in Knowledge Bases

Definition 9. Let Δ be a KB with its set of constants C. Let n be a positive integer, and let $a, b \in C^n$ be two tuples of constants. Then a and b are *equivalent*[4] if

$$(\mathsf{P} \circ \rho)(a) = (\mathsf{P} \circ \rho)(b) \tag{4}$$

for all atoms $\mathsf{P} \circ \rho$ acting on n variables in Δ. Let $\sim$ denote this equivalence relation. We can also extend this to an equivalence relation for C^∞ by adding that tuples of different lengths are never equivalent. Finally, a *projection* is a map $\pi : C^n \to C^n/\!\sim$ such that $\pi(a) = [a]$ for any $a \in C^n$ (for $n = 1, \ldots, \infty$).

Informally, two tuples of constants are equivalent if they have the same length, and, given any fact in the KB, we can replace any combination of constants from one tuple with the corresponding constants from the other tuple and get another fact in the KB.

Example 2. Let Δ_1 and Δ_2 be KBs defined as follows:

$$\begin{aligned}\Delta_1 \coloneqq \{&\mathsf{Husband}(\mathit{joffrey}, \mathit{margaery}), \\ &\mathsf{Husband}(\mathit{tommen}, \mathit{margaery}), \\ &\mathsf{Husband}(\mathit{renly}, \mathit{margaery}), \\ &\mathsf{Parent}(\mathit{cersei}, \mathit{joffrey}), \mathsf{Parent}(\mathit{cersei}, \mathit{myrcella}), \\ &\mathsf{Parent}(\mathit{cersei}, \mathit{tommen}), \mathsf{Parent}(\mathit{tywin}, \mathit{cersei})\},\end{aligned} \tag{5}$$

$$\begin{aligned}\Delta_2 \coloneqq \{&\mathsf{Female}(\mathit{cersei}), \mathsf{Female}(\mathit{margaery}), \\ &\mathsf{Female}(\mathit{myrcella})\}.\end{aligned} \tag{6}$$

Let C be the set of all constants mentioned in Eqs. (5) and (6), and let $\sim$ and $\approx$ be the equivalence relations of Δ_1 and Δ_2, respectively. Finally, let $\pi_1 : C^\infty \to C^\infty/\!\sim$ and $\pi_2 : C^\infty \to C^\infty/\!\approx$ be the respective projections of $\sim$ and $\approx$.

To efficiently identify equivalence classes, we can look at pairs of constants that appear as arguments at the same position of the same predicate. For example, *joffrey* and *tommen* both appear as the first argument to the predicate Husband. We then look for a fact in Δ_1 that would contradict their equivalence, e.g., an atom with constant *joffrey* such that replacing *joffrey* with *tommen* results in a fact not in Δ_1. In this case, there is no such fact, so we have that

$$\mathit{joffrey} \sim \mathit{tommen}. \tag{7}$$

If we take *joffrey* and *renly*, for example, their equivalence is contradicted by the fact $\mathsf{Parent}(\mathit{cercei}, \mathit{joffrey})$. Equivalence (7) is, indeed, the only equivalence of individual constants in Δ_1. The situation with Δ_2 is much more straightforward where $C/\!\approx$ consists of two equivalence classes:

$$\pi_2^{-1}(c) = \{\mathit{cersei}, \mathit{margaery}, \mathit{myrcella}\}$$

and $\pi_2^{-1}(d) = C \setminus \pi_2^{-1}(c)$.

In the rest of this section, we will develop a few propositions, some of which are interesting on their own, and some of which will be used in Section 5. Let n, m be positive integers, and let Δ be a KB with its set of constants C, equivalence relation $\sim$, and its projection $\pi : C^\infty \to C^\infty/\!\sim$.

Lemma 2. *Any realisation function can be represented as a composition of four types of* elementary *functions:*

duplication: $(x_1, \ldots, x_n) \mapsto (x_1, \ldots, x_i, x_i, \ldots, x_n)$,
omission: $(x_1, \ldots, x_n) \mapsto (x_1, \ldots, x_{i-1}, x_{i+1}, \ldots, x_n)$,
permutation: $(x_1, \ldots, x_n) \mapsto (x_1, \ldots, x_{i+1}, x_i, \ldots, x_n)$,
insertion: $(x_1, \ldots, x_n) \mapsto (x_1, \ldots, x_n, a)$.

[4] One can easily check that this is indeed an equivalence relation.

Proposition 1. *Let $\sigma : C^n \to C^m$ be a realisation function. Then, for any $a, b \in C^n$, if $a \sim b$, then*[5] *$\sigma(a) \sim \sigma(b)$.*

Proof sketch. For any predicate P/l in Δ and any elementary function $\sigma : C^n \to C^m$ from Lemma 2, one can construct the set of all possible realisation functions $\rho' : C^m \to C^l$ such that

$$(\mathsf{P} \circ \rho' \circ \sigma)(a) = (\mathsf{P} \circ \rho' \circ \sigma)(b)$$

from the set of all realisation functions $\rho : C^n \to C^l$ such that $(\mathsf{P} \circ \rho)(a) = (\mathsf{P} \circ \rho)(b)$. □

Remark. Note that the converse statement is not necessarily true because the omission operation can destroy crucial information. For example, if $(a, b) \sim (a', b')$, then $a \sim a'$, but if $a \sim a'$, it may or may not be the case that $(a, b) \sim (a', b')$.

Proposition 2. *Let $c \in C^n/\!\sim$ be an equivalence class of n-tuples for $n > 1$. Then, for any positive integer $l < n$, there exist unique equivalence classes $d \in C^l/\!\sim$ and $e \in C^{n-l}/\!\sim$ such that*

$$\pi^{-1}(c) = \pi^{-1}(d) \times \pi^{-1}(e).$$

Proof. Let $a \in \pi^{-1}(c)$ be arbitrary, and let $\rho : C^n \to C^l$ and $\sigma : C^n \to C^{n-l}$ be realisation functions composed purely of omission operations such that $a = (\rho(a), \sigma(a))$. Then set $d \coloneqq [\rho(a)]$ and $e \coloneqq [\sigma(a)]$. We will first show that

$$\pi^{-1}(c) \subseteq \pi^{-1}(d) \times \pi^{-1}(e).$$

Clearly $a \in \pi^{-1}(d) \times \pi^{-1}(e)$. For any other $b \sim a$, by Proposition 1 we have that $\rho(b) \sim \rho(a)$ and $\sigma(b) \sim \sigma(a)$, so $\rho(b) \in \pi^{-1}(d)$ and $\sigma(b) \in \pi^{-1}(e)$, so $b \in \pi^{-1}(d) \times \pi^{-1}(e)$. Finally, note that d and e are unique by definition, as a single element such as $\rho(a)$ cannot belong to multiple equivalence classes.

Conversely, let $r, s \in C^\infty$ be such that $r \sim \rho(a)$ and $s \sim \sigma(a)$. Then $(r, s) \in \pi^{-1}(d) \times \pi^{-1}(e)$, so we just need to show that $(r, s) \sim a$. Let $\mathsf{P} \circ \tau$ be any atom in Δ, and let $\upsilon(x) = (x, \sigma(a))$ be a realisation function composed solely of insertions. Then

$$\begin{aligned}(\mathsf{P} \circ \tau)(a) &= (\mathsf{P} \circ \tau)(\rho(a), \sigma(a)) = (\mathsf{P} \circ \tau \circ \upsilon)(\rho(a)) \\ &= (\mathsf{P} \circ \tau \circ \upsilon)(r) = (\mathsf{P} \circ \tau)(r, \sigma(a)) \\ &= \cdots = (\mathsf{P} \circ \tau)(r, s),\end{aligned}$$

where the skipped steps replace $\sigma(a)$ with s the same way $\rho(a)$ was replaced with r. □

In other words, Proposition 1 says that each equivalence class of tuples is a Cartesian product of 'smaller' equivalence classes. Despite this observation, it remains convenient to reason about equivalences of tuples in many occasions. Having defined constant equivalence and outlined some of the key properties, we end the section with two lemmas that will be useful in the next section.

[5]Formally, this means that realisation functions are morphisms from $\sim$ to itself.

Lemma 3. *Let $\pi : C^n \to C^n/\!\sim$ be the projection map of $\sim$. For any atom $\mathsf{P} \circ \rho$ acting on n variables, we can find a collection of equivalence classes $(c_i)_{i \in I}$ in $C^n/\!\sim$ such that the subset of C^n instantiating $\mathsf{P} \circ \rho$ can be expressed as*

$$\bigcup_{i \in I} \pi^{-1}(c_i).$$

Lemma 4. *Let S be a set of literals acting on n variables, and let F be a formula defined by*

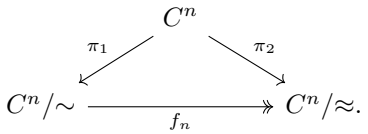
$$\mathsf{F} \coloneqq \bigwedge_{\mathsf{L} \in S} \mathsf{L}.$$

Then, for any $a, b \in C^n$, if $\Delta \models \mathsf{F}(a)$ and $a \sim b$, then $\Delta \models \mathsf{F}(b)$.

5 Refinements and Logic Programs

Now that we have developed the basic tools for reasoning about equivalences in KBs, we can build up to Theorem 2 via Propositions 3 and 4 where we represent each refinement relationship by a map between quotient sets and consider how each equivalence class can be captured with a formula.

Proposition 3. *Let Δ be a KB with its set of constants C and two equivalence relations $\sim$, $\approx$ (as defined in Definition 9) with their respective projections π_1 and π_2. Then $\approx$ is coarser than $\sim$ if and only if, for every positive integer n, there is a map $f_n : C^n/\!\sim \to C^n/\!\approx$ that makes the following diagram commute:*



We can also extend this to $f : C^\infty/\!\sim \to C^\infty/\!\approx$ by considering C^∞ as a disjoint union, i.e.,

$$C^\infty = \coprod_{n=1}^{\infty} C^n.$$

Then f is just a coproduct, i.e., $f = [f_1, f_2, \dots]$.

Proof. Given such an $f : C^\infty/\!\sim \to C^\infty/\!\approx$,

$$\begin{aligned}a \sim b &\iff \pi_1(a) = \pi_1(b) \\ &\implies (f \circ \pi_1)(a) = (f \circ \pi_1)(b) \\ &\iff \pi_2(a) = \pi_2(b) \iff a \approx b.\end{aligned}$$

Conversely, suppose that $\approx$ is coarser than $\sim$, and let n be an arbitrary positive integer. We need to define $f_n : C^n/\!\sim \to C^n/\!\approx$ such that

$$(f_n \circ \pi_1)(c) = \pi_2(c)$$

for all $c \in C^n$. Let $c \in C^n/\!\sim$ be arbitrary. By Theorem 1 and Lemma 1, there is a unique $d \in C^n/\!\approx$ such that $\pi_1^{-1}(c) \subseteq \pi_2^{-1}(d)$, so we can set $f_n(c) \coloneqq d$. □

Remark. Note that f_n must be surjective because otherwise there would be a nonempty equivalence class defined by $\approx$ contradicting the commutativity of the triangle.

Algorithm 1: Capturing an equivalence class

Data:

- a KB Δ with:
  - its set of constants C,
  - and its equivalence relation $\sim$,
- and an n-tuple of constants a.

Result: a set of literals S.

1 $S \leftarrow \emptyset$;
2 **foreach** *atom*[6] $\mathsf{P} \circ \rho$ *acting on* n *variables in* Δ **do**
3 **if** $\Delta \models (\mathsf{P} \circ \rho)(a)$ **and**[7] $\exists b \in C^n$ *s.t.* $b \not\sim a$ **and** $\Delta \not\models (\mathsf{P} \circ \rho)(b)$ **then**
4 add $\mathsf{P} \circ \rho$ to S;
5 **else if** $\Delta \not\models (\mathsf{P} \circ \rho)(a)$ **and** $\exists b \in C^n$ *s.t.* $b \not\sim a$ **and** $\Delta \models (\mathsf{P} \circ \rho)(b)$ **then**
6 add $\neg\mathsf{P} \circ \rho$ to S;

Example 2 (continued)**.** As $\{joffrey, tommen\} \subset \pi_2^{-1}(d)$, $\approx$ is coarser than $\sim$. We can then define $f_1 : C/{\sim} \to C/{\approx}$ as

$$f_1(\pi_1(a)) \coloneqq c \quad \text{for } a \in \pi_2^{-1}(c)$$

and

$$f_1(\pi_1(a)) \coloneqq d \quad \text{for } a \in \pi_2^{-1}(d).$$

Note that a similar definition would not work in the opposite direction ($C/{\approx} \to C/{\sim}$) as some values in the domain would be mapped to multiple values in the codomain. One could similarly define $f_2 : C^2/{\sim} \to C^2/{\approx}$ as well.

Corollary 1. *Let C be a set of constants with two equivalence relations $\sim$ and $\approx$ and their respective projections π_1 and π_2. Furthermore, suppose that $\approx$ is coarser than $\sim$ as exemplified by $f : C^\infty/{\sim} \to C^\infty/{\approx}$. Then, for any $c \in C^\infty/{\approx}$,*

$$\pi_2^{-1}(c) = \bigcup_{c' \in f^{-1}(c)} \pi_1^{-1}(c').$$

Proof sketch. An immediate consequence of Proposition 3. □

Proposition 4. *Let Δ be a KB over a set of constants C inducing an equivalence relation $\sim$. For any positive integer n and equivalence class $c \in C^n/{\sim}$, one can construct a formula that is instantiated by c and only c.*

Proof. Let $a \in C^n$ be any n-tuple of constants such that $[a] = c$, and consider the set S of predicates composed with realisation functions generated by Algorithm 1. We claim that c and only c instantiates

$$\mathsf{R} = \bigwedge_{\mathsf{L} \in S} \mathsf{L}.$$

By the definition of S, $\Delta \models \mathsf{R}(a)$, and so Lemma 4 already tells us that every element of c instantiates R. It remains to show that nothing outside c can instantiate R.

[6] The loop terminates because the number of such atoms is finite.

[7] The second part of the condition is not necessary, but it makes the set S much smaller.

We will show that if $b \not\sim a$, then it cannot be the case that $\Delta \models \mathsf{R}(b)$ using a proof by contradiction and splitting the proof into cases. Let $b \in C^n$ be such that $\Delta \models \mathsf{R}(b)$, and suppose there is an atom $\mathsf{P} \circ \rho$ acting on n variables such that

$$(\mathsf{P} \circ \rho)(a) \neq (\mathsf{P} \circ \rho)(b). \tag{8}$$

Case 1. $\mathsf{P} \circ \rho \in S$. Then, by the definition of S, we have that $\Delta \models (\mathsf{P} \circ \rho)(a)$. Since $\Delta \models \mathsf{R}(b)$, we also have that $\Delta \models (\mathsf{P} \circ \rho)(b)$. But then

$$(\mathsf{P} \circ \rho)(a) = (\mathsf{P} \circ \rho)(b)$$

which contradicts Assumption (8).

Case 2. $\neg\mathsf{P} \circ \rho \in S$. By the same argument as in Case 1,

$$(\mathsf{P} \circ \rho)(a) = (\mathsf{P} \circ \rho)(b) = \bot$$

which also contradicts Assumption (8).

Case 3. $\mathsf{P} \circ \rho \notin S$ and $\neg\mathsf{P} \circ \rho \notin S$. In this case, we know that conditions on Lines 3 and 5 of Algorithm 1 must be false.

Case 3.1. $\Delta \models (\mathsf{P} \circ \rho)(a)$. Line 3 of the algorithm then says that for any $b' \in C^n$, either $b' \sim a$ or $\Delta \models (\mathsf{P} \circ \rho)(b')$. Since $b \not\sim a$, we must have that $\Delta \models (\mathsf{P} \circ \rho)(b)$. But then

$$(\mathsf{P} \circ \rho)(a) = (\mathsf{P} \circ \rho)(b) = \top$$

which contradicts Assumption (8).

Case 3.2. $\Delta \not\models (\mathsf{P} \circ \rho)(a)$. Similarly, Line 5 says that for any $b' \in C^n$, either $b' \sim a$ or $\Delta \models (\mathsf{P} \circ \rho)(b')$, and a similar argument ensures a contradiction.

□

Theorem 2. *Let C be a set of constants, and let P_1, P_2 be two sets of predicates. Let $\Delta_1 \in \mathcal{KB}(P_1, C)$ and $\Delta_2 \in \mathcal{KB}(P_2, C)$ be two KBs, and let $\sim$, $\approx$ be their respective equivalence relations on C^∞. Then there is a logic program $\mathcal{L} : \mathcal{KB}(P_1, C) \to \mathcal{KB}(P_2, C)$ such that $\mathcal{L}(\Delta_1) = \Delta_2$ if and only if $\approx$ is coarser than $\sim$.*

Proof. Suppose that $\approx$ is coarser than $\sim$ as exemplified by $f : C^\infty/{\sim} \to C^\infty/{\approx}$. Let P/n be an arbitrary predicate in P_2. Then, by Lemma 3, there is a collection of equivalence classes $(c_i)_{i \in I}$ in $C^n/{\approx}$ such that the tuples of constants instantiating P can be expressed as

$$P = \bigcup_{i \in I} \pi_2^{-1}(c_i).$$

Then, by Corollary 1,

$$P = \bigcup_{i \in I} \bigcup_{c_i' \in f^{-1}(c_i)} \pi_1^{-1}(c_i').$$

For every such $\pi_1^{-1}(c_i')$, we can construct a clause with P as the head and the formula given by Proposition 4 as the body. These clauses collectively define P to be instantiated by precisely the required tuples of constants. Repeating the process for other predicates in P_2 produces a logic program $\mathcal{L}$ such that $\mathcal{L}(\Delta_1) = \Delta_2$.

Conversely, suppose there is a logic program $\mathcal{L} : \mathcal{KB}(P_1, C) \to \mathcal{KB}(P_2, C)$ such that $\mathcal{L}(\Delta_1) = \Delta_2$. Let n be a positive integer, and consider two tuples of constants $a, b \in C^n$ such that $a \sim b$. We want to show that $a \approx b$. Let $\mathsf{P} \circ \rho$ be an atom acting on n variables in Δ_2 such that $\Delta_2 \models (\mathsf{P} \circ \rho)(a)$, and let m be the arity of P. Because of symmetry, it is enough to show that $\Delta_2 \models (\mathsf{P} \circ \rho)(b)$. If $\Delta_2 \models (\mathsf{P} \circ \rho)(a)$, then there must be a clause in $\mathcal{L}$ that generated this fact. Let

$$\mathsf{P} \circ \sigma \leftarrow \bigwedge_{i=1}^{L} \mathsf{L}_i \tag{9}$$

be such a clause. Here, $(\mathsf{L}_i)_{i=1}^{L}$ are literals in Δ_1, and $\mathsf{P} \circ \sigma$ is an atom in Δ_2. Suppose that Clause (9) acts on l variables, for some positive integer l that is in no way related to n or m. The input to this clause that generates $(\mathsf{P} \circ \rho)(a)$ can be represented as $\tau(a)$ for a realisation function with constants $\tau : C^n \to C^l$ such that $\rho = \sigma \circ \tau$. Indeed, only one restriction is imposed by this choice, namely that at least one element of a is assigned to a variable in Clause (9). Clause (9) can then be represented by the following diagram:

$$\begin{array}{ccccccc} C^n & \xrightarrow{\tau} & C^l & \xrightarrow{\prod_{i=1}^{L} \mathsf{L}_i} & \mathbb{B}^L & \xrightarrow{\wedge} & \mathbb{B} \\ & \searrow^{\rho} & \downarrow{\scriptstyle \sigma} & & & \nearrow_{\mathsf{P}} & \\ & & C^m & & & & \end{array} \tag{10}$$

with the property that, for any $c \in C^n$, if the top path leads to $\top$, then $(\mathsf{P} \circ \sigma \circ \tau)(c) = \top$, and, since the left triangle commutes by definition, this also implies that $(\mathsf{P} \circ \rho)(c) = \top$. Therefore, it remains to show that the top path in Diagram (10) leads to $\top$ for $b \in C^n$, but this follows directly from $a \sim b$ since, for each i, $\mathsf{L}_i \circ \tau$ is just another literal in Δ_1, so b instantiates it if and only if a does. □

Example 2 (continued)**.** Given the KBs Δ_1 and Δ_2, one possible program $\mathcal{L}$ such that $\mathcal{L}(\Delta_1) = \Delta_2$—as generated by Theorem 2 and Algorithm 1—is:

$$\mathsf{Female}(X) \leftarrow \mathsf{Husband}(\mathit{joffrey}, X), \tag{11}$$

$$\mathsf{Female}(X) \leftarrow \mathsf{Parent}(X, \mathit{joffrey}),$$

$$\mathsf{Female}(X) \leftarrow \mathsf{Parent}(\mathit{cersei}, X) \wedge \neg\mathsf{Husband}(X, \mathit{margaery}). \tag{12}$$

Let us remark that the constants in Clauses (11) and (12) could be replaced with new variables to make the program more general (e.g., writing $\mathsf{Husband}(Y, X)$ instead of $\mathsf{Husband}(\mathit{joffrey}, X)$), but such literals would not be considered by Algorithm 1.

6 From Logic to Probabilities

An important extension of logic programs to reason about uncertainty takes the form of probabilistic logic programs, as represented by languages such as ProbLog [Raedt *et al.*, 2007]. Our work can be extended to probabilistic KBs with a small extension to the language. One would have to make the following changes:

- A KB now assigns a probability to each fact.
- Each clause $\mathsf{A} \leftarrow \mathsf{F}$ also has an associated probability p such that $\Pr(\mathsf{A}) = p \times \Pr(\mathsf{F})$.
- We replace $\mathbb{B}$ with $[0, 1]$, so that each predicate can now be represented by a map that assigns a probability to each tuple of constants.

This way, the definition of a logic program extends to the definition of a probabilistic logic program, and the definition of equivalence remains valid. In order to adapt Algorithm 1 to a probabilistic setting, one would have to be able to add a condition to any clause $\mathsf{A} \leftarrow \mathsf{F}$, saying that the clause is only 'activated' if $\Pr(\mathsf{F})$ is in a given interval because otherwise there would be no way to distinguish structurally equivalent facts with different probabilities, e.g., as in $\{0.5 : \mathsf{P}(a), 0.49 : \mathsf{P}(b)\}$. With this addition, we can construct clauses that only apply to tuples of constants with the same $\Pr(\mathsf{F})$. This probability can then be increased or decreased as needed by changing the probability associated with the clause and considering multiple copies of the same clause if needed[8].

Our work is related to exchangeability of ground atoms (interpreted as random variables) [Niepert and den Broeck, 2014], although the two settings are difficult to compare because in this paper we do not consider the structure (e.g., a probabilistic logic program or a Markov logic network) that generated the KB. However, by identifying two constants as equivalent, Definition 9 gives us a set of pairs of ground atoms such that each pair is guaranteed to have the same probability. By considering how equivalence of constants relates to the structure generating the KB, one should be able to show how the equivalence also induces an exchangeable decomposition, although the details are left for future work.

7 Conclusion

In this paper, we described how the equivalence relation of constants induced by a KB Δ can be used to describe Δ in a fundamental way. We also developed a new way to interpret acyclic logic programs, and identified a number of important properties of these equivalence relations. Our work proved the existence of and developed a way to construct logic programs that transform a refinement of a KB to its coarser version. In the context of auto-encoding logic programs [Dumancic *et al.*, 2019] among other cases, it would also be interesting to consider how one could efficiently find an approximate transformation back, i.e., a logic program that takes the coarser KB to something 'similar' to the original (finer) KB.

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[8] In an extended report / journal paper, we will expand on these observations and also report on the application of our framework for auto-encoding logic programs [Dumancic *et al.*, 2019].

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Generating Random Logic Programs Using Constraint Programming

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Abstract

We present a novel approach to generating random logic programs and random probabilistic logic programs using constraint programming. The generated programs are useful in empirical testing of inference algorithms, random data generation, and program learning. This approach has a major advantage in that one can easily add additional conditions for the generated programs. As an example of this, we introduce a new constraint for predicate independence with efficient propagation and entailment algorithms, allowing one to generate programs that have a certain independence structure. To generate valid probabilistic logic programs, we also present a new constraint for negative cycle detection. Finally, we provide a combinatorial argument for correctness and describe how the parameters of the model affect the empirical difficulty of the program generation task.

1 INTRODUCTION

Unifying logic and probability is a long-standing challenge in artificial intelligence (Russell, 2015), and, in that regard, statistical relational learning (SRL) has developed into an exciting area that mixes machine learning and symbolic (logical and relational) structures. In particular, logic programs and probabilistic logic programs—including languages such as PRISM (Sato and Kameya, 1997), ICL (Poole, 1997), and ProbLog (De Raedt et al., 2007)—are promising frameworks for codifying complex SRL models. With the enhanced structure, however, inference becomes more challenging as algorithms have to correctly handle hard and soft logical constraints. At the moment, we have no precise way of evaluating and comparing different inference algorithms. Incidentally, if one were to survey the literature, one often finds that an inference algorithm is only tested on 1–4 data sets (Kimmig et al., 2011; Bruynooghe et al., 2010; Vlasselaer et al., 2015), originating from areas such as social networks, citation patterns, and biological data. But how confidently can we claim that an algorithm works well if it is only tested on a few types of problems?

About thirty years ago, SAT solving technology was dealing with a similar lack of clarity (Selman et al., 1996). This changed with the study of generation of random SAT instances against different input parameters (e.g., clause length and total number of variables) to better understand the behaviour of algorithms and their ability to solve random synthetic problems. Unfortunately, in the context of probabilistic logic programming, most current approaches to random instance generation are very restrictive, e.g., limited to clauses with only two literals (Namasivayam and Truszczynski, 2009), or to clauses of the form $a \leftarrow \neg b$ (Wen et al., 2016), although some are more expressive, e.g., defining a program only by the (maximum) number of atoms in the body and the total number of rules (Zhao and Lin, 2003).

In this work, we introduce a constraint model for generating random logic programs according to a number of user-specified parameters on the structure of the program. In fact, the same model can generate both probabilistic programs directly in the syntax of ProbLog (De Raedt et al., 2007) and non-probabilistic Prolog programs. For generated probabilistic programs to be valid, we use a custom constraint to detect negative cycles. A major advantage of our constraint-based approach is that one can easily add additional constraints to the model. To demonstrate that, we present a custom constraint with propagation and entailment algorithms that can ensure predicate independence. We also present a combinatorial argument for correctness, counting the number of programs that the model produces for various parame-

ter values. Finally, we show how the model scales when tasked with producing more complicated programs and identify the relationships between parameter values and the empirical hardness of the program generation task.

Overall, our main contributions are concerned with logic programming-based languages and frameworks, which capture a major fragment of SRL (De Raedt et al., 2016). However, since probabilistic logic programming languages are closely related to other areas of machine learning, including (imperative) probabilistic programming (De Raedt and Kimmig, 2015), our results can lay the foundations for exploring broader questions on generating models and testing algorithms in machine learning.

2 PRELIMINARIES

The basic primitives of logic programs are *constants*, *(logic) variables*, and *predicates*. Each predicate has an *arity* that defines the number of terms that it can be applied to. A *term* is either a variable or a constant, and an *atom* is a predicate of arity n applied to n terms. A *formula* is a grammatically-valid expression that connects atoms using conjunction ($\wedge$), disjunction ($\vee$), and negation ($\neg$). A *clause* is a pair of a *head* (which is an atom) and a *body* (which is a formula). A *(logic) program* is a multiset of clauses. Given a program $\mathscr{P}$, a *subprogram* $\mathscr{R}$ of $\mathscr{P}$ is a subset of the clauses of $\mathscr{P}$ and is denoted by $\mathscr{R} \subseteq \mathscr{P}$.

In the world of constraint satisfaction, we also have *(constraint) variables*, each with its own *domain*, whose values are restricted using *constraints*. All constraint variables in the model are integer or set variables, however, if an integer refers to a logical construct (e.g., a logical variable or a constant), we will make no distinction between the two and often use names of logical constructs to refer to the underlying integers. We say that a constraint variable is *(fully) determined* if its domain (at the given moment in the execution) has exactly one value. We will often use $\square$ as a special domain value to indicate a 'disabled' (i.e., fixed and ignored) part of the model. We write $\texttt{a}[b] \in c$ to mean that $\texttt{a}$ is an array of variables of length b such that each element of $\texttt{a}$ has domain c. Similarly, we write $\texttt{c} : \texttt{a}[b]$ to denote an array $\texttt{a}$ of length b such that each element of $\texttt{a}$ has type $\texttt{c}$. Finally, we assume that all arrays start with index zero.

2.1 PARAMETERS OF THE MODEL

We begin defining the parameters of our model by initialising sets and lists of the primitives used in constructing logic programs: a list of predicates $\mathcal{P}$, a list of their corresponding arities $\mathcal{A}$ (so $|\mathcal{A}| = |\mathcal{P}|$), a set of variables $\mathcal{V}$, and a set of constants $\mathcal{C}$. Either $\mathcal{V}$ or $\mathcal{C}$ can be empty, but we assume that $|\mathcal{C}| + |\mathcal{V}| > 0$. Similarly, the model supports zero-arity predicates but requires at least one predicate to have non-zero arity. For notational convenience, we also set $\mathcal{M}_{\mathcal{A}} \coloneqq \max \mathcal{A}$.

We also define a measure of how complicated a body of a clause can become. As each body is represented by a tree (see Section 4), we set $\mathcal{M}_{\mathcal{N}} \geq 1$ to be the maximum number of nodes in the tree representation of any clause. We also set $\mathcal{M}_{\mathcal{C}}$ to be the maximum number of clauses in a program. We must have that $\mathcal{M}_{\mathcal{C}} \geq |\mathcal{P}|$ because we require each predicate to have at least one clause that defines it. The model supports eliminating either all cycles or just negative cycles (see Section 8) and enforcing predicate independence (see Section 7), so a set of independent pairs of predicates is another parameter. Since this model can generate probabilistic as well as non-probabilistic programs, each clause is paired with a probability which is randomly selected from a given multiset (i.e., our last parameter). For generating non-probabilistic programs, one can set this list equal to $\{1\}$. Finally, we define $\mathcal{T} = \{\neg, \wedge, \vee, \top\}$ as the set of tokens that (together with atoms) form a clause. All decision variables of the model can now be divided into $2 \times \mathcal{M}_{\mathcal{C}}$ separate groups, treating the body and the head of each clause separately. We say that the variables are contained in two arrays: $\texttt{Body} : \texttt{bodies}[\mathcal{M}_{\mathcal{C}}]$ and $\texttt{Head} : \texttt{heads}[\mathcal{M}_{\mathcal{C}}]$. Since the order of the clauses does not change the meaning of the program, we can also state our first constraint:

Constraint 1. *Clauses are sorted.*

Here and henceforth, the exact ordering is immaterial: we only impose an order to eliminate permutation symmetries.

3 HEADS OF CLAUSES

Definition 1. The *head* of a clause is composed of a $\texttt{predicate} \in \mathcal{P} \cup \{\square\}$, and $\texttt{arguments}[\mathcal{M}_{\mathcal{A}}] \in \mathcal{C} \cup \mathcal{V} \cup \{\square\}$.

Here, we use $\square$ to denote either a disabled clause that we choose not to use or disabled arguments if the arity of the $\texttt{predicate}$ is less than $\mathcal{M}_{\mathcal{A}}$. The reason why we need a separate value for the latter (i.e., why it is not enough to fix disabled arguments to a single already-existing value) will become clear in Section 5.

Definition 2. The $\texttt{predicate}$'s $\texttt{arity} \in [0, \mathcal{M}_{\mathcal{A}}]$ can then be defined using the $\texttt{table}$ constraint as the arity of the $\texttt{predicate}$ if $\texttt{predicate} \in \mathcal{P}$, and zero otherwise.

Having defined arity, we can now fix the superfluous arguments:

Constraint 2. *For* $i = 0, \ldots, \mathcal{M}_\mathcal{A} - 1$*,*

$$\texttt{arguments}[i] = \square \iff i \geq \texttt{arity}.$$

We can also add a constraint that each predicate $\mathsf{P} \in \mathcal{P}$ should have at least one clause with P at its head:

Constraint 3. *Let*

$$P = \{h.\texttt{predicate} \mid h \in \texttt{heads}\}.$$

Then $\texttt{nValues}(P) = |\mathcal{P}|$ *if* $\texttt{count}(\square, P) = 0$ *and* $|\mathcal{P}| + 1$ *otherwise, where* $\texttt{nValues}(P)$ *counts the number of unique values in* P*.*

4 BODIES OF CLAUSES

As was briefly mentioned before, the body of a clause is represented by a tree.

Definition 3. The *body* of a clause has two parts. First, we have the $\texttt{structure}[\mathcal{M}_\mathcal{N}] \in [0, \mathcal{M}_\mathcal{N} - 1]$ array that encodes the structure of the tree using the following two rules: $\texttt{structure}[i] = i$ means that the i-th node is a root, and $\texttt{structure}[i] = j$ (for $j \neq i$) means that the i-th node's parent is node j. The second part is the array $\texttt{Node} : \texttt{values}[\mathcal{M}_\mathcal{N}]$ such that $\texttt{values}[i]$ holds the value of the i-th node.

We can use the `tree` constraint (Fages and Lorca, 2011) to forbid cycles in the `structure` array and simultaneously define $\texttt{numTrees} \in \{1, \ldots, \mathcal{M}_\mathcal{N}\}$ to count the number of trees. We will view the tree rooted at the zeroth node as the main tree and restrict all other trees to single nodes. For this to work, we need to make sure that the zeroth node is indeed a root:

Constraint 4. $\texttt{structure}[0] = 0$.

Definition 4. For convenience, we also define $\texttt{numNodes} \in \{1, \ldots, \mathcal{M}_\mathcal{N}\}$ to count the number of nodes in the main tree. We define it as

$$\texttt{numNodes} = \mathcal{M}_\mathcal{N} - \texttt{numTrees} + 1.$$

Example 1. Let $\mathcal{M}_\mathcal{N} = 8$. Then

$$\neg\mathsf{P}(X) \vee (\mathsf{Q}(X) \wedge \mathsf{P}(X))$$

corresponds to the tree in Fig. 1 and can be encoded as:

$$\begin{aligned} \texttt{structure} &= [0, 0, 0, \quad 1, \quad 2, \quad 2, \quad 6, 7], \\ \texttt{values} &= [\vee, \neg, \wedge, \mathsf{P}(X), \mathsf{Q}(X), \mathsf{P}(X), \top, \top], \\ \texttt{numNodes} &= 6, \\ \texttt{numTrees} &= 3. \end{aligned}$$

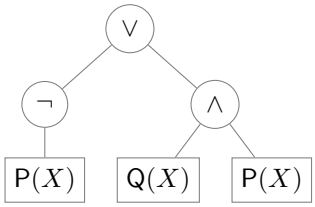

Figure 1: A tree representation of the formula from Example 1

Here, $\top$ is the value we use for the remaining one-node trees. The elements of the `values` array are nodes:

Definition 5. A *node* has a $\texttt{name} \in \mathcal{T} \cup \mathcal{P}$ and $\texttt{arguments}[\mathcal{M}_\mathcal{A}] \in \mathcal{V} \cup \mathcal{C} \cup \{\square\}$. The node's `arity` can then be defined analogously to Definition 2.

Furthermore, we can use Constraint 2 to again disable the extra arguments.

Example 2. Let $\mathcal{M}_\mathcal{A} = 2$, $X \in \mathcal{V}$, and let P be a predicate with arity 1. Then the node representing atom $\mathsf{P}(X)$ has:

$$\begin{aligned} \texttt{name} &= \mathsf{P}, \\ \texttt{arguments} &= [X, \square], \\ \texttt{arity} &= 1. \end{aligned}$$

We need to constrain the forest represented by the `structure` array together with its `values` to eliminate unnecessary symmetries and adhere to our desired format. First, we can recognise that the order of the elements in the `structure` array does not matter, i.e., the structure is only defined by how the elements link to each other, so we can add a constraint saying that:

Constraint 5. `structure` *is sorted.*

Next, since we already have a variable that counts the number of nodes in the main tree, we can fix the structure and the values of the remaining trees to some constant values:

Constraint 6. *For* $i = 1, \ldots, \mathcal{M}_\mathcal{N} - 1$*, if* $i \geq \texttt{numNodes}$*, then*

$$\texttt{structure}[i] = i, \quad \textit{and} \quad \texttt{values}[i].\texttt{name} = \top,$$

else $\texttt{structure}[i] < i$*.*

The second part of this constraint states that every node in the main tree except the zeroth node cannot be a root and must have its parent located to the left of itself. Next, we classify all nodes into three classes: predicate (or empty) nodes, negation nodes, and conjunction/disjunction nodes based on the number of children (zero, one, and two, respectively).

Constraint 7. *For $i = 0, \ldots, \mathcal{M}_\mathcal{N} - 1$, let C_i be the number of times i appears in the* `struture` *array with index greater than i. Then*

$$C_i = 0 \iff \texttt{values}[i].\texttt{name} \in \mathcal{P} \cup \{\top\},$$
$$C_i = 1 \iff \texttt{values}[i].\texttt{name} = \neg,$$
$$C_i > 1 \iff \texttt{values}[i].\texttt{name} \in \{\wedge, \vee\}.$$

The value $\top$ serves a twofold purpose: it is used as the fixed value for nodes outside the main tree, and, when located at the zeroth node, it can represent a clause with no body. Thus, we can say that only root nodes can have $\top$ as the value:

Constraint 8. *For $i = 0, \ldots, \mathcal{M}_\mathcal{N} - 1$,*

$$\texttt{structure}[i] \neq i \implies \texttt{values}[i].\texttt{name} \neq \top.$$

Finally, we add a way to disable a clause by setting its head predicate to $\square$:

Constraint 9. *For $i = 0, \ldots, \mathcal{M}_\mathcal{C} - 1$, if* `heads`$[i]$.`predicate` $= \square$*, then*

$$\texttt{bodies}[i].\texttt{numNodes} = 1,$$

and

$$\texttt{bodies}[i].\texttt{values}[0].\texttt{name} = \top.$$

5 VARIABLE SYMMETRIES

Given any clause, we can permute the variables in that clause without changing the meaning of the clause or the entire program. Thus, we want to fix the order of variables to eliminate unnecessary symmetries. Informally, we can say that variable X goes before variable Y if the first occurrence of X in either the head or the body of the clause is before the first occurrence of Y. Note that the constraints described in this section only make sense if $|\mathcal{V}| > 1$. Also, note that all definitions and constraints here are on a per-clause basis.

Definition 6. Let $N = \mathcal{M}_\mathcal{A} \times (\mathcal{M}_\mathcal{N} + 1)$, and let $\texttt{terms}[N] \in \mathcal{C} \cup \mathcal{V} \cup \{\square\}$ be a flattened array of all arguments in a particular clause.

Then we can use a channeling constraint to define $\texttt{occ}[|\mathcal{C}|+|\mathcal{V}|+1]$ as an array of subsets of $\{0, \ldots, N-1\}$ such that for all $i = 0, \ldots, N-1$, and $t \in \mathcal{C} \cup \mathcal{V} \cup \{\square\}$,

$$i \in \texttt{occ}[t] \iff \texttt{terms}[i] = t$$

Next, we introduce an array that, for each variable, holds the position of its first occurrence:

Definition 7. Let $\texttt{intros}[|\mathcal{V}|] \in \{0, \ldots, N\}$ be such that for $v \in \mathcal{V}$,

$$\texttt{intros}[v] = \begin{cases} 1 + \min \texttt{occ}[v] & \text{if } \texttt{occ}[v] \neq \emptyset \\ 0 & \text{otherwise.} \end{cases}$$

Here, a value of zero means that the variable does not occur in the clause. The reason why we want to use specifically zero for this will become clear with Constraint 12. Because of this choice, the definition of `intros` shifts all indices by one. Lastly, we add the constraint that eliminates variable symmetries:

Constraint 10. `intros` *are sorted.*

In other words, we constrain the model so that the variable listed first in whatever order $\mathcal{V}$ is presented in has to occur first in our representation of a clause.

Example 3. Let $\mathcal{C} = \emptyset$, $\mathcal{V} = \{X, Y, Z\}$, $\mathcal{M}_\mathcal{A} = 2$, $\mathcal{M}_\mathcal{N} = 3$, and consider the clause

$$\mathsf{sibling}(X, Y) \leftarrow \mathsf{parent}(X, Z) \wedge \mathsf{parent}(Y, Z).$$

Then

$$\texttt{terms} = [X, Y, \square, \square, X, Z, Y, Z],$$
$$\texttt{occ} = [\{0, 4\}, \{1, 6\}, \{5, 7\}, \{2, 3\}],$$
$$\texttt{intros} = [0, 1, 5],$$

where the $\square$'s correspond to the conjunction node.

5.1 REDUNDANT CONSTRAINTS

We add a number of redundant constraints to make search more efficient. First, we can state that the positions occupied by different terms must be different:

Constraint 11. *For $u \neq v \in \mathcal{C} \cup \mathcal{V} \cup \{\square\}$,*

$$\texttt{occ}[u] \cap \texttt{occ}[v] = \emptyset.$$

The reason why we used zero to represent an unused variable is so that we could efficiently rephrase Constraint 11 for the `intros` array:

Constraint 12. `allDifferentExcept0(intros)`.

We can also add another link between `intros` and `occ` that essentially says that the smallest element of a set is an element of the set:

Constraint 13. *For $v \in \mathcal{V}$,*

$$\texttt{intros}[v] \neq 0 \iff \texttt{intros}[v] - 1 \in \texttt{occ}[v].$$

Finally, we define an auxiliary set variable to act as a set of possible values that `intros` can take:

Definition 8. Let $\texttt{potentials} \subseteq \{0, \ldots, N\}$ be such that for $v \in \mathcal{V}$, $\texttt{intros}[v] \in \texttt{potentials}$.

Using this new variable, we can add a constraint saying that non-predicate nodes in the tree representation of a clause cannot have variables as arguments:

Constraint 14. *For* $i = 0, \ldots, \mathcal{M}_\mathcal{N} - 1$*, let*

$$S = \{\mathcal{M}_\mathcal{A} \times (i+1) + j + 1 \mid j = 0, \ldots, \mathcal{M}_\mathcal{A} - 1\}.$$

If $\texttt{values}[i].\texttt{name} \notin \mathcal{P}$*, then* $\texttt{potentials} \cap S = \emptyset$.

6 COUNTING PROGRAMS

To demonstrate the correctness of the model and explain it in more detail, in this section we are going to derive combinatorial expressions for counting the number of programs with up to $\mathcal{M}_\mathcal{C}$ clauses and up to $\mathcal{M}_\mathcal{N}$ nodes per clause, and arbitrary $\mathcal{P}$, $\mathcal{A}$, $\mathcal{V}$, and $\mathcal{C}$[1]. To simplify the task, we only consider clauses without probabilities and disable (negative) cycle elimination. We also introduce the term *total arity* of a body of a clause to refer to the sum total of arities of all predicates in the body.

We will first consider clauses with gaps, i.e., without taking variables and constants into account. Let $T(n, a)$ denote the number of possible clause bodies with n nodes and total arity a. Then $T(1, a)$ is the number of predicates in $\mathcal{P}$ with arity a, and the following recursive definition can be applied for $n > 1$:

$$T(n,a) = T(n-1,a) + 2 \sum_{\substack{c_1+\cdots+c_k=n-1,\\ 2\le k\le \frac{a}{\min \mathcal{A}},\\ c_i\ge 1 \text{ for all } i}} \sum_{\substack{d_1+\cdots+d_k=a,\\ d_i\ge \min \mathcal{A} \text{ for all } i}} \prod_{i=1}^{k} T(c_i, d_i).$$

The first term here represents negation, i.e., negating a formula consumes one node but otherwise leaves the task unchanged. If the first operation is not negation, then it must be either conjunction or disjunction (hence the coefficient '2'). In the first sum, k represents the number of children of the root node, and each c_i is the number of nodes dedicated to child i. Thus, the first sum iterates over all possible ways to partition the remaining $n - 1$ nodes. Similarly, the second sum considers every possible way to partition the total arity a across the k children nodes.

[1]We checked that our model agrees with the derived combinatorial formula in close to a thousand different scenarios. The details of this empirical investigation are omitted as they are not crucial to the thrust of this paper.

We can then count the number of possible clause bodies with total arity a (and any number of nodes) as

$$C(a) = \begin{cases} 1 & \text{if } a = 0 \\ \sum_{n=1}^{\mathcal{M}_\mathcal{N}} T(n,a) & \text{otherwise.} \end{cases}$$

Here, the empty clause is considered separately.

The number of ways to select n terms is

$$P(n) = |\mathcal{C}|^n + \sum_{\substack{1\le k\le |\mathcal{V}|,\\ 0=s_0<s_1<\cdots<s_k<s_{k+1}=n+1}} \prod_{i=0}^{k} (|\mathcal{C}| + i)^{s_{i+1}-s_i-1}.$$

The first term is the number of ways select n constants. The parameter k is the number of variables used in the clause, and $s_1, \ldots, s_k$ mark the first occurrence of each variable. For each gap between any two introductions (or before the first introduction, or after the last introduction), we have $s_{i+1} - s_i - 1$ spaces to be filled with any of the $|\mathcal{C}|$ constants or any of the i already-introduced variables.

Let us order the elements of $\mathcal{P}$, and let a_i be the arity of the i-th predicate. The number of programs is then:

$$\sum_{\substack{\sum_{i=1}^{|\mathcal{P}|} h_i = n,\\ |\mathcal{P}|\le n\le \mathcal{M}_\mathcal{C},\\ h_i\ge 1 \text{ for all } i}} \prod_{i=1}^{|\mathcal{P}|} \left(\left(\begin{matrix} \sum_{a=0}^{\mathcal{M}_\mathcal{A}\times\mathcal{M}_\mathcal{N}} C(a)P(a+a_i) \\ h_i \end{matrix} \right) \right),$$

where

$$\left(\left(\begin{matrix} n \\ k \end{matrix} \right) \right) = \binom{n+k-1}{k}$$

counts the number of ways to select k out of n items with repetition (and without ordering). Here, we sum over all possible ways to distribute $|\mathcal{P}| \le n \le \mathcal{M}_\mathcal{C}$ clauses among $|\mathcal{P}|$ predicates so that each predicate gets at least one clause. For each predicate, we can then count the number of ways to select its clauses out of all possible clauses. The number of possible clauses can be computed by considering each possible arity a, and multiplying the number of 'unfinished' clauses $C(a)$ by the number of ways to select the required $a + a_i$ terms in the body and the head of the clause.

7 PREDICATE INDEPENDENCE

In this section, we define a notion of predicate independence as a way to constrain the probability distributions defined by the generated programs. We also describe efficient algorithms for propagation and entailment checking.

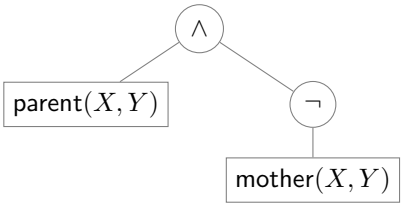

Figure 2: A tree representation of the body of Clause (1)

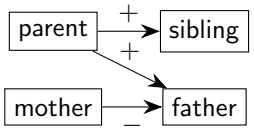

Figure 3: The predicate dependency graph of the program in Example 4. Positive edges are labelled with '+', and negative edges with '−'.

Definition 9. Let $\mathscr{P}$ be a probabilistic logic program. Its *predicate dependency graph* is a directed graph $G_{\mathscr{P}} = (V, E)$ with the set of nodes V consisting of all predicates in $\mathscr{P}$. For any two different predicates P and Q, we add an edge from P to Q if there is a clause in $\mathscr{P}$ with Q as the head and P mentioned in the body. We say that the edge is *negative* if there exists a clause with Q as the head and at least one instance of P at the body such that the path from the root to the P node in the tree representation of the clause passes through at least one negation node. Otherwise, it is *positive*. We say that $\mathscr{P}$ (or $G_{\mathscr{P}}$) has a *negative cycle* if $G_{\mathscr{P}}$ has a cycle with at least one negative edge.

Labelling the edges as positive/negative will be immaterial for predicate independence, but the same graph will play a crucial role in negative cycle detection in the next section.

Definition 10. Let P be a predicate in a program $\mathscr{P}$. The set of *dependencies* of P is the smallest set D_{P} such that $\mathsf{P} \in D_{\mathsf{P}}$, and, for every $\mathsf{Q} \in D_{\mathsf{P}}$, all direct predecessors of Q in $G_{\mathscr{P}}$ are in D_{P}.

Definition 11. Two predicates P and Q are *independent* if $D_{\mathsf{P}} \cap D_{\mathsf{Q}} = \emptyset$.

Example 4. Consider the following (fragment of a) program:

$$\mathsf{sibling}(X, Y) \leftarrow \mathsf{parent}(X, Z) \wedge \mathsf{parent}(Y, Z),$$
$$\mathsf{father}(X, Y) \leftarrow \mathsf{parent}(X, Y) \wedge \neg \mathsf{mother}(X, Y) \quad (1)$$

Its predicate dependency graph is in Fig. 3. Because of the negation in Clause (1) (as seen in Fig. 2), the edge from mother to father is negative, while the other two edges are positive.

We can now list the dependencies of each predicate:

$$D_{\mathsf{parent}} = \{\mathsf{parent}\},\ D_{\mathsf{sibling}} = \{\mathsf{sibling}, \mathsf{parent}\},$$
$$D_{\mathsf{mother}} = \{\mathsf{mother}\}, D_{\mathsf{father}} = \{\mathsf{father}, \mathsf{mother}, \mathsf{parent}\}.$$

Hence, we have two pairs of independent predicates, i.e., mother is independent of parent and sibling.

We can now add a constraint to define an adjacency matrix for the predicate dependency graph but without positivity/negativity:

Definition 12. An $|\mathcal{P}| \times |\mathcal{P}|$ adjacency matrix $\mathbf{A}$ with $\{0, 1\}$ as its domain is defined by stating that $\mathbf{A}[i][j] = 0$ if and only if, for all $k \in \{0, \ldots, \mathcal{M}_{\mathcal{C}} - 1\}$, either

$$\texttt{heads}[k].\texttt{predicate} \neq j$$

or $i \notin \{a.\texttt{name} \mid a \in \texttt{bodies}[k].\texttt{values}\}$.

Given an undetermined model, we can classify all dependencies of a predicate P into three categories based on how many of the edges on the path from the dependency to P are undetermined. In the case of zero, we call the dependency *determined*. In the case of one, we call it *almost determined*. Otherwise, it is *undetermined*. In the context of propagation and entailment algorithms, we define a *dependency* as the sum type:

$$\langle \textit{dependency} \rangle ::= \Delta(p) \mid \Upsilon(p) \mid \Gamma(p, s, t)$$

where each alternative represents a determined, undetermined, and almost determined dependency, respectively. Here, $p \in \mathcal{P}$ is the name of the predicate which is the dependency of P, and—in the case of Γ—$(s, t) \in \mathcal{P}^2$ is the one undetermined edge in $\mathbf{A}$ that prevents the dependency from being determined. For a dependency d—regardless of its exact type—we will refer to its predicate p as d.predicate. In describing the algorithms, we will use an underscore to replace any of p, s, t in situations where the name is unimportant.

Algorithm 1: Entailment for independence

Data: predicates p_1, p_2
$D \leftarrow \{(d_1, d_2) \in \texttt{deps}\,(p_1,\, 1) \times \texttt{deps}\,(p_2,\, 1)$
$\quad \mid d_1.\mathsf{predicate} = d_2.\mathsf{predicate}\}$;
if $D = \emptyset$ **then return** TRUE;
if $\exists(\Delta\ \_, \Delta\ \_) \in D$ **then return** FALSE;
return UNDEFINED;

Each entailment algorithm returns one out of three different values: TRUE if the constraint is guaranteed to hold, FALSE if the constraint is violated, and UNDEFINED if whether the constraint will be satisfied or not depends on

the future decisions made by the solver. Algorithm 1 outlines a simple entailment algorithm for the independence of two predicates p_1 and p_2. First, we separately calculate all dependencies of p_1 and p_2 and look at the set D of dependencies that p_1 and p_2 have in common. If there are none, then the predicates are clearly independent. If they have a dependency in common that is already fully determined (Δ) for both predicates, then they cannot be independent. Otherwise, we return UNDEFINED.

Algorithm 2: Propagation for independence

Data: predicates p_1, p_2; adjacency matrix $\mathbf{A}$

1 **for** $(d_1, d_2) \in \texttt{deps}\,(p_1, 0) \times \texttt{deps}\,(p_2, 0)$ *such that* d_1.predicate $= d_2$.predicate **do**

2 **if** d_1 **is** $\Delta(\_)$ **and** d_2 **is** $\Delta(\_)$ **then** `fail()`;

3 **if** d_1 **is** $\Delta(\_)$ **and** d_2 **is** $\Gamma(\_, s, t)$ **or** d_2 **is** $\Delta(\_)$ **and** d_1 **is** $\Gamma(\_, s, t)$ **then**

4 $\mathbf{A}[s][t]$.`removeValue(1)`;

Propagation algorithms have two goals: causing a contradiction (failing) in situations where the corresponding entailment algorithm would return FALSE, and eliminating values from domains of variables that are guaranteed to cause a contradiction. Algorithm 2 does the former on Line 2. Furthermore, for any dependency shared between predicates p_1 and p_2, if it is determined (Δ) for one predicate and almost determined (Γ) for another, then the edge that prevents the Γ from becoming a Δ cannot exist–Lines 3 and 4 handle this possibility.

Algorithm 3: Dependencies of a predicate

Data: adjacency matrix $\mathbf{A}$

Function `deps`$(p,$ allDependencies$)$**:**

 $D \leftarrow \{\Delta(p)\}$;

 while `true` **do**

  $D' \leftarrow \emptyset$;

  for $d \in D$ **and** $q \in \mathcal{P}$ **do**

   edge $\leftarrow \mathbf{A}[q][d.\text{predicate}] = \{1\}$;

   if edge **and** d **is** $\Delta(\_)$ **then**

    $D' \leftarrow D' \cup \{\Delta(q)\}$

   else if edge **and** d **is** $\Gamma(\_, s, t)$ **then**

    $D' \leftarrow D' \cup \{\Gamma(q, s, t)\}$;

   else if $|\mathbf{A}[q][d.\text{predicate}]| > 1$ **and** d **is** $\Delta(r)$ **then**

    $D' \leftarrow D' \cup \{\Gamma(q, q, r)\}$;

   else if $|\mathbf{A}[q][d.\text{predicate}]| > 1$ **and** allDependencies **then**

    $D' \leftarrow D' \cup \{\Upsilon(q)\}$;

  if $D' = D$ **then return** D;

  $D \leftarrow D'$;

$$\begin{array}{c} \\ \text{father} \\ \text{mother} \\ \text{parent} \\ \text{sibling} \end{array} \begin{pmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & \{0, 1\} & \{0, 1\} & \{0, 1\} \\ 0 & 0 & 0 & 0 \end{pmatrix}$$

Figure 4: The adjacency matrix defined using Definition 12 for Example 5

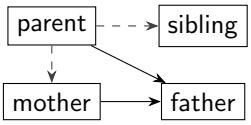

Figure 5: The predicate dependency graph that corresponds to Fig. 4. Dashed edges are undetermined—they may or may not exist.

The function `deps` in Algorithm 3 calculates D_p for any predicate p. It has two versions: `deps`$(p, 1)$ returns all dependencies, while `deps`$(p, 0)$ returns only determined and almost-determined dependencies. It starts by establishing the predicate p itself as a dependency and continues to add dependencies of dependencies until the set D stabilises. For each dependency $d \in D$, we look at the in-links of d in the predicate dependency graph. If the edge from some predicate q to d.predicate is fully determined and d is determined, then q is another determined dependency of p. If the edge is determined but d is almost determined, then q is an almost-determined dependency. The same outcome applies if d is fully determined but the edge is undetermined. Finally, if we are interested in collecting all dependencies regardless of their status, then q is a dependency of p as long as the edge from q to d.predicate is possible. Note that if there are multiple paths in the dependency graph from q to p, Algorithm 3 could include q once for each possible type (Δ, Υ, and Γ), but Algorithms 1 and 2 would still work as intended.

Example 5. Consider this partially determined (fragment of a) program:

$$\square(X, Y) \leftarrow \mathsf{parent}(X, Z) \wedge \mathsf{parent}(Y, Z),$$
$$\mathsf{father}(X, Y) \leftarrow \mathsf{parent}(X, Y) \wedge \neg\mathsf{mother}(X, Y)$$

where $\square$ indicates an unknown predicate with domain

$$D_\square = \{\mathsf{father}, \mathsf{mother}, \mathsf{parent}, \mathsf{sibling}\}.$$

The predicate dependency graph without positivity/negativity (as defined in Definition 12) is represented in Figs. 4 and 5.

Suppose we have a constraint that mother and parent must be independent. The lists of potential dependencies

for both predicates are:

$$D_{\mathsf{mother}} = \{\Delta(\mathsf{mother}), \Gamma(\mathsf{parent}, \mathsf{parent}, \mathsf{mother})\},$$
$$D_{\mathsf{parent}} = \{\Delta(\mathsf{parent})\}.$$

An entailment check at this stage would produce UNDEFINED, but propagation replaces the boxed value in Fig. 4 with zero, eliminating the potential edge from parent to mother. This also eliminates mother from $D_{\square}$, and, although some undetermined variables remain, this is enough to make Algorithm 1 return TRUE.

8 NEGATIVE CYCLES

Having no negative cycles in the predicate dependency graph is a requirement of ProbLog that makes the program well-defined (Kimmig et al., 2009). Ideally, we would like to design a constraint for negative cycles similar to the constraint for independence in the previous section. However, the difficulty with creating a propagation algorithm for negative cycles is that there seems to be no good way to extend Definition 12 so that the adjacency matrix captures positivity/negativity. Thus, we settle for an entailment algorithm with no propagation.

Algorithm 4: Entailment for negative cycles

Data: a program $\mathscr{P}$
Let $\mathscr{R} \subseteq \mathscr{P}$ be the largest subprogram of $\mathscr{P}$ with its `structure` and predicates in both body and head fully determined[2];
if `hasNegativeCycles` $(G_{\mathscr{R}})$ **then**
  return FALSE;
if $\mathscr{R} = \mathscr{P}$ **then return** TRUE;
return UNDEFINED;

The algorithm takes all clauses whose structure and predicates have been fully determined and uses them to construct a full dependency graph. In our implementation, `hasNegativeCycles` function is just a simple extension of the backtracking cycle detection algorithm that 'travels' around the graph following edges and checking if each vertex has already been visited or not. Alternatively, one could assign weights to the edges (e.g., 1 for positive and $-\infty$ for negative edges), thus reducing our negative cycle detection problem to what is typically known as the negative cycle detection problem in the literature, and use an algorithm such as Bellman-Ford (Shimbel, 1954).

If the algorithm finds a negative cycle in this fully-determined part of the program, then we must return FALSE. If there was no negative cycle and the entire program is (sufficiently) determined, then there cannot be any negative cycles. In all other cases, it is too early to tell.

[2]The arguments (whether variables or constants) are irrelevant to our definition of independence.

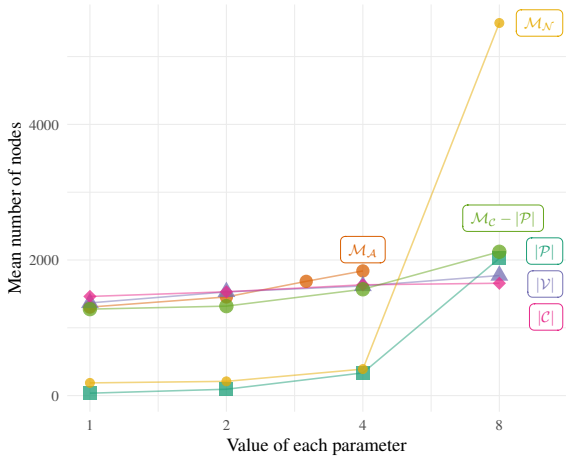

Figure 6: The mean number of nodes in the binary search tree for each value of each experimental parameter. Note that the horizontal axis is on a $\log_2$ scale.

9 EMPIRICAL PERFORMANCE

Along with constraints, variables, and their domains, two more design decisions are needed to complete the model: heuristics and restarts. By trial and error, the variable ordering heuristic was devised to eliminate sources of thrashing, i.e., situations where a contradiction is being 'fixed' by making changes that have no hope of fixing the contradiction. Thus, we partition all decision variables into an ordered list of groups, and require the values of all variables from one group to be determined before moving to the next group. Within each group, we use the 'fail first' variable ordering heuristic. The first group consists of all head predicates. Afterwards, we handle all remaining decision variables from the first clause before proceeding to the next. The decision variables within each clause are divided into: 1. the `structure` array, 2. body predicates, 3. head arguments, 4. (if $|\mathcal{V}| > 1$) the `intros` array, 5. body arguments. For instance, in the clause from Example 3, all visible parts of the clause would be decided in this order:

$$\overset{1}{\mathsf{sibling}}(\overset{3}{X}, \overset{3}{Y}) \leftarrow \overset{2}{\mathsf{parent}}(\overset{4}{X}, \overset{4}{Z}) \overset{2}{\wedge} \overset{2}{\mathsf{parent}}(\overset{4}{Y}, \overset{4}{Z}).$$

We also employ a geometric restart policy, restarting after $10, 20, 40, 80, \ldots$ contradictions.

We ran close to 400 000 experiments, investigating whether the model is efficient enough to generate

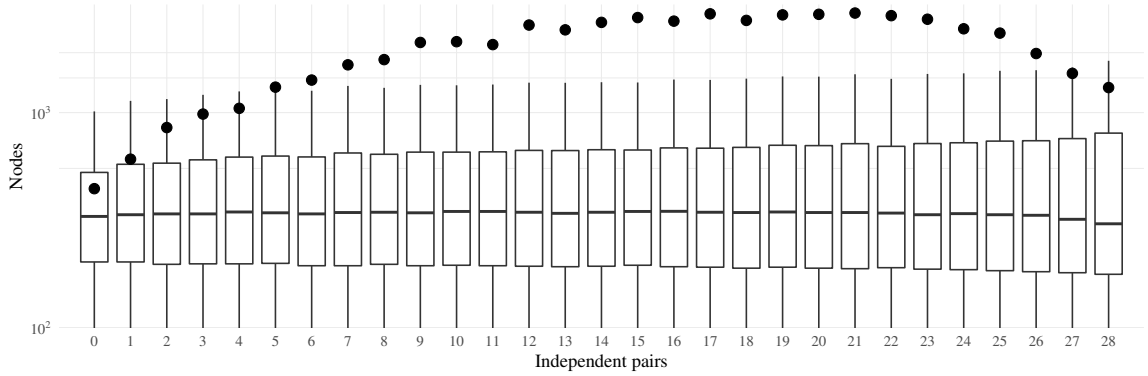

Figure 7: The distribution of the number of nodes in the binary search tree as a function of the number of independent pairs of predicates for $|\mathcal{P}| = 8$. Outliers are hidden, the dots denote mean values, and the vertical axis is on a $\log_{10}$ scale.

reasonably-sized programs and gaining insight into what parameter values make the constraint satisfaction problem harder. For these experiments, we use Choco 4.10.2 (Prud'homme et al., 2017) with Java 8. For $|\mathcal{P}|$, $|\mathcal{V}|$, $|\mathcal{C}|$, $\mathcal{M}_\mathcal{N}$, and $\mathcal{M}_\mathcal{C} - |\mathcal{P}|$ (i.e., the number of clauses in addition to the mandatory $|\mathcal{P}|$ clauses), we assign all combinations of 1, 2, 4, 8. $\mathcal{M}_\mathcal{A}$ is assigned to values 1–4. For each $|\mathcal{P}|$, we also iterate over all possible numbers of independent pairs of predicates, ranging from 0 up to $\binom{|\mathcal{P}|}{2}$. For each combination of the above-mentioned parameters, we pick ten random ways to assign arities to predicates (such that $\mathcal{M}_\mathcal{A}$ occurs at least once) and ten random combinations of independent pairs. We then run the solver with a $60\,\mathrm{s}$ timeout.

The majority ($97.7\,\%$) of runs finished in under $1\,\mathrm{s}$, while four instances timed out: all with $|\mathcal{P}| = \mathcal{M}_\mathcal{C} - |\mathcal{P}| = \mathcal{M}_\mathcal{N} = 8$ and the remaining parameters all different. This suggests that—regardless of parameter values—most of the time a solution can be identified instantaneously while occasionally a series of wrong decisions can lead the solver into a part of the search space with no solutions.

In Fig. 6, we plot how the mean number of nodes in the binary search tree grows as a function of each parameter (the plot for the median is very similar). The growth of each curve suggest how well/poorly the model scales with higher values of the parameter. From this plot, it is clear that $\mathcal{M}_\mathcal{N}$ is the limiting factor. This is because some tree structures can be impossible to fill with predicates without creating either a negative cycle or a forbidden dependency, and such trees become more common as the number of nodes increases. Likewise, a higher number of predicates complicates the situation as well.

Fig. 7 takes the data for $|\mathcal{P}| = 8$ (almost $300\,000$ observations) and shows how the number of nodes in the search tree varies with the number of independent pairs of predicates. The box plots show that the median number of nodes stays about the same while the dots (representing the means) draw an arc. This suggests a type of phase transition, but only in mean rather than median, i.e., most problems remain easy, but with some parameter values hard problems become more likely. On the one hand, with few pairs of independent predicates, one can easily find the right combination of predicates to use in each clause. On the other hand, if most predicates must be independent, this leaves fewer predicates that can be used in the body of each clause (since all of them have to be independent with the head predicate), and we can either quickly find a solution or identify that there is none.

10 CONCLUSIONS

We were able to design an efficient model for generating both logic programs and probabilistic logic programs. The model avoids unnecessary symmetries, generates valid programs, and can ensure predicate independence. Our constraint-driven approach is advantageous in that one can easily add additional conditions on the structure and properties of the program, although the main disadvantage is that there are no guarantees about the underlying probability distribution from which programs are sampled.

In addition, note that our model treats logically equivalent but syntactically different formulas as different. This is so in part because designing a constraint for logical equivalence fell outside the scope of this work and in part because in some situations one might want to enumerate all ways to express the same probability distribution or knowledge base, e.g., to investigate whether inference algorithms are robust to changes in representation.

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A EXAMPLE PROGRAMS

In this appendix, we provide examples of probabilistic logic programs generated by various combinations of parameters. In all cases, we use $\{0.1, 0.2, \ldots, 0.9, 1, 1, 1, 1, 1\}$ as the multiset of probabilities. Each clause is written on a separate line and ends with a full stop. The head and the body of each clause are separated with `:-` (instead of $\leftarrow$). The probability of each clause is prepended to the clause, using `::` as a separator. Probabilities equal to one and empty bodies of clauses can be omitted. Conjunction, disjunction, and negation are denoted by commas, semicolons, and '`\+`', respectively. Parentheses are used to demonstrate precedence, although many of them are redundant.

By setting $\mathcal{P} = [\mathtt{p}]$, $\mathcal{A} = [1]$, $\mathcal{V} = \{\mathtt{X}\}$, $\mathcal{C} = \emptyset$, $\mathcal{M}_\mathcal{N} = 4$, and $\mathcal{M}_\mathcal{C} = 1$, we get fifteen one-line programs, six of which are without negative cycles (as highlighted below). Only the last program has no cycles at all.

1. `0.5 :: p(X) :- (\+(p(X))), (p(X)).`
2. `0.8 :: p(X) :- (\+(p(X))); (p(X)).`
3. `0.8 :: p(X) :- (p(X)); (p(X)).`
4. `0.7 :: p(X) :- (p(X)), (p(X)).`
5. `0.6 :: p(X) :- (p(X)), (\+(p(X))).`
6. `p(X) :- (p(X)); (\+(p(X))).`
7. `0.1 :: p(X) :- (p(X)); (p(X)); (p(X))`
8. `0.8 :: p(X) :- (p(X)), (p(X)), (p(X))`
9. `p(X) :- \+(p(X)).`
10. `0.1 :: p(X) :- \+(\+(p(X))).`
11. `p(X) :- \+((p(X)); (p(X))).`
12. `0.4 :: p(X) :- \+((p(X)), (p(X))).`
13. `0.4 :: p(X) :- \+(\+(\+(p(X)))).`
14. `0.7 :: p(X) :- p(X).`
15. `p(X).`

Note that:

- A program such as Program 14, because of its cyclic definition, defines a predicate that has probability zero across all constants. This can more easily be seen as solving equation $0.7x = x$.
- Programs 10 and 14 are not equivalent (i.e., double negation does not cancel out) because Program 10 has a negative cycle and is thus considered to be ill-defined.

To demonstrate variable symmetry reduction in action, we set $\mathcal{P} = [\mathtt{p}]$, $\mathcal{A} = [3]$, $\mathcal{V} = \{\mathtt{X}, \mathtt{Y}, \mathtt{Z}\}$, $\mathcal{C} = \emptyset$, $\mathcal{M}_\mathcal{N} = 1$, $\mathcal{M}_\mathcal{C} = 1$, and forbid all cycles. This gives us the following five programs:

- `0.8 :: p(Z, Z, Z).`
- `p(Y, Y, Z).`
- `p(Y, Z, Z).`
- `p(Y, Z, Y).`
- `0.1 :: p(X, Y, Z).`

This is one of many possible programs with $\mathcal{P} = [\mathtt{p}, \mathtt{q}, \mathtt{r}]$, $\mathcal{A} = [1, 2, 3]$, $\mathcal{V} = \{\mathtt{X}, \mathtt{Y}, \mathtt{Z}\}$, $\mathcal{C} = \{\mathtt{a}, \mathtt{b}, \mathtt{c}\}$, $\mathcal{M}_\mathcal{N} = 5$, $\mathcal{M}_\mathcal{C} = 5$, and without negative cycles:

```
p(b) :- \+((q(a, b)), (q(X, Y)), (q(Z, X))).
0.4 :: q(X, X) :- \+(r(Y, Z, a)).
q(X, a) :- r(Y, Y, Z).
q(X, a) :- r(Y, b, Z).
r(Y, b, Z).
```

Finally, we set $\mathcal{P} = [\mathtt{p}, \mathtt{q}, \mathtt{r}]$, $\mathcal{A} = [1, 1, 1]$, $\mathcal{V} = \emptyset$, $\mathcal{C} = \{\mathtt{a}\}$, $\mathcal{M}_\mathcal{N} = 3$, $\mathcal{M}_\mathcal{C} = 3$, forbid negative cycles, and constrain predicates `p` and `q` to be independent. The resulting search space contains thousands of programs such as:

- ```
  0.5 :: p(a) :- (p(a)); (p(a)).
  0.2 :: q(a) :- (q(a)), (q(a)).
  0.4 :: r(a) :- \+(q(a)).
  ```
- ```
  p(a) :- p(a).
  0.5 :: q(a) :- (r(a)); (q(a)).
  r(a) :- (r(a)); (r(a)).
  ```
- ```
  p(a) :- (p(a)); (p(a)).
  0.6 :: q(a) :- q(a).
  0.7 :: r(a) :- \+(q(a)).
  ```
  ```