Constrained Bayesian Networks: Theory, Optimization, and Applications

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Abstract

We develop the theory and practice of an approach to modeling and probabilistic inference in causal networks that is suitable when application-specific or analysis-specific constraints should inform such inference or when little or no data for the learning of causal network structure or probability values at nodes are available. Constrained Bayesian Networks generalize a Bayesian Network such that probabilities can be symbolic, arithmetic expressions and where the meaning of the network is constrained by finitely many formulas from the theory of the reals. A formal semantics for constrained Bayesian Networks over first-order logic of the reals is given, which enables non-linear and non-convex optimization algorithms that rely on decision procedures for this logic, and supports the composition of several constrained Bayesian Networks. A non-trivial case study in arms control, where few or no data are available to assess the effectiveness of an arms inspection process, evaluates our approach. An open-access prototype implementation of these foundations and their algorithms uses the SMT solver Z3 as decision procedure, leverages an open-source package for Bayesian inference to symbolic computation, and is evaluated experimentally.

Keywords: Bayesian Belief Network. Imprecise Probabilities. Lack of Prior Data. Non-Linear Optimization. Confidence Building in Nuclear Arms Control.

1 Introduction

Bayesian Networks (BN) are a prominent, well established, and widely used formalism for expressing discrete probability distributions in terms of directed, acyclic graphs (DAG) that encode conditional independence assumptions of distributions. Bayesian Networks have a wide range of applications – for example, trouble shooting, design of experiments, and digital forensics to support legal reasoning. Their graph-based formalism and automated support for probabilistic inference seem to lower adaption hurdles for a diverse set of users with different technical backgrounds. Bayesian Networks are also appealing since we may combine, within the same Bayesian Network, different aspects such as subjective beliefs expressed in probabilities, implicit trust assumptions reflected in a bias of information processing or the combinatorial logic of a process. Probabilistic inference for such combinations is supported, including belief updates based on observed evidence.

Bayesian Networks also come with methodological support for learning an appropriate graph structure as well as appropriate prior probability values at nodes in such graphs from
pre-existing data (see for example [29, 19]). The appropriateness of chosen prior probability values may depend on a variety of factors: the quality and quantity of data used for learning these values or the trust we place in experts who determine such values subjectively – to give two examples. We would therefore like reassurance that the prior distributions represented by such values are robust enough in that small changes to such values only result in small changes of posterior distributions of interest. This naturally leads to the consideration of robust Bayesian statistics [9, 10].

A popular idea here is to approximate prior probabilities with intervals and to then calculate – somehow – the intervals that correspond to posterior probabilities. A good conceptual explanation of this is Good’s black box model [26, 27], in which interval information of priors is submitted into a black box that contains all the usual methods associated with precise computations in Bayesian Networks, and where the box then outputs intervals of posteriors without limiting any interpretations or judgments on those output intervals.

Our engagement with a problem owner in arms control made us realize the benefits of Good’s black box model and made us identify opportunities for extending it to increase the confidence that users from such problem domains can place in models and their robustness. Specifically, we want to be able to

R1 re-interpret compactly a BN as a possibly infinite set of BNs over the same graph, with robustness being analyzable over that re-interpretation

R2 add logical constraints to capture domain knowledge or dependencies, and reflect constraints in robustness analyses in a coherent manner

R3 compare models, within a composition context, to determine any differences in the robustness that they may offer for supporting decision making

R4 parametrize the use of such a box so that it can produce outputs for any quantitative measure of interest definable as an arithmetic term

R5 retain the “blackness” of the box so that the user neither has to see nor has to understand its inner workings

R6 interpret outputs of the black box within the usual methodology of Bayesian Networks in as far as this may be possible.

We believe that these requirements are desired or apt in a wide range of problem domains, in addition to the fact that they should enhance usability of such a methodology in practice. We develop constrained Bayesian Networks in this paper and show that they meet the above requirements. This development is informed by advances made in areas of Symbolic Computation [34] and Automated Theorem Proving [23] (with its applications to Non-Linear, Non-Convex Optimization [8]), Three-Valued Model Checking [13], and Abstract Interpretation [15]. Concretely, we allow prior probabilities to be arithmetic expressions that may contain variables, and we enrich this model with logical constraints expressed in the theory of the reals.

We draw comparisons to related work, including Credal Networks [16, 22, 33] and Constraint Networks [24]. We then highlight similarities, differences, and complementary value of our approach to this previous work.
Contributions and methodology of the paper We develop a formal syntax and semantics of constrained Bayesian Networks which denote an empty, finite or infinite set of Bayesian Networks over the same directed acyclic graph. We support this concept with a composition operator in which two or more constrained Bayesian Networks with different or “overlapping” graphs may be combined for cross-model analysis, subject to constraints that are an optional parameter of that composition. We formulate a three-valued semantics of the theory of the reals over constrained BNs that captures the familiar duality of satisfiability and validity but over the set of Bayesian Networks that a constrained Bayesian Network denotes. This semantics is used to reduce the computation of its judgments to satisfiability checks in the first-order logic over the reals. We then apply that reduction to design optimization algorithms that can compute, for any term definable in that logic, infima and suprema up to a specified accuracy – for example for terms that specify the meaning of marginal probabilities symbolically. These optimization algorithms and their term parameter allow us to explore or verify the robustness of a constrained Bayesian Network including, but not limited to, the robustness of posterior distributions. We demonstrate the use of such extended robustness analyses on a non-trivial case study in the domain of arms control. We also report a tool prototype that we have implemented and used to conduct these analyses; it uses an SMT solver as a feasibility checker to implement these optimization algorithms; and it adapts an open-source package for Bayesian inference to symbolic computations.

Our principal theoretical contribution is the introduction of the concept of a Constrained Bayesian Network itself, as well as its intuitive yet formal semantics. Our theoretical results, such as those for computational complexity and algorithm design, follow rather straightforwardly from these definitions. This is because the latter allow us to appeal directly to existing results from the existential theory of the reals and optimization based thereupon.

Our main practical contribution is the successful integration of a number of disparate techniques and approaches into a coherent semantic framework and tool prototype that supports a range of modelling and analysis capabilities, and does so in a highly automated manner.

2 Background on Bayesian Networks

A Bayesian Network (BN) is a graph-based statistical model for expressing and reasoning about probabilistic uncertainty. The underlying graph is directed and acyclic, a DAG. Nodes in this DAG represent random variables defined by discrete probability distributions that are also a function of the random variables represented by the parent nodes in the DAG. In other words, a random variable is conditioned on the random variables of its parent nodes.

We can use a BN to compute probabilities for events of interest over these random variables. Bayesian inference also allows us to revise such probabilities when additional observations of “evidence” have been made.

Figure 1 shows a simple BN, which is part of the folklore of example Bayesian Networks. It depicts the possible causes of wet grass on two neighbours’ lawns. For example, the probabilities of Holmes’ Grass Wet is conditioned on its parents’ output – whether It Rains and Holmes’ Sprinkler is turned On or Off. The probability of Holmes’ Grass Wet = T, given that Holmes’ Sprinkler = Off, Rain = F, for instance, is computed to be 0.05, and is formally
Figure 1: A BN with a 4-node DAG in the center and probability tables next to the respective nodes. This BN models beliefs about possible causes of wet grass on two neighbours’ lawns. This BN allows us to reason about, for example, whether Holmes’ lawn being wet is due to rain or Holmes’ sprinkler – using observed evidence about a neighbour’s lawn.

stated as:

\[ p(\text{Holmes’ Grass Wet} = T \mid \text{Sprinkler} = \text{Off}, \text{Rain} = \text{F}) = 0.05 \]

This approach naturally gives cause to computations of the “overall” probability of an event happening, referred to as the marginal probability. In the Bayesian approach, the Junction Tree Algorithm (JTA) (see e.g. Chapter 6 in [6] for further details) may be used to revise a marginal of a BN because of “hard”, respectively “soft”, evidence – the definite, respectively probabilistic, observation of an additional or new event.

We now formalize BNs and use this below to enrich BNs with modeling and reasoning capabilities that realize the aforementioned requirements.

**Definition 1**

1. A Bayesian network (BN) is a pair \((G, \pi)\) where \(G\) is a finite, directed, acyclic graph \(G = (N, E)\) of nodes \(N\) and edge relation \(E \subset N \times N\), and where \(\pi\) is a tuple \((\pi_n)_{n \in N}\) of formal probability tables.

2. The formal probability table \(\pi_n\) is defined as follows. Let \(\text{pnt}(n) = \{n' \in N \mid (n', n) \in E\}\) be the (possibly empty) set of parents of \(n\) in DAG \(G\) and \(O_n\) the set of outcomes of the random variable at node \(n\). Then \(\pi_n\) is a discrete probability distribution, a function \(\pi_n\) of type \((\prod_{n' \in \text{pnt}(n)} O_{n'}) \times O_n \to [0,1]\) such that its mass \(\sum_e \pi_n(e)\) equals 1.

Above, it is understood that \(\prod_{n' \in \emptyset} O_{n'}\) equals \(\{\}\); in that case, \(\pi_n\) has type isomorphic to \(O_n \to [0,1]\).
3 Constrained Bayesian Networks

Informally, a constrained BN is obtained from a BN by replacing one or more probabilities in its probability tables with symbolic expressions, and by adding constraints for variables used in these expressions or in quantitative terms of interest, and for variables that refer to marginal probabilities of interest. We write $B^C_X$ for constrained BN with set of constraints $C$ and variable set $X$.

To illustrate, in Figure 2 the probability tables for two nodes Sprinkler and Rain of the BN in Figure 1 are made symbolic with a variable $x$ to obtain a constrained BN. This allows us to model strict uncertainty (also known as Knightian uncertainty) in the actual value of such probabilities. Our approach allows variables to be shared across such tables, as $x$ is shared across the tables for Sprinkler and Rain. This is certainly useful, e.g., to express that a certain subjective probability is twice as likely as another one.

We use variables $mp_H$ and $mp_W$ to refer to marginal probabilities

$$p(\text{Holmes' Grass Wet} = \text{True})$$  \hspace{1cm} (1)

$$p(\text{Holmes' Grass Wet} = \text{True} \mid \text{Watson's Grass Wet} = \text{True})$$ \hspace{1cm} (2)

respectively. The constraints we then consider are $0 \leq x \leq 1$, to ensure that symbolic expressions still specify probability distributions, as well as the symbolic meaning of the marginal probabilities $mp_H$ and $mp_W$ which are captured in two non-linear equations in $x$ as

$$mp_H = 0.495*x*x + 0.5*x*(-0.95*x + 0.95) + 0.7*x*(-0.5*x + 1) + 1.0*(-0.5*x + 1)*(-0.05*x + 0.05)$$ \hspace{1cm} (3)

$$mp_W = (0.35*x*x + 0.025*x*(-0.95*x + 0.95) + 0.7*x*(-x*0.5 + 1) + 0.025*x*(-0.05*x + 0.05) + 0.05*(-0.05*x + 0.05)) = (0.3465*x*x + 0.025*x*(-0.95*x + 0.95) + 0.49*x*(-x*0.5 + 1) + 0.05*(-x*0.5 + 1)*(-0.05*x + 0.05))$$ \hspace{1cm} (4)

The above equations are constructed through symbolic interpretations of computations of marginals, for example of the Junction Tree Algorithm, and subsequent elimination of...
\[ t ::= c \mid mp \mid x \mid t + t \mid t * t \]
\[ \varphi ::= \text{true} \mid t \leq t \mid t < t \mid \neg \varphi \mid \varphi \land \varphi \]
\[ \phi ::= \varphi \mid \exists x : \phi \mid \neg \phi \mid \phi \land \phi \]

Figure 3: BNF grammars for real-valued terms \( t \), constraints \( \varphi \), and queries \( \phi \) where \( x \) are variables from set \( X_x \), \( c \) are constant reals, \( mp \) are variables from set \( X_{mp} \) denoting marginal probabilities, and \( \text{true} \) denotes logical truth.

division operators. The latter computes a normal form of rational terms from which these equations are easily derived.

### 3.1 Theoretical Foundations

We begin the formal development by defining grammars for symbolic expressions that occur in probability tables and for properties that contain such expressions as arguments. Figure 3 shows definitions for real-valued terms \( t \), where \( c \) ranges over real constants, and \( x \) and \( mp \) are real variables ranging over variable sets \( X_x \) and \( X_{mp} \), respectively. The distinction between \( mp \) and \( x \) is one of modelling intent. Variables \( mp \) refer to marginal probabilities of a constrained BN \( B \subset X \). The meaning of these symbolic marginals is defined via constraints in \( C \). Variables in \( X_x \) may occur in symbolic expressions in probability tables of nodes or denote any quantitative measures of interest. We write \( X = X_x \cup X_{mp} \) for the disjoint union of such variable sets.

Constraints \( \varphi \) are quantifier-free formulas built from inequalities over terms \( t \), logical truth constant \( \text{true} \), and propositional operators. Queries \( \phi \) are built out of constraints and first-order quantifiers.

**Definition 2** We write \( \mathcal{T}[X] \) for the set of all terms \( t \), \( \mathcal{C}[X] \) for the set of all constraints \( \varphi \) generated in this manner, and we write \( \mathcal{Q}[X] \) for the set of all queries \( \phi \) generated in this manner from variable set \( X \).

We write \( \mathcal{T}, \mathcal{C}, \) and \( \mathcal{Q} \) whenever \( X \) is clear from context and write \( \lor, \land, =, > \) and so forth for derived logical, arithmetic, and relational operators.

We may think of a constrained BN \( B \subset X \) as a BN \( B \) in which entries in probability tables of nodes may not only be concrete probabilities but terms \( t \) of the grammar in Figure 3 over variable set \( X_x \), and where the BN is enriched with a finite set of constraints \( C = \{ \varphi_i \mid 1 \leq i \leq n \} \). The intuition is that \( B \subset X \) denotes a set of BNs that all have the same graph and the same structure of probability tables but where probability values may be uncertain, modelled as arithmetic terms, and subject to application-specific or analysis-specific constraints. The only difference in two BNs from that set may be in the real number entries in those probability tables, and those real numbers are instantiations of the specified arithmetic terms such that all constraints are met. We formalize this:

**Definition 3** A constrained BN of type \( (X_x, X_{mp}) \) – denoted as \( X = X_x \cup X_{mp} \) by abuse of notation – is a triple \( (G, C, \pi) \) where \( G = (N, E) \) is a finite DAG, \( C \) a finite set of constraints from \( \mathcal{C}[X] \), and \( \pi \) a tuple \( (\pi_n)_{n \in N} \) of symbolic probability tables with \( O_n \) as the
set of outcomes of random variable at node $n$:

$$\pi_n: \left( \prod_{\nu \in \text{pt}(n)} O_{n^\nu} \right) \times O_n \to \mathcal{T}[X_x]$$

Note that a symbolic probability table has the same input type as a formal probability table, but its output type is a set of terms not the unit interval. Let us first define syntactic restrictions for constrained BNs.

**Definition 4** 1. A constrained BN $(G, C, \pi)$ of type $X$ is well-formed if
   
   (a) $X = X_x \cup X_{mp}$ equals the set of variables that occur in $C$
   
   (b) all $mp$ in $X_{mp}$ have exactly one defining equation $mp = t$ or $mp \ast t = t'$ in $C$ where neither $t$ nor $t'$ contain variables from $X_{mp}$.

2. When $G$ and $\pi$ are determined by context, we refer to a well-formed, constrained BN $(G, C, \pi)$ of type $X$ as $B^C_X$.

Item 1(a) says that all variables in $X$ occur in some constraint from $C$. Item 1(b) ensures all variables $mp$ that model marginal probabilities have a defined meaning in $C$. Note that item 1(b) is consistent with having other constraints on such variables in $C$, for example a constraint saying that $0.1 \leq mp \leq x \ast y$. These items create a two-level term language, with variables in $X_x$ informing meaning of variables in $X_{mp}$.

A sound, constrained BN has a semantic requirement about its concretizations, which we now formalize using assignments for quantifier-free formulas.

**Definition 5** 1. An assignment $\alpha$ is a function $\alpha: X \to \mathbb{R}$. For $c$ in $\mathbb{R}$ and $x$ in $X$, assignment $\alpha[x \mapsto c]$ equals $\alpha$ except at $x$, where it outputs $c$.

2. The meaning $\alpha(t)$ of term $t$ in $\mathcal{T}$ under $\alpha$, as well as the judgment $\alpha \models \phi$ for all $\phi$ in $Q$, are defined in Figure 4.

Note that $\alpha(t)$ extends $\alpha: X \to \mathbb{R}$ to type $\mathcal{T}[X] \to \mathbb{R}$. The judgment $\alpha \models \phi$ is satisfaction of first-order logic over the reals. We use these judgments to define the set of concretizations of a well-formed, constrained BN:

**Definition 6** Let $B^C_X = (G, C, \pi)$ be a well-formed, constrained BN where $G = (N, E)$. Let $\alpha: X \to \mathbb{R}$ be an assignment.

1. We write $B^C_X[\alpha]$ for the BN $(G, \pi[\alpha])$ that forgets $C$ from $B^C_X$ and has formal probability table $\pi[\alpha]_n$ for each node $n$ with $\pi[\alpha]_n = \lambda e: \alpha(\pi_n(e))$.

2. The set $\mathbb{B}^C_X$ of BNs that $B^C_X$ denotes, its set of concretizations, is

$$\mathbb{B}^C_X = \{ B^C_X[\alpha] \mid \alpha: X \to \mathbb{R} \text{ and } \alpha \models \bigwedge_{\varphi \in C} \varphi' \}$$

Note that the formal probability table $\pi[\alpha]_n$ computes $\pi[\alpha]_n(e)$ as $\alpha(t)$ where $t$ is the term $\pi_n(e)$ in $\mathcal{T}[X_x]$. We can now define sound constrained BNs.
\[ \alpha(c) = c \quad \text{constants denote themselves} \]
\[ \alpha(x) = \alpha(x) \quad \text{for all } x \text{ in } X, \text{overloading of notation} \]
\[ \alpha(t_1 + t_2) = \alpha(t_1) + \alpha(t_2) \]
\[ \alpha(t_1 \ast t_2) = \alpha(t_1) \ast \alpha(t_2) \]

\[ \alpha \models \text{true} \quad \text{holds} \]
\[ \alpha \models t_1 \leq t_2 \iff \alpha(t_1) \leq \alpha(t_2) \]
\[ \alpha \models t_1 < t_2 \iff \alpha(t_1) < \alpha(t_2) \]
\[ \alpha \models \neg \phi \iff \text{not } \alpha \models \phi \]
\[ \alpha \models \varphi_1 \land \varphi_2 \iff (\alpha \models \varphi_1 \text{ and } \alpha \models \varphi_2) \]
\[ \alpha \models \exists x : \phi \iff \alpha[x \mapsto e] \models \phi \text{ for some real number } c \]
\[ \alpha \models \neg \phi \iff \text{not } \alpha \models \phi \]
\[ \alpha \models \varphi_1 \land \varphi_2 \iff (\alpha \models \varphi_1 \text{ and } \alpha \models \varphi_2) \]

Figure 4: Top: meaning of terms for an assignment \( \alpha \), where we identify constants with their meaning, and use the same symbol \( + \) for syntax and semantics, and similarly for \( \ast \). Bottom: Semantics of judgment \( \alpha \models \phi \) for an assignment \( \alpha : X \to \mathbb{R} \) and \( \phi \) from \( Q \). This uses the meaning \( \alpha(t) \) from Figure 4 and uses \( \leq \) both as syntax and semantics, similarly for \(<\).

**Definition 7** Let \( B^C_X = (G, C, \pi) \) be a well-formed, constrained BN. Then \( B^C_X \) is sound if for all \( B^C_X[\alpha] \) that are concretizations of \( B^C_X \) we have, for all nodes \( n \) and inputs \( e \) of \( \pi[\alpha]_n \), that \( \pi[\alpha]_n(e) \) is in \([0, 1]\) and \( \sum_e \pi[\alpha]_n(e) = 1 \).

Soundness is saying that all concretizations of a well-formed, constrained BN are actually BNs: for each such \( B^C_X[\alpha] \) and node \( n \) in it, \( \pi[\alpha]_n \) is a discrete probability distribution.

**Assumption 1** All constrained BNs used in this paper are sound.

It is important to know whether \( \| B^C_X \| \) is non-empty.

**Definition 8** A constrained \( B^C_X \) is consistent iff \( \| B^C_X \| \neq \emptyset \).

The techniques developed in the next Section \( \ref{semantic-judgments} \) will also allow us to decide whether a constrained BN is consistent.

### 3.2 Semantic Judgments

How should we best reason about a set of BNs \( \| B^C_X \| \)? We propose two semantic judgments that allow us to explore worst-case and best-case properties of \( B^C_X \). A judicious combination of these judgments also enables us to express optimizations over the imprecision and probabilistic uncertainty inherent in \( B^C_X \), whilst reflecting any application-specific or analysis-specific constraints. Both semantic judgments rest on a satisfaction relation between concretization BNs and queries. We define this formally.
Definition 9 Let $B_X^C$ be a constrained BN. For all $\phi$ in $Q$, the two semantic judgments $\models^\text{must}$ and $\models^\text{may}$ are defined as

\begin{align*}
B_X^C &\models^\text{must} \phi \iff \text{ for all } B_X^C[\alpha] \text{ in } B_X^C \text{ we have } \alpha \models \phi \quad (6) \\
B_X^C &\models^\text{may} \phi \iff \text{ for some } B_X^C[\alpha] \text{ in } B_X^C \text{ we have } \alpha \models \phi \quad (7)
\end{align*}

The definition in (6) allows us to discover invariants: truth of $B_X^C\models^\text{must} \phi$ implies that $\phi$ holds no matter what concrete instance in $\{B_X^C\}$ the modeller may face, a form of worst-case reasoning. Dually, the truth of $B_X^C\models^\text{may} \phi$ in (7) implies it is possible that the modeller faces a BN in $\{B_X^C\}$ that satisfies $\phi$, a form of best-case reasoning. We may formalize this duality.

Theorem 1 For all constrained BNs $B_X^C$ and $\phi$ in $Q$ we have

1. $B_X^C\models^\text{must} \phi$ iff not $B_X^C\models^\text{may} \neg \phi$
2. $B_X^C\models^\text{may} \phi$ iff not $B_X^C\models^\text{must} \neg \phi$
3. $B_X^C\models^\text{must} \phi_1 \land \phi_2$ iff ($B_X^C\models^\text{must} \phi_1$ and $B_X^C\models^\text{must} \phi_2$)
4. $B_X^C\models^\text{may} \phi_1 \lor \phi_2$ iff ($B_X^C\models^\text{may} \phi_1$ or $B_X^C\models^\text{may} \phi_2$)

We illustrate this formalization of constrained BNs with an example.

Example 1 The constrained BN from Figures 7 and 2 is sound and consistent. Consider the query $\varphi_H$ being $mp_H < 0.3$ where we use variable $mp_H$ to denote the marginal probability $p(\text{Holmes’ Grass Wet} = \text{True})$. We mean to compute whether $B_X^C\models^\text{must} \varphi_H$ and $B_X^C\models^\text{may} \varphi_H$ hold for this constrained BN. We conclude that $B_X^C\models^\text{must} \varphi_H$ does not hold: $p(\text{Holmes’ Grass Wet} = \text{True})$ equals 0.35255 for $\alpha(x) = 0.3$ and so $\alpha(mp_H) = 0.35255$ as well, and we have $\alpha \models \bigwedge_{\varphi \in C} \varphi'$ and 0.35255 $\not\leq$ 0.3. On the other hand, $B_X^C\models^\text{may} \varphi_H$ holds since for $\alpha'(x) = 0.1$ we have $\alpha' \models \bigwedge_{\varphi \in C} \varphi'$ and $\alpha'(mp_H) = 0.15695$ is less than or equal to 0.3.

Observing additional hard evidence that Watson’s grass is wet, we similarly evaluate judgments $B_X^C\models^\text{may} \varphi$ and $B_X^C\models^\text{must} \varphi$ when $\varphi$ contains $mp_W$ which refers to marginal

$$p(\text{Holmes’ Grass Wet} = \text{True} \mid \text{Watson’s Grass Wet} = \text{True})$$

3.3 Consistent constrained BNs

It is important to understand how the semantic judgments $\models^\text{may}$ and $\models^\text{must}$ relate to consistent or inconsistent constrained BNs. We can characterize consistency through properties of these semantic judgments:

Theorem 2 Let $B_X^C$ be a constrained BN. Then the following are all equivalent:

1. $B_X^C\models^\text{may} \text{true}$ holds.
2. $B_X^C$ is consistent.
3. For all $\phi$ in $Q$, we have that $B_X^C\models^\text{must} \phi$ implies $B_X^C\models^\text{may} \phi$. 
4. For all $\phi$ in $Q$, we have that $B_X^C \models \text{may } \phi \lor \neg \phi$ holds.

5. For all $\phi$ in $Q$, we have that $B_X^C \models \text{must } \phi \land \neg \phi$ does not hold.

We stress that it is vital to check the consistency of $B_X^C$ prior to relying on any findings of its further analysis. If $B_X^C$ is inconsistent, then $\| B_X^C \|$ is empty and so $B_X^C \models \text{must } \phi$ holds trivially for all $\phi$ in $Q$ since the universal quantification of its defining semantics in $[6]$ ranges over the empty set. Not detecting such inconsistency may thus lead to unintended and flawed reasoning. In our tool, this is a non-issue as it uses these judgments within optimization algorithms that either report a concretization as witness or report a discovered inconsistency.

Consistency checking is NP-hard: checking the satisfiability of constraints in logic $C$ is NP-hard. And so this hardness is inherited for any notion of size of a constrained BN that includes the sum of the sizes of all its constraints.

### 3.4 Reducing $\models \text{may}$ and $\models \text{must}$ to satisfiability checking

Our case studies involving constrained BNs suggest that it suffices to consider elements of $C$, i.e. to consider formulas of $Q$ that are quantifier-free. The benefit of having the more expressive logic $Q$, however, is that its quantifiers allow us to reduce the decisions for $B_X^C \models \text{may } \varphi$ and $B_X^C \models \text{must } \varphi$ for quantifier-free formulas $\varphi$ to satisfiability checking, respectively validity checking in the logic $Q$ – which we now demonstrate. For sound, constrained BNs $B_X^C$, the judgment $B_X^C \models \text{may } \varphi$ asks whether there is an assignment $\alpha : X \rightarrow \mathbb{R}$ such that $\alpha \models \bigwedge_{\varphi' \in C} \varphi'$ and $\alpha \models \varphi$ both hold. Since $C$ is contained in $Q$, we may capture this meaning within the logic $Q$ itself as a satisfiability check. Let set $X$ equal $\{x_1, \ldots, x_n\}$. Then, asking whether $\alpha \models \bigwedge_{\varphi' \in C} \varphi'$ and $\alpha \models \varphi$ hold, asks whether the formula in (8) of logic $Q$ is satisfiable:

$$\exists x_1 : \ldots : \exists x_n : \varphi \land \bigwedge_{\varphi' \in C} \varphi'$$

(8)

**Definition 10** For a constrained BN $B_X^C$ and $\varphi$ in $C$, we write $\text{Ex}(B_X^C, \varphi)$ to denote the formula defined in (8).

Note that $\text{Ex}(B_X^C, \varphi)$ depends on $B_X^C$: namely on its set of variables $X$ and constraint set $C$, the latter reflecting symbolic meanings of marginal probabilities. Let us illustrate this by revisiting Example 1.

**Example 2** For $\varphi_H$ as in Example 1 with type $X = \{x\} \cup \{mp_H\}$, the formula we derive for $B_X^C \models \text{may } \varphi_H$ is

$$\exists mp_H : \exists x : (mp_H < 0.3) \land (0.1 \leq x) \land (x \leq 0.3) \land (0.5 \times x + (1 - 0.5 \times x) = 1) \land (x + (1 - x) = 1) \land (mp_H = t)$$

where $t$ is the term on the righthand side of the equation in (3).

We can summarize this discussion, where we also appeal to the first item of Theorem 1 to get a similar characterization for $\models \text{must}$. 

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Theorem 3  Let $B^C_X$ be a constrained BN and $\varphi$ in $C$. Then we have:

1. Formula $\text{Ex}(B^C_X, \varphi)$ in $[8]$ is in $Q$ and in the existential fragment of $Q$.
2. Truth of $B^C_X \models \text{may} \varphi$ is equivalent to the satisfiability of $\text{Ex}(B^C_X, \varphi)$ in $Q$.
3. $B^C_X \models \text{may} \varphi$ can be decided in PSPACE in the size of formula $\text{Ex}(B^C_X, \varphi)$.
4. $B^C_X \models \text{must} \varphi$ can be decided in PSPACE in the size of formula $\text{Ex}(B^C_X, \neg \varphi)$.

This result of deciding semantic judgments in polynomial space pertains to the size of formulas $\text{Ex}(B^C_X, \varphi)$ and $\text{Ex}(B^C_X, \neg \varphi)$, and these formulas contain equations that define the meaning of marginals symbolically. There is therefore an incentive to simplify such symbolic expressions prior to their incorporation into $C$ and these formulas, and we do such simplifications in our implementation.

3.5 Constrained Union Operator

We also want the ability to compare two or more constrained BNs or to discover relationships between them. This is facilitated by a notion of composition of constrained BNs, which we now develop. Consider two constrained BNs $B^C_{X_1}$ and $B^C_{X_2}$. Our intuition for composition is to use a disjoint union of the graphs of each of these constrained BNs such that each node in this unioned DAG still has its symbolic probability table as before. This union operator renames nodes that appear in both graphs so that the union is indeed disjoint. As a set of constraints for the resulting constrained BN, we then consider $C_1 \cup C_2$.

It is useful to make this composition depend on another set of constraints $C$. The idea is that $C$ can specify known or assumed relationships between these BNs. The resulting composition operator $\cup$ defines the composition

$$B^C_{X_1} \cup B^C_{X_2}$$

as the constrained BN with graph and probability tables obtained by disjoint union of the graphs and symbolic probability tables of $B^C_{X_1}$ and $B^C_{X_2}$, where the set of constraints for this resulting constrained BN is now $C_1 \cup C_2 \cup C$.

This composition operator has an implicit assumption for being well defined, namely that $C$ does not contain any equations that (re)define the (symbolic) meaning of marginal probabilities given in $C_1 \cup C_2$.

We give an example of such a union of constrained BNs that already illustrates some reasoning capabilities to be developed in this paper:

Example 3  Figure 5 specifies a constrained BN $B^C_{X_0}$ that is similar to constrained BN $B^C_{X_0}$ defined in Figure 2 but that models rain with more specificity. Variables $y$ and $z$ are used in symbolic probabilities, and variables $mp_H$ and $mp_W$ refer to the marginals in $[1]$ and $[2]$ respectively. The constraint $0.1 \leq 5 \cdot y \leq 0.3$ in $C_0$ corresponds to the constraint $0.1 \leq x \leq 0.3$ in $C_0$ and so term $5 \cdot y$ in some way reflects $x$, that it rains according to $B^C_{X_0}$.

The constraint set $C$ that binds the two models together is $\{2 \cdot z = x\}$, which ensures that the probability for the sprinkler to be on is the same in both models. In the constrained
| Sprinkler   | Off | On  |
|------------|-----|-----|
| z          | 1 - z |
| Rain       |     |     |
| Heavy      | y   | y   |
| Light      | 4y  | 1 - 5y |

| Sprinkler/Rain | Holmes’ Sprinkler/Rain |
|----------------|-------------------------|
| Off            | 0.05 0.95               |
| Off            | 0.65 0.35               |
| Off            | 0.9 0.1                 |
| On             | 0.95 0.05               |
| On             | 0.95 0.05               |
| On             | 0.99 0.01               |

| Watson’s Rain | T   | F   |
|---------------|-----|-----|
| Off           | N   | 0.05 0.95 |
| Off           | L   | 0.65 0.35 |
| Off           | H   | 0.9 0.1   |
| On            | N   | 0.95 0.05 |
| On            | L   | 0.95 0.05 |
| On            | H   | 0.99 0.01 |

Figure 5: Symbolic probability tables for a constrained BN $B_{X_0}^{C_0}$ that has the same DAG as $B_{X_0}^{C_0}$ of Figure 2 but is more complex: rain is modelled to a greater degree of specificity. Variable set $X_0'$ is \{y, z\} $\cup$ \{mp\'_H, mp\'_W\}. The constraint set $C_0'$ includes $0.1 \leq 5 * y \leq 0.3$, equations that define the meaning of marginals $mp\'_W$ and $mp\'_W$ in terms of y and z (not shown), and equations that ensure that all tables specify probability tables.

BN $B_{X_0}^{C_0} \cup B_{X_0}^{C_0'}$, we want to understand the difference in the marginal probabilities $mp_W$ and $mp\'_W$, expressed by term $\text{diff} = mp_W - mp\'_W$.

Subtraction $-$ and equality $=$ are derived operations in Q. The methods we will develop in this paper allow us to conclude that the maximal value of $\text{diff}$ is in the closed interval $[0.134079500198, 0.134079508781]$, with $\text{diff}$ being $0.134079500198$ when

$$x = 0.299999999930, z = 0.149999999965, y = 0.020000000003$$

$$mp_W = 0.663714285678, mp\'_W = 0.529634782614$$

Similarly, we may infer that the minimum of $\text{diff}$ is in the closed interval $[-0.164272228181, -0.164272221575]$ with $\text{diff}$ being $-0.164272221575$ when

$$x = 0.100000000093, z = 0.050000000046, y = 0.059999999855$$

$$mp_W = 0.472086956699, mp\'_W = 0.636359183424$$

In particular, the absolute value of the difference of the marginal probability (2) in those constrained BNs is less than 0.1643, attained for the values just shown.

These union operators are symmetric in that $B_{X_1}^{C_1} \cup B_{X_2}^{C_2}$ and $B_{X_2}^{C_2} \cup B_{X_1}^{C_1}$ satisfy the same judgments $\models \text{must}$ and $\models \text{may}$ for all $\phi$ in Q. Idempotency won’t hold in general as unions may introduce a new set of constraints $C$. Associativity holds, assuming all compositions in (11) give rise to sound constrained BNs:

$$(B_{X_1}^{C_1} \cup B_{X_2}^{C_2}) \cup B_{X_3}^{C_3} \text{ is equivalent to } B_{X_1}^{C_1} \cup (B_{X_2}^{C_2} \cup B_{X_3}^{C_3})$$  (11)

Assumption 2 All composed, constrained BNs $B_{X_1}^{C_1} \cup B_{X_2}^{C_2}$ used in this paper are sound.
3.6 Non-Linear Optimization

We next relate the judgments $\models^{\text{may}}$ and $\models^{\text{must}}$ to optimization problems that seek to minimize or maximize values of terms $t$ of interest in a constrained BN $B^C_X$, and where $B^C_X$ itself may well be the result of a composition of constrained BNs as just described. We define the set of “concretizations” of term $t$ for $B^C_X$:

**Definition 11** Let $t$ be a term whose variables are all in $X$ for a constrained BN $B^C_X$. Then $\{ \| t \| \} \subseteq \mathbb{R}$ is defined as set $\{ \alpha(t) \mid B^C_X[\alpha] \in \| B^C_X \| \}$.

Note that $\{ \| t \| \}$ does depend on $C$ and $X$ as well, but this dependency will be clear from context. We can compute approximations of $\sup \{ \| t \| \}$ and $\inf \{ \| t \| \}$, assuming that these values are finite. To learn that $\sup \{ \| t \| \}$ is bounded above by a real high, we can check whether $B^C_X \models^{\text{must}} t \leqslant \text{high}$ holds. To learn whether $\sup \{ \| t \| \}$ is bounded below by a real low, we can check whether $B^C_X \models^{\text{may}} \text{low} \leqslant t$ holds. Gaining such knowledge involves both judgments $\models^{\text{must}}$ and $\models^{\text{may}}$. So we cannot compute approximations of $\sup \{ \| t \| \}$ directly in the existential fragment of $Q$ but search for approximations by repeatedly deciding such judgments.

We want to do this without making any assumptions about the implementation of a decision procedure for logic $Q$ or its existential fragment. This can be accommodated through the use of *extended binary search*, as seen in Figure 6, to derive an algorithm $\text{Sup}$ for computing a closed interval $[\text{low}, \text{high}]$ of length at most $\delta > 0$ such that $\sup \{ \| t \| \}$ is guaranteed to be in $[\text{low}, \text{high}]$. This algorithm has as input a constrained BN $B^C_X$ with $X$ as set of variables for constraint set $C$, a term $t$ in $\mathcal{T}[X]$, and a desired accuracy $\delta > 0$. This algorithm assumes that $B^X_C$ is consistent and that $0 < \sup \{ \| t \| \}/\infty$. We explain below how we can weaken those assumptions to $\sup \{ \| t \| \}/\infty$.

Algorithm $\text{Sup}$ first uses a satisfiability witness $\alpha$ to compute a real value $\alpha(t)$ that $t$ can attain for some $B^C_X[\alpha]$ in $\| B^C_X \|$ such that $\alpha(t) > 0$. It then stores this real value in a cache and increases the value of cache each time it can find a satisfiability witness that makes the value of $t$ at least twice that of the current cache value. Since $\sup \{ \| t \| \}/\infty$, this while loop terminates. The subsequent assignments to low and high establish an invariant that there is a value in $\{ \| t \| \}$ that is greater or equal to low, but that there is no value in $\{ \| t \| \}$ that is greater or equal to high.

The second while statement maintains this invariant but makes progress using bisection of the interval $[\text{low}, \text{high}]$. This is achieved by deciding whether there is a value in $\{ \| t \| \}$ that is greater or equal to the arithmetic mean of low and high. If so, that mean becomes the new value of low, otherwise that mean becomes the new value of high. By virtue of these invariants, the returned closed interval $[\text{low}, \text{high}]$ contains $\sup \{ \| t \| \}$ as desired. We capture this formally:

**Theorem 4** Let $B^C_X$ be a consistent constrained BN and $\delta > 0$. Let $0 < \sup \{ \| t \| \}/\infty$. Then we have:

1. Algorithm $\text{Sup}(t, \delta, B^C_X)$ terminates, $\sup \{ \| t \| \}$ is in the returned closed interval $[l, h]$ of length $\leqslant \delta$, and $B^C_X \models^{\text{may}} t \geqslant l$ is true.

2. Let $c$ be the initial value of cache. Then the algorithm makes at most $\lceil 2 \log_2(\sup \{ \| t \| \}) \rceil - \log_2(c) - \log_2(\delta) + 1$ satisfiability checks for formulas $\text{Ex}(B^C_X, t \geqslant r)$ or $\text{Ex}(B^C_X, t > r)$,
Sup$(t, \delta, B^C_X) \{ 
    \text{let } \alpha : X \rightarrow \mathbb{R} \text{ make } \text{Ex}(B^C_X, t > 0) \text{ true;}
    \text{cache} = \alpha(t); 
    \text{while (Ex}(B^C_X, t \geq 2 \times \text{cache}) \text{ satisfiable) \{ }
        \text{let } \alpha' : X \rightarrow \mathbb{R} \text{ make } \text{Ex}(B^C_X, t \geq 2 \times \text{cache}) \text{ true;}
        \text{cache} = \alpha'(t); 
    \} 
    \text{low} = \text{cache}; \text{ high} = 2 \times \text{cache}; 
    \text{assert ((Ex}(B^C_X, t \geq \text{low}) \text{ satisfiable) \&\& (Ex}(B^C_X, t \geq \text{high}) \text{ unsatisfiable))}; 
    \text{while (| high - low | > } \delta) \{ 
        \text{if (Ex}(B^C_X, t \geq \text{low + | high - low | / 2}) \text{ satisfiable) \{ }
            \text{low} = \text{low + | high - low | / 2}; 
            \text{assert ((Ex}(B^C_X, t \geq \text{low}) \text{ satisfiable) \&\& (Ex}(B^C_X, t \geq \text{high}) \text{ unsatisfiable))}; 
        \} 
        \text{else \{ }
            \text{high} = \text{low + | high - low | / 2}; 
            \text{assert ((Ex}(B^C_X, t \geq \text{low}) \text{ satisfiable) \&\& \text{Ex}(B^C_X, t \geq \text{high}) \text{ unsatisfiable))}; 
        \} 
    \} 
    \text{return [low, high];} 
\}

Figure 6: Algorithm for approximating sup \{| t |\} up to \delta > 0 for a consistent, constrained BN $B^C_X$ and term $t$ with variables in $X$ when $0 < \sup \{| t |\} < \infty$. The returned closed interval $[\text{low, high}]$ has length $\leq \delta$ and contains sup $\{| t |\}$. Key invariants are given as asserts

\[ \text{and these formulas only differ in the choice of comparison operator and in the value of real constant } r. \]

We now give an example of using algorithm Sup. Our specifications of optimization algorithms such as that of algorithm Sup in Figure 6 do not return witness information, we omitted such details for sake of simplicity.

Example 4 For constrained BN $B^C_{X_0}$ of Figure 2 Sup$(mp_W, \delta, B^C_{X_0})$ terminates for $\delta = 0.000000001$ with output $[0.663714282364, 0.663714291751]$. The value 0.663714282364 is attained when $x$ equals 0.299999999188.

An algorithm Inf$(t, \delta, B^C_X)$ is defined in Figure 7. It assumes that $B^C_X$ is consistent and that $\text{inf} \{| t |\}$ is a subset of $\mathbb{R}^+_0$ and contains a positive real – conditions we will weaken below. In that case, it terminates and returns a closed interval $[l, h]$ such that $\text{inf} \{| t |\}$ is in $[l, h]$. We prove this formally:

Theorem 5 Let $B^C_X$ be a consistent constrained BN and $\delta > 0$. Let $\{| t |\} \subseteq \mathbb{R}^+_0$ contain a positive real. Then we have:

1. Algorithm Inf$(t, \delta, B^C_X)$ terminates and $\text{inf} \{| t |\}$ is in the returned interval $[l, h]$ such that $h - l \leq \delta$ and $B^C_X|_{\text{may} =} t \leq h$ are true.
\[ \inf(t, \delta, B_X^C) \{ \\
  \text{let } \alpha : X \to \mathbb{R} \text{ make } \text{Ex}(B_X^C, t > 0) \text{ true}; \\
  \text{cache } = \alpha(t); \\
  \text{while } (\text{Ex}(B_X^C, t \leq 0.5 \cdot \text{cache}) \text{ satisfiable and } 0.5 \cdot \text{cache} > \delta) \{ \\
    \text{let } \alpha' : X \to \mathbb{R} \text{ make } \text{Ex}(B_X^C, t \leq 0.5 \cdot \text{cache}) \text{ true}; \\
    \text{cache } = \alpha'(t); \\
  \} \\
  \text{if } (\text{Ex}(B_X^C, t \leq 0.5 \cdot \text{cache}) \text{ satisfiable}) \{ \text{return } [0, 0.5 \cdot \text{cache}]; \} \\
  \text{low } = 0.5 \cdot \text{cache}; \text{ high } = \text{cache}; \\
  \text{assert } (\text{Ex}(B_X^C, t \leq \text{low}) \text{ unsatisfiable}) \& \& (\text{Ex}(B_X^C, t \leq \text{high}) \text{ satisfiable}); \\
  \text{while } (|\text{high} - \text{low}| > \delta) \{ \\
    \text{if } (\text{Ex}(B_X^C, t \leq \text{low} + |\text{high} - \text{low}|/2) \text{ satisfiable}) \{ \\
      \text{high } = \text{low} + |\text{high} - \text{low}|/2; \\
      \text{assert } ((\text{Ex}(B_X^C, t \leq \text{low}) \text{ unsatisfiable}) \& \& (\text{Ex}(B_X^C, t \leq \text{high}) \text{ satisfiable})); \\
    \} \text{ else } \{ \\
      \text{low } = \text{low} + |\text{high} - \text{low}|/2; \\
      \text{assert } ((\text{Ex}(B_X^C, t \leq \text{low}) \text{ unsatisfiable}) \& \& (\text{Ex}(B_X^C, t \leq \text{high}) \text{ satisfiable})); \\
    \} \\
  \} \\
  \text{return } [\text{low}, \text{high}]; \\
\}

Figure 7: Algorithm for approximating \( \inf \{ |t| \} \) up to \( \delta > 0 \) for a consistent, constrained BN \( B_X^C \) and term \( t \) in \( T[X] \) when \( \{ |t| \} \subseteq \mathbb{R}_0^+ \) contains a positive real.

2. Let \( c \) be the initial value of cache. Then the algorithm makes one satisfiability check \( \text{Ex}(B_X^C, t > 0) \) and at most \( |2 \cdot \log_2(c) - \log_2(\min(\delta, \inf \{ |t| \}))| \) satisfiability checks for formulas \( \text{Ex}(B_X^C, t \leq r) \), and these formulas only differ in the size of real constant \( r \).

We now show how we can relax the conditions of \( B_X^C \) being consistent and of \( 0 < \sup \{ |t| \} < \infty \) to \( \sup \{ |t| \} < \infty \). In Figure 8, we see this modified algorithm \( \text{Sup}^* \) which relies on both \( \text{Sup} \) and \( \text{Inf} \). It returns a closed interval with the same properties as that returned by \( \text{Sup} \) but where \( \sup \{ |t| \} \) only need be finite. We state the correctness of this algorithm formally:

**Theorem 6** Let \( B_X^C \) be a constrained BN, \( \delta > 0 \), and \( \sup \{ |t| \} < \infty \). Then \( \text{Sup}^*(t, \delta, B_X^C) \) terminates and its calls to \( \text{Sup} \) and \( \text{Inf} \) meet their preconditions. Moreover, it either correctly identifies that \( B_X^C \) is inconsistent, that \( 0 \) is the maximum of \( \{ |t| \} \) or it returns a closed interval \([l, h]\) such that \( \sup \{ |t| \} \) is in that interval, \( h - l \leq \delta \) is less than or equal to \( \delta \), and \( B_X^C \models \max t \geq l \) holds.

We conclude this section by leveraging \( \text{Sup}^* \) to an algorithm \( \text{Inf}^* \), seen in Figure 9. Algorithm \( \text{Inf}^* \) relaxes that \( \{ |t| \} \) contains a positive real and is a subset of \( \mathbb{R}_0^+ \) to a more general pre-condition \( \neg \infty < \inf \{ |t| \} \), and it has correct output for inconsistent, constrained BNs. We formalize this:
Sup*(t, δ, BCX) {
  if (Ex(BCX, t > 0) satisfiable) {
    return Sup(t, δ, BCX);
  }
  elseif (Ex(BCX, t = 0) satisfiable) {
    return 0 as maximum for t;
  }
  elseif (Ex(BCX, t < 0) satisfiable) {
    let [l, h] = Inf(−t, δ, BCX);
    return [−h, −l];
  }
  return BCX is inconsistent;
}

Figure 8: Algorithm Sup* uses algorithms Sup and Inf and terminates whenever sup {∥t∥} < ∞. It either recognizing that 0 is the maximum of {∥t∥}, returns a closed interval [l, h] with h − l ≤ δ such that sup {∥t∥} is in [l, h], or it detects that BCX is inconsistent

Inf*(t, δ, BCX) {
  let x = Sup*(−t, δ, BCX);
  if (x reports that BCX is inconsistent) { return BCX is inconsistent; }
  elseif (x reports 0 as maximum for −t) { return 0 as minimum for t; }
  elseif (x reports interval [l, h]) { return [−h, −l]; }
}

Figure 9: Algorithm Inf* uses algorithm Sup* and terminates whenever −∞ < inf {∥t∥}. It either recognizes that 0 is the minimum of {∥t∥}, returns a closed interval [l, h] with h − l ≤ δ such that inf {∥t∥} is in [l, h], or it detects that BCX is inconsistent
Theorem 7 Let $B_C^X$ be a constrained BN, $\delta > 0$, and $t$ a term with $-\infty < \inf \{|t|\}$. Then $\text{Inf}^*(t, \delta, B_C^X)$ terminates and either correctly identifies that $B_C^X$ is inconsistent, that $0$ is the minimum of $\{|t|\}$ or it returns a closed interval $[l, h]$ of length $\leq \delta$ such that $\inf \{|t|\}$ is in $[l, h]$ and $B_C^X \mid \text{may} t \leq h$ holds.

Let us revisit Example 3 to illustrate use of $\text{Sup}^*$.

Example 5 Let $\tilde{C}_0$ be $C_0 \cup \{0.1 \leq x \leq 0.2\}$. For constrained BN $B_{X_0}^{\tilde{C}_0} \cup B_{X_0}^{C_0}$, we maximise $\text{diff}$ using $\text{Sup}^*(\text{diff}, 0.000000001, B_{X_0}^{\tilde{C}_0} \cup B_{X_0}^{C_0})$, which returns the interval $[-0.055219501217, -0.0552194960809]$ arising from the third case of $\text{Sup}^*$ as both $\text{Ex}(B_C^X, t > 0)$ and $\text{Ex}(B_C^X, t = 0)$ are unsatisfiable, but formula $\text{Ex}(B_C^X, t < 0)$ is satisfiable. It shows that marginal $m_{p_W}$ is always smaller than marginal $m_{p'_W}$ in this constrained BN, in contrast to the situation of Example 3.

4 Detailed Case Study

We now apply and evaluate the foundations for constrained BNs on a case study in the context of arms control. Article VI of the Treaty on the Non-Proliferation of Nuclear Weapons (NPT) [1] states that each treaty party

“undertakes to pursue negotiations in good faith on effective measures relating to cessation of the nuclear arms race at an early date and to nuclear disarmament, and on a treaty on general and complete disarmament under strict and effective international control.”

One important aspect of meeting such treaty obligations may be the creation and execution of trustworthy inspection processes, for example to verify that a treaty-accountable item has been made inoperable. Designing such processes is challenging as it needs to guarantee sufficient mutual trust between the inspected and inspecting party in the presence of potentially conflicting interests. Without such trust, the parties might not agree to conduct such inspections.

The potential benefit of mathematical models for the design and evaluation of such inspection processes is apparent. Bayesian Networks can capture a form of trust – through an inherent bias of processing imperfect information – and different degrees of beliefs – expressed, e.g., in subjective probabilities. Bayesian Networks can also represent objective data accurately, and their graphical formalism may be understood by domain experts such as diplomats. These are good reasons for exploring Bayesian Networks for modeling and evaluating inspection processes. But Bayesian Networks do not seem to have means of building confidence in their adequacy and utility, especially in this domain in which prior data for learning both graph structure and probabilities at nodes in such a graph are hard to find. We now show how constrained BNs can be used to build such confidence in mathematical models of an inspection process.
Figure 10: Prototype of an information barrier (IB), photo taken from [3], that the inspecting nation might build. The IB would output either a green or red light to inspectors based on physical measurements made within the IB that verify the presence of nuclear material.

4.1 An Arms Control Inspection Process

Consider the situation of two fictitious nation states. The inspecting nation is tasked with identifying whether an item belonging to the host nation, available to inspect in a controlled inspection facility and declared by the host nation to be a nuclear weapon, is indeed a nuclear weapon. This situation is similar to a scenario that had been explored in the UK/Norway initiative in 2007 [3, 4].

Given the nations’ non-proliferation obligations and national security concerns, the design details of the inspected item must be protected: the inspecting nation will have no visual access to the item. Instead the nations agree that the to-be-inspected item contain Plutonium with the isotopic ratio 240Pu:239Pu below a certain threshold value, which they set at 0.1.

In order to draw conclusions about whether an item presented for inspection is a weapon, the inspecting nation uses an information barrier (IB) system comprising a HPGe detector and bespoke electronics with well-understood performance characteristics (see Figure 10, [3]) to conduct measurements on the item while the item is concealed in a box. The IB system displays a green light if it detects a gamma-ray spectrum indicative of the presence of Plutonium with the appropriate isotopic ratio; if it does not detect this spectrum for whatever reason, it shows a red light. No other information is provided, and weapon-design information is thus protected [4].

The inspecting nation believes that it may be possible for the host nation to spoof a radioactive signal – or in some way provide a surrogate – to fool the detector, or that the host nation may have just placed Plutonium with the appropriate isotopic ratio in the box rather than a weapon. These subjective assessments should be reflected in the mathematical model alongside the error rates of the IB system that reflect the reliability of that device.

In order to deter cheating, the inspecting nation is allowed to choose the IBs used in the verification from a pool of such devices provided by the host nation, and may choose one or two IBs to that end. From that same pool of devices, the inspecting nation may take some unused IBs away for authentication – activities designed to assess whether the host nation tampered with the IBs. But the inspecting nation must not inspect any used IBs, to prevent it from exploiting any residual information still present in such used IBs to its advantage.

This selection process of IBs is therefore designed to ensure that a nefarious host nation
is held at risk of detection should it decide to tamper with the IBs used in verification: it would run the risk of one or more tampered IBs being selected for authentication by the inspecting nation. Although such authentication cannot be assumed to be perfect – and this fact, too, should be modelled – the prospect of detection may deter such a host.

We model this inspection process through constrained BNs that are abstracted from a sole BN with DAG shown in Figure 11 and based on a design developed by the Arms Control Verification Research group at AWE. This DAG depicts different aspects of the verification procedure in four key areas:

- the selection of the IBs for inspection or authentication purposes,
- the workings of the IB in the inspection itself,
- authentication of (other) IBs, and
- the combination of these aspects to assess any possibility of cheating overall, be it through IB tampering, surrogate nuclear sources, and so forth.

The selection of the IBs starts with the IB pool size; a selection of IBs built by the host nation, from which there will be a Number of IBs picked for authentication and Number of IBs picked for use by the inspecting nation. Should a Number of tampered IBs exist, then the selection process (blind to such a tamper) follows a Hypergeometric distribution and will probabilistically determine whether such tampered IBs make it into use in the verification process, authentication process or neither. The choice of distribution reflects that IBs – once chosen for either verification or authentication – cannot be used for any other purpose.

The IBs picked for either authentication or verification help the inspecting nation to judge whether the item under inspection is a weapon. A weapon or a Surrogate Pu source determine physical nuclear properties about the Isotopic ratio of Plutonium elements. Our mathematical model captures a possible inspector judgment that a surrogate source would only be used if the host felt that it was extremely likely to pass the IBs verification tests. Therefore, any surrogate source would have isotopic properties at least as good as those of a real weapon.

We stress that the probabilities chosen for each isotopic ratio, conditioned on whether the item under test is or is not a weapon, are not derived from real-world weapons data, but instead reflect in broad terms that Plutonium with a higher isotopic ratio than the chosen threshold is less likely to be found in a nuclear weapon. A bespoke algorithm is used by the IB system on the collected gamma-ray spectrum to test whether both the Peaks are in the expected locations and the Peak aspect ratio are as expected. If all 5 peaks are present and the Ratio of 240/239 isotopes is acceptable, then one or both of the First IB result or Second IB result are reported, conditional on any tampering and depending on whether or not two IBs are used to test the same item.

A mathematical model cannot hope to reflect each potential tamper. Therefore, we model authentication as an assessment of the Inspector’s authentication capabilities: the better these are, the more likely the Tamper will be found, and this requires that at least one tampered IB exists and was selected for authentication. This is controlled by the parent nodes: the aforementioned Hypergeometric distribution, and a node Chance of picking a tampered IB for authentication.
Figure 11: A BN [7] which details aspects of an arms inspection process. Aspects of the 1-2 IB devices used for verification are modeled in blue and green nodes, respectively. The assessment of cheating and the operation of the inspection in other ways are shown in orange nodes, and authentication procedures are modeled in purple nodes. Mathematical or logical computations are represented in grey nodes.
The mathematical model is drawn together by the overarching question of “Is the Host cheating?” If so, we then determine a Cheating method, which reflects the understanding of the inspecting nation about the possible ways that the host nation could try to cheat, as outlined above, and the prior beliefs of the inspecting nation about the relative likelihood of the use of each method if the host nation were to be cheating.

Finally, we check whether a Portal monitor is used to stop transportation of radioactive material – which could be used as a surrogate source – in and out of the facility, although we do not model this aspect in greater detail.

The probabilities used in this BN stem from a variety of sources. Some are somewhat arbitrarily selected, as described above, and therefore need means of building confidence in their choice. Probabilities relating to the performance of the IB system are derived from experimental analysis of the UKNI IB [4, 3].

The size of the probability tables for nodes of the BN in Figure 11 range from small (a few or tens of entries), to medium (hundreds of entries) and larger ones (thousands of entries). Given that complexity, we refrain from specifying more details on these tables within the paper itself.

Our evaluation of the methods developed in Section 3 will abstract the BN described above (see Figure 11) into constrained BNs, and demonstrate that these abstractions can inform decision support given the sparsity or lack of prior data that informed its choices of probabilities.

**Assumption 3** For convenience, this case study will not explicitly list or show the constraints that define the meaning of marginals symbolically. These meanings are included in the open-access research code cited on page 34.

### 4.2 Impact of Cheating Method on Tamper Detection

We want to understand how the choice of cheating method can impact the probability of detecting a tamper. The uncertainty about what cheating method the host nation will adopt is modelled in a constrained BN $B^C_{X_1}$ that takes the BN from Figure 11 and replaces the probability table for its node Cheating Method as specified in Figure 12. We use variables $x$, $y$, and $u$ to denote, respectively, the probability of IB tamper only, Surrogate source tamper only, and both IB tamper and surrogate source tamper. The variable $mp_{tf}$ refers to the marginal probability $p(\text{Will tamper be found?} = \text{Yes})$.

We compute the interval $[l, h] = [0.197137598548, \ldots, 0.00000001]$ as output of the function call $\text{Sup}^* (mp_{tf}, 0.00000001)$ of $B^C_{X_1}$. The witness information for the existentially quantified variables $x$, $y$, and $u$ and $mp_{tf}$ pertains to value $l = 0.197137598548$:

\[
x = 0.000000010001153 \quad y = 0.00000010001153 \quad u = 0.99999979997693
\]

We compute the interval $[\tilde{l}, \tilde{h}] = [5.875158e-09, 1.1750316e-08]$ as output of function call $\text{Inf}^* (mp_{tf}, 0.00000001)$ of $B^C_{X_1}$ and we get

\[
x = 0.000000030265893 \quad y = 0.99999939468212 \quad u = 0.00000030265893
\]
Cheating Method

| Cheating Method                      | Is cheating | Is not cheating |
|--------------------------------------|-------------|-----------------|
| None                                 | 0           | 1               |
| IB tamper only                       | $x$         | 0               |
| Surrogate source only                | $y$         | 0               |
| IB tamper & surrogate source         | $u$         | 0               |

Figure 12: Probability table for node Cheating Method in constrained BN $B_{X_1}^{C_1}$ where $C_1$ contains $\{0 < x, y, u < 1.0, x + y + u = 1.0\}$, $X_x = \{x, y, u\}$, $X_{mp} = \{mpf\}$, $X_1 = X_x \cup X_{mp}$, and the BN graph and all other probability tables for $B_{X_1}^{C_1}$ are as for the BN in Figure 11.

We may combine this information, for example to bound the range of values that $mpf$ can possibly attain, as the interval

$$[\bar{l}, h] = [0.00000000587, 0.197137608314]$$

We therefore conclude that this marginal probability can only vary by less than 0.19714 in the given strict uncertainty of the model.

Let us now ask for what values of $x$ can $mpf$ be within 0.01 of the lower bound $l = 0.197137598548$ returned for $\text{Sup}^*$ above. To that end, we consider the constrained BN $B_{X_1}^{C_1}$ where $C_1' = C_1 \cup \{|mpf - 0.197137598548| \leq 0.01\}$ and compute lower and upper bounds for $x$ in this constrained BN:

$$[\bar{l}^x, h^x] = \text{Sup}^*(x, 0.00000001, B_{X_1}^{C_1'}) = [0.99999994824, 1.00000000196]$$

$$[\bar{l}^x, h^x] = \text{Inf}^*(x, 0.00000001, B_{X_1}^{C_1'}) = [7.4505805e--09, 1.4901161e--08]$$

From this we can learn that

$$\forall x : [(1.4901161e--08 \leq x \leq 0.99999994824) \land \bigwedge C_1] \rightarrow \ |mpf - 0.197137598548| \leq 0.01 \quad (12)$$

is logically valid: whenever $x$ is in that value range and all constraints in $C_1$ are satisfied (which is true for all concretizations of $B_{X_1}^{C_1}$), then the marginal $mpf$ is within 0.01 of the lower bound for its maximal value.

Repeating these optimizations above for variables $y$ and $u$, we determine similar formulas that are logically valid:

$$\forall y : [(1.209402e--08 \leq y \leq 0.0507259986533) \land \bigwedge C_1] \rightarrow \ |mpf - 0.197137598548| \leq 0.01$$

$$\forall u : [(1.4901161e--08 \leq u \leq 0.99999998164) \land \bigwedge C_1] \rightarrow \ |mpf - 0.197137598548| \leq 0.01$$

These results say that the marginal $mpf$ is insensitive to changes to $x$, which is able to vary across the whole range $(0.0, 1.0)$ without having much impact on the results; the
| Authentication Capabilities | Good | Medium | Poor |
|-----------------------------|------|--------|------|
|                            | 0.3333 | 0.6667 - x |

Figure 13: Probability table for node Authentication Capabilities in constrained BN $B_{X_2}^{C_2}$ that is like that BN in Figure 11 except that the symbolic probability table for node Authentication Capabilities is as above, $X_x = \{x\}$, $X_{mp} = \{mp_{tf_2}\}$, and $C_2$ contains $\{0 \leq x \leq 0.6667, x + 0.3333 + (0.6667 - x) = 1\}$. Variable $mp_{tf_2}$ denotes the marginal in (14). Constrained BN $B_{X_2}^{C_2}$ is a “copy” of $B_{X_2}^{C_2}$ that replaces all occurrences of $x$ with $y$ and has $X_{mp} = \{mp_{tf_2}\}$ where $mp_{tf_2}$ denotes the marginal in (15).

situation is very similar for variable $u$. For variable $y$, the range at which $mp_{tf}$ is not too sensitive on changes of $y$ is much smaller – just over 0.05. Overall, we conclude that the model remains in the area of highest probability for detecting tampering as long as $x$ or $u$ are large.

Our analysis shows that the “tamper” cheating method is the one for which there is the highest chance of detecting cheating. However, our results also highlight that unless both tamper and surrogate source, or tamper on its own are used, there are limited ways in which to detect cheating through these nodes. From this we learn that use of a portal monitor is advisable, as any increase in $y$ moves the marginal out of the region of highest probability of detecting cheating, and decreases the chance of cheating being detected otherwise. Related to this is that the range of $y$ gives potential insight into future work required on tamper detection for the inspecting nation. Despite contributing neither to an IB tamper nor detection, $y$ can vary by over 0.05 – over five times that of the movement away from the marginal $mp_{tf}$’s maximum point by only 0.01. This suggests there are other limiting factors to tamper detection, such as capability, that could be better reflected in a mathematical model.

4.3 Comparing two BN models

We now illustrate the benefits of composing two constrained BNs (see Section 3.5). Two constrained BNs, $B_{X_2}^{C_2}$ and $B_{X_2}^{C_2}$, are defined in Figure 13. Both have symbolic and equivalent probability tables for node Authentication Capabilities but consider different hard evidence for the probability of a tamper to be found. In $B_{X_2}^{C_2}$, there is 1 IB machine picked for authentication whereas in $B_{X_2}^{C_2}$ there are 5 IB machines picked to that end, resulting in the respective marginals

$$ p(\text{Will tamper be found?} = \text{Yes} \mid \text{Host cheating} = \text{Yes}, \text{Number of IBs picked for authentication} = 1) $$

$$ p(\text{Will tamper be found?} = \text{Yes} \mid \text{Host cheating} = \text{Yes}, \text{Number of IBs picked for authentication} = 5) $$

In both models, the probability for state “Good” is bounded by 0.6667 so that there is a “gradient” pivoting around Medium capabilities fixed at 0.3333.
Figure 14: The surface in blue shows the values of $\text{diff}$ in (15) for the sample points defined in (16). The plane $\text{diff} = 0$ is shown in red. Its intersection with the blue surface marks the boundary of where decision support would favor running 1 IB authentication (above the red plane) and 5 IB authentications (below the red plane). The linear equation defining this boundary line is $0 = -0.212884507399337 \cdot x + 0.354426098468987 \cdot y - 0.16515544651$.

We seek decision support on how much to prioritise research into IB authentication capabilities, each of $B_{X_2}^{C_2}$ and $B_{X_2}^{C'_{Y}}$ representing a different capability scenario. Of interest here is the change in the likelihood that a tamper will be found. We can simply model this by defining a new term

$$\text{diff} = mp_{y_2} - mp_{y_2'}$$  \hspace{1cm} (15)

Variable $\text{diff}$ is in $X_x$ for the constrained BN $B_{X_2}^{C_2} \subseteq B_{X_2}^{C'_{Y}}$ where the constraint set $C$ for this combination is $\{ \text{diff} = mp_{y_2} - mp_{y_2'} \}$. We compute the value of $\text{diff}$ for each combination of values $(x, y)$ from set

$$S = \{(0.0 + 0.01 \cdot a, 0.0 + 0.01 \cdot b) \mid 0 \leq a, b \leq 67\}$$  \hspace{1cm} (16)

and linearly interpolate the result as a surface seen in Figure 14. The linear relationship between the symbolic probabilities of node Authentication Capability to that of its child node Will the tamper be found? make this surface flat.

We can now use the method familiar from our earlier analyses to assess the value range of term $\text{diff}$ in this composed, constrained BN. The function call $\text{Sup}^*(\text{diff}, 0.00000001, B_{X_2}^{C_2} \subseteq B_{X_2}^{C'_{Y}})$ returns the interval

$$[l, h] = [0.0711404333363, 0.0711404338663]$$

Next, $\text{Inf}^*(\text{diff}, 0.00000001, B_{X_2}^{C_2} \subseteq B_{X_2}^{C'_{Y}})$ is computed as the interval

$$[\tilde{l}, \tilde{h}] = [-0.307085548061, -0.307085547533]$$

In particular, the values of $\text{diff}$ for all concretizations of $B_{X_2}^{C_2} \subseteq B_{X_2}^{C'_{Y}}$ lie in the interval

$$[-0.307085548061, 0.0711404338663]$$
The blue surface of $\text{diff}$ in Figure 14 is mostly negative (below the red plane). This shows that the case of testing 5 IBs for tampers is nearly always better, irrespective of the confidence one may have in one’s ability to find a tamper. This is true, other than for the most extreme cases when there is the least confidence in authentication capabilities when testing five IBs (for $y = 0$) and most confidence when testing one (for $x = 0.667$).

Let us next explore a situation in which the inspector believes to have high authentication capabilities, regardless of whether 1 or 5 IBs are picked for authentication. We can easily model this by setting $C'_1 = C \cup \{0.467 \leq x, y \leq 0.667\}$ and refining the composed model using $C''$. We compute the output of $\text{Sup}^*(\text{diff, } 0.00000001, B^C_{X_2} \cup B^C_{X_2'})$ to be the interval

$$[l, h] = [-0.0282766319763, -0.0282766314489]$$

and $\text{Inf}^*(\text{diff, } 0.00000001, B^C_{X_2} \cup B^C_{X_2'})$ to be the interval

$$[\tilde{l}, \tilde{h}] = [-0.141568560141, -0.141568559299]$$

Now $\text{diff}$ is in $[-0.141568560141, -0.0282766314489]$ and the largest absolute difference between picking 1 and 5 IBs for authentication is greater than 0.14, witnessed when the inspector has a particularly high capability in authenticating 5 IBs, (when $y = 0.667$ and $mp_{2} = 0.24932$) compared with only inspecting one IB with more moderate capability (when $x = 0.467$, $mp_{2} = 0.10696$).

A decision maker could vary the use of the above approach in order to weigh the cost of IB production against the cost of developing and employing more advanced authentication capabilities. He or she could also query in detail how the results of such cost-benefit analyses might change as new information is learned or new techniques deployed. This capability might help decision makers to balance their priorities and to gain the best assurance possible within a cost budget that the verification regime they implement is effective.

### 4.4 Determining equivalent decision support

We assess the consistency of two different constrained BNs of equal intent of decision support. Constrained BNs $B^C_{X_3}$ and $B^C_{X_3'}$ are identical to $B^C_{X_1}$ and its symbolic probability table for node Cheating Method as in Figure 12 except that $th$ is an additional variable used to model decision support. Variable set $X_{mp}$ also changes. For $B^C_{X_3}$ we have $X_{mp} = \{mp_{f3}\}$ and for $B^C_{X_3'}$ we set $X_{mp} = \{mp_{f3}\}$ instead. Variable $mp_{f3}$ denotes marginal probabilities for hard evidence that Initial Pool Size = 10 IBs in (17), whereas variable $mp_{f3}$ denotes a marginal for hard evidence Initial Pool Size = 20 IBs in (18):

$$p(\text{Will tamper be found?} = \text{Yes} | \text{Initial Pool Size} = 10) \quad (17)$$

$$p(\text{Will tamper be found?} = \text{Yes} | \text{Initial Pool Size} = 20) \quad (18)$$

These are marginal probabilities that the nation which is authenticating IBs will find a tamper. A decision – for example that an IB has been tampered with – may then be supported if such a marginal is above a certain threshold $th$. We now want to understand whether the
two constrained BNs would support decisions in the same manner, and for what values or value ranges of \( th \).

For any value \( th \), consider the constraint \( \varphi_{th} \) in \( Q \) given by

\[
-\left[ \left( (th < m_{p_{f_3}}) \wedge (m_{p_{f_3}} \leq th) \right) \vee \left( (th < m_{p_{f_3}'} \wedge (m_{p_{f_3}'} \leq th) \right) \right]
\]

We can now analyze whether both constrained BNs will always support decisions through threshold \( th \) by evaluating

\[
B_{X_3}^{C_3} \cup B_{X_3}^{C_3'} \models_{\text{must}} \varphi_{th}
\]

where \( C \) equals \( \{0 < th < 1\} \). By Theorem 1, judgment (19) is equivalent to

\[
\text{not } B_{X_3}^{C_3} \cup B_{X_3}^{C_3'} \models_{\text{max}} \left( (th < m_{p_{f_3}}) \wedge (m_{p_{f_3}} \leq th) \right) \vee \left( (th < m_{p_{f_3}'} \wedge (m_{p_{f_3}'} \leq th) \right)
\]

Setting \( \varphi_1 \equiv (th < m_{p_{f_3}}) \wedge (m_{p_{f_3}} \leq th) \) and \( \varphi_2 \equiv (th < m_{p_{f_3}'} \wedge (m_{p_{f_3}'} \leq th) \), the same theorem tells us that (20) is equivalent to

\[
[\text{not } B_{X_3}^{C_3} \cup B_{X_3}^{C_3'} \models_{\text{max}} \varphi_1] \text{ and } [\text{not } B_{X_3}^{C_3} \cup B_{X_3}^{C_3'} \models_{\text{max}} \varphi_2]
\]

Using our tool, we determine that \( \text{Ex}(B_{X_3}^{C_3} \cup B_{X_3}^{C_3'}, \varphi_1) \) is unsatisfiable and so – by appeal to Theorem 3 – the first proof obligation of (21) holds. Similarly, we evaluate the satisfiability of \( \text{Ex}(B_{X_3}^{C_3} \cup B_{X_3}^{C_3'}, \varphi_2) \). Our tool reports this to be satisfiable and so the two constrained BNs do not always support the same decision. We now want to utilize our non-linear optimization method to compute ranges of the \( th \) itself for which both models render the same decision. Understanding such a range will be useful to a modeller as both models are then discovered to be in agreement for all values of \( th \) in such a range.

Since \( \text{Ex}(B_{X_3}^{C_3} \cup B_{X_3}^{C_3'}, \varphi_1) \) is unsatisfiable, we use \( C' = \{0 < th < 1, \varphi_2\} \) which forces truth of \( \varphi_2 \), and compute \( \text{Sup}^*(th, 0.00000001, B_{X_3}^{C_3} \cup B_{X_3}^{C_3'}) \) to maximise expression \( th \). This obtains the interval

\[
[l, h] = [0.259147588164, 0.259147588909]
\]

Computing \( \text{Inf}^*(th, 0.00000001, B_{X_3}^{C_3} \cup B_{X_3}^{C_3'}) \) outputs the interval

\[
[\tilde{l}, \tilde{h}] = [-9.31322e-10, -4.65661e-10]
\]

For the given accuracy \( \delta \), the interval \( [\tilde{l}, \tilde{h}] \) may be interpreted as 0. Thus, we can say that for all \( th \) in \( [0, 0.259147588909] \) the use of either \( B_{X_3}^{C_3} \) or \( B_{X_3}^{C_3'} \) could support different decisions. More importantly, we now know that both constrained BNs always support the same decision as described above when the value of the threshold \( th \) for decision making is greater or equal to 0.2592, say.

The range of \( th \) for which both models can support different decisions may seem rather large and it may be surprising that it goes down to zero. But this is a function of the chance and capability of finding a tamper in an IB. Intuitively, the models tend to disagree most in situations where the chance of cheating by tampering is highest, when \( x = 1 \), and thus where
Cheating Method

| Cheating Method                  | Is cheating | Is not cheating |
|----------------------------------|-------------|-----------------|
| None                             | 0           | 1               |
| IB tamper only                   | x           | 0               |
| Surrogate source only            | 0.6666 - x  | 0               |
| IB tamper & surrogate source     | 0.3334      | 0               |

Figure 15: Probability table for node Cheating Method in constrained BN $B_{X_4}^{C_4}$ where $C_4$ contains $\{0 < x < 0.6666, 0 + x + (0.6666 - x) + 0.3334 = 1.0\}$, $X_x = \{x\}$, $X_{mp} = \{mpf\}$, $X_4 = X_x \cup X_{mp}$, and where the BN graph is that of Figure 11. All other symbolic probability tables for $B_{X_4}^{C_4}$ are as for the BN in Figure 11.

authenticating the IB has benefit. Our approach gave a decision maker safe knowledge that any threshold for decision making outside the range $[-9.31322e-10, 0.259147588909]$ would statistically agree and lead to the same decision regarding finding tampers, irrespective of the initial number of IBs – either 10 or 20 – in the pool. Dependent on the nations involved, and the tolerances for decision making they are willing to set, it could be decided – for instance – that building only 10 IBs per inspection would be enshrined in the treaty to avoid unnecessary expense and so forth. This would undoubtedly be an important data-driven decision for diplomats and negotiators to make.

4.5 Symbolic sensitivity analysis

It is well known that BNs may be sensitive to small changes in probability values in tables of some nodes. Sensitivity analyses have therefore been devised as a means for assessing the degree of such sensitivities and the impact this may have on decision support. See, e.g., the sensitivity value defined in [32, 31].

We now leverage such analyses to our approach by computing such sensitivity measures symbolically as terms of the logic $Q$. Then we may analyze such terms using the methods Sup* and Inf* as before to understand how such sensitivity measures may vary across concretizations of a constrained BN. We illustrate this capability for constrained BN $B_{X_4}^{C_4}$, which is similar to $B_{X_1}^{C_1}$ but has probability table for node Cheating Method as shown in Figure 15.

The sensitivity value describes the change in the posterior output of the hypothesis for small variations in the likelihood of the evidence under study. The larger the sensitivity value, the less robust the posterior output of the hypothesis. In other words, a likelihood value with a large sensitivity value is prone to generate an inaccurate posterior output. If the sensitivity value is less than 1, then a small change in the likelihood value has a minimal effect on the result of the posterior output of the hypothesis.

A modeller may be uncertain about the sensitivity of event Will tamper be found? = Yes to the authentication of IBs if probabilities in node Authentication Capability of the IB were to change. Our tool can compute such a sensitivity value $s$ symbolically for the sensitivity of event Will tamper be found? = Yes to small perturbations in probabilities of node Authentication Capability.
The sensitivity value \( s \) is defined in this instance as

\[
s = \frac{PO \cdot (1 - POx) \cdot Px}{(PO \cdot PxO + (1 - POx) \cdot Px)^2}
\]  

(22)

where terms \( PO, Px, POx \) and \( PxO \) are defined as

\[
PO \equiv p(\text{Authentication Capability} = \text{Low})
\]

\[
Px \equiv p(\text{Finding a tamper in IB} = \text{Yes})
\]

\[
POx \equiv p(\text{Authentication Capability} = \text{Low} | \text{Finding a tamper in IB} = \text{Yes})
\]

\[
PxO \equiv p(\text{Finding a tamper in IB} = \text{Yes} | \text{Authentication Capability} = \text{Low})
\]

All three marginals of \( \text{Authentication Capability} \) are considered using just two functions \( POx \) and \( 1 - POx \). In (23), \( PO \) is a modelling choice that combines the states of Medium and High into one state \( 1 - POx \). Term \( 1 - POx \) accounts for situations in which an inspector is relatively good at authentication, with \( POx \) representing situations in which they are less capable. Other modelling choices would lead to a marginally small difference in \( s \).

Our tool can compute an explicit function of \( s \) in variable \( x \), as defined in (22). This symbolic expression for \( s \) is depicted in Figure 16 and shown as a function of \( x \) in Figure 17. This confirms that as the value of \( x \) increases, and thus the probability of “IB tamper only” seen in Figure 15 decreases, the marginal of interest for \( \text{Will tamper be found?} = \text{Yes} \) becomes less sensitive to changes in the probabilities of the node \( \text{Authentication Capability} \) of IB.

We can now determine the worst-case sensitivity value by computing the interval returned by function call \( \text{Sup}^*(t_s, 0.00000001, B_{X_4}^{C_1}) \) as \([3.5838265468, 3.5838265475]\) where \( t_s \) is the term in the righthand side of the equation in Figure 16 that describes \( s \) as a function of \( x \). Thus we learn that this sensitivity cannot be larger than 3.5838265475 for all concretizations of constrained BN \( B_{X_4}^{C_1} \). As is evident from the graph, there are no valid values of \( x \) where the sensitivity value drops below 1.0 – the aforementioned bound at which a sensitivity score, and therefore its corresponding marginal probability, is deemed to be robust.

The output \([1.17313380051, 1.17313380116]\) of \( \text{Inf}^*(s, 0.00000001, B_{X_4}^{C_1}) \) confirms this, and shows that \( s \) is always above 1.17313380051 for all concretizations of constrained BN \( B_{X_4}^{C_1} \). Knowing this may indicate to a decision-maker that potential deviations in the real domain from the model of node \( \text{Authentication Capability} \) will require close attention, irrespective of the value of \( x \) and thus of the perceived marginal probabilities of the states of node \( \text{Cheating Method} \).
5 Implementation and Evaluation

5.1 Software Engineering

The numerical results reported in previous sections were computed by a prototype implementation of the approach developed in this paper. This implementation uses Python to capture a data model for Bayesian Networks and constraints, to formulate marginals of interest, and to interface with the SMT solver Z3 [23]. The latter we use as a decision procedure for logic \( \mathcal{Q} \) that also returns witness information for all variables. The computation of symbolic meaning of marginals relies on the Junction Tree Algorithm and is achieved through software from an open-source Python package provided in [5].

Python also supports a lightweight and open-source library for symbolic computation, sympy [34], which we can employ to run the Junction Tree Algorithm in [5] fully symbolically. The generated symbolic expressions are then simplified using a method of sympy before they are put into constraints such as in (3) and added to the SMT solver for analysis.

5.2 Validation and Evaluation

Some symbolic marginals that we generated for analyses but not reported in our case study were too large to be handled by the SMT solver we used: the string representation of the symbolic meaning was about 25 Megabytes. We performed linear regression on those symbolic expressions and then validated that this approximation has higher precision than the accuracy \( \delta \), before defining the meaning of marginal variables as these regressed expressions. Our open-access research data, discussed on page 34, contains details on these analyses.

We evaluated the performance of the symbolic interpretation of the JTA as implemented in
on randomly generated constrained BNs. This does not evaluate our approach per se, but the manner in which we interpreted an existing inference implementation symbolically. We refer to our open-access data repository for more details on model generation: key parameters are the number of nodes $|N|$, the number of variables $|X_x|$, and a random choice of the number of states for each node (between 1 and 10 uniformly at random). Terms in probability tables have form $c, x$ or $1-x$ for constants $c$ or $x$ in $X_x$. In generated models, a random node was picked to determine hard evidence – its first state having probability 1. The JTA was run for that hard evidence, and the time to complete it was recorded. These automated test suites ran on an institutional server with 64 Intel Xeon E5/Core i7 processors, on Ubuntu 14.04.

Many of these tests terminated very quickly. Though, as the number of nodes per graph and the number of states per node increased, the running times increased on some but not all tests. The size of $X_x$ seemed to have a limited effect, possibly indicating that the additional overhead of our approach to running the JTA implementation of [5] symbolically in Python is not huge.

Figure 18 shows plots for the computation times (in seconds) of 1000 such test cases against the number of nodes, the size of $X_x$, the number of node states in total (a summation over all nodes) and the average length over all nodes of the outputted marginal text string in characters.

For this randomized test suite, there was a small trend for the running times to increase with the size of the DAG. But computations were still quicker for many of the BNs of larger size compared to smaller ones. The size of $X_x$ appears to have little impact on computation time, nor any strong correlation to the length of the computed symbolic marginal. This suggests that use of symbolic probabilities may not in and of itself increase such empirical complexity.

6 Discussion

Our approach advocates the use of constrained Bayesian Networks as a means of gaining confidence into Bayesian Network modelling and inference in the face of little or no data. A modeler may thus start with a BN, turn it into several constrained BNs and subject them to analysis, and perhaps modify the BN based on such findings. Witness information computed in analyses could, in principle, be fed back into a BN modeling tool so that users can see a concrete BN that would, for example, explain how a marginal of interest can attain a certain value in a constrained BN.

The ability to represent witness information as a concrete BN is also a means of testing whether the computation of symbolic meaning of marginals is free of errors. We have indeed conducted such tests to gain confidence into the correctness of our tool and the packages that it depends upon. Note also that errors in the symbolic meaning of marginals are likely to create numerical inconsistencies, so our analyses would detect such an inconsistent, constrained BN.

The algorithms that we devised for non-linear optimization made no assumptions about the internal workings of the decision procedure used and its witness information apart from that such results would be semantically correct. Knowledge of such internal details could,
Figure 18: Plots for the time the symbolic Junction Tree Algorithm takes to run (in seconds, on the $y$-axis) against properties of various randomly generated BNs, on the $x$-axis. We assess (from left-to-right, top-to-bottom) the effect on the computation time by the number of nodes, the number of variables in $X_x$, the number of states (a summation of the number of states in each of the nodes) and the average length of the text string in the resulting marginal computation. In this last graph, we embed the closeup of the datapoint in the larger graph.
however, be exploited to speed up computation. For example, such a method is used in
the SMT solver Z3 to optimize linear objective functions. One could therefore run different
methods in parallel or even let them share information in between search iterations.

Our tool prototype interprets the JTA implementation provided in [5] symbolically, and
symbolic meanings of marginal variables may contain divisions. Of course, we could translate
away all division operators without changing meaning – to match this with the formal setting
of Section 3. We did not do this since our foundations apply equally to $\mathcal{Q}$ extended with
division, such translations would increase the size of these terms, and the SMT solver we
used, Z3, was able to process and reason with such or suitably simplified terms.

7 Related Work

In [21], it is shown how probabilistic inference in Bayesian Networks can be represented
through the evaluation and formal differentiation of a “network polynomial”. The size of the
polynomial can be reduced by its representation in an arithmetic circuit, in which evaluation
and differentiation are more efficient. It would be of interest to determine whether this work
can be extended to make the computation of symbolic marginals generated in our approach
more efficient.

For Bayesian Networks there are methods for learning the structure of a DAG and for
learning the probabilities within nodes of such a graph (see e.g. [29, 19]) – based on existing
empirical data. We assumed in this paper that little or no data are available, ruling out the
effective use of such learning methods. But our approach is consistent with settings in which
plenty of data are available.

Bayesian Networks have tool support such as the software JavaBayes [2], which is able
to perform robustness analysis. But this software can neither cope with the Knightian un-
certainty of our approach, nor fuse networks of different structures together with non-trivial
constraints.

Our work in [8] reported early attempts of developing the approach presented in this
paper: in [8], a much simpler Bayesian Network of a nuclear inspection process is presented
and some analyses with preliminary versions of our tool are discussed; but that work offered
neither formal foundations nor greater technical details for the methods it used. The more
detailed Bayesian Network we studied in Section 4 was discussed in [7], along with a non-
technical summary of our general approach and some of its analysis findings.

Credal networks – see e.g. [16] – refer to the theory and practice of associating a convex
set of probability measures with directed, acyclic graphs. Credal networks are also referred
to as the Theory of Imprecise Probabilities [39] or as the Quasi-Bayesian Theory [25].

The generalization of probability measures to sets of such measures can accommodate a
formal notion of probabilistic independence, rooted in axioms of preferences as developed in
[16]. The approach is based on constraints for such convex sets of probability measures. In-
fERENCE algorithms and their approximations are bespoke for an interpretation of constraints;
an interpretation is called an “extension” in [16].

To compare this to our approach, we follow Good’s black box model in that our semantics
and optimizations reflect Bayesian inference – even though this is done symbolically. Another
difference is that a constrained Bayesian Network may have nodes with non-convex sets of
probability measures as meaning, for example when logical constraints on variables rule out certain points in intervals. Our approach is also more practical in outlook, since we rely on reductions to known and tried techniques, such as satisfiability checking for the existential theory of the reals. In contrast, theoretical results for Credal Networks range from different evidence propagation and inference methods (see e.g. [17][20]) to deep relationships to logic programming and its semantics [18].

In [11], a methodology is developed for assessing sensitivity of lower and upper probabilities in Credal networks. It is shown that for some classes of parameters in Bayesian networks one may replace the Credal sets of probability measures associated with such parameters with a sole such measure. It would be of interest to determine whether these or similar results are attainable for suitable classes of constrained Bayesian Networks.

Constraint Networks [24] are graphical representations that are meant to guide solution strategies for constraint satisfaction problems. In our tool prototype, we decoupled the choice of graph structure for a constrained Bayesian Network from the use of strategies for solving satisfiability problems over the existential theory of the reals. It may be beneficial to couple graph structure and satisfiability checking in tool support of our approach that relies on constraint satisfaction solvers.

8 Conclusions

This work was motivated by the fact that some problem domains have little or no data that one could use to learn the structure of a causal network or the probabilities for nodes within that structure – whatever the reasons for such sparsity of data may be in such a domain. This led us to consider suitable generalizations of Bayesian Networks. Ideally, we wanted a formalism that those who already use Bayesian Networks for modeling and analysis would find easy to adopt. In particular, we sought to preserve – as much as possible – the manner in which probabilistic inference is done in Bayesian Networks. Crucially, we wanted a set of methods whose use could help us to build sufficient confidence into the quality, suitability or robustness of models expressed in such a formalisms in the face of little or no empirical data.

We propose constrained Bayesian Networks as such a formalism. The derivation of that concept is a contribution in and of itself, and it used first-order logic and its semantics as well as syntactic criteria for wellformedness. But it also required methods from three-valued logic to define a precise yet intuitive semantics for a constrained BN.

We also developed meta-properties of this semantics, including checks for the consistency of a constrained Bayesian Network. These properties were needed to prove the correctness of our optimization algorithms, which can compute suprema or infima of bounded arithmetic terms up to a specific accuracy. These optimization algorithms are non-standard in that they rely on a decision procedure for the theory of reals and in that the optimization problems are generally non-linear and non-convex.

The marginals in a constrained Bayesian Network are computed symbolically, but computed in the same manner as the marginals for a Bayesian Network – a concretization of that constrained Bayesian Network. This is appealing as it allows reuse of known and trusted methods such as the Junction Tree Algorithm. But it also creates a potential computational bottleneck with scope for future work that may extend an approach in [21] to our setting.
We implemented our approach in a tool prototype, which benefitted from the significant advances in symbolic computation and in the implementation of theorem provers such as SMT solvers. We evaluated this prototype through stress tests and a non-trivial case study in the domain of nuclear arms control. The latter is a domain in which the availability of data is very limited and where any means of building confidence into the trustworthiness of mathematical models are expected to have positive impact on arms reduction efforts.

We used this case study to illustrate some pertinent types of analyses of a constrained Bayesian Network that our approach can accommodate: a range analysis that computes infima and suprema for a term of interest to determine their robustness, the comparison of two or more constrained Bayesian Networks to assess modeling impact, the ability to determine ranges of threshold values that would render equivalent decision support, and the symbolic computation of a sensitivity measure for a given node – with the ability to optimize this to understand worst-case sensitivities. We trust that the approach presented in this paper will be useful for other applications in the arms-control domain, as well as in other domains – particularly those with a lack of data.

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Open Access: The Python and SMT code for the queries and models of this paper and raw SMT analysis results are found in the public data repository

bitbucket.org/pjbeaumont/beaumonthuthcbns/

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A Mathematical Proofs

Proof of Theorem 1

1. We have that $B^C_X \models \text{must } \phi$ holds iff for all concretizations $B^C_X[\alpha]$ of $B^C_X$ we have that $\alpha \models \phi$ holds iff for all concretizations $B^C_X[\alpha]$ of $B^C_X$ we have that $\alpha \models \neg \phi$ does not hold iff $B^C_X \models \text{may } \neg \phi$ does not hold.

2. We have that $B^C_X \models \text{may } \phi$ holds iff there is some concretization $B^C_X[\alpha]$ of $B^C_X$ such that $\alpha \models \phi$ holds iff there is some concretization $B^C_X[\alpha]$ of $B^C_X$ such that $\alpha \models \neg \phi$ does not hold iff $B^C_X \models \text{must } \neg \phi$ does not hold.

3. (a) Let $B^C_X \models \text{must } \phi_1 \land \phi_2$ hold. Let $B^C_X[\alpha]$ be a concretization of $B^C_X$. Then we know that $\alpha \models \phi_1 \land \phi_2$ holds. This implies that $\alpha \models \phi_i$ holds for $i = 1, 2$. But then both $B^C_X \models \text{must } \phi_1$ and $B^C_X \models \text{must } \phi_2$ hold since $B^C_X[\alpha]$ was an arbitrary concretization of $B^C_X$. 

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(b) Let both \( B^C_X \models \text{must } \phi_1 \) and \( B^C_X \models \text{must } \phi_2 \) hold. Let \( B^C_X[\alpha] \) be a concretization of \( B^C_X \). Then \( B^C_X \models \text{must } \phi_1 \) implies that \( \alpha \models \phi_i \) holds for \( i = 1, 2 \). Therefore, we get that \( \alpha \models \phi_1 \land \phi_2 \) holds as well. Since \( B^C_X[\alpha] \) was an arbitrary concretization of \( B^C_X \), this gives us that \( B^C_X \models \text{must } \phi_1 \land \phi_2 \) holds.

4. (a) Let \( B^C_X \models \text{may } \phi_1 \lor \phi_2 \) hold. Then there is some concretization \( B^C_X[\alpha] \) of \( B^C_X \) such that \( \alpha \models \phi_1 \lor \phi_2 \) holds. This implies that \( \alpha \models \phi_i \) holds for some \( i = 1, 2 \). But then \( B^C_X \models \text{may } \phi_i \) holds as claimed.

(b) Let one of \( B^C_X \models \text{may } \phi_1 \) and \( B^C_X \models \text{may } \phi_2 \) hold, say \( B^C_X \models \text{may } \phi_i \). Then there is some concretization \( B^C_X[\alpha] \) of \( B^C_X \) such that \( \alpha \models \phi_i \) holds. This implies that \( \alpha \models \phi_1 \lor \phi_2 \) holds as well. Since \( B^C_X[\alpha] \) is a concretization of \( B^C_X \), we get that \( B^C_X \models \text{may } \phi_1 \lor \phi_2 \) holds.

\[ \square \]

Proof of Theorem 2

- **Item 1 implies item 2.** Let \( B^C_X \models \text{may true} \) hold. By definition of \( \models \text{may} \), there then is some concretization \( B^C_X[\alpha] \) of \( B^C_X \) such that \( \alpha \models \text{true} \) holds. Therefore the set of concretizations of \( B^C_X \) is non-empty and so \( B^C_X \) is consistent.

- **Item 2 implies item 3.** Let \( B^C_X \) be consistent. Suppose that \( \phi \) is in \( Q \) such that \( B^C_X \models \text{must } \phi \) holds. Since \( B^C_X \) is consistent, there is some concretization \( B^C_X[\alpha] \) of \( B^C_X \) such that \( \alpha \models \text{must } \phi \) holds. Since \( B^C_X \models \text{must } \phi \) holds, we get that \( \alpha \models \phi \) holds. But then we have \( B^C_X \models \text{may } \phi \) by definition of \( \models \text{may} \).

- **Item 3 implies item 4.** Let \( B^C_X \models \text{must } \phi \) imply \( B^C_X \models \text{may } \phi \) for all \( \phi \) in \( Q \). Let \( \psi \) be in \( Q \). We claim that \( B^C_X \models \text{may } \psi \lor \neg \psi \) holds. By Theorem 4, it suffices to show that \( B^C_X \models \text{may } \psi \) or \( B^C_X \models \text{may } \neg \psi \) holds. If the former holds, we are done. Otherwise, we have that \( B^C_X \models \text{may } \psi \) does not hold. By Theorem 2, this implies that \( B^C_X \models \text{must } \neg \psi \) holds.

- Next, we show that \( B^C_X \) has to be consistent: note that \( B^C_X \models \text{must true} \) holds by the definitions of \( \models \text{must} \) and \( \models \). Therefore, we get that \( B^C_X \models \text{may true} \) holds by item 3 – and we already showed that this implies that \( B^C_X \) is consistent.

Let \( B^C_X[\alpha] \) be a concretization of \( B^C_X \), which exists as \( B^C_X \) is consistent. Since we showed \( B^C_X \models \text{must } \neg \phi \), the latter implies that \( \alpha \models \neg \phi \). But then \( B^C_X \models \text{may } \neg \phi \) follows given the definition of \( \models \text{may} \).

- **Item 4 implies item 5.** Let \( B^C_X \models \text{may } \phi \lor \neg \phi \) hold for all \( \phi \) in \( Q \). Let \( \psi \) be in \( Q \). Then we have that \( B^C_X \models \text{may } \psi \lor \neg \psi \) holds, and we need to show that \( B^C_X \models \text{must } \psi \land \neg \psi \) does not hold. Proof by contradiction: assume that \( B^C_X \models \text{must } \psi \land \neg \psi \) holds. Since \( B^C_X \models \text{may } \psi \lor \neg \psi \) holds, we know that there is some concretization \( B^C_X[\alpha] \) of \( B^C_X \) such that \( \alpha \models \psi \land \neg \psi \) holds. Since \( B^C_X \models \text{must } \psi \land \neg \psi \) holds, we know that \( B^C_X \models \text{must } \psi \) and \( B^C_X \models \text{must } \neg \psi \) hold by Theorem 3. We do a case analysis on the truth of judgment \( \alpha \models \psi \lor \neg \psi \):

- Let \( \alpha \models \psi \). Since \( B^C_X \models \text{must } \neg \psi \) holds, this implies that \( \alpha \models \neg \psi \) holds. This contradicts that \( \alpha \models \psi \) holds.
Proof of Theorem 3

1. Constraints $\varphi'$ in $C$ and $\varphi$ are quantifier-free formulas of $Q$ with variables contained in $X$, which equals $\{x_1, x_2, \ldots, x_n\}$. Therefore, the formula in (8) is in $Q$, and contains only existential quantifiers and all in front of the formula.

2. We prove this claim by structural induction over $\varphi$:
   
   - Let $\varphi$ be true. Then $\text{Ex}(B^C_X, \text{true})$ equals $\exists x_1: \ldots: \exists x_n: \text{true} \land \bigwedge_{\varphi' \in C} \varphi'$ and this is satisfiable iff there is an assignment $\alpha$ such that $\alpha \models \bigwedge_{\varphi' \in C} \varphi'$ and $\alpha \models \text{true}$ both hold (the latter holding by definition) iff there is a concretization $B^C_X[\alpha]$ of $B^C_X$ if $B^C_X$ is consistent iff (by Theorem 1.2) $B^C_X \models \text{maytrue}$ holds.
   
   - Let $\varphi$ be $t_1 \leq t_2$. Then $\text{Ex}(B^C_X, t_1 \leq t_2)$ equals $\exists x_1: \ldots: \exists x_n: (t_1 \leq t_2) \land \bigwedge_{\varphi' \in C} \varphi'$ and this is satisfiable iff there is an assignment $\alpha$ such that $\alpha \models \bigwedge_{\varphi' \in C} \varphi'$ and $\alpha \models t_1 \leq t_2$ both hold iff there is a concretization $B^C_X[\alpha]$ of $B^C_X$ such that $\alpha \models t_1 \leq t_2$ holds iff $B^C_X \models \text{mayt}_1 \leq t_2$ holds.
   
   - Let $\varphi$ be $t_1 < t_2$. Then $\text{Ex}(B^C_X, t_1 < t_2)$ equals $\exists x_1: \ldots: \exists x_n: (t_1 < t_2) \land \bigwedge_{\varphi' \in C} \varphi'$ and this is satisfiable iff there is an assignment $\alpha$ such that $\alpha \models \bigwedge_{\varphi' \in C} \varphi'$ and $\alpha \models t_1 < t_2$ both hold iff there is a concretization $B^C_X[\alpha]$ of $B^C_X$ such that $\alpha \models t_1 < t_2$ holds iff $B^C_X \models \text{mayt}_1 < t_2$ holds.
   
   - Let $\varphi$ be $\neg \psi$. Then $\text{Ex}(B^C_X, \neg \psi)$ equals $\exists x_1: \ldots: \exists x_n: \neg \psi \land \bigwedge_{\varphi' \in C} \varphi'$ and this is satisfiable iff there is an assignment $\alpha$ such that $\alpha \models \bigwedge_{\varphi' \in C} \varphi'$ and $\alpha \models \neg \psi$ both hold iff there is a concretization $B^C_X[\alpha]$ of $B^C_X$ such that $\alpha \models \neg \psi$ holds iff $B^C_X \models \text{may} \neg \psi$ holds.
   
   - Let $\varphi$ be $\varphi_1 \land \varphi_2$. Then $\text{Ex}(B^C_X, \varphi_1 \land \varphi_2)$ equals $\exists x_1: \ldots: \exists x_n: \varphi_1 \land \varphi_2 \land \bigwedge_{\varphi' \in C} \varphi'$ and this is satisfiable iff there is an assignment $\alpha$ such that $\alpha \models \bigwedge_{\varphi' \in C} \varphi'$ and $\alpha \models \varphi_1 \land \varphi_2$ both hold iff there is a concretization $B^C_X[\alpha]$ of $B^C_X$ such that $\alpha \models \varphi_1 \land \varphi_2$ holds iff $B^C_X \models \text{may} \varphi_1 \land \varphi_2$ holds.

3. By the previous item, we may decide $B^C_X \models \text{may} \varphi$ by deciding whether formula $\text{Ex}(B^C_X, \varphi)$ is satisfiable. By item 1 above, that formula is in the existential fragment of $Q$. By [13], deciding the satisfiability (truth) of such formulas is in PSPACE in the size of such formulas.
4. By Theorem 1, we have that $B_X^C \models \text{must} \varphi$ holds iff $B_X^C \models \text{may} \neg \varphi$ does not hold. By item 2 above, the latter is equivalent to $\text{Ex}(B_X^C, \neg \varphi)$ not being satisfiable. By 14, this can be decided in PSPACE in the size of formula $\text{Ex}(B_X^C, \neg \varphi)$.

Proof of Theorem 4: The arguments below make use of Theorems 1 and 3 without explicit reference to them. Note that consistency of $B_X^C$ and $0 < \sup \{| t |\}$ guarantee that the first let statement in Sup can find such a $\alpha$. In particular, we see that $0 < cache$ becomes an invariant and so $\text{cache} < 2 \cdot \text{cache}$ is another invariant.

First, we show that the asserts hold prior to the execution of the second while loop. Note that cache is always assigned real of form $\eta(t)$ for some concretization $B_X^C[\eta]$ of $B_X^C$. So when low is initialized with the last updated value of cache, then $B_X^C \models \text{may} t \leq low$ clearly holds after the first assignment to low (witnessed by the assignment that gave rise to the last value of cache) and prior to its reassignment. By definition of the initial value of high, we have that $B_X^C \models \text{may} t \geq high$ does not hold after that initial assignment and prior to the reassignment of high. Therefore, both asserts in front of the second while loop hold, and we get that $low \leq high$ is an invariant.

Second, we show that each iteration of the second while loop preserves the asserts. This is clear as the Boolean guard of the if statement tests for preservation of these asserts, and makes the correct, invariant-preserving assignment accordingly.

Third, let $[l, h]$ be the returned closed interval. It is clear that $h - l \leq \delta$ holds as required. We argue that $\sup \{| t |\}$ is in $[l, h]$. Since the asserts hold for $l$ and $h$, we know that $B_X^C \models \text{may} t \geq l$ holds, but $B_X^C \models \text{may} t \geq h$ does not hold. Let $c$ be in $\{| t |\}$. Then there is some $\alpha$ with $c = \alpha(t)$. Since $B_X^C \models \text{may} t \geq h$ does not hold, we get that $\alpha(t) < \alpha(h) = h$. Therefore, $h$ is an upper bound of $\{| t |\}$ which implies $\sup \{| t |\} \leq h$. Since $B_X^C \models \text{may} t \geq l$ holds, we have some concretization $B_X^C[\alpha']$ with $\alpha' \models t \geq l$. This means $\alpha'(t) \geq l$. But $\sup \{| t |\} \geq \alpha'(t)$ as the latter is an element of $\{| t |\}$. Thus, $l \leq \sup \{| t |\}$ follows.

2. Let $s$ be $\sup \{| t |\}$. For the first while loop, we have at least $k$ iterations if $s \geq 2^k \cdot c$, i.e. if $s \cdot c^{-1} \geq k$, i.e. if $k \leq \log_2(s) - \log_2(c)$. So the real number $\log_2(s) - \log_2(c)$ is an upper bound on the number of iterations of the first while loop.

To get an upper bound for the number of iterations of the second while loop, we know that high is of form $2^{l+1} \cdot c$ and so low equals $2^l \cdot c$. But then high – low equals $2^l \cdot c$. Since this is monotone in $l$, we may use the upper bound for the number of iterations of the first while loop as an upper bound of $l$, to get $2^{\log_2(s) - \log_2(c)} \cdot c = s \cdot c^{-1} \cdot c = s$ as an upper bound on the value of $| high - low |$ before the Boolean guard of the second while is first evaluated. This allows us to derive an upper bound on the number of iterations of the second while loop, since the larger that value is, the more iterations take place. Based on the bisection in each iteration, there are at least $k$ iterations if $s \cdot 2^{-k} > \delta$, i.e. if $k < \log_2(s) - \log_2(\delta)$. Therefore, the total number of iterations of both while loops combined is $(\log_2(s) - \log_2(c)) + (\log_2(s) - \log_2(\delta))$. The claim now follows given that each iteration makes exactly one satisfiability check and since there is an initial satisfiability check as well.
Proof of Theorem 5:

1. The argument is similar to the one for Theorem 4 but there are important differences. Note that cache > 0 is also here an invariant, guaranteed by the fact that \(|t|\) contains a positive real. We know that \((0.5^n \cdot \text{cache})_{n \in \mathbb{N}}\) converges to 0 for any positive constant cache. Since \(0 < \delta\) and since \(\alpha'(t) \leq 0.5 \cdot \text{cache}\) for the \(\alpha'(t)\) assigned to cache, there is some \(n_0\) such that \(0.5^{n_0} \cdot \text{cache} \leq \delta\). This proves that the first while statement terminates.

(a) Suppose that the return statement in the line after the first while loop is executed. Then \(\text{Ex}(B_X^C, t \leq 0.5 \cdot \text{cache})\) is satisfiable and so there is some concretization \(B_X^C[\alpha]\) such that \(\alpha(t) \leq 0.5 \cdot \text{cache}\). But then \(\inf \{|t|\} \leq 0.5 \cdot \text{cache}\) as well. From \(\{|t|\} \subseteq \mathbb{R}_0^+\), we get \(0 \leq \inf \{|t|\}\). Therefore, \(\inf \{|t|\}\) is in the returned interval \([0, 0.5 \cdot \text{cache}]\) and \(B_X^C[\text{may}t] \leq 0.5 \cdot \text{cache}\) is true. Moreover, the length of the interval is \(0.5 \cdot \text{cache}\), which must be less than or equal to \(\delta\) as the first while loop just terminated and the first conjunct of its Boolean guard is true – forcing \(0.5 \cdot \text{cache} > \delta\) to be false.

(b) Otherwise, \(\text{Ex}(B_X^C, t \leq 0.5 \cdot \text{cache})\) is not satisfiable but the formula \(\text{Ex}(B_X^C, t \leq \text{cache})\) is satisfiable. From that, it should then be clear that the asserts in front of the second while statement hold when they are reached. That each iteration of the second while statement maintains these two asserts is reasoned similarly as for Sup.

So we have that \(B_X^C[\text{may}t] \leq h\) and \(B_X^C[\text{must}t] > l\) are invariants. This means that \(l\) is a lower bound of \(|t|\) and \(\alpha(t) \leq h\) for some \(\alpha(t)\) in \(\{|t|\}\). But then \(l \leq \inf \{|t|\} \leq \alpha(t) \leq h\) shows that \(\inf \{|t|\}\) is in \([l, h]\).

2. Let \(i = \inf \{|t|\}\). We derive an upper bound on the number of iterations for the first while loop. Because we are interested in upper bounds, we may assume that the \(\alpha'(t)\) assigned to cache equals \(0.5 \cdot \text{cache}\) for the current value of cache. We then have at least \(k\) iterations if \(\delta < c \cdot 2^{-k}\) and \(i < c \cdot 2^{-k}\). Since we are interested in upper bounds on that number of iterations, we get at least \(k\) iterations if both \(\delta < c \cdot 2^{-k}\) and \(i < c \cdot 2^{-k}\) hold, i.e. if \(\min(\delta, i) < c \cdot 2^{-k}\). But this is equivalent to \(k \leq \log_2(c) - \log_2(\min(i, \delta))\).

We now derive an upper bound on the number of iterations of the second while loop. The initial value of high – low equals cache–0.5-cache = 0.5-cache for the current value of cache when entering that loop. The value of cache is monotonically decreasing during program execution and so \(c/2\) is an upper bound of high – low. We may therefore use \(c/2\) as initial value of high – low since this can only increase the number of iterations, for which we seek an upper bound. There are now at least \(k\) iterations if \((c/2) \cdot 2^{-k} > \delta\) which is equivalent to \(k < \log_2(c) - 1 - \log_2(\delta)\).

The total number of iterations for both while loops is therefore \((\log_2(c) - \log_2(\min(i, \delta))) + (\log_2(c) - 1 - \log_2(\delta)) = 2 \cdot \log_2(c) - \log_2(\min(i, \delta)) - 1\). From this the claim follows since each iteration has exactly one satisfiability check of the stated form, and there is one more satisfiability check between the first and second while loop.
Proof of Theorem 6

1. We do a case analysis:

(a) If algorithm $\text{Sup}$ is called, then consistency of $B_X^C$ and $0 < \sup \{|t|\}$ follow from the Boolean guard that triggered the call. Since $\sup \{|t|\} < \infty$ is assumed, we get $0 < \sup \{|t|\} < \infty$ and so $\text{Sup}$ terminates by Theorem 4.

(b) If 0 is returned as a maximum, the algorithm clearly terminates and no preconditions are needed.

(c) If $\text{Inf}$ is called, we have to show that $\{|t|\}$ is a subset of $\mathbb{R}^+$ that contains a positive real. Since the first two return statements were not reached, we know that $B_X^C$ is consistent and $\{|t|\}$ is a subset of $\mathbb{R}^-$. But then $\{|-t|\}$ is a subset of $\mathbb{R}^+$.

2. If the algorithm reports that 0 is the maximum for $t$, then we know that $\{|t|\}$ cannot contain a positive real (first if-statement), and that it contains 0 (second if-statement). Clearly, this means that 0 is the supremum of $\{|t|\}$ and so also its maximum as 0 is in $\{|t|\}$.

3. Let $\text{Sup}^*(t, \delta, B_X^C)$ return an interval $[-h, -l]$. Then $[l, h]$ is the interval returned by a call to $\text{Inf}(-t, \delta, B_X^C)$. By the first item and Theorem 5, we get that $B_X^C \models \text{may } -t \leq h$ holds, $\inf \{|-t|\}$ is in $[l, h]$, and $h - l \leq \delta$. Therefore, we conclude that $B_X^C \models \text{may } -h$ holds as claimed. Moreover, since $\inf \{|-t|\}$ equals $\sup \{|t|\}$, this implies that $\sup \{|t|\}$ is in the closed interval $[-h, -l]$, whose length is that of $[l, h]$ and so $\leq \delta$.

4. If the algorithm returns saying that $B_X^C$ is inconsistent, then all three formulas $\text{Ex}(B_X^C, t > 0)$, $\text{Ex}(B_X^C, t = 0)$, and $\text{Ex}(B_X^C, t < 0)$ are unsatisfiable. But then we know that the three judgments $B_X^C \models \text{may } t > 0$, $B_X^C \models \text{may } t = 0$, and $B_X^C \models \text{may } t < 0$ do not hold, by Theorem 3. This means that $B_X^C$ is inconsistent: for all concretization $B_X^C[\alpha]$ we have that $\alpha \models (t > 0) \lor (t = 0) \lor (t < 0)$ holds as that query is a tautology over the theory of reals; and then Theorem 3.4 yields a contradiction to $B_X^C$ being consistent.

Proof of Theorem 7. The correctness of the first two claims in that theorem (inconsistency and minimum) follow from the corresponding items of Theorem 6. The general identity $\inf \{x_i \mid i \in I\} = -\sup \{-x_i \mid i \in I\}$ shows that $-\infty < \inf \{x_i \mid i \in I\}$ iff $-\sup \{-x_i \mid i \in I\} < \infty$ and so preconditions are also met. Finally, to see the correctness of $\text{Inf}^*$ when interval $[l, h]$ is returned, note that this means that interval $[-h, -l]$ is returned for the call $\text{Sup}^*(-t, \delta, B_X^C)$ and so $B_X^C \models \text{may } -t \geq -h$ holds by Theorem 6. But this implies that $B_X^C \models \text{may } t \leq h$ holds as claimed.

B Quantitative Information about the BN of Figure 11

Table 1 shows quantitative information about the size and complexity of the BN in Figure 11.
Table 1: The probability tables for the BN in Figure 11 are too large to be specified explicitly in the paper. Here we want to convey the structural and resulting computational complexity of this BN in tabular form. For each node shown in the leftmost column we list its number of parents (\# Parents) in the BN graph, its number of input combinations (\# Rows) which is $\max(1, \prod_{i=1}^{k} n_i)$ where $n_i$ is the number of outputs any of the $0 \leq k$ parents $i$ can have, whereas in \# Columns we list the number of output values that node itself can have. Rightmost column Table Size depicts the size of the support of the probability distribution of that node.

| Node name                                         | # Parents | # Rows | # Columns | Table Size |
|---------------------------------------------------|-----------|--------|-----------|------------|
| Number of IBs picked for use in treaty             | 0         | 1      | 2         | 2          |
| Is a portal monitor used?                         | 0         | 1      | 2         | 2          |
| Is the host cheating?                             | 0         | 1      | 2         | 2          |
| Inspector authentication capabilities             | 0         | 1      | 3         | 3          |
| Is item under test a weapon?                      | 1         | 2      | 2         | 4          |
| Number of IBs picked for authentication            | 0         | 1      | 5         | 5          |
| Cheating method                                   | 1         | 2      | 4         | 8          |
| Initial IB pool size                              | 0         | 1      | 11        | 11         |
| Are 5 peaks present?                             | 2         | 6      | 2         | 12         |
| Are the peaks in the expected locations?          | 2         | 6      | 2         | 12         |
| Are the peak aspect ratios as expected?           | 2         | 6      | 2         | 12         |
| Will tamper be found?                             | 2         | 6      | 2         | 12         |
| Surrogate Pu source deployment successful?        | 2         | 8      | 3         | 24         |
| Which IB has been tampered with?                  | 2         | 6      | 4         | 24         |
| Isotopic ratio judged acceptable by IB 1?          | 1         | 14     | 2         | 28         |
| Isotopic ratio judged acceptable by IB 2?          | 1         | 14     | 2         | 28         |
| Chance of picking a tampered IB for authentication| 1         | 21     | 2         | 42         |
| Number of tampered IBs picked for use             | 1         | 20     | 3         | 60         |
| Isotopic ratio of the item under test             | 2         | 6      | 14        | 84         |
| First IB result                                   | 5         | 64     | 2         | 128        |
| Second IB result                                  | 6         | 128    | 3         | 384        |
| IB Pool after authentication                      | 2         | 55     | 15        | 825        |
| Number of IBs host has tampered                   | 2         | 44     | 21        | 924        |
| Number of tampered IBs after authentication        | 2         | 441    | 21        | 9261       |
| Hypergeometric distribution                       | 3         | 630    | 20        | 12600      |
| Hypergeometric distribution (2)                   | 3         | 1355   | 21        | 24255      |

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