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## Most Probable Explanations in Bayesian Networks: complexity and tractability

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#### Abstract

An overview is given of definitions and complexity results of a number of variants of the problem of probabilistic inference of the most probable explanation of a set of hypotheses given observed phenomena.

## 1 Introduction

Bayesian or probabilistic inference of the most probable explanation of a set of hypotheses given observed phenomena lies at the core of many problems in diverse fields. For example, in a decision support system that facilitates medical diagnostics (like the systems described in [1], [2], [3], or [4]) one wants to find the most likely diagnosis given clinical observations and test results. In a weather forecasting system as in [5] or [6] one aims to predict precipitation based on meteorological evidence. But the problem is often also key in the computational models of economic processes [7, 8, 9], sociology [10], and cognitive tasks as vision or goal inference [11, 12]. Although these tasks may superficially appear different, the underlying computational problem is the same: given a probabilistic network, describing a set of stochastic variables and the (in)dependencies between them, and observations (or evidence) of the values for some of these variables, what is the most probable joint value assignment to (a subset of) the other variables?

Since probabilistic (graphical) models have made their entrance in domains like cognitive science (see e.g. the editorial of the special issue on probabilistic models of cognition in the *TRENDS in Cognitive Sciences* journal [13]), this problem now becomes more and more interesting for other investigators than those traditionally involved in probabilistic reasoning. However, the problem comes in many variants (e.g., with either full or partial evidence) and has many names (e.g., MPE, MPA, and MAP which may or may not refer to the same problem variant) that may obscure the novice reader in the field. Apart from the naming conventions, even the question *how an explanation should be defined* depends on the author (compare e.g. the approaches in [14], [15], [16], and [17]). Furthermore, some computational complexity results may be counter-intuitive at first sight.

For example, finding the best (i.e., most probable) explanation is NP-hard and thus intractable in general, but so is finding a *good enough* explanation for any reasonable formalization of 'good enough'. So the argument that is is sometimes found in the literature (e.g. in [13]) and that can be paraphrased as "Bayesian abduction is NP-hard, but we'll assume that the mind approximates these results, so we're fine" is fundamentally flawed. However, when constraints are imposed on the structure of the network or on the probability distribution, the problem may become tractable. In order words: the optimization criterion is not a *source of complexity* [18] of the problem, but the network structure *is*, in the sense that unconstrained structures lead to intractable models in general, while imposing constraints to the structure sometimes leads to tractable models.

With this paper we intend to provide the computational modeler, who describes phenomena in cognitive science, economics, sociology, or elsewhere, an overview of complexity and tractability results in this problem, in order to assist her in identifying sources of complexity. An example of such an approach can be found in [19]. Here the Bayesian Inverse Planning model for goal inference [11] was examined and the conditions under which the model becomes intractable, respectively remains tractable were identified, allowing the modelers to investigate the (psychological) plausibility of these conditions.

While good introductions to explanation problems in Bayesian networks exist (see, e.g., [20] for an overview of explanation methods and algorithms), these papers appear to be aimed at the user-focused knowledge engineer, rather than at the computational modeler, and thus pay less attention to complexity issues. In this paper, we aim to bridge that gap, and focus on *tractability issues* in explanation problems, i.e., we address the question under which circumstances problem variants are tractable or intractable. We present definitions and complexity results related to Bayesian inference of the most probable explanation, including some new or previously unpublished results. The paper starts with some needed preliminaries from probabilistic networks, graph theory, and computational complexity theory. In the following sections the computational complexity of a number of problem variants is discussed. The final section concludes the paper and summarizes the results.

## 2 Preliminaries

In this section, we give a concise overview of a number of concepts from probabilistic networks, graph theory, and complexity theory, in particular definitions of probabilistic networks and treewidth, some background on complexity classes defined by probabilistic Turing Machines and oracles, and fixedparameter tractability. For a more thorough discussion of these concepts, the reader is referred to textbooks like [15], [21], [22], [23], [24], [25], and [26].

#### 2.1 Bayesian Networks

A probabilistic network  $\mathcal{B}$  is a graphical structure that models a set of stochastic variables, the (in-) dependencies among these variables, and a joint probability distribution over these variables.  $\mathcal{B}$  includes a directed acyclic graph  $\mathbf{G} = (\mathbf{V}, \mathbf{A})$ , modeling the variables and (in-) dependencies in the network, and a set of parameter probabilities  $\Gamma$  in the form of conditional probability tables (CPTs), capturing the strengths of the relationships between the variables. The network models a joint probability distribution  $\Pr(\mathbf{V}) = \prod_{i=1}^{n} \Pr(v_i | \pi(V_i))$  over its variables, where  $\pi(V)$  denotes the parents of V in  $\mathbf{G}$ . We will use upper case letters to denote individual nodes in the network, upper case bold letters to denote sets of nodes, lower case letters to denote value assignments to nodes, and lower case bold letters to denote joint value assignments to sets of nodes. We will use  $\mathbf{E}$  to denote a set of evidence nodes, i.e., a set of nodes for which a particular joint value assignment is observed.

Throughout this chapter, we will refer to the *Brain tumor* network, shown in Figure 1, as a running example. This network, adapted from Cooper [27], captures some fictitious and incomplete medical knowledge related to metastatic cancer.. The presence of metastatic cancer (modeled by the node MC) typically induces the development of a brain tumor (*B*), and an increased level of serum calcium (*ISC*). The latter can also be caused by Paget's disease (*PD*). A brain tumor is likely to increase the severity of headaches (*H*). Long-term memory (*M*) is probably impaired, or even malfunctioning. Furthermore, it is likely that a CT-scan (*CT*) of the head will reveal a tumor if it is present, but it may also reveal other anomalies like a fracture or a lesion, which might explain an increased serum calcium.

Every (posterior) probability of interest in Bayesian networks can be computed using well known lemmas in probability theory, like Bayes' theorem  $(\Pr(H \mid E) = \frac{\Pr(E|H)\Pr(H)}{\Pr(E)})$ , marginalization  $(\Pr(H) = \sum_{g_i} \Pr(H \land G = g_i))$ , and the property that  $\Pr(\mathbf{V}) = \prod_{i=1}^{n} \Pr(v_i \mid \pi(V_i))$ . For example, from the definition of the Brain Tumor network we can compute that  $\Pr(b \mid M = \operatorname{imp} \land CT =$ fract) = 0.04 and that  $\Pr(mc \land \neg pd \mid M = \operatorname{norm} \land H = \operatorname{abs}) = 0.16$ .

An important structural property of a probabilistic network is its *treewidth*. Treewidth is a graph-theoretical concept, which can be loosely described as a measure on the *locality* of the dependencies in the network. Formally, the treewidth of a probabilistic network, denoted by  $tw(\mathcal{B})$ , is defined as the minimal width over all tree-decompositions of the moralization of **G**. The moralization  $\mathbf{M}_{\mathbf{G}}$  of a directed graph **G** is the undirected graph, obtained by iteratively connecting the parents of all variables and then dropping the arc directions. The moral graph of the *Brain Tumor* network is shown in Figure 2.

A tree-decomposition of an undirected graph is defined as follows [22]:

**Definition 2.1 (tree-decomposition).** A tree-decomposition of an undirected graph  $\mathbf{G} = (\mathbf{V}, \mathbf{E})$  is a pair  $\langle T, \mathcal{X} \rangle$ , where T = (I, F) is a tree and  $\mathcal{X} = \{\mathbf{X}_i \mid i \}$ 



ISC	$\Pr(mc)$ $\Pr(pd)$	= 0.20 = 0.10
	$\Pr(b \mid mc) \ \Pr(b \mid mc)$	= 0.20 = 0.05
CT)	$\begin{aligned} &\Pr(M = \operatorname{norm}   b) \\ &\Pr(M = \operatorname{imp}   b) \\ &\Pr(M = \operatorname{malf}   b) \\ &\Pr(M = \operatorname{norm}   \overline{b}) \\ &\Pr(M = \operatorname{imp}   \overline{b}) \\ &\Pr(M = \operatorname{malf}   \overline{b}) \end{aligned}$	$= 0.50 \\= 0.40 \\= 0.10 \\= 0.70 \\= 0.25 \\= 0.05$
	$\begin{aligned} &\Pr(H = \operatorname{sev} b) \\ &\Pr(H = \operatorname{mod} b) \\ &\Pr(H = \operatorname{abs} b) \\ &\Pr(H = \operatorname{sev} \overline{b}) \\ &\Pr(H = \operatorname{mod} \overline{b}) \\ &\Pr(H = \operatorname{abs} \overline{b}) \end{aligned}$	$= 0.70 \\= 0.25 \\= 0.05 \\= 0.30 \\= 0.20 \\= 0.50$
$\Pr(isc \mid mc, pd)$ $\Pr(isc \mid mc, pd)$ $\Pr(isc \mid \overline{mc}, pd)$ $\Pr(isc \mid \overline{mc}, pd)$	= 0.95 = 0.80 = 0.70 = 0.20	
$\begin{aligned} &\Pr(CT = \operatorname{tum}   b, isc \\ &\Pr(CT = \operatorname{tum}   b, isc \\ &\Pr(CT = \operatorname{tum}   \overline{b}, isc \\ &\Pr(CT = \operatorname{tum}   \overline{b}, isc \\ &\Pr(CT = \operatorname{tum}   \overline{b}, isc \\ & \end{aligned}$	$ \begin{array}{l} &= 0.80 \\ &= 0.90 \\ &= 0.05 \\ &= 0.10 \end{array} $	
$\begin{array}{l} \Pr(CT = \operatorname{fract} \mid b, isc \\ \end{array} \end{array}$	$\begin{array}{l} (2) &= 0.18 \\ (3) &= 0.01 \\ (2) &= 0.55 \\ (3) &= 0.40 \end{array}$	
$\begin{aligned} &\Pr(CT = \operatorname{les} b, isc) \\ &\Pr(CT = \operatorname{les} b, isc) \\ &\Pr(CT = \operatorname{les} b, isc) \\ &\Pr(CT = \operatorname{les} b, isc) \end{aligned}$	$= 0.02 \\= 0.09 \\= 0.40 \\= 0.50$	

Figure 1: The Brain tumor network



Figure 2: The moral graph obtained from the Brain Tumor network



Figure 3: A tree-decomposition of the moralization of the Brain Tumor network

 $i \in I$  is a family of subsets (called bags) of V, one for each node of T, such that

- $\bigcup_{i \in I} \mathbf{X}_i = \mathbf{V}$ ,
- for every edge  $(V, W) \in \mathbf{E}$  there exists an  $i \in I$  with  $V \in \mathbf{X_i}$  and  $W \in \mathbf{X_i}$ , and
- for every  $i, j, k \in I$ : if j is on the path from i to k in T, then  $\mathbf{X}_{i} \cap \mathbf{X}_{k} \subseteq \mathbf{X}_{i}$ .

The width of a tree-decomposition  $\langle (I, F), \{ \mathbf{X_i} \mid i \in I \} \rangle$  is  $\max_{i \in I} \mid \mathbf{X_i} \mid -1$ .

Treewidth is defined such that a tree (an undirected graph without cycles) has treewidth 1. A polytree (a directed acyclic graph that has no undirected cycles as well) with at most k parents per node has treewidth k. A tree-decomposition of the moralization of the *Brain Tumor* network is shown in Figure 3. The width of this tree-decomposition is 2, since this decomposition has at most 3 variables in each bag.

#### 2.2 Computational Complexity

In the remainder, we assume that the reader is familiar with basic concepts of computational complexity theory, such as Turing Machines, the complexity classes P and NP, and NP-completeness proofs. For more background we refer to classical textbooks like [24] and [25]. In addition to these basic concepts, to describe the complexity of various problems we will use the *probabilistic* class PP, oracles, and fixed-parameter tractability.

The class PP contains languages L accepted in polynomial time by a *Prob*abilistic Turing Machine. Such a machine augments the more traditional nondeterministic Turing Machine with a probability distribution associated with each state transition, e.g. by providing the machine with a tape, randomly filled with symbols [28]. If all choice points are binary and the probability of each transition is  $\frac{1}{2}$ , then the *majority* of the computation paths accept a string s if and only if  $s \in L$ . This majority, however, is not fixed and may depend on the input, e.g., a problem in PP may accept 'yes'-instances with size n with probability  $\frac{1}{2} + \frac{1}{2^n}$ . This makes problems in PP intractable in general, in contrast to the related complexity class BPP which is associated with problems which allow for efficient randomized computation. BPP, however, accepts 'yes'-inputs with a bounded majority (say  $\frac{3}{4}$ ). This means we can amplify the probability of a correct answer arbitrary close to one by running the algorithm a polynomial amount of times and taking a majority vote on the outcome. This approach failes for unbounded majorities as  $\frac{1}{2} + \frac{1}{2^n}$  as allowed by the class PP: here an exponential number of simulations (with respect to the input size) is needed to meet a constant treshold on the probability.

The canonical PP-complete problem is MAJSAT: given a Boolean formula  $\phi$ , does the majority of the truth instantiations satisfy  $\phi$ ? Indeed it is easily shown that MAJSAT encodes SATISFIABILITY: take a formula  $\phi$  with n variables and construct  $\psi = \phi \lor x_{n+1}$ . Now, the majority of truth assignments satisfy  $\psi$  if and only if  $\phi$  is satisfiable, thus NP  $\subseteq$  PP. In the field of probabilistic networks, the problem of determining whether the probability  $\Pr(\mathbf{X} = \mathbf{x}) \ge q$  (known as the INFERENCE problem) is PP-complete.

A Turing Machine  $\mathcal{M}$  has oracle access to languages in the class A, denoted as  $\mathcal{M}^{A}$ , if it can "query the oracle" in one state transition, i.e., in  $\mathcal{O}(1)$ . We can regard the oracle as a 'black box' that can answer membership queries in constant time. For example, NP<sup>PP</sup> is defined as the class of languages which are decidable in polynomial time on a non-deterministic Turing Machine with access to an oracle deciding problems in PP. Informally, computational problems related to probabilistic networks that are in NP<sup>PP</sup> typically combine some sort of selecting with probabilistic inference. The canonical NP<sup>PP</sup>-complete satisfiability variant is E-MAJSAT: given a formula  $\phi$  with variable sets  $X_1 \dots X_k$  and  $X_{k+1} \dots X_n$ , is there an instantiation to  $X_1 \dots X_k$  such that the majority of the instantiations to  $X_{k+1} \dots X_n$  satisfy  $\phi$ ? Likewise, P<sup>NP</sup> and P<sup>PP</sup> denote classes of languages decidable in polynomial time on a deterministic Turing Machine with access to an oracle for problems in NP and PP, respectively. The canonical satisfiability variants for P<sup>NP</sup> and P<sup>PP</sup> are LEXSAT and MIDSAT (given  $\phi$ , what is the lexicographically first, respectively middle, satisfying truth assignment). These classes are associated with finding optimal solutions or enumerating solutions.

In complexity theory, we are often interested in *decision problems*, i.e., problems for which the answer is *yes* or *no*. Well-known complexity classes like P and NP are defined for decision problems and are formalized using Turing Machines. In this paper we will also encounter *function problems*, i.e., problems for which the answer is a function of the input. For example, the problem of determining whether a solution to a 3SAT instance exists, is in NP; the problem of actually *finding* such a solution is in the corresponding function class FNP. Function classes are defined using Turing Transducers, i.e., machines that not only halt in an accepting state on a satisfying input on its input tape, but also return a result on an output tape.

A problem is called fixed parameter tractable for a parameter l [26] if it can be solved in time, exponential only in l and polynomial in the input size n, i.e. when the running time is  $\mathcal{O}(f(l) \cdot n^c)$  for an arbitrary function f and a constant c, independent of n. In practice, this means that problem instances can be solved efficiently, even when the problem is NP-hard in general, if l is known to be small. If an NP-hard problem  $\Pi$  is fixed parameter tractable for a parameter l then l is denoted a source of complexity of  $\Pi$  [18].

## 3 Computational Complexity

The problem of finding the most probable explanation for a set of variables in Bayesian networks has been discussed in the literature using many names, like Most Probable Explanation (MPE) [29], Maximum Probability Assignment (MPA) [30], Scenario-Based Explanation [31], (Partial) Abductive Inference or Maximum A Posteriori hypothesis (MAP) [32]. MAP also doubles to denote the set of variables for which an explanation is sought [30]; for this set, also the term *explanation set* is coined [32]. In recent years, more or less consensus is reached to use the terms MPE and Partial MAP to denote the problem with full, respectively partial evidence. We will use the term *explanation set* to denote the set of variables to be explained, and *intermediate nodes* to denote the variables that constitute neither evidence nor the explanation set. The formal definition of the canonical variants of these problems is as follows.

#### MPE

**Instance:** A probabilistic network  $\mathcal{B} = (\mathbf{G}, \Gamma)$ , where  $\mathbf{V}$  is partitioned into a set of evidence nodes  $\mathbf{E}$  with a joint value assignment  $\mathbf{e}$ , and an explanation set  $\mathbf{M}$ .

**Output:** The most probable joint value assignment  $\mathbf{m}$  to the nodes in  $\mathbf{M}$  with evidence  $\mathbf{e}$ , or  $\perp$  if  $\Pr(\mathbf{m}, \mathbf{e}) = 0$  for every joint value assignment  $\mathbf{m}$  to  $\mathbf{M}$ .

#### Partial MAP

**Instance:** A probabilistic network  $\mathcal{B} = (\mathbf{G}, \Gamma)$ , where **V** is partitioned into a set of evidence nodes **E** with a joint value assignment **e**, a set of intermediate

nodes  $\mathbf{I}$ , and an explanation set  $\mathbf{M}$ .

**Output:** The most probable joint value assignment **m** to the nodes in **M** given evidence **e**, or  $\perp$  if  $Pr(\mathbf{m}|\mathbf{e}) = 0$  for every joint value assignment **m** to **M**.

We assume that the problem instance is encoded using a *reasonable* encoding as is customary in computational complexity theory. For example, we expect that numbers are encoded using binary notation (rather than unary), that probabilities are encoded using rational numbers, and that the number of values for each node in the network is bounded. In principle, it is possible to "cheat" on the complexity results by completely discarding the structure in a network  $\mathcal{B}$ and encode *n* stochastic binary variables using a single node with  $2^n$  values that each represent a particular joint value assignment in the original network. The CPT of this node in the thus created network  $\mathcal{B}'$  (and thus the input size of the problem) is exponential in the number of variables in the original network, and thus many computational problems will run in time, polynomial in the input size, which of course does not reflect the actual intractability of this approach.

In the next sections we will discuss the complexity of MPE and PARTIAL MAP, respectively. We then enhance both problems to *enumeration* variants: instead of finding the most probable assignment to the explanation set, we are interested in the complexity of finding the k-th most probable assignment for arbitrary values of k. Lastly, we discuss the complexity of *approximating* MPE and PARTIAL MAP and their *parameterized* complexity.

### 4 MPE and variants

Shimony [33] first addressed the complexity of the MPE problem. He showed that the decision variant of MPE was NP-complete, using a reduction from VERTEX COVER. As already pointed out by Shimony, reductions from several problems are possible, yet using VERTEX COVER allows particular constraints on the structure of the network to be preserved. In particular, it was shown that MPE remains NP-hard, even if all variables are binary and both indegree and outdegree of the nodes is at most two [33].

An alternative proof, using a reduction from SATISFIABILITY, will be given below. In this proof, we need to relax the constraint on the outdegree of the nodes, however, in this variant MPE remains NP-hard when all variables have either uniformly distributed prior probabilities (i.e., Pr(V = TRUE) = Pr(V =FALSE) =  $\frac{1}{2}$ ) or have deterministic conditional probabilities (Pr(V = TRUE | $\pi(V)$ ) is either 0 or 1). The main merit of this alternative proof is, however, that a reduction from SATISFIABILITY may be more familiar for readers not acquainted with graph problems. We first define the decision variant of MPE:

#### MPE-D

**Instance:** A probabilistic network  $\mathcal{B} = (\mathbf{G}, \Gamma)$ , where **V** is partitioned into a set of evidence nodes **E** with a joint value assignment **e**, and an explanation set **M**; a rational number  $0 \le q < 1$ .



Figure 4: The probabilistic network corresponding to  $\neg(X_1 \lor X_2) \land \neg X_3$ 

**Question:** Is there a joint value assignment **v** to the nodes in **M** with evidence **e** with probability  $Pr(\mathbf{v}, \mathbf{e}) > q$ ?

Let  $\phi$  be a Boolean formula with n variables. We construct a probabilistic network  $\mathcal{B}_{\phi}$  from  $\phi$  as follows. For each propositional variable  $X_i$  in  $\phi$ , a binary stochastic variable  $X_i$  is added to  $\mathcal{B}_{\phi}$ , with possible values TRUE and FALSE and a uniform probability distribution. These variables will be denoted as truthsetting variables  $\mathbf{X}$ . For each logical operator in  $\phi$ , an additional binary variable in  $\mathcal{B}_{\phi}$  is introduced, whose parents are the variables that correspond to the input of the operator, and whose conditional probability table is equal to the truth table of that operator. For example, the value TRUE of a stochastic variable mimicking the *and*-operator would have a conditional probability of 1 if and only if both its parents have the value TRUE, and 0 otherwise. These variables will be denoted as truth-maintaining variables  $\mathbf{T}$ . The variable in  $\mathbf{T}$  associated with the top-level operator in  $\phi$  is denoted as  $V_{\phi}$ . The explanation set  $\mathbf{M}$  is  $\mathbf{V} \setminus V_{\phi}$ . In Figure 4 the network  $\mathcal{B}_{\phi_{ex}}$  is shown for the formula  $\phi_{ex} = \neg(X_1 \vee X_2) \wedge \neg X_3$ .

Now, for any particular truth assignment  $\mathbf{x}$  to the set of truth-setting variables  $\mathbf{X}$  in the formula  $\phi$  we have that the probability of the value TRUE of  $V_{\phi}$ , given the joint value assignment to the stochastic variables matching that truth assignment, equals 1 if  $\mathbf{x}$  satisfies  $\phi$ , and 0 if  $\mathbf{x}$  does not satisfy  $\phi$ . With evidence  $V_{\phi} = \text{TRUE}$ , the probability of any joint value assignment to  $\mathbf{M}$  is 0 if the assignment to  $\mathbf{X}$  does not satisfy  $\phi$ , or the assignment to  $\mathbf{T}$  does not match the constraints imposed by the operators. However, the probability of any satisfying (and matching) joint value assignment to  $\mathbf{M}$  is  $\frac{\#_{\phi}}{2^n}$ , where  $\#_{\phi}$  is the number of satisfying truth assignments to  $\phi$ . Thus there exists an instantiation  $\mathbf{m}$  to  $\mathbf{M}$  such that  $\Pr(\mathbf{m}, V_{\phi} = \text{TRUE}) > 0$  if and only if  $\phi$  is satisfiable. Note that the above network  $\mathcal{B}_{\phi}$  can be constructed from  $\phi$  in polynomial time.

**Result 4.1.** MPE-D is NP-complete, even when all variables are binary, the indegree of all variables is at most two, and either the outdegree of all variables is

two or the probabilities of all variables are deterministic or uniformly distributed.

#### Corollary 4.2. MPE is NP-hard under the same constraints as above.

The exact complexity of the *functional* variant of MPE is discussed in [34]. The proof uses a similar construction as above, however, the prior probabilities of the truth-setting variables is not uniform, but depends on the index of the variable. More in particular, the prior probabilities  $p_1, \ldots, p_i, \ldots, p_n$  for the variables  $X_1, \ldots, X_i, \ldots, X_n$  are such that  $p_i = \frac{1}{2} - \frac{2^k - 1}{2n+1}$ . This ensures that a joint value assignment  $\mathbf{x}$  to  $\mathbf{X}$  is more probable than  $\mathbf{x}'$  if and only if the corresponding truth assignment  $\mathbf{x}_{\phi}$  to  $X_1, \ldots, X_n$  is *lexicographically* ordered before  $\mathbf{x}'_{\phi}$ . Using this construction, Kwisthout [34] reduced MPE from the LEXSAT-problem of finding the lexicographically first satisfying truth assignment to a formula  $\phi$ . This shows that MPE is FPNP-complete and thus in the same complexity class as the functional variant of the TRAVELING SALESMAN-problem [35].

**Result 4.3 ([34]).** MPE is FP<sup>NP</sup>-complete, even when all variables are binary and the indegree of all variables is at most two.

Kwisthout [34, p. 70] furthermore argued that the proposed decision variant MPE-D does not capture the essential complexity of the functional problem, and suggested the alternative decision variant MPE-D': given  $\mathcal{B}$  and a designated variable  $M \in \mathbf{M}$  with designated value m, does M have the value m in the most probable joint value assignment  $\mathbf{m}$  to  $\mathbf{M}$ ? This problem turns out to be  $\mathsf{P}^{\mathsf{NP}}$ -complete, using a reduction from the decision variant of LEXSAT.

**Result 4.4 ([34]).** MPE-D' is  $P^{NP}$ -complete, even when all variables are binary and the indegree of all variables is at most two.

Bodlaender et al. [30] used a reduction from 3SAT in order to prove a number of complexity results for related problem variants. A 3SAT instance (U, C), where U denotes the variables and C the clauses, was used to construct a probabilistic network  $\mathcal{B}_{(U,C)}$  with explanatory set  $\mathbf{X} \cup Y$ . The construction was such that for any joint value instantiation  $\mathbf{x}$  to  $\mathbf{X} \cup Y$  that set Y to TRUE,  $\mathbf{x}$ was the most probable explanation for  $\mathcal{B}_{(U,C)}$  if (U,C) was not satisfiable, and the second most probable explanation if if (U,C) was satisfiable. Using this construction, they proved (among others) the following complexity results.

**Result 4.5 ([30]).** The IS-AN-MPE problem (given a network  $\mathcal{B} = (G, \Gamma)$ , an explanatory set  $\mathbf{M}$ , evidence  $\mathbf{e}$ , and an joint value assignment  $\mathbf{m}$  to  $\mathbf{M}$ : is  $\mathbf{m}$  the most probable joint value assignment<sup>1</sup> to  $\mathbf{M}$ ) is co-NP-complete.

**Result 4.6 ([30]).** The BETTER-MPE problem (given a network  $\mathcal{B} = (G, \Gamma)$ , an explanatory set  $\mathbf{M}$ , evidence  $\mathbf{e}$ , and an joint value assignment  $\mathbf{m}$  to  $\mathbf{M}$ : find a joint value assignment  $\mathbf{m}'$  to  $\mathbf{M}$  which has a higher probability than to  $\mathbf{m}$ ) is NP-hard.

 $<sup>^{1}</sup>$ Or one of the most probable assignments in case of a tie.

## 5 Partial MAP

Park and Darwiche [36] showed that the decision variant of PARTIAL MAP is NP<sup>PP</sup>-complete, using a reduction from MAJSAT (given a Boolean formula  $\phi$  partitioned in two sets  $\mathbf{X}_{\mathbf{A}}$  and  $\mathbf{X}_{\mathbf{B}}$ : is there an truth instantiation to  $\mathbf{X}_{\mathbf{A}}$  such that the majority of the truth instantiations to  $\mathbf{X}_{\mathbf{B}}$  satisfies  $\phi$ ?). The proof structure is similar to the hardness proof of MPE, however, the nodes modeling truth setting variables are partitioned into the evidence set  $\mathbf{X}_{\mathbf{A}}$  and a set of intermediate variables  $\mathbf{X}_{\mathbf{B}}$ . Furthermore, q is set to  $\frac{1}{2}$ . Using this structure NP<sup>PP</sup>-completeness is proven with the same constraints on the network structure as in Result 4.1. However, Park and Darwiche also prove a considerably strengthened theorem, using an other (and notably more technical) proof:

**Result 5.1 ([36]).** PARTIAL MAP-*D* remains NP<sup>PP</sup>-complete when the network has depth 2, there is no evidence, all variables are binary, and all probabilities lie in the interval  $\left[\frac{1}{2} - \epsilon, \frac{1}{2} + \epsilon\right]$  for any fixed  $\epsilon > 0$ .

Park and Darwiche [36] show that a number of restricted problem variants remain hard. If there are no intermediate variables, the problem degenerates to MPE-D and thus remains NP-complete. On the other hand, if the explanation set is empty, then the problem degenerates to INFERENCE and thus remains PP-complete. If the number of variables in the explanation set is logarithmic in the total number of variables the problem is in  $\mathsf{P}^{\mathsf{PP}}$  since we can iterate over all joint value assignments of the explanation set in polynomial time and infer the joint probability using an oracle for INFERENCE. If the number of intermediate variables is logarithmic in the total number of variables the problem is in NP since we can verify in polynomial time whether the probability of any given assignment to the variables in the explanation set exceeds the threshold, by summing over the polynomially bounded number of joint value assignments of the other variables. However, when the number of variables in the explanation set or the number of intermediate variables is  $\mathcal{O}(n^{\epsilon})$  the problem remains NP<sup>PP</sup>-complete, since we can 'blow up' the general proof construction with a polynomial number of unconnected and deterministic dummy variables such that these constraints are met. Lastly, the problem remains NP-complete when the network is restricted to a polytree.

**Result 5.2 ([36]).** PARTIAL MAP-D remains NP-complete when restricted to polytrees.

It follows as a corollary that the functional problem variant PARTIAL MAP is NP<sup>PP</sup>-hard in general with the same constraints as the decision variant. In addition, Kwisthout [34] shows that PARTIAL MAP is FP<sup>NP<sup>PP</sup></sup>-complete and remains FP<sup>NP</sup>-complete on polytrees. This result shares the constraints with Result 4.3.

**Result 5.3 ([34]).** PARTIAL MAP is  $\mathsf{FP}^{\mathsf{NP}^{\mathsf{PP}}}$ -complete, even when all variables are binary and the indegree of all variables is at most two.

**Result 5.4 ([34]).** PARTIAL MAP remains  $\mathsf{FP}^{\mathsf{NP}}$ -complete on polytrees, even when all variables are binary and the indegree of all variables is at most two.

Some variants of PARTIAL MAP can be formulated. For example, in [37] the COND MAP-D problem was defined as follows: Given a probabilistic network  $\mathcal{B} = (\mathbf{G}, \Gamma)$ , with explanation set  $\mathbf{M}$  and designated variable C with designated value c, and a rational number q; is there a joint value assignment  $\mathbf{m}$  to  $\mathbf{M}$  such that  $\Pr(C = c | \mathbf{m}) > q$ ?

It can be easily shown that the hardness proofs of Park and Darwiche [36] for PARTIAL MAP-D can also be applied, with trivial adjustments, to COND MAP-D.

**Result 5.5 ([37, 36]).** COND MAP-D is NP<sup>PP</sup>-complete, even when all variables are binary and the indegree of all variables is at most two.

**Result 5.6.** COND MAP-D remains NP-complete on polytrees, even when all variables are binary and the indegree of all variables is at most two.

## 6 Enumeration variants

In practical applications, one often wants to find a number of different joint value assignments with a high probability, rather than just the most probable one [38, 39]. For example, in medical applications, one wants to suggest alternative (but also likely) explanations to a set of observations. One might like to prescribe medication that treats a number of plausible (combinations of) diseases, rather than just the most probable combination. It may also be useful to examine the second-best explanation to gain insight in *how good* the best explanation is, relative to other solutions, or how sensitive it is to changes in the parameters of the network [40].

Kwisthout [41] addressed the computational complexity of MPE and PAR-TIAL MAP when extended to the k-th most probable explanation, for arbitrary values of k. The construction for the hardness proof of KTH MPE is similar to that of Result 4.3, however, the reduction is made from KTHSAT (given a Boolean formula  $\phi$ , what is the lexicographically k-th satisfying truth assignment?) rather than LEXSAT. It is thus shown that KTH MPE is FP<sup>PP</sup>-complete and has a P<sup>PP</sup>-complete decision variant, even if all nodes have indegree at most two. Finding the k-th MPE is thus considerably harder (i.e., complexitywise) than MPE, and also harder than the PP-complete INFERENCE-problem in Bayesian networks. The computational power of P<sup>PP</sup> and FP<sup>PP</sup> (and thus the intractability of KTH MPE) is illustrated by Toda's theorem [42] which states that P<sup>PP</sup> includes the entire Polynomial Hierarchy (PH).

**Result 6.1 ([41]).** KTH MPE is  $FP^{PP}$ -complete and has a  $P^{PP}$ -complete decision variant, even if all nodes have indegree at most two.

The KTH PARTIAL MAP-problem is even harder than that, under usual

assumptions<sup>2</sup> in complexity theory. Kwisthout proved [41] that a variant of the problem with *bounds* on the probabilities (BOUNDED KTH PARTIAL MAP) is  $\mathsf{FP}^{\mathsf{PP}^\mathsf{PP}}$ -complete and has a  $\mathsf{P}^{\mathsf{PP}^\mathsf{PP}}$ -complete decision variant, using a reduction from the KTHNUMSAT-problem (given a Boolean formula  $\phi$  whose variables are partitioned in two subsets  $\mathbf{X}_{\mathbf{A}}$  and  $\mathbf{X}_{\mathbf{B}}$  and an integer l, what is the lexicographically k-th satisfying truth assignment to  $\mathbf{X}_{\mathbf{A}}$  such that exactly l truth assignments to  $\mathbf{X}_{\mathbf{B}}$  satisfy  $\phi$ ?). The proof of Park and Darwiche [36] that shows that PARTIAL MAP remains NP-complete on polytrees, mentioned in the previous section, can be easily modified to reduce KTH PARTIAL MAP on polytrees from the  $\mathsf{FP}^{\mathsf{PP}}$ -complete problem KTH3SAT [44], hence finding the k-th Partial MAP on polytrees remains  $\mathsf{FP}^{\mathsf{PP}}$ -complete.

**Result 6.2 ([41]).** KTH PARTIAL MAP is  $\mathsf{FP}^{\mathsf{PP}}$ -complete and has a  $\mathsf{P}^{\mathsf{PP}}$ -complete decision variant, even if all nodes have indegree at most two.

**Result 6.3 ([41]).** KTH PARTIAL MAP remains FP<sup>PP</sup>-complete on polytrees, even if all nodes have indegree at most two.

## 7 Approximation Results

While sometimes NP-hard problems can be efficiently approximated in polynomial time (e.g., algorithms exist that find a solution that may not be optimal, but nevertheless is guaranteed to be within a certain bound), no such algorithms exist for the MPE and PARTIAL MAP problems. In fact, Abdelbar and Hedetniemi showed that there can not exist an algorithm that is guaranteed to find a joint value assignment within any fixed bound of the most probable assignment, unless P = NP [45]. That does not imply that heuristics play no role in finding assignments; however, if no further restrictions are assumed on the graph structure or probability distribution, no approximation algorithm is guaranteed to find a solution (in polynomial time) that has a probability of at least  $\frac{1}{r}$  times the probability of the best explanation, for any fixed r.

In fact, it can be easily shown that no algorithm can guarantee *absolute* bounds as well. As we have seen in Section 4, deciding whether there exist a joint value assignment with a probability larger than q is NP-hard for any q larger than 0. Thus, finding a solution which is 'good enough' is NP-hard in general, where 'good enough' may be defined as a ratio of the probability of the best explanation or as an absolute threshold.

Observe that MPE is a special case of PARTIAL MAP, in which the set of intermediate variables **I** is empty, and that the intractability of approximating MPE extends to PARTIAL MAP. Furthermore, Park and Darwiche [36] proved that approximating PARTIAL MAP on polytrees within a factor of  $2^{n^{\epsilon}}$  is NP-hard for any fixed  $\epsilon, 0 \leq \epsilon < 1$ , where *n* is the size of the problem.

**Result 7.1 ([45]).** MPE cannot be approximated within any fixed ratio unless P = NP.

 $<sup>^2\</sup>mathrm{To}$  be more precise, the assumptions that the inclusions in the Counting Hierarchy [43] are strict.

**Result 7.2 ([33]).** MPE cannot be approximated within a fixed bound unless P = NP.

## 8 Fixed Parameter Results

In the previous sections we saw that finding the best explanation in a probabilistic network is NP-hard and NP-hard to approximate as well. These intractability results hold *in general*, i.e., when no further constraints are put on the problem instances. However, polynomial-time algorithms are possible for MPE if certain *problem parameters* are known to be small. In this section, we present known results and corollaries that follow from these results. In particular, we discuss the following parameters: probability (PROBABILITY-L MPE, PROBABILITY-L PARTIAL MAP), treewidth (TREEWIDTH-L MPE, TREEWIDTH-L PARTIAL MAP), and, for PARTIAL MAP, the number of intermediate variables (INTER-MEDIATE-L PARTIAL MAP). In all of these problems, the input is a probabilistic network and the parameter l as mentioned. Also, for the PARTIAL MAP variants combinations of these parameters will be discussed, in particular probability and treewidth (PROBABILITY-L TREEWIDTH-M PARTIAL MAP) and probability and number of intermediate variables (PROBABILITY-L INTERMEDIATE-M PARTIAL MAP).

Bodlaender et al. [30] presented an algorithm to decide whether the most probable explanation has a probability larger than q, but where q is seen as a fixed parameter rather than part of the input. The algorithm has a running time of  $\mathcal{O}(2^{\frac{\log q}{\log 1-q}} \cdot n)$ , where n denotes the number of variables. When q is a fixed parameter (and thus assumed constant), this is linear in n; moreover, the running time decreases when q increases, thus for problem instances where the most probable explanation has a high probability, deciding the problem is tractable. The problem is easily enhanced to a functional problem variant where the most probable assignment (rather than TRUE or FALSE) is returned.

#### Result 8.1 ([30]). PROBABILITY-L MPE is fixed-parameter tractable.

**Corollary 8.2.** Finding the most probable explanation can be done efficiently if the probability of that explanation is high.

Sy [29] first introduced an algorithm for finding the most probable explanation, based on junction tree techniques, which in multiply connected graphs runs in time, exponential only in the maximum number of node states of the compound variables. Since the size of the compound variables in the junction tree is equal to the treewidth of the network plus one, this algorithm is exponentially only in the treewidth of the network<sup>3</sup>. Hence, if treewidth is seen as a fixed parameter, then the algorithm runs in polynomial time.

<sup>&</sup>lt;sup>3</sup>Note that the number of values per variable may be high, thus rendering the algorithm intractable even for networks with low treewidth. However, the conditional probability distribution of each variable is part of the problem instance, so even when there are many values per variable, the algorithm still runs in time, polynomial in the input size.

Result 8.3 ([29]). TREEWIDTH-L MPE is fixed-parameter tractable.

**Corollary 8.4.** Finding the most probable explanation can be done efficiently if the treewidth of the network is low.

Sy's algorithm [29] in fact finds the k most probable explanations (rather than only the most probable) and has a running time of  $\mathcal{O}(k \cdot n^{|C|})$ , where |C| denotes the maximum number of node states of the compound variables. Since k may become exponential in the size of the network this is in general not polynomial, even with low treewidth; however, if k is regarded as parameter then fixed parameter tractability follows as a corollary.

Result 8.5 ([29]). TREEWIDTH-L KTH MPE is fixed-parameter tractable.

**Corollary 8.6.** Finding the k-th most probable explanation can be done efficiently if both k and the treewidth of the network are low.

When we consider PARTIAL MAP then restricting either the probability or the treewidth is insufficient to render the problem tractable. This latter result follows from the NP-completeness result of Park and Darwiche [36] for PARTIAL MAP restricted to polytrees with at most 2 parents per node, i.e., networks with treewidth at most 2. Furthermore, it is easy to see that deciding PARTIAL MAP includes solving the INFERENCE problem, even if l, the probability of the most probable explanation, is very high. Assume we have a network  $\mathcal{B}$ with designated binary variable V. Deciding whether  $\Pr(V = \text{TRUE}) > \frac{1}{2}$  is PP-complete in general (see e.g. [34, p.19-21] for a completeness proof, using a reduction from MAJSAT). We now add a binary variable C to our network, with V as its only parent, and probability table  $\Pr(C = \text{TRUE} | V = \text{TRUE}) = l + \epsilon$ and  $\Pr(C = \text{TRUE} | V = \text{FALSE}) = l - \epsilon$  for an arbitrary small value  $\epsilon$ . Now,  $\Pr(C = \text{TRUE}) > l$  if and only if  $\Pr(V = \text{TRUE}) > \frac{1}{2}$ , so determining whether the most probable explanation of C has a probability larger than l boils down to deciding INFERENCE which is PP-complete.

**Result 8.7** ([36]). TREEWIDTH-L PARTIAL MAP is NP-complete for  $l \geq 2$ .

**Result 8.8.** PROBABILITY-L PARTIAL MAP is PP-complete independent of the probability l of the most probable explanation.

However, the algorithm of Bodlaender et al. [30] can be adapted to find partial MAPs as well. The algorithm iterates over a topological sort  $1, \ldots, i, \ldots, n$ of the nodes of the network. At one point, the algorithm computes  $\Pr(V_{i+1} | \mathbf{v})$ for a particular joint value assignment  $\mathbf{v}$  to  $V_1, \ldots, V_i$ . In the paper it is concluded that this can be done in polynomial time since all values of  $V_1, \ldots, V_i$  are known at iteration step *i*. To obtain an algorithm for finding partial MAPs, we just skip any iteration step *i* if  $V_i$  is an intermediate variable, and we compute  $\Pr(V_{i+1})$  by computing the probability distribution over the 'missing' values  $V_i$ . This can be done in polynomial time if either the number of intermediate variables is fixed or the treewidth of the network is fixed. A similar result can be shown for the COND MAP problem variant. **Result 8.9 (adapted from [30]).** PROBABILITY-L TREEWIDTH-M PARTIAL MAP and PROBABILITY-L INTERMEDIATE-M PARTIAL MAP are fixed-parameter tractable.

**Corollary 8.10.** Finding the Partial MAP can be done efficiently if both the probability of the most probable explanation is high, and either the treewidth of the network or the number of intermediate variables is low.

## 9 Conclusion

Inference of the most probable explanation is hard in general. Approximating the most probable explanation is hard as well. Furthermore, various problem variants, like finding the k-th MPE, finding a better explanation than the one that is given, and finding best explanations when not all evidence is available is hard. Many problems remain hard under severe constraints.

However, this need not to be 'all bad news' for the computational modeler. MPE *is* tractable when the probability of the most probable explanation is high or when the treewidth of the underlying graph is low. PARTIAL MAP *is* tractable when both constraints are met, to name a few examples. The key question for the modeler is: are these constraints plausible with respect to the phenomenon one wants to model? Is it reasonable to suggest that the phenomenon does not occur when the constraints are violated? For example, when cognitive processes like goal inference are modeled as finding the most probable explanation of a set of variables given partial evidence, is it reasonable to suggest that humans have difficulty inferring actions when the probability of the most probable explanation is low, as suggested by [19]?

We do not claim to have answers to such questions. However, the overview of known results in this paper may aid the computational modeler in finding potential sources of intractability. Whether the outcome is received as a blessing (because empirical results may *confirm* those sources of intractability, thus attributing more credibility to the model) or a curse (because empirical results *refute* those sources of intractability, thus providing counterexamples to the model) is beyond our control.

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