# **Query-driven PAC-Learning for Reasoning**

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#### Abstract

We consider the problem of learning rules from a data set that support a proof of a given query, under Valiant's PAC-Semantics. We show how any backward proof search algorithm that is sufficiently oblivious to the contents of its knowledge base can be modified to learn such rules while it searches for a proof using those rules. We note that this gives such algorithms for standard logics such as chaining and resolution.

## 1 Introduction

Machine learning, coupled with plentiful data, promises an approach to the problem of constructing the large knowledge bases needed for AI. Whereas traditional knowledge engineering by hand, as exemplified by the CYC project [Lenat, 1995], proved difficult to scale, machine learning holds the promise of producing a large and consistently interpreted knowledge base. Of course, any kind of inductive learning faces the danger of incorrect generalization, and thus such knowledge must use a semantics that is weaker than classical logic. Valiant [2000] proposed PAC-Semantics as a semantics for classical logics that is liberal enough to tolerate the imperfect rules produced by models of machine learning [Valiant, 1984]. Subsequently, Valiant [2006] also demonstrated that a large knowledge base can be soundly learned from a reasonable size data set. Michael and Valiant [2008] demonstrated the use of such knowledge bases on a sentence completion task, and a system using this approach [Isaak and Michael, 2016] was tied for top performance in the first Winograd Schema Challenge competition [Davis et al., 2017].

Although Valiant [2006] showed that there is no *statistical* barrier to learning a large knowledge base, *computational* issues from representing and accessing such a large knowledge base may still arise. One way of avoiding these issues was proposed by Juba [2013], building on Khardon and Roth's *learning to reason* approach [Khardon and Roth, 1997]: instead of representing a knowledge base explicitly, Juba decides a query using the data directly, and guarantees that the result is sufficient to distinguish queries that have low validity from queries with small proofs using knowledge that *could* have been learned from the data. Thus, the query is answered

using a knowledge base that is only *implicitly* learned. Crucially, this approach applies to settings where some attributes are not observed in the examples used for learning, and therefore some reasoning may be required. These attributes may still be mentioned in the background knowledge and query. For example, we may observe medical test results, but not whether a given patient actually has a given disease.

A drawback of Juba's approach, however, is that it provides no explicit representation of what knowledge could have been learned to support the query. It only provides a set of proofs for specific examples from the data set. This may not be adequately interpretable for human oversight of the system; if possible, we would like to inspect the knowledge that is being used to provide answers to our queries. Moreover, there are applications for which we are more interested in what knowledge could have been used to derive the conclusion than we are in the conclusion itself. For example, such algorithms might be applied to learn a screening rule for fraud detection as follows: Given a definition of behavior that is legitimate and a set of example transaction histories that are known to be legitimate, we could seek to learn what properties (if any) of the observed portions of these transactions can be used to guarantee that they are legitimate by using the definition of legitimate behavior as our query. We can then check whether or not these learned properties are observed to hold on future transactions to decide whether or not they warrant further inspection. Note that in this case the query is presumed to hold, and the interesting part is what properties we can discover to justify the query. We will discuss a similar but more easily formalized application to learning input filters later.

In this work, we show how for a large class of *oblivious* backward search algorithms for reasoning, we can explicitly identify rules that suffice to answer queries. Thus, we explicitly identify a sufficient set of relevant rules from this "implicit" knowledge base in a goal-driven fashion. *Obliviousness* means that the only effect of the knowledge base on the search is to terminate branches early when the subgoal is already present in the knowledge base. We observe that this suffices to learn such rules for logics such as chaining and treelike resolution where there are natural oblivious (or nearly oblivious) algorithms, e.g., DPLL-like algorithms [Davis and Putnam, 1960; Davis et al., 1962]. This is achieved by deeming subgoals to be successful by adding them to the knowledge base when they are supported by the data; if the search

is obvlivious, then we obtain the same results as if those formulas had belonged to the knowledge base all along.

Our algorithms resemble algorithms arising in inductive logic programming (ILP) [Muggleton and De Raedt, 1994], in particular work by Muggleton and Buntine [1988] that constructed rules for resolution; although Muggleton [1991] anticipated that a connection to PAC-Learning should exist, ILP learning theory is quite different. The main distinction here is conceptual: ILP treats the input examples as defining a domain for which we seek to synthesize a description. By contrast, in PAC-Semantics, we are only seeking to bound the probability our formulas are true with respect to some probability distribution D over valuations. Relatedly, the examples are simply drawn from D, and thus only statistically representative of it. We thus do not have complete knowledge of D nor do we even have access to the valuation of every formula in any given example. Although this bounding of probability is similar to a probability logic (e.g., as discussed by Nilsson [1986] for propositional logic or Halpern [1990] for first-order), we stress that the logical languages we use are simple Boolean logics such as chaining and resolution, and the probability bounds appear only in our semantics.

# 2 **Problem formulation**

We now describe the framework we use for learning and reasoning from partial examples (interpretations). First, we describe learning from partial examples, and give the key definition of concealment that captures when a credulous strategy for learning from partial examples will succeed. (Skeptical learning is considered later.) We then define a family of backward search algorithms, the family of algorithms for which we will be able to introduce query-driven learning. Since our guarantees will have the form of ensuring that these reasoning algorithms are as successful as if they had started their search with the learned knowledge given up-front, we will need a technical condition that the search algorithms are not too sensitive to the contents of the knowledge base they are given up-front-that is, "oblivious" to the knowledge base. Indeed, this definition will guarantee that we can introduce learned knowledge as the search proceeds without harming its performance, which is our main strategy.

#### 2.1 Learning and reasoning in PAC-Semantics

Following Valiant [2000], we will describe our logic in terms of the linear threshold connective (a common generalization of the usual AND and OR connectives). The linear threshold connective has the advantage that it can capture softened versions of AND and OR.

**Definition 1 (Threshold connective)** A threshold connective for a list of k formulas  $\varphi_1, \ldots, \varphi_k$  is given by a list of k + 1 integers,  $c_1, \ldots, c_k, b$ . The formula  $[\sum_{i=1}^k c_i \varphi_i \ge b]$  is interpreted as follows: given a Boolean interpretation for the k formulas, the connective is true if  $\sum_{i:\varphi_i=1}^{k} c_i \ge b$ .

A threshold connective expresses a k-ary AND connective by taking the  $c_i = 1$ , and b = k, and expresses a k-ary OR by taking  $c_1, \ldots, c_k, b = 1$ . Negation corresponds to  $c_i < 0$ .

Although we could have taken the weights to be realvalued, on account of the  $\varphi_i$ 's essentially taking values from  $\{0,1\}$ , any real-valued threshold connective has an equivalent integer connective. We use integers as they are simpler to represent and reason about.

**Example 2** Suppose we have one, unary relation symbol R and six elements in our domain,  $x_1, x_2, x_3, x_4, x_5$  and  $x_6$ . Now, an example of a formula using a threshold connective is

$$[5R(x_1) + R(x_2) + R(x_3) + R(x_4) + R(x_5) - R(x_6) \ge 4],$$

*i.e.*, with formulas  $\psi_i = R(x_i)$ , weights  $c_1 = 5$ ,  $c_6 = -1$ , and  $c_2, \ldots, c_5 = 1$ , and a threshold of b = 4.

We will assume a finite domain, and hence a finite (but possibly large) number of ground atomic formulas, N. Thus, our setting is essentially propositional. We will formulate our exposition in terms of a simplified first-order language without functions, in which free variables are taken to be universally quantified; these quantified formulas are of course equivalent to a quantifier-free (propositional) formula given by an AND (expressed by a threshold connective) over copies of the formula with each possible binding of the free variables. This is an example of the standard "propositionalization" transformation, and a suitable family of formulas for these purposes is described by Valiant [2000]. Nevertheless, this representation captures standard settings of (function-free) resolution and chaining with Horn KBs.

The main feature of PAC-Semantics is a probability distribution D on interpretations of the relation symbols, i.e., assignments of truth values to their groundings. Equivalently, we take each ground atomic formula as a Boolean-valued random variable. We stress that we do not assume independence (or any other relationship) between these random variables. Given an interpretation drawn from D, the semantics of a formula are then defined classically.  $KB \models \varphi$  denotes that  $\varphi$  is a (classically) valid formula given the knowledge base (set of formulas) KB. We denote the truth value of a formula  $\varphi$  under an interpretation x as  $\varphi|_x$ . We may view an interpretation as a Boolean vector indexed by the set of ground atomic formulas. Following Valiant [2000], we refer to interpretations of the ground atomic formulas as scenes.

**Definition 3**  $((1 - \epsilon)$ **-valid**) A sentence (i.e., formula with no free variables)  $\varphi$  is said to be  $(1 - \epsilon)$ -valid under D if the probability that  $\varphi$  evaluates to true under an interpretation drawn from D is at least  $1 - \epsilon$ . If  $\epsilon = 0$ , we say that  $\varphi$  is perfectly valid.

Now, an *obscured scene* is a *partial* interpretation of the ground atomic formulas of the logic:

**Definition 4 (Obscured scene)** A obscured scene  $\rho$  is a mapping taking ground atomic formulas to  $\{0, 1, *\}$  where \* denotes an "unknown" value. We say that an obscured scene  $\rho$  is consistent with an interpretation if whenever  $\rho$  assigns an ground atomic formula a value other than \*, the interpretation agrees with  $\rho$ .

We need obscured scenes because frequently our knowledge base will refer to atomic formulas that are not observed in the data we use for learning. Sometimes these unobserved atomic formulas take the form of properties we wish to reason about or predict with learned rules. Following Rubin [1976] and Michael [2010], we suppose that a "masking process" takes interpretations drawn from the distribution D and hides some ground atomic formulas, producing obscured scenes.

Definition 5 (Masking process) A mask is a function mapping interpretations to obscured scenes that are consistent with the respective interpretations. A masking process M is a mask-valued random variable (i.e., a random function). We denote the probability distribution over obscured scenes obtained by applying a masking process M to a distribution Dover interpretations by M(D).

Some natural examples of masking processes that don't use the full expressive power of the formalism are the following.

**Example 6** Consider masking processes that always produce a mask m that hides the values of a subset of the ground atomic formulas, and never hide the rest. Such masking processes capture the information available in a (learningdriven) program analysis application where the examples specify an input and nothing else. The hidden formulas would then encode the omitted trace of the program's execution. It also captures the information available in typical statistical studies in which a subset of the attributes of sampled members of a population are (reliably) recorded, and the rest are omitted from the data.

**Example 7** Consider a masking process that independently tosses a fair coin to decide whether or not to hide the value of each ground atomic formula in a given scene. So M produces m by sampling a set S at random by tossing a fair coin for each ground atomic formula, and then the corresponding m is of the type described in Example 6 - it hides the ground atomic formulas in the random set S and no others. This captures a setting where, due to noise corrupting a transmission, only portions of a scene can be decoded.

These examples do not use the ability of a masking process to optionally hide an atom depending on the underlying truth value, but our definition allows this.

**Example 8** Consider a setting where in a survey, participants are allowed to decline to answer a question. Naturally, one might find that when participants have (for example) atypically high or low income, or where they possess minority political opinions, or suffer from certain kinds of diseases, they might be less inclined to provide an answer. Thus, in such a setting, the survey responses would be more naturally modeled by a masking process in which, given that the sampled member of the population falls into one of these categories, the probability of the value being obscured is much higher than otherwise. Indeed, the model also allows for the decision to mask to depend on more than one attribute of the example (note that m(x) is allowed to depend on the entire interpretation x) – e.g., m(x) may omit the value of the formulas encoding the political inclinations only if they are relatively inconsistent with some other attributes of the respondent encoded by x.

For a given ground atomic formula  $\alpha$ , a PAC-Learning algorithm could be used to learn a formula  $\varphi$  that predicts  $\alpha$ , in which case the formula  $[\varphi \equiv \alpha]$  is  $(1-\epsilon)$ -valid with probability  $1 - \delta$  over the random example scenes (for  $\delta$  given to the algorithm): if we may take the truth value of  $\alpha$  as a *label* and the truth values of the ground atomic formulas as attributes for the example scenes, then PAC-Learning uses such examples to produce precisely such a formula  $\varphi$  as output. Using such a rule, we could hope to infer the value of  $\alpha$  in examples in which it is obscured. Such an approach was proposed by Valiant [2000], and we will return to it later.

Following Juba [2013], we will consider the following operation that uses obscured scenes to partially evaluate quantifier-free formulas defined using linear threshold connectives. Again, these could have been obtained from firstorder formulas by propositionalization. Note that the recursive definition corresponds to a linear-time algorithm for computing these partially evaluated formulas:

Definition 9 (Partial evaluation and witnessing) Given an obscured scene  $\rho$  and a quantifier-free formula  $\varphi$ , the partial evaluation of  $\varphi$  under  $\rho$ , denoted  $\varphi|_{\rho}$ , is recursively defined as follows; when the partial evaluation produces a Boolean constant, we say that the formula is witnessed:

- A ground atomic formula  $\varphi$  is replaced by its value under  $\rho$  (i.e., it is witnessed) unless this value is \*, in which case it remains  $\varphi$ .
- If  $\varphi = \neg \psi$  and  $\psi$  is not witnessed in  $\rho$ , then  $\varphi|_{\rho} =$  $\neg(\psi|_{\rho})$ ; otherwise,  $\varphi|_{\rho}$  is witnessed to be  $\neg(\psi|_{\rho})$ .
- For  $\varphi = [\sum_{i=1}^{k} c_i \psi_i \ge b]$ ,  $\varphi$  is witnessed true if  $\sum_{i:\psi_i \text{ witnessed true } c_i + \sum_{i:\psi_i \text{ not witnessed } \min\{0, c_i\} \ge b$ ,  $\varphi$  is witnessed false if  $\sum_{i:\psi_i \text{ witnessed true } c_i + \sum_{i:\psi_i \text{ not witnessed } \max\{0, c_i\} < b$ ,

  - and otherwise, supposing that  $(\psi_i, \psi_i) < 0$ , and otherwise, supposing that  $\psi_1, \ldots, \psi_\ell$  are witnessed in  $\rho$  (and  $\psi_{\ell+1}, \ldots, \psi_k$  are not witnessed),  $\varphi|_{\rho}$  is  $[\sum_{i=\ell+1}^k c_i(\psi_i|_{\rho}) \ge d]$  where  $d = b \sum_{i:\psi_i|_{\rho}=1} c_i$ .

Example 10 Continuing Example 2, in any partial scene in which  $R(x_1)$  is witnessed true, we find that  $\sum_{i:\psi_i \text{ witnessed true } c_i + \sum_{i\psi_i \text{ not witnessed}} \min\{c_i, 0\} \text{ is at least} \\ 5 - 1 = 4, \text{ so the formula will be witnessed true. Likewise,}$ if  $R(x_2), \ldots, R(x_5)$  are true and  $R(x_6)$  is false, then the formula is again witnessed true. But, if  $R(x_1)$  is false and  $R(x_6)$  is true, then the formula is witnessed false, as it is if  $R(x_1)$  is false and any of  $R(x_2), \ldots, R(x_5)$  are false. Finally, the formula is not witnessed if, for example,  $R(x_1)$  and  $R(x_6)$  are both false, and any proper subset of  $R(x_2),\ldots,R(x_5)$  are true.

Following Michael [2010], we consider learning from example obscured scenes, provided that the value of  $\alpha$  is not obscured in too many of the examples. Essentially we distinguish formulas that are perfectly valid under the unknown distribution from those that are not even  $(1-\epsilon)$ -valid for some given  $\epsilon > 0$ . The main finding is that the learnability of such rules is controlled by the probability of observing counterexamples to flawed rules under the masking process.

**Definition 11 (Concealment)** We say that a masking process M is (at most)  $(1 - \eta)$ -concealing with respect to a set of formulas C and a distribution over interpretations D if

$$\forall \varphi \in \mathcal{C} \Pr_{x \in D, m \in M} [\varphi \text{ witnessed on } m(x) \mid \varphi \mid_x = 0 ] \geq \eta.$$

We observe that the degree of concealment of a family of formulas depends on the family of formulas, the distribution over scenes, and the masking process.

**Example 12** In the masking process of Example 6, in which a fixed subset of the ground atomic formulas is never hidden and the rest are always hidden, the degree of concealment depends on whether or not the formula in question is ever falsified on the distribution, and if so, which ground atomic formulas in the scene it refers to. Generally, for formulas that only refer to the observed ground atomic formulas, the masking process is 0-concealing (i.e.,  $\eta = 1$ , no discounting) but for formulas that only refer to the unobserved ground atomic formulas, the masking process is 1-concealing ( $\eta = 0$ ) and learning is, strictly speaking, impossible. It may still be possible to infer the values of these attributes by reasoning, however, e.g., in the program analysis example we may be able to use the program code to infer the values of the program state from an example input.

**Example 13** In the case of the masking process of Example 7, where the ground atomic formulas are hidden uniformly at random, the degree of concealment may be bounded by the number of distinct ground atomic formulas: if we observe all k of the ground atomic formulas we certainly observe the formula being falsified, and this occurs with probability  $1/2^k$ . Thus, the masking process in this case would be  $(1 - 1/2^k)$ -concealing  $(\eta = 1/2^k)$ . In this case, we can take the number of ground atomic formulas that appear in a formula as a measure of its complexity. Some natural fragments of logics, such as bounded-width resolution, limit the number of atomic formulas that may appear in the lines of a proof, and would thus control the degree of concealment for lines of the proof for this masking process.

In the statement of our main theorem, we include the size of the input query formula as a parameter, and we suppose that the degree of concealment may depend on this parameter. This is because it is sometimes possible to bound the number of distinct formulas that can appear in proofs by the number of proofs, which may be bounded similar Lemma 22, below. The number of proofs may sometimes depend, in turn, on the number and complexity of the premises which are encoded in the query – consider for example, proofs with a bounded number of lines. We have included this parameterization to facilitate the application of our theorem in such situations.

Bounded concealment justifies a "credulous" learning strategy: rules are satisfactory as long as we do not observe counterexamples to them.

**Proposition 14 (Theorem 2.2 of [Michael, 2010])** For any distribution D over interpretations, masking process M, and class C of formulas, if M is  $(1 - \eta)$ -concealing with respect to C and D and  $\varphi \in C$  is not  $(1 - \epsilon)$ -valid, then  $\Pr_{\rho \in M(D)}[\varphi|_{\rho} = 0] \ge \eta \epsilon$ . Conversely, if M is not  $(1 - \eta)$ -concealing with respect to C and D then there exists  $\varphi \in C$  such that  $\Pr_{\rho \in M(D)}[\varphi|_{\rho} = 0] \le \eta \Pr_{x \in D}[\varphi|_x = 0]$  (where, note,  $\varphi$  is  $(1 - \Pr_{x \in D}[\varphi|_x = 0]$ )-valid).

That is, the degree of concealment controls the discounting of the probability of observing counterexamples to formulas from C. We have actually modified the definitions slightly

from the original version by including the distribution in the definition of concealment, and moreover, by using a notion of witnessed evaluation (as opposed to the value merely being *determined* by the obscured scene) but the proof is similar.

In the above formulation of PAC-Learning using equivalence rules, this means that for any incorrect hypothesis in our representation class, the value of  $\alpha$  should be witnessed (by the masking process) on an example where the hypothesis is incorrect with probability at least  $\eta$ . It turns out that for many classes of interest, learning is still possible as long as the masking process features an  $\eta$  bounded away from zero.

In this work, we are interested in reasoning problems, in which we only consider proofs of bounded complexity. For simplicity our formulation is again presented in terms of ground formulas, which could have been obtained by propositionalization. Formally, we consider the following family of problems:

**Definition 15 (Search problem)** Fix a logic, and let  $\mathcal{P}$  be a set of proofs in the logic (e.g., a fragment of bounded complexity). The search problem for  $\mathcal{P}$  is then the following promise problem: given as input a formula  $\varphi$  with no free variables and a set of formulas KB such that either there is a proof of  $\varphi$  in  $\mathcal{P}$  from KB or else KB  $\not\models \varphi$ , return such a proof in the former case, and return "Fail" in the latter.

Our first example of such a fragment is a mild generalization of the usual forward-chaining system that was presented by Valiant [2000]. It is designed to utilize rules of the form  $[\varphi \equiv \alpha]$  in which  $\alpha$  is an atomic formula, i.e., of the sort obtained from PAC-Learning algorithms. The main inference rule is *chaining*: given a formula of the form  $[\varphi \equiv \alpha]$  in which  $\alpha$  is a ground atomic formula, and a consistent set of literals (atomic formulas or their negations)  $\{\ell_1, \ldots, \ell_k\}$  such that for the obscured scene  $\rho$  that satisfies  $\ell_1, \ldots, \ell_k$  (and leaves every ground atomic formula not appearing in this list unassigned)  $\varphi|_{\rho} \in \{0, 1\}$ , if  $\varphi|_{\rho} = 0$ , infer  $\neg \alpha$ , and otherwise (i.e., if  $\varphi|_{\rho} = 1$ ) infer  $\alpha$ .

In chaining, it is typical to distinguish ground atomic formulas ("facts") and "rules" of the form  $[\varphi \equiv \alpha]$ ; in some formulations, we suppose that only the facts appear as lines of the proof and take the rules to be rules of inference. This limits the complexity of the proofs that may appear in the fragment: they are just ordered lists of facts. In particular, recall that one often considers augmenting the axioms of a logic with a set of additional formulas – "hypotheses" – that capture a specific domain or a specific scene one wishes to reason about. Typically, these hypotheses are the contents of the knowledge base. In the case of forward-chaining, for example, often these hypotheses are restricted to be just a set of (additional) facts. We will suppose in particular that the set of proofs  $\mathcal{P}$  parameterizing our search problem may restrict the formulas that may be used as hypotheses in this way.

### 2.2 A model of backward search algorithms

Informally, "backward" (goal-directed) algorithms start with a goal query and repeatedly generate sets of subgoal queries such that if all of the subgoal queries succeed - i.e., if proofs can be found for all of these subgoal queries - then the algorithm can construct a proof of the goal query. Although

this informal description suggests a recursive algorithm, it is highly desirable to cache the results of subgoal queries when they are answered—beyond the obvious time-efficiency improvements, it is often possible for a naïve recursive algorithm to get stuck following a circular sequence of subgoals. Thus, our model of such algorithms will be stated in terms of a graph indicating the dependency structure among the (sub)goals considered by the algorithm.

This graph would conventionally be an "AND-OR" graph: a query would be associated with an OR node, with edges to various alternative lists of subgoal queries, represented by AND nodes with edges to the OR nodes corresponding to the queries in the list. The success of the algorithm corresponds to the goal query node evaluating to 'true' in the natural interpretation of such a graph when one more generally associates success at finding a proof of a (subgoal) query with a node evaluating to 'true.' Given our interest in using rules expressed using linear threshold connectives, though, we will find it natural and convenient to replace the AND nodes with more general "linear threshold" nodes, expressing that success at the node is achieved if an appropriate subset of the subgoals are successful.

**Definition 16 (Subgoal dependency graph)** A subgoal dependency graph is a (possibly infinite) directed graph G in which the vertices are either query nodes labeled with a formula or are labeled with an integer threshold and have outgoing edges labeled by integer weights. A partial subgoal dependency graph also contains, for each threshold vertex, weights  $w_+$  and  $w_-$ . Given sets of successful nodes S and unsuccessful nodes U in the partial graph G', each node v is considered successful using S, U if there is an acyclic subgraph of G' featuring v as the (unique) source with sinks from  $S \cup U$  such that v has a path to every sink and at every nonquery node, the sum of the weights on the outgoing edges to vertices in S plus  $w_{-}$  and the negative weights on outgoing edges to vertices outside S or U is at least the threshold. Similarly, v is unsuccessful if the sum of the weights on outgoing edges to vertices in S plus  $w_+$  and the positive weights of edges to vertices outside S and U is less than its threshold.

Our rule for determining when a vertex is successful or unsuccessful match our rules for witnessing connectives true and false, respectively. The weights  $w_+$  and  $w_-$  will allow us to determine witnessing with (unwitnessed) unrepresented vertices. They represent the total weight of unrepresented vertices with positive coefficients and negative coefficients, respectively; note that the definition of witnessing uses one to establish a formula is witnessed true and the other to establish that it is witnessed false. Our successful vertices will intuitively represent either a provable query, or an applicable inference.

The backward search algorithm is now a meta-algorithm (Algorithm 1) parameterized by three sub-algorithms. One algorithm, GENERATE, generates the subgoal dependency graph, and another, EXPLORE, chooses edges in the dependency graph to explore (as long as the algorithm is not done). The third algorithm, TEST, generates a proof of the query if enough of the subgoal dependency graph has been revealed so that the original goal vertex was successful (given the ax-

**input** : Query formula  $\varphi$ , set of formulas *KB* **begin** 

```
if \varphi \in KB then
     return Trivial proof of \varphi
    end
    G \leftarrow vertex labeled by \varphi, marked "unexplored"
    while \text{TEST}(G, \varphi, KB) = FAIL \operatorname{do}
        if v \leftarrow \text{EXPLORE}(G, \varphi, KB) is not FAIL then
             if G' \leftarrow \text{GENERATE}(G, v) is not "fully
             explored" then
                 if G' contains a vertex not in G, not
                 labeled with \psi \in KB then
                     Mark the new vertex "unexplored."
                 end
                 G \leftarrow G'
             end
             else Remove "unexplored" mark from v
        end
        else return Fail
    end
    return TEST(G, \varphi, KB)
end
```

Algorithm 1: Backward search meta-algorithm

ioms and a knowledge base as successful vertices), or else indicates that the search is not successful yet. Thus, the algorithm explores the subgoal dependency graph (starting from the original query) until an appropriate collection of successful subgoals is discovered or the search algorithm gives up.

**Definition 17 (Backward search algorithm)** *A* backward search algorithm *is given by an instantiation of Algorithm 1 with three algorithms:* 

- An algorithm EXPLORE that, given a finite partial subgoal dependency graph G with a source labeled by  $\varphi$ and a subset of vertices marked "unexplored," and set of formulas KB, chooses an unexplored vertex  $v \in G$ or outputs "FAIL."
- An algorithm GENERATE that, given a partial subgoal dependency graph G and a vertex v ∈ G either returns "fully explored" or returns a subgoal dependency graph G' that extends G by adding one new edge starting from v, possibly to a new vertex, and reducing w<sub>+</sub> or w<sub>-</sub> by its weight if it is positive or negative, respectively.
- An algorithm TEST that, given a partial subgoal dependency graph G, a query formula  $\varphi$  labeling some vertex of G, and a set of formulas KB, either returns a proof of  $\varphi$  from KB, or if the vertex labeled by  $\varphi$  is not successful using KB and the axioms of the logic, returns "FAIL."

A key property possessed by instantiations of the backward-search paradigm is that the graph generation algorithm is often *oblivious* to which queries are successful, the algorithm exploring the graph only "terminates early" when it encounters a vertex labeled by a successful query, and the algorithm recovering the proof depends only on the portion of the subgoal dependency graph revealed thus far (and the formulas appearing on query vertices appearing in it). We will restrict our attention to such *oblivious* algorithms.

# Definition 18 (Oblivious backward search algorithm) We

say that a backward search algorithm is oblivious if:

- 1. For any partial subgoal dependency graph G, query  $\varphi$  (contained as a label in G), and set of formulas  $\Phi$  not appearing as labels of query nodes in G,  $\text{TEST}(G, \varphi, KB) = \text{TEST}(G, \varphi, KB \cup \Phi)$ .
- 2. For any query  $\varphi$  and sets of formulas KB and  $\Phi$ , the execution of the algorithm on input  $\varphi$  and  $KB \cup \Phi$  differs from the execution on input  $\varphi$  and KB only in that the sequence of vertices proposed by EXPLORE on input  $\varphi$  and  $KB \cup \Phi$  is the subsequence of vertices proposed on input  $\varphi$  and KB that omits (skips) exploring vertices in the sequence that are successful from  $KB \cup \Phi$  in the partial subgoal dependency graph used by the algorithm in the corresponding step.

#### An example: oblivious backward chaining

We briefly note that standard backward-chaining algorithms (for Horn KBs on ground atomic formulas) are oblivious backward search algorithms in the sense of Definition 18: recall that a *Horn clause* is a formula of the form  $[\alpha_1 \land \cdots \land \alpha_k] \Rightarrow \alpha_{k+1}$  where each  $\alpha_i$  is a ground atomic formula.  $\alpha_{k+1}$  is the *head* whereas  $\alpha_1 \land \cdots \land \alpha_k$  is the *body*. The knowledge base then consists of such clauses and a set of ground atomic formulas. The query is a conjunction of ground atomic formulas, represented as a threshold vertex with a threshold equal to the number of atomic formulas in the conjunction.

The oblivious backward chaining algorithm works as follows: EXPLORE performs a depth-first search of the subgoal dependency graph, terminating a search early only when it encounters an atomic formula in KB. GENERATE, on the other hand, when given a vertex corresponding to a ground atomic formula, returns an edge to a threshold vertex corresponding to the next clause in KB with the given atomic formula appearing in the head (in some fixed ordering), with a threshold equal to the number of atomic formulas in the body; when given a vertex corresponding to one of the clauses of KB (or the goal conjunction), it returns an edge to the vertex labeled with the next atomic formula in the body (also in some fixed ordering) of weight 1. Finally, TEST uses a dynamic programming algorithm to check if the query is successful from KB and return a chaining proof if it is. The running time is bounded by a polynomial in the size of *KB*: it runs for a linear number of iterations, and TEST may take quadratic time on each iteration.

**Example 19** We now illustrate the backward search algorithm for chaining of Horn rules. Let's consider the following simple domain, concerning fragile objects. The relations are fragile(x), broken(x), hard(x), crushed(x), and hit(x, y). We have a KB containing rules  $[crushed(x) \land fragile(x)] \Rightarrow broken(x)$  and  $[hit(x, y) \land fragile(x) \land hard(y)] \Rightarrow broken(x)$ . Let's suppose that the domain of objects consists of sculpture, crate, floor, and sidewalk. As an example, we might indicate that a fragile sculpture is crushed – fragile(sculpture) and crush(sculpture) are given – and we wish to know if broken(sculpture) holds. The full subgoal dependency graph is depicted in Figure 1.

A short execution of the backward search algorithm

starts with the query node, broken(sculpture). TEST on broken(sculpture) determines that this fact is not given, so the algorithm invokes EXPLORE which determines that the vertex broken(sculpture) is not yet fully explored. So, the algorithm invokes GENERATE on broken(sculpture) which begins generating the rules that could produce broken(x) in the head with sculpture substituted for x. For simplicity, let's suppose that it first considers the rule  $[crushed(x) \land$  $fragile(x)] \Rightarrow broken(x)$ , which is such a rule. This threshold vertex represents an AND on two conjuncts, so it has a threshold of 2. As the graph is partial, it has values  $w_{+} = 2$ since both of the conjuncts (yet to be generated) have a weight of 1 > 0 and  $w_{-} = 0$  since this threshold formula does not use negative weights. Note that none of the nodes are yet witnessed, so TEST will continue to the next iteration.

EXPLORE would, if it is a depth-first exploration, choose the new rule to explore. So it would invoke GENERATE on the rule, which would first yield the subgoal node crushed(sculpture) and reduce the value of  $w_+$  for the threshold by 1 (since one of these nodes is now represented in the graph). Note that crushed(sculpture) is in the KB, so this vertex will not be marked "unexplored." Furthermore, this node is successful, since it is in the KB. But, the rule that uses crushed(sculpture) is not yet witnessed since it also needs fragile(sculpture), so TEST will continue to the next iteration.

Now, since the new node is not marked "unexplored," the depth-first EXPLORE would return to the rule, and GENERATE next generates the subgoal fragile(sculpture), which is also in the KB, and reducing  $w_+$  (at the rule's vertex) by 1 to 0. At this point, TEST will discover that crushed(sculpture) and fragile(sculpture) suffice to witness the linear threshold corresponding to [crushed(sculpture)  $\wedge$  fragile(sculpture)], so this node is successful, which in turn witnesses that the original goal broken(sculpture) is successful. Thus, TEST returns the chaining proof of the query

- 1. crushed(sculpture) (hypothesis)
- 2. fragile(sculpture) (hypothesis)
- 3. broken(sculpture) (chaining, 1 & 2,  $[crushed(x) \land fragile(x)] \Rightarrow broken(x)/x = sculpture)$

Needless to say, the execution would be rather longer if the search had first started exploring the various domain substitutions for y in the rule  $[hit(x, y) \land fragile(x) \land$  $hard(y)] \Rightarrow broken(x)$ . A breadth-first search of the graph would have been similarly longer. Note that there are no rules with hit(x, y) or hard(x) in the head, so although these nodes will initially be marked "unexplored" (in contrast to, say, fragile(sculpture)), when GENERATE considers these nodes it will immediately report that they are "fully explored." Thus, after exploring these rules, the search will eventually return to exploring  $[crushed(x) \land fragile(x)] \Rightarrow broken(x)$ and succeed as described above, even in these cases.

Now, suppose that the sculpture hits the floor, so hit(sculpture, floor) holds instead of crushed(sculpture). Now, we are not given hard(floor) (the floor may be carpeted) so there is no proof of broken(sculpture). In this case, the backward search algorithm will generate the entire subgoal dependency graph, before determining that the query



Figure 1: A (AND-OR) subgoal dependency graph for the query *broken*(*sculpture*) with backward chaining using our Horn KB. The threshold nodes are labeled with the corresponding groundings of the rules of the KB. ANDs are represented by arcs connecting edges.

is not provable, and terminate with Fail.

## **3** Query-driven learning in backward search

The relative blindness of oblivious algorithms to the contents of the knowledge base allows us to add new members as the search proceeds, and obtain the same result as if we had started with them. As some algorithms may consider families of formulas that scale with the size of the query, in our theorem we will parameterize our bounds on the proof size B and degree of concealment  $\eta$  by the size of the query  $\ell$  (in bits). For example, adding clauses to a query for resolution generally increases the variety of clauses that may be derived. For larger families, we expect that the bounds grow weaker. We will use  $|\varphi|$  for a formula  $\varphi$  to denote its representation size (in bits), and |KB| to denote the representation size of the KB, again in bits. We assume the KB is represented in a way that ensures  $|KB \cup H| \leq |KB| + |H|$ , e.g., if it is represented as a string in which the elements are separated by special symbols, and terminated by another symbol.

**Theorem 20** Let  $\mathcal{P}$  be a set of proofs such that proofs of queries of length  $\ell$  only have proofs with  $B(\ell)$ -bit encodings in  $\mathcal{P}$  (in some fixed encoding scheme). Suppose there is an oblivious backward search algorithm for the search problem for  $\mathcal{P}$  that on input  $\varphi$  and KB over N ground atomic formulas, runs in time  $T(N, |\varphi|, |KB|)$  (for a function T that is monotone increasing in |KB|). Let D be a distribution over scenes and M be a masking process that is at most  $(1-\eta(\ell))$ concealing for the set of formulas  $\Phi$  that may be hypotheses in proofs of formulas of length  $\ell$  in  $\mathcal{P}$ . Then for any  $\delta, \epsilon \in (0, 1)$ , on input  $\varphi$  and KB and  $\Theta(\frac{1}{\epsilon\eta(|\varphi|)}(B(|\varphi|) + \log 1/\delta))$  example obscured scenes, Algorithm 2 using the same EXPLORE, GENERATE, and TEST as the given algorithm runs in time  $O(\frac{B(|\varphi|)}{\epsilon\eta(|\varphi|)}(B(|\varphi|) + \log 1/\delta)T(N, |\varphi|, C))$  (for  $C = |KB| + T(N, |\varphi|, |KB|)$ ), and with probability  $1 - \delta$ 

- returns "Fail" if  $[KB \Rightarrow \varphi]$  is not  $(1 \epsilon)$ -valid with respect to D, or
- returns a proof of  $\varphi$  from  $KB \cup H'$  for a set of formulas  $H' = \{h'_1, \ldots, h'_k\}$  such that  $h'_1 \wedge \cdots \wedge h'_k$  is  $(1 \epsilon)$ -valid if there exists a set of perfectly valid formulas H such that there is a proof of  $\varphi$  from  $KB \cup H$  in  $\mathcal{P}$ .

We remark that the cases are *not* exhaustive, for two reasons. First, for many logics, the fragments for which proof search can be considered tractable are not complete. Second, it may be that the query formula is indeed  $(1 - \epsilon)$ -valid, but that there is not a set of formulas that we can learn in support of it. For example, in chaining it may be that we have  $p \rightarrow r$  and  $q \rightarrow r$ , and we never observe r but we do observe either p or q to be true, half of the time each. So, we know r is always true, but since neither p nor q is consistently true, neither one can be learned.

**Proof:** First suppose that there is a set of perfectly valid formulas H such that there is a proof of the query  $\varphi$  from  $KB \cup H$  in  $\mathcal{P}$ . Since we have assumed that the given backward search algorithm solves the search problem for  $\mathcal{P}$ , on input  $\varphi$  and  $KB \cup H$ , the given backward search algorithm

```
input : Query formula \varphi, set of formulas KB, list of obscured scenes \rho_1 \dots, \rho_m
```

```
begin
```

```
G \leftarrow vertex labeled by \varphi, marked "unexplored"
while TEST(G, \varphi, KB) = FAIL do
    if v \leftarrow \texttt{EXPLORE}(G, \varphi, KB) is not FAIL then
        if G' \leftarrow \text{GENERATE}(G, v) is not "fully
        explored" then
             if G' contains a query vertex labeled by
             a formula h not in G and for no \rho_i is
             h|_{\rho_i} = 0 then KB \leftarrow KB \cup \{h\}
             if G' contains a vertex not in G, not
             labeled with \psi \in KB then
                 Mark the new vertex "unexplored."
            end
             G \leftarrow G'
        end
        else Remove "unexplored" mark from v
    end
    else return Fail
end
return TEST(G, \varphi, KB)
```

end

Algorithm 2: Backward search with query-driven learning

would return a proof of  $\varphi$  from  $KB \cup H$ . Suppose this occurs after  $t^*$  iterations.

Now, consider the sets  $KB'_t$  and subgoal dependency graphs  $G'_t$  used on each respective iteration t by Algorithm 2. If we consider the runs of the given algorithm using  $KB'_t$ , we see that since it is assumed to be oblivious, on each step up to t, it proposes the same vertex to explore as Algorithm 2 (i.e., it only omits the vertices that are successful from  $KB'_t$ ) and thus generates the subgoal dependency graph  $G'_t$  on the tth step. Furthermore, we note that since  $KB'_t$  contains the subset of  $KB \cup H$  that appears as labels in  $G'_t$ , every vertex of  $G'_t$  that is not deemed successful from  $KB'_t$  is likewise not successful from  $KB \cup H$  in the graph generated on the *t*th step on input  $\varphi$  and  $KB \cup H$ . Therefore, if Algorithm 2 runs for  $t^*$  iterations,  $\varphi$  is successful from  $KB'_{t^*}$ . Moreover, as EXPLORE continues to propose the vertices of  $G'_t$  not successful from  $KB'_t$  on each step (since it is oblivious) until the vertex labeled by  $\varphi$  is successful, another unsuccessful vertex must exist. Therefore the algorithm can only terminate before  $t^*$  iterations if TEST returns a proof and so either way Algorithm 2 returns a proof of  $\varphi$  in  $\mathcal{P}$  from some  $KB'_t$ .

The running time is bounded as follows: we see that the algorithm runs for no more iterations than before, and the final size of  $KB'_t$  is at most |KB| plus the algorithm's running time, since the algorithm creates vertices representing each formula added to  $KB'_t$ . Ignoring the time to test the proposed vertices for membership in  $KB'_t$ , the running time may be at most  $T(N, |\varphi|, |KB'_t|) \leq T(N, |\varphi|, |KB| + T(N, |\varphi|, |KB|))$ . Now, each formula tested appears as a premise in some proof in  $\mathcal{P}$  and therefore has a representation of size at most  $B(|\varphi|)$ . Since we can determine the witnessed value of a formula on a given obscured scene in linear time the time bound follows.

We now argue that with probability  $1 - \delta$  over the example obscured scenes provided to the algorithm as input, any proof that could be returned by Algorithm 2 uses a knowledge base  $KB \cup H'$  such that the formula  $h'_1 \wedge \cdots \wedge h'_k$  (for  $H' = \{h'_1, \ldots, h'_k\}$ ) is  $(1 - \epsilon)$ -valid. This will establish the theorem as the existence of such a proof guarantees that the query  $\varphi$  is  $(1 - \epsilon)$ -valid, so if the first case holds, the algorithm cannot produce a proof except with probability  $\delta$ ; and likewise, in the second case, the proof returned by the algorithm is satisfactory with probability  $1 - \delta$ .

To this end, we note that since M is assumed to be  $(1 - \eta(|\varphi|))$ -concealing with respect to the premises that may appear on any proof of  $\varphi$  in  $\mathcal{P}$ , for any proof using a set of premises that is *not*  $(1 - \epsilon)$ -valid, Proposition 14 shows that each example produces an obscured scene  $\rho$  for which  $h'_i|_{\rho} = 0$  for some  $h'_i$  used as a premise with probability at least  $\epsilon \eta(|\varphi|)$ . Therefore, in a sample of  $\Omega(\frac{1}{\epsilon \eta(|\varphi|)}(B(|\varphi|) +$  $\log (1/\delta)$  independent obscured scenes, the probability that no premise of such a proof has  $h'_i|_{\rho} = 0$  for any  $\rho$  in the sample is at most  $\delta \cdot 2^{-B(|\varphi|)}$ ; as the proofs in  $\mathcal{P}$  for  $\varphi$  have encodings of at most  $B(|\varphi|)$  bits, a union bound over these proofs gives that the overall probability of some proof having no  $\rho$  in the sample for which  $h'_i|_{\rho} = 0$  for some premise in the proof is at most  $\delta$ . Now, as the algorithm only returns proofs using premises contained in the sets  $KB'_t$  which in particular do not contain formulas h' such that  $h'|_{\rho} = 0$  for any  $\rho$ in the sample, we see that with probability  $1 - \delta$ , the algorithm does not return a proof with a set of premises that is not  $(1 - \epsilon)$ -valid, as needed.

### Example: backward chaining

If we represent chaining proofs by the sequence of inferred ground atomic formulas (using  $\log N$  bits for each), then since any proof needs only write down an atomic formula at most once, we can use the bound  $B = N \log N$  in the statement of Theorem 20. (The size of the query  $\ell$  is always the length of a single ground atomic formula,  $\log N$  bits.) So, after applying the transformation depicted in Algorithm 2 to the standard backward-chaining algorithm, Theorem 20 establishes that this modified backward chaining algorithm finds chaining proofs of queries using not only ground atomic formulas from the explicitly given KB, but also additional formulas that are almost always true. The modified algorithm automatically supplements a given KB with any such additional ground atomic formulas that suffice to complete some chaining proof of a query if one exists, provided further that the masking process has bounded concealment with respect to ground atomic formulas-meaning here, the masking process leaves the value of each ground atomic formula present with some bounded probability when it is false.

Chaining does not feature a rule of inference that allows new rules to be derived, so chaining algorithms never need to consider rules outside KB. Hence, the proposed generic transformation does not learn such rules. Other logics such as resolution, which allow richer kinds of formulas to be derived, yield more interesting query-driven learning. In principle one could also consider a variant of backward-chaining in which rules are learned as well. The difficulty with such a variant lies in controlling the complexity of the search.

#### 3.1 Skeptical query-driven learning

Theorem 20 relies on an assumption of bounded concealment, and uses a credulous learning strategy of searching for hypotheses for which we do not possess counterexamples. A more conservative strategy would replace the condition "for no  $\rho_i$  is  $h|_{\rho_i} = 0$ " in Algorithm 2 with the condition "for all  $\rho_i$ ,  $h|_{\rho_i} = 1$ ." An *h* that is witnessed true with probability 1 will pass this condition. Moreover, if  $h|_{\rho_i} = 1$  for  $\rho_i = m_i(x_i)$  (where  $m_i$  is drawn from *M* and  $x_i$  is drawn from *D*), then  $h|_{x_i} = 1$  as well. Thus, the probability that an *h* that is *not*  $(1 - \epsilon)$ -valid with respect to *D* passes this test for *m* examples is less than  $(1 - \epsilon)^m$ . We can use this observation in place of Proposition 14 to finish an analogous proof, given that we are searching for an *H* that is always *witnessed* rather than one that is merely perfectly *valid*. We leave further details to an interested reader.

#### **Example application: learning input filters**

We note that our transformation for skeptical learning of rules could be applied to static program analysis algorithms to automate the generation of sound and approximately complete input filters. For example, the SIFT system [Long *et al.*, 2014] is based on a set of sound transformation rules for analyzing integer overflow errors in a given program. Its associated static analysis algorithm uses the knowledge base given by these transformation rules and the program code to generate symbolic expressions that are propagated backwards from integer operations that might produce overflows, until they refer only to program inputs. The condition expressed by these expressions may then be used to filter out inputs that do not satisfy the condition. The soundness of SIFT's transformation rules ensures that no input that passes this condition generates an integer overflow error.

We can interpret SIFT as taking the safety property of "no integer overflows occur at the given point in the program" as a query, and seeking a proof of this query using a property of the input, together with the transformation rules and program code. Note that once SIFT generates expressions that refer only to input values, the conditions they express are witnessed against example inputs, if they are  $(1 - \epsilon)$ -valid for inputs in practice. Thus, we can apply the transformation of the skeptical variant of Algorithm 2 to the static analysis algorithm used by SIFT, and we would obtain an algorithm with a similar termination condition, with the added requirement that the condition found must be witnessed on a set of given examples.

Thus, the distinction between the approach taken by Long et al. and our transformation is that SIFT has no guarantee that it produces a rule that is testable on real inputs.<sup>1</sup> SIFT does not use any training data, and simply terminates once it finds a rule that refers only to the input; thus, while this rule is sound – inputs that satisfy it provably do not generate integer overflow errors – it has no guarantee of completeness, approximate or otherwise. Indeed, SIFT conservatively considers all possible execution paths and relatedly uses some hard-coded limits on, for example the number of loop iterations it considers in search of loop invariants, to ensure termination. If this limit is exceeded because the loop potentially relies on an unbounded number of values (for example), then SIFT simply fails to find a condition. Thus, there is scope for a backtracking variant of SIFT's static analysis algorithm to obtain greater completeness by iteratively refining a symbolic condition. Under our transformation, we would then obtain an algorithm that searches for a condition on the inputs that empirically satisfies witnessing for a large fraction of a training set of benign inputs.

### 3.2 Query-driven learning in treelike resolution

Recall that *resolution* is a logic that operates on *clauses* (ORs of literals), using two kinds of inference rules: *cut* and (optionally) *weakening*. Cut takes two clauses  $C = C' \lor \alpha$  and  $D = D' \lor \neg \alpha$  and produces a clause of the form  $C' \lor D'$ . (More general variants use substitutions to unify distinct atomic formuals  $\alpha$  and  $\neg \alpha'$ .) Weakening, by contrast, simply adds new literals to the clause. Resolution is typically used to prove a DNF (an OR of ANDs) by deriving an (unsatisfiable) empty clause from its negation, a CNF.

DPLL [Davis and Putnam, 1960; Davis *et al.*, 1962] is another example of such a goal-directed search algorithm. In particular, bounded variants of DPLL that (efficiently) solve the proof search problem for space-bounded treelike resolution are known [Kullmann, 1999; Esteban and Torán, 2001]. This is the fragment of resolution refutations that can be derived while (*i*) storing at most *s* clauses in memory simultaneously and (*ii*) "forgetting" a clause as soon as it is used in a proof step (so that it must be derived again if it is needed again). This is a second example of an algorithm into which we can introduce query-driven explicit learning along the lines of Theorem 20. The algorithm will be more interesting because it will discover a CNF that suffices to complete the proof out of an exponentially large (in terms of the number of ground atomic formulas) set of possible such formulas.

Unfortunately, we cannot apply Theorem 20 directly, as the standard algorithm is not actually *oblivious* in our strict sense. The difficulty is that the base case of the recursive algorithm involves a search for a hypothesis clause for which we can derive the current clause via weakening. This "looking ahead" into the hypothesis set means that the algorithm may not engage in exactly the same search pattern if we modify the hypothesis set during the search. Nevertheless, the use is innocuous enough that essentially the same technique can be used to give a variant of the algorithm that learns an explicit set of clauses from the data.

Our analysis of explicit query-driven learning (following Theorem 20) still requires a bound on the lengths of the proofs in terms of the space (and number of ground atomic formulas). We will need the observation that DPLL-like algorithms produce *normal* resolution proofs:

**Definition 21 (Normal)** We will say that a resolution proof is normal if in its corresponding DAG:

- 1. All outgoing edges from Cut nodes are directed to Cut nodes.
- 2. The clauses labeling any path to the sink from a Cut node contain literals using every variable along the path.

<sup>&</sup>lt;sup>1</sup>Nevertheless, it has been empirically demonstrated that for a certain piece of software, SIFT produces rules that are satisfied by real inputs with high probability on a natural distribution [Juba *et al.*, 2015].

**input** : CNF  $\varphi$ , integer space bound  $s \ge 1$ , current clause C, list of obscured scenes  $\rho^{(1)}, \ldots, \rho^{(m)}$ . Learn+SearchSpace $(\varphi, s, C, (\rho^{(1)}, \ldots, \rho^{(m)}))$ begin if No  $\rho^{(i)}$  has  $C|_{\rho^{(i)}} = 0$  then | **return** A proof asserting C (from H). end else if C is a superset of some clause C' of  $\varphi$  then **return** *The weakening derivation of C from C*′*.* end else if s > 1 then **foreach** Literal  $\ell$  such that neither  $\ell$  nor  $\overline{\ell}$  is in C do **if**  $\Pi_1 \leftarrow \text{Learn+SearchSpace}$  $(\varphi, s - 1, C \lor \ell, (\rho^{(i)} : \ell|_{\rho^{(i)}} \neq 1))$  does not *return* none **then**  $\textbf{if}\,\Pi_2 \leftarrow \texttt{Learn+SearchSpace}$  $(\varphi, s, C \vee \overline{\ell}, (\rho^{(i)} : \ell|_{\rho^{(i)}} \neq 0))$  does not return none then **return** Derivation of C from  $\Pi_1$  and  $\Pi_2$ end else return none end end end return none end

Algorithm 3: Space-bounded resolution with learning

3. A given variable is used in at most one cut step and at most one weakening step along every path from a source to a Cut node.

Our bound is now given in the following lemma, slightly modified from the work of Ehrenfeucht and Haussler [1989].

#### Lemma 22 (Lemma 1, Ehrenfeucht and Haussler 1989)

Let k be the number of nodes in a space-s normal treelike resolution proof over N ground atomic formulas where  $N \ge s \ge 1$ . Then,

- $I. 2^{s} 1 \le k \le 2(eN/(s-1))^{s-1}$  where e is the base of the natural logarithm.
- 2. There are at most  $(8N)^{(eN/(s-1))^{s-1}}$  space-s normal treelike proofs that do not use weakening.

**Theorem 23** Let a clause C and a (KB) CNF  $\varphi$  be given. Suppose the examples are drawn from a masking process that is  $(1 - \eta)$ -concealing with respect to CNFs of size  $(eN/s - 1)^{s-1}$  for the distribution D; suppose further that  $\varphi$ is perfectly valid with respect to D and there exists some other perfectly valid CNF H for which there is a space-s treelike resolution proof of C from  $\varphi \wedge H$ . Then, Algorithm 3 run on  $\varphi$ and C with parameter s on a sample of size  $\Theta((N^{s-1} \log N + \log \frac{1}{\delta})) \frac{1}{\eta\epsilon})$  runs in time  $O(\frac{N^{2(s-1)}|\varphi|}{\eta\epsilon}(N^{s-1} \log N + \log \frac{1}{\delta}))$ and returns a proof of C from  $\varphi \wedge H'$  for some CNF H' of size  $O(N^{s-1})$  that is  $(1 - \epsilon)$ -valid with respect to D with probability  $1 - \delta$ . Similarly, if  $[\varphi \Rightarrow C]$  is not  $(1 - \epsilon)$ -valid, Algorithm 3 rejects in the same time bound using the same

### number of examples.

**Proof:** First, consider the (possibly exponential size) formula  $\tilde{H}$  consisting of all clauses that are consistent with the obscured scenes  $\rho^{(1)}, \ldots, \rho^{(m)}$ . Noting we don't need to use weakening for clauses from  $\tilde{H}$  since any clause that would be derived by weakening is also in  $\tilde{H}$ , the standard analysis of algorithms for space-bounded treelike resolution [Kullmann, 1999] establish that Algorithm 3 finds a normal space-s treelike resolution proof of the input C from  $\varphi \wedge \tilde{H}$  and runs in time  $O(m|\varphi|N^{2(s-1)})$  on a sample of size m. When a 1-valid space-s treelike proof is assumed to exist, it is in particular consistent with every sample with probability 1, so the algorithm outputs some proof in this case. It remains only to show that, for a sample of size  $\Theta(\frac{1}{\eta\epsilon}(N^{(s-1)}\log N + \log \frac{1}{\delta}))$ , any such proof has its leaves labeled with a  $(1-\epsilon)$ -valid CNF with probability at least  $1 - \delta$  (and so in particular, the algorithm cannot return a proof if  $[\varphi \Rightarrow C]$  is not  $(1 - \epsilon)$ -valid).

Consider any space-s normal treelike resolution proof that has leaves that are *not* labeled by a  $(1 - \epsilon)$ -valid CNF. Since, by part 1 of Lemma 22, this CNF has at most  $O(N^{s-1})$ clauses, Proposition 14 shows that each example produces a counterexample to this CNF with probability at least  $\eta \epsilon$ . Thus, in a sample of size  $\Omega(\frac{1}{\eta\epsilon}(N^{s-1}\log N + \log \frac{1}{\delta}))$ , the probability that this CNF is consistent with the sample is at most  $\delta N^{-\Omega(N^{s-1})}$ . Now, by part 2 of Lemma 22, there are at most  $N^{O(N^{s-1})}$  possible proofs (up to weakening steps), where we notice that Algorithm 3 introduces weakening steps iff the clause is consistent with some clause of the (fixed) input CNF  $\varphi$ . Therefore, the algorithm indeed considers at most  $N^{O(N^{s-1})}$  distinct proofs, so for a suitable choice of constant in the sample size, a union bound gives the probability that Algorithm 3 encounters some proof from a CNF that is not  $(1 - \epsilon)$ -valid but consistent with the sample is at most  $\delta$ . Since the algorithm only outputs proofs that are consistent with the sample, we therefore find that any proof it outputs is derived from a CNF that is  $(1 - \epsilon)$ -valid with respect to D with probability at least  $1 - \delta$ , establishing the claim.

Lemma 22 also shows treelike proofs of size k are necessarily space- $\log(k + 1)$ , so this gives a quasipolynomial time and sample complexity algorithm for general treelike proofs.

# **4** Directions for future work

One main direction for future work concerns a slightly relaxed variant of the skeptical learning strategy, in which we try to learn rules that are simultaneously witnessed true with maximum frequency, which may be less than 1. What makes this formulation challenging is that it cannot be achieved by just seeking that the formulas at the individual nodes are each witnessed with some probability  $1 - \epsilon$ : it matters which  $\epsilon$ fraction of example scenes are not witnessed across the various rules, since we are interested in how many examples in total fail to witness at least one of the hypotheses used in the proof. This formulation seems to be a much harder computational problem, so it makes sense to ask what kind of approximate solutions can be obtained.

Another direction for work concerns relational reasoning

algorithms. The usual algorithms for backward search in relational reasoning generate substitutions during the search, rather than generating grounded versions of the rules as we do here. Although this creation of substitutions may create a "non-oblivious" search (as viewed on the ground atomic formulas), we suspect that it may again be innocuous enough that our main theorem will still hold, as in the example of weakening in resolution. Such algorithms would be much more efficient, of course. The main difference is that we now need to identify unifiers against the set of (all) example scenes (in addition to formulas in the KB).

A related question, along the lines of the above but perhaps more ambitious is, can we learn universally quantified expressions in infinite or open domains? Again, our current method generates ground expressions, and so we can only consider domains with a reasonable number of elements. But, the credulous bounded concealment definition at least raises the possibility that we might be able to infer a universally quantified statement based merely on the lack of observed counterexamples. Of course, such inferences lean heavily on the bounded concealment assumption.

A final direction is the development of further applications of such algorithms. In addition to the natural application of the algorithm in extracting knowledge that is suitable for human inspection in query driven learning, we have identified two domains in which the kind of sound and approximately complete rules our method generates would provide a useful filtering criterion. It is natural to ask if there are any others.

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