On the non-efficient PAC learnability of conjunctive queries

Balder ten Cate[a,1], Maurice Funk[b], Jean Christoph Jung[c], Carsten Lutz[b]

[a] *ILLC, University of Amsterdam, Postbus 94242, Amsterdam, 1090 GE, The Netherlands*
[b] *Leipzig University, Augustusplatz 10, Leipzig, 04109, Germany*
[c] *TU Dortmund University, August-Schmidt-Straße 1, Dortmund, 44227, Germany*

Abstract

This note serves three purposes: (i) we provide a self-contained exposition of the fact that conjunctive queries are not efficiently learnable in the *Probably-Approximately-Correct (PAC)* model, paying clear attention to the complicating fact that this concept class lacks the *polynomial-size fitting property*, a property that is tacitly assumed in much of the computational learning theory literature; (ii) we establish a strong negative PAC learnability result that applies to many restricted classes of conjunctive queries (CQs), including acyclic CQs for a wide range of notions of acyclicity; (iii) we show that CQs (and UCQs) are efficiently PAC learnable with membership queries.

Keywords: Computational Learning Theory, Conjunctive Queries, Inductive Logic Programming

1. Introduction

Conjunctive queries (CQs) are an extensively studied database query language that plays a prominent role in database theory. CQs correspond precisely to Datalog programs with a single non-recursive rule and to the positive-existential-conjunctive fragment of first-order logic. Since the evaluation problem for conjunctive queries is NP-complete, various tractable subclasses have been introduced and studied. These include different variants of acyclicity, such as α-acyclicity, β-acyclicity, γ-acyclicity, and Berge-acyclicity, which form a strict hierarchy with Berge-acyclicity being most restrictive [15]. A landmark result by Grohe states that a class of CQs is tractable if and only if the treewidth of all CQs in it is bounded by a constant (under certain assumptions) [18, 24].

In this note, we consider the learnability of CQs from labeled examples, in Valiant's well-known *Probably Approximately Correct* (PAC) learning model [28]. We give a self-contained proof that the class of all CQs as well as all classes of acyclic CQs mentioned above are *not* efficiently PAC learnable. While the general idea of our proof is due to [23, 19], we strengthen the result in several respects and present it in a form that is easily accessible to modern-day database theorists.

The result $q(I)$ of evaluating a k-ary CQ q on a database instance I is a set of k-tuples of values from the active domain of I. An *example*, then, is most naturally taken to be a pair $(I, \mathbf{a})$ where I is a database instance and $\mathbf{a}$ is a k-tuple of values from the active domain of I. The example is *positive* if $\mathbf{a} \in q(I)$ and *negative* otherwise.

An *efficient PAC algorithm* is a (possibly randomized) polynomial-time algorithm that takes as input a set of examples drawn from an unknown probability distribution D and labeled as positive/negative according to an unknown target CQ q^* to be learned, and that outputs a CQ q, such that, if the input sample is sufficiently large, then with probability at least $1 - \delta$, q has expected error at most ϵ, meaning that if we draw an example e from D, then with probability $1 - \epsilon$, q and q^* assign the same label to e (cf. Figure 1). The required number of examples must furthermore be bounded by a function polynomial in $|q^*|$, $1/\delta$, $1/\epsilon$, and the example size. We give a precise definition in Section 2. Note that since a PAC algorithm does not know the example distribution D, it must perform well for *all* distributions D. In this sense, the PAC model captures a strong form of distribution-independent learning.

Our main result is the following, stated, for simplicity, for unary CQs:

Theorem 1.1. *(assuming RP $\neq$ NP) Let C be any class of unary CQs over a fixed schema $\mathbf{S}$ that contains at least one binary relation symbol and one unary relation symbol. If C includes all path-CQs, then C is not efficiently PAC learnable, even w.r.t. single-instance example distributions.*

Here, RP denotes the class of problems solvable by a randomized algorithm with one-sided error that runs in polynomial time, and by a *path-CQ* we mean a unary CQ of the form

$$q(x_1) \coloneq \exists x_2 \ldots x_n (R(x_1, x_2) \land \cdots \land R(x_{n-1}, x_n) \\ \land P(x_{j_1}) \land \cdots \land P(x_{j_m}))$$

where R is a binary relation symbol and P is a unary relation symbol. That is, a path-CQ is a very simple type

[1] Research supported by the European Union's Horizon 2020 research and innovation programme (MSCA-101031081). We thank Victor Dalmau for helpful feedback on an early version of this note.

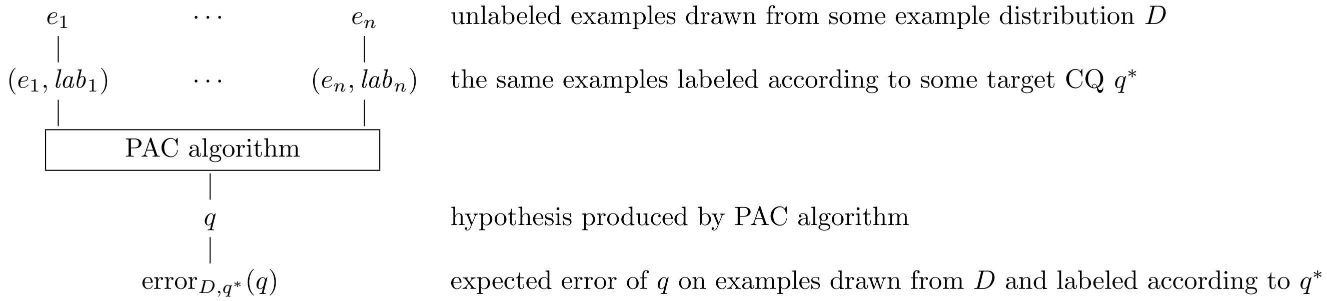

e_1
$\cdots$
e_n
unlabeled examples drawn from some example distribution D
(e_1, lab_1)
$\cdots$
(e_n, lab_n)
the same examples labeled according to some target CQ q^*
PAC algorithm
q
hypothesis produced by PAC algorithm
$\text{error}_{D,q^*}(q)$
expected error of q on examples drawn from D and labeled according to q^*

Figure 1: Graphical depiction of a PAC algorithm

of CQ that describes an outgoing directed path decorated with a single unary relation symbol.

With a *single-instance example distribution*, we mean an example distribution D such that for some database instance I, D assigns non-zero probability mass only to examples of the form $(I, \mathbf{a})$. This captures the natural scenario of learning CQs from positive and negative examples that all pertain to a single given database instance. Clearly, efficient PAC learnability w.r.t. all example distributions implies efficient PAC learnability w.r.t. single-instance distributions.

Note that efficient PAC learnability is not an anti-monotone property of query classes, and Theorem 1.1 says more than just that path-CQs are not efficiently PAC learnable. In particular, Theorem 1.1 implies that *the class of all CQs* is not efficiently PAC learnable, and the same is true for all classes of acyclic CQs mentioned above since path-CQs belong to all of these classes. Theorem 1.1 also implies non-efficient PAC learnability of concept expressions in the description logics $\mathcal{EL}$ and $\mathcal{ELI}$ (even in the absence of a TBox), see e.g. [17] and references therein.

It is worth comparing the notion of a *PAC learning algorithm* to that of a *fitting algorithm*. Both types of algorithms take as input a set of labeled examples. A fitting algorithm decides the existence of a CQ that agrees with the labels of the input examples. The fitting problem is coNExpTime-complete for CQs [29, 5] and, in fact, is known to be hard already for some more restricted classes of acyclic CQs [5, 16, 17]. A PAC algorithm, on the other hand, produces a CQ that, with high probability, has a low expected error, but is not required to fit the input examples. Despite these differences, it is well-known that for concept classes that are both polynomial-time evaluable and have the polynomial-size fitting property (defined in Section 2), NP-hardness of the fitting problem implies the non-existence of an efficient PAC learning algorithm [26], see Proposition 2.6 below. Unfortunately, the concept class of CQs has neither of these properties. A main difficulty of our proof of Theorem 1.1 (which is nevertheless based on a reduction from an NP-hard fitting problem) is to find a way around this.

We also prove that PAC learnability of CQs can be recovered by extending the PAC model with membership queries, known from Angluin's [1] model of exact learning. In a membership query, the learner chooses an example $(I, \mathbf{a})$ and asks an oracle to provide, in unit time, the positive or negative labeling of $(I, \mathbf{a})$ according to the target query. In Angluin's model of exact learning, CQs are known to not be efficiently learnable with membership queries alone, but they are efficiently learnable when also equivalence queries are admitted (the learner may give a hypothesis query to the oracle and ask whether it is equivalent to the target query, requesting a counterexample if this is not the case). The latter is implicit in [6], an explicit proof can be found in [7], cf. also [3].

As pointed out in [6], the fact that CQs are efficiently exactly learnable with membership and equivalence queries implies PAC learnability with membership queries and an NP-oracle (cf. [1]), where the NP-oracle is used for evaluating hypotheses on examples. It was left open whether CQs are efficiently PAC learnable with membership queries *without* an NP-oracle. We give an affirmative answer to this question and show that it also extends to UCQs, that is, to disjunctions of conjunctive queries.

Theorem 1.2. *Fix any schema* $\mathbf{S}$ *and* $k \geq 0$. *The class of all* k*-ary CQs over* $\mathbf{S}$ *is efficiently PAC learnable with membership queries. The same is true for the class of all* k*-ary UCQs over* $\mathbf{S}$.

1.1. Related work

Haussler [19] shows that the class of Boolean CQs over a schema that contains an unbounded number of unary relation symbols is not efficiently PAC-learnable (unless RP = NP). The essential part of the proof is to show that the fitting problem for the same concept class is NP-complete. Over a schema that consists of unary relation symbols only, every CQ is trivially Berge-acyclic. Therefore, this implies that efficient PAC learnability fails for acyclic Boolean CQs, for any of the aforementioned notions of acyclicity. The fact that Haussler's result is stated for Boolean CQs and Theorem 1.1 is stated for unary CQs is an inessential difference (cf. [23]). The fact that the proof in [19] uses an unbounded number of unary relation symbols, however, is an important difference. Indeed, if one was to consider Boolean queries over a fixed finite schema that consists of unary relation symbols only, then the resulting concept class would be finite and trivially PAC learnable.

Kietz [23] proves that the class of unary CQs over a schema that contains a single binary relation symbol and an unbounded number of unary relation symbols is not PAC-learnable (unless RP = NP). Again the essential part of the proof is to show that the fitting problem is NP-complete. Kietz's result already applies to path-CQs of length 1 with multiple unary relation symbols. This is only possible because of the infinite schema, as, otherwise, the concept class is again finite and trivially PAC learnable.

Cohen [12] proves that the class of unary CQs over a schema that contains two binary relation symbols is not PAC-predictable unless certain assumptions from the field of cryptography fail. In *PAC prediction*, the output of the algorithm is not required to be a concept from the concept class, but instead must be any polynomial-time evaluable concept such as a polynomial-time algorithm. PAC learnability implies PAC predictability for concept classes that are polynomial-time evaluable (cf. Remark 6.3). Cohen's result already applies to path-CQs (defined slightly differently than above, using two binary relation symbols and no unary relation symbol – this difference is inessential). As a consequence, Cohen's result yields the restriction of Theorem 1.1 to polynomial-time evaluable classes C (such as the class of all acyclic CQs, under any of the mentioned notions of acyclicity), under cryptographic assumptions. Moreover, in contrast to PAC learnability, PAC predictability is an anti-monotone property of concept classes. Thus, Cohen's result also yields Theorem 1.1 for efficient PAC predictability in place of efficient PAC learnability, again under cryptographic assumptions.

In an earlier paper [11], Cohen had proved a related but weaker result that requires relation symbols of arity three. The work of Hirata [21], in a similar vain, shows that there is even a fixed database on which efficient PAC prediction (and thus also learning) of acyclic CQs is impossible – a stronger condition than single-instance example distributions. The result, however, requires ternary relation symbols and CQs of unbounded arity. We also remark that it follows from general results of Schapire, see Section 6.3 of [27], that any class of CQs that is NP-hard to evaluate is not efficiently PAC-predictable unless NP $\subseteq$ P/poly.

We consider, in this note, classes of CQs defined through acyclicity conditions. In the literature on inductive logic programming (ILP) various positive and negative PAC learnability results have been obtained for classes of CQs defined by different means (e.g., limitations on the use of existential variables, determinacy conditions pertaining to functional relations, and restricted variable depth). These are orthogonal to acyclicity. An overview can be found in [25, Chapter 18].

In [6], the authors study learnability of *GAV schema mappings*, which are closely related to *Unions of Conjunctive Queries (UCQs)*. Specifically, it was proved in [6] that GAV schema mappings are not efficiently PAC learnable, assuming RP $\neq$ NP, on source schemas that contain at least one relation symbol of arity at least two, using a reduction of the non-PAC-learnability of propositional formulas in positive DNF. This result immediately implies that, for any schema $\mathbf{S}$ containing a relation symbol of arity at least two, and for each $k \geq 0$, the class of k-ary UCQs over $\mathbf{S}$ is not efficiently PAC learnable, assuming RP $\neq$ NP. Additionally, in [6], the authors completely map out the (non-)learnability of restricted classes of UCQs definable by conditions on their Gaifman graph.

There is also another line of work on PAC learnability of conjunctive queries [13, 14, 10] that is somewhat different in nature: one fixes a schema $\mathbf{S}$ and an $\mathbf{S}$-instance I and defines a concept class where the concepts are now all relations over the active domain of I definable by a k-ary CQ (as evaluated in I). PAC learning for various classes of Boolean formulas, such as 3-CNF, can be seen as a special case of this framework, for a specific choice of schema $\mathbf{S}$ and (two-element) instance I, where k then corresponds to the number of Boolean variables. Since, for a fixed choice of k, this yields a finite concept class, in this setting, one is interested in the complexity of PAC learning as a function of k. The mentioned papers establish effective dichotomies, showing that, depending on the choice of $\mathbf{S}$ and I, this concept class is either efficiently PAC learnable in k or is not even efficiently PAC predictable with membership queries in k (under suitable cryptographic assumptions). See also Remark 6.3 below.

2. Preliminaries

2.1. Conjunctive Queries

A *schema* $\mathbf{S}$ is a finite set of relation symbols with associated arity. An *instance* I over schema $\mathbf{S}$ is a finite set of facts over $\mathbf{S}$, where a *fact* is an expression of the form $R(a_1, \ldots, a_n)$ where $R \in \mathbf{S}$ is an n-ary relation symbol and $a_1, \ldots, a_n$ are *values*. The *active domain* of an instance I, denoted by $\mathrm{adom}(I)$ is the (finite) set of values that occur in the facts of I.

A k-ary *conjunctive query (CQ)* over a schema $\mathbf{S}$, for $k \geq 0$, is an expression of the form

$$q(\mathbf{x}) :- \exists \mathbf{y}(\alpha_1 \wedge \cdots \wedge \alpha_n)$$

where $\mathbf{x}, \mathbf{y}$ are tuples of variables, $\mathbf{x}$ has length k, and each conjunct α_i is an atomic formula that uses a relation symbol from $\mathbf{S}$ and only variables from $\mathbf{x}$ and $\mathbf{y}$, such that each variable from $\mathbf{x}$ occurs in some conjunct. We denote by $q(I)$ the set of all k-tuples $\mathbf{a}$ such that $I \models q(\mathbf{a})$.

We will not define in depth the various notions of acyclicity that have been mentioned in the introduction, but we reiterate here that they form a hierarchy with Berge-acyclicity being most restrictive, and that all mentioned classes of acyclic queries are polynomial-time evaluable, meaning that given a CQ $q(\mathbf{x})$ from the class, an instance I and a tuple $\mathbf{a}$ of elements of the active domain of I, we can decide in polynomial time whether $\mathbf{a} \in q(I)$.

The definition of *path-CQs* was given in Section 1.

Example 2.1. *An example of a path-CQ is the query*

$$q(x) :- \exists yzu(R(x, y) \wedge R(y, z) \wedge R(z, u) \wedge P(y) \wedge P(u)).$$

Every path-CQ is Berge-acyclic and hence polynomial-time evaluable, see e.g. the classic paper where this is proved for α-acyclic queries [15].

2.2. Computational Learning Theory

A *concept class* is a triple $C = (\Phi, Ex, \models)$, where Φ is a set of concepts, Ex is a set of examples, and $\models \subseteq Ex \times \Phi$ represents whether an example is a positive or a negative example for a given concept. We also denote by $lab_\phi(e)$ the *label* of e according to ϕ, that is, $lab_\phi(e) = +$ if $e \models \phi$ and $lab_\phi(e) = -$ otherwise. Two concepts $\phi, \phi' \in \Phi$ are said to be *equivalent* if $lab_\phi(e) = lab_{\phi'}(e)$ for all $e \in Ex$.[2]

A *labeled example* is a pair (e, s) with $e \in Ex$ and $s \in \{+, -\}$. A concept $\phi \in \Phi$ *fits* a set of labeled examples E if $lab_\phi(e) = s$ for all $(e, s) \in E$.

We only consider countable concept classes. Concepts and examples are assumed to have an effective representation and a corresponding notion of size, which is denoted by $|\phi|$ and $|e|$, respectively. We also denote the set of all concepts (examples) of size at most n by $\Phi_{(n)}$ (respectively, $Ex_{(n)}$). For a finite set of (possibly labeled) examples E, $||E|| = \sum_{e \in E} |e|$.

The following two properties of concept classes will be important for us later on:

Definition 2.2 (Polynomial-time evaluability). *A concept class is* polynomial-time evaluable *if there exists a polynomial-time algorithm that, given $\phi \in \Phi$ and $e \in Ex$, outputs a Boolean indicating whether $e \models \phi$.*

Definition 2.3 (Polynomial-size fitting property). *A concept class has the* polynomial-size fitting property *if for every finite set of labeled examples E, the existence of a concept that fits E implies that there exists a fitting concept whose size is bounded by a polynomial in $||E||$.*

We now define the two algorithmic problems mentioned in the introduction, namely fitting and PAC learning.

Definition 2.4 (Fitting problem). *The* fitting problem *(also known as* consistency problem *or* separability problem*) for a concept class C is the problem to decide, given a finite set of labeled examples E, whether there exists a concept in C that fits E.*

In order to define PAC algorithms, we first need to introduce some terminology and notation. An *example distribution* for a concept class $C = (\Phi, Ex, \models)$ is a probability distribution D over Ex. Given concepts $\phi, \phi^* \in \Phi$ and an example distribution D,

$$\text{error}_{D,\phi^*}(\phi) = \Pr_{e \in D}(lab_\phi(e) \neq lab_{\phi^*}(e))$$

is the expected error of ϕ relative to ϕ^* and D.

Definition 2.5 (Efficient PAC learnability). *An* efficient PAC algorithm *for a concept class C is a pair (A, f) where*

- *A is a randomized polynomial-time algorithm that takes as input a set of labeled examples and outputs a concept from C, and*
- *$f(\cdot,\cdot,\cdot,\cdot)$ is a polynomial function, such that, for all $\delta, \epsilon \in (0, 1)$, all $n, m \in \mathbb{N}$, all example distributions D over $Ex_{(m)}$, and all $\phi^* \in \Phi_{(n)}$, if the input consists of at least $f(1/\delta, 1/\epsilon, n, m)$ examples drawn from D and labeled according to ϕ^*, then with probability at least $1 - \delta$, A outputs a concept ϕ with $\text{error}_{\phi^*,D}(\phi) \leq \epsilon$.*

If such an algorithm exists, we say that C is efficiently PAC learnable*. If the function f depends only on δ and ϵ and not on n, m, then we say that (A, f) is a* strongly efficient *PAC algorithm, and that the concept class C is* strongly efficiently PAC learnable.

This definition of efficient PAC algorithms is modeled after the one in the textbook [2], in line with the literature on inductive logic programming (cf., e.g., [25]). Our results also apply to the alternative oracle-based definition.[3] We prefer the above definition as it exhibits more clearly the relationship to fitting algorithms.

The following proposition relates the two algorithmic problems (fitting and PAC learning) to each other.

Proposition 2.6 (Pitt and Valiant [26]). *Let C be a polynomial-time evaluable concept class with the polynomial-size fitting property. If C is efficiently PAC learnable, then the fitting problem for C is in RP.*

[2] This deviates slightly from the standard convention, which defines a concept class to be a pair (Ex, C) where $C \subseteq \wp(Ex)$ (and, for $c \in C$, $|c|$ to be the size of the smallest representation of c). The difference is non-essential. We prefer this presentation as it makes it easier to spell out unambiguously the algorithmic problems that we consider (e.g., Definition 2.2)

[3] Following the oracle-based presentation in, e.g., [22], one can define an efficient PAC learning algorithm for a concept class C to be a randomized polynomial-time algorithm that takes as input $\delta, \epsilon \in (0, 1)$ and a bound $n \in \mathbb{N}$ on the size of the target concept ϕ^*, and that has access to an oracle $EX_{\phi^*,D}$ which, when called, returns (in unit time) a random example drawn from D and labeled according to ϕ^*. For every choice of δ, ϵ, $\phi^* \in \Phi$, $n \geq |\phi^*|$, and for every example distribution D, the algorithm must terminate in time polynomial in $1/\delta, 1/\varepsilon$, n, and the size of the largest example returned by the oracle. Furthermore, it must return a concept that with probability $1 - \delta$ satisfies $\text{error}_{\phi^*,D}(\phi) < \epsilon$.

Note that, under this definition, not only the running time of the algorithm but also the number of examples drawn from the distribution may depend on the size of examples: if the learning algorithm encounters a large example e, it may follow up by requesting a number of additional examples that is polynomial in the size of e.

Efficient PAC learnability in the above sense implies efficient PAC learnability in the sense of Definition 2.5: one can turn an oracle-based learning algorithm into a learning algorithm according to Definition 2.5 by drawing examples uniformly at random from the input batch to answer EX oracle calls. (To guarantee polynomial-time termination, even on inputs where a fitting concept does not exist, we can maintain a counter and terminating after $p(n)$ steps, where p is the polynomial that bounds the running time of the oracle-based learner on consistent inputs). Our negative learnability results thus apply also to the oracle-based definition. A classic paper that shows equivalence of different PAC learning models is [20].

This is a well-known fact (cf. also [2, Thm 6.2.1]), although not in this precise formulation, as, usually, polynomial evaluability and the polynomial-size fitting property are tacitly assumed (which has sometimes led to mistakes, e.g., in the derivation of Corollary 15 in [23]). To be self-contained, we outline the proof of Proposition 2.6 here.

Proof. (of Proposition 2.6) Assume that there is an efficient PAC algorithm (A, f) for C. We use it to solve the fitting problem for C in randomized polynomial time. Assume that a set E of k labeled examples is given as the input. Let $n = p(||E||)$, where p is the polynomial witnessing the fact that C has the polynomial-size fitting property. Let D be the uniform distribution on E (where each example in E gets probability mass $1/k$), and let m be the maximum size of an example in E. Pick $\delta < .5$ and $\epsilon < 1/k$. We generate a new (polynomial-sized) collection of labeled examples E' by drawing $f(1/\delta, 1/\epsilon, n, m)$ samples from distribution D, and run algorithm A on it. Finally, we check that the output of A is a fitting concept for E. If so, we answer Yes. Otherwise, we answer No.

Clearly, if there is no fitting concept, the output will be No. If, on the other hand, there is a fitting concept, then there is one of size at most n, and hence, with probability $1 - \delta$, the algorithm will output a concept with error less than ϵ. This in fact implies that the error is 0 (because if the query misclassifies an example to which D assigns non-zero mass, then it will have error at least $1/k$). Hence, with probability $1 - \delta > 0.5$ the algorithm outputs Yes. □

A variation on the same argument shows:

Proposition 2.7. *If a concept class is strongly efficiently PAC learnable, then it has the polynomial-size fitting property.*

Proof. The proof uses the same construction as before, except that the sample size now does not depend on n. Furthermore, we omit the verification step where we confirm that the produced concept fits the input examples. Instead, we just output the result of the learning algorithm. In this way, we obtain a randomized polynomial-time algorithm that has a non-zero probability of outputting a fitting concept for given input labeled examples, whenever a fitting concept exists. The polynomial-size fitting property immediately follows from this (the run that outputs a fitting concept does so in polynomial time). □

We also make use of the following trivial fact:

Proposition 2.8. *If a concept class $(\Phi, Ex, \models)$ is efficiently PAC learnable, then, for every $Ex' \subseteq Ex$, the concept class $(\Phi, Ex', \models)$ is also efficiently PAC learnable.*

Indeed, this follows from the fact that every example distribution over $Ex'_{(n)}$ is in particular also an example distribution over $Ex_{(n)}$ (that assigns no probability mass to any example in $Ex \setminus Ex'$).

Finally, we use a well known connection between PAC algorithms and *Occam algorithms*.

Definition 2.9 (Occam algorithm). *An* Occam algorithm *for a concept class $C = (\Phi, Ex, \models)$, with parameters $\alpha < 1$ and $k \geq 1$, is an algorithm that takes as input a set of labeled examples E and outputs a concept $\phi \in \Phi$ with $|\phi| \leq |E|^\alpha |\phi^*|^k$ that fits E provided that any concept from Φ does. Furthermore, the running time is required to be bounded by a polynomial in $|\phi^*|$ and $||E||$.*

Blumer *et al.* [4] proved that every Occam algorithm A yields an efficient PAC algorithm, namely $A' = (A, f)$, where the sample-size polynomial f is chosen such that

$$f(1/\delta, 1/\epsilon, n, m) = \left(\frac{n^k \ln 2 + \ln(2/\delta)}{\epsilon}\right)^{1/(1-\alpha)}.$$

Note that f does not depend on its fourth component m (i.e., the example size bound). Moreover, every Occam algorithm gives rise to an efficient PAC algorithm, not only in the sense of Definition 2.5 as explained above, but, by the same arguments, also when considering the oracle-based presentation of PAC algorithms (cf. Footnote 3).

Theorem 2.10 ([4]). *Every concept class for which there is an Occam algorithm is efficiently PAC learnable.*

3. Classes of CQs as Concept Classes

Each class of CQs can be naturally viewed as a concept class. Fix a schema $\mathbf{S}$, an arity $k \geq 0$, and a class C of k-ary CQs over $\mathbf{S}$. In the associated concept class $(C, Ex, \models)$, Ex is the class of all pairs $(I, \mathbf{a})$ with I an $\mathbf{S}$-instance and $\mathbf{a}$ a k-tuple of elements of the active domain of I, and $\models$ describes query answers, that is, $(I, \mathbf{a}) \models q(\mathbf{x})$ iff $\mathbf{a} \in q(I)$, for all $q(\mathbf{x}) \in C$ and $(I, \mathbf{a}) \in Ex$. We may abuse notation and refer to this concept class $(C, Ex, \models)$ simply as C when no ambiguity arises. The following theorem summarizes some basic properties.

Theorem 3.1 ([5, 8]). *Fix any schema $\mathbf{S}$ that contains at least one binary relation symbol, and some $k \geq 0$.*

1. *The concept class of k-ary CQs over $\mathbf{S}$ is not polynomial-time evaluable (unless P = NP). Indeed, its evaluation problem is NP-complete.*[4]
2. *The concept class of k-ary CQs over $\mathbf{S}$ lacks the polynomial-size fitting property. Indeed, the smallest fitting CQ for a given set of labeled examples is in general exponentially large.*
3. *The fitting problem for k-ary CQs over $\mathbf{S}$ is coNExpTime-complete.*

Let us now consider restricted classes of (unary) CQs that still include path-CQs. We will see in the next section that *every* such class of CQs has an NP-hard fitting problem (cf. Theorem 5.6). We observe here that every such class of CQs lacks the polynomial-size fitting property:

[4] The evaluation problem takes as input ϕ and e and asks if $e \models \phi$.

Theorem 3.2. *Fix a schema* $\mathbf{S}$ *that contains at least a binary and a unary predicate, and let* C *be any class of unary CQs over* $\mathbf{S}$ *that includes all path-CQs. Then* C *lacks the polynomial-size fitting property.*

Proof. Let $R \in \mathbf{S}$ be binary and $P \in \mathbf{S}$ unary. For $m \geq 1$, let L_m denote the "lasso" instance, with active domain $a_0^m, \ldots, a_{2m-1}^m$ consisting of the facts $R(a_i^m, a_{i+1}^m)$ for all $i < 2m-1$ and $R(a_{2m-1}^m, a_m^m)$ and $P(a_m^m)$.

For $i \geq 1$, let p_i be the i-th prime number (where $p_1 = 2$). By the prime number theorem, $p_i = O(i \log i)$.

Finally, for $n \geq 1$, let I_n be the disjoint union of L_{p_i} for $i = 1, \ldots, n$, extended with the fact $R(b, b)$ for a fresh value b. We now construct our set of examples E_n as follows:

- Positive example $(I_n, a_0^{p_i})$ for $i = 1 \ldots n$.
- Negative example (I_n, b).

It is easy to see that a fitting path-CQ for E_n exists, namely the query

$$q(x_1) :- \exists x_2 \ldots x_k (R(x_1, x_2) \wedge \cdots \wedge R(x_{k-1}, x_k) \wedge P(x_k))$$

where $k = \Pi_{i=1\ldots n}(p_i)$.

We claim that every CQ that fits the examples must be of size at least 2^n. Let $q(x)$ be any CQ that fits the examples. Since positive and negative examples are based on the same instance, we may assume that q is connected. First of all, note that q must contain a conjunct of the form $P(y)$ (otherwise it would fail to fit the negative example). Furthermore, y is not the free variable x and q uses only the relation symbols P and R (otherwise it would fail to fit any positive example). Consider the directed graph where the vertices are the variables of q and there is an edge from variable z to variable z' iff the atom $R(z, z')$ occurs in q. Since q is connected, there is an undirected path connecting x to y. Take any such path of minimal length. We can represent it as a sequence

$$x = x_0, \alpha_0, x_1, \alpha_1, \ldots, x_\ell = y$$

where for each $i < \ell$, α_i is an atom that occurs in q that is either $R(x_i, x_{i+1})$ (then α_i is a "forward edge") or $R(x_{i+1}, x_i)$ (then α_i is a "backward edge"). We define the net-length of this path to be the number of forward edges minus the number of backward edges.

Clearly, in order for the query q to be satisfied in a lasso instance L_m, the net length of the above path must be divisible by m. Therefore, since q fits all the examples constructed above, the net-length must be divisible by p_i, for all $i = 1 \ldots n$, and thus at least $\prod_{i=1\ldots n}(p_i)$. It follows, then, that also the length (in the ordinary sense) of the path must be at least $\prod_{i=1\ldots n}(p_i)$. Therefore, every CQ that fits the above examples must have at least $\prod_{i=1\ldots n}(p_i)$ variables, which exceeds 2^n. □

4. Failure of Strong PAC Learnability

By Proposition 2.7, Theorem 3.2 implies:

Corollary 4.1. *Fix any schema* $\mathbf{S}$ *that contains at least a binary relation symbol and a unary relation symbol. Let* C *be any class of unary CQs over* $\mathbf{S}$ *that includes all path-CQs. Then* C *is not strongly efficiently PAC learnable.*

Alternatively, Corollary 4.1 can be shown using a VC-dimension argument. In fact, we may then even drop the 'efficiently' from the statement. We define *strong PAC learnability* in the same way as *strongly efficient PAC learnability* (cf. Definition 2.5) except that A is not required to run in polynomial time and f is not required to be a polynomial function.

Theorem 4.2. *Fix any schema* $\mathbf{S}$ *that contains at least a binary relation symbol and a unary relation symbol. Let* C *be any class of unary CQs over* $\mathbf{S}$ *that includes all path-CQs. Then* C *is not strongly PAC learnable.*

Proof. Let us recall the definition of VC-dimension. We say that a concept class C *shatters* a set of examples S if for every subset $S' \subseteq S$ there is a $c \in C$ such that $S' = \{e \in S \mid e \models c\}$. The *VC-dimension* of C is the cardinality of the largest set of examples that is shattered by C, or infinite if arbitrarily large sets can be shattered. The fundamental theorem of statistical machine learning says that a concept class is strongly PAC learnable iff it has finite VC dimension [4].

Let $\mathbf{S}$ be a schema that contains a unary relation symbol P and a binary relation symbol R, and let C be a class of unary CQs over $\mathbf{S}$ that contains all path-CQs. We show that C has infinite VC-dimension.

Let $n > 0$. We construct a set S that contains n examples $(I_1, a_1), \ldots, (I_n, a_1)$. Each instance I_i contains an R-path of length $n-1$ starting at a_1, that is, $\text{adom}(I_i) = \{a_1, \ldots, a_n\}$ and $R(a_j, a_{j+1}) \in I_i$ for all $j \in \{1, \ldots, n-1\}$. Moreover, we include in I_i all facts $P(a_j)$ for $j \neq i$.

To show that C shatters S, let $S' \subseteq S$ be an arbitrary subset of S and let $X \subseteq \{1, \ldots, n\}$ be such that $S' = \{(I_i, a_1) \in S \mid i \in X\}$ and set $\overline{X} = \{1, \ldots, n\} \setminus X$. Let $q(x_1)$ be the path-CQ

$$q(x_1) :- \exists x_2 \ldots x_n (\bigwedge_{i=1\ldots n-1} R(x_i, x_{i+1}) \ \wedge \bigwedge_{j \in \overline{X}} P(x_j)).$$

One may verify that $S' = \{(I_i, a_1) \in S \mid q(a_1) \in I_i\}$. □

The concept class of path-CQs *is* polynomial-time evaluable, as follows from the fact that it forms a subclass of the class of α-acyclic CQs, which is polynomial-time evaluable [30]. We make use of this in the next section.

Theorem 4.3 ([30]). *Fix any schema* $\mathbf{S}$. *The concept class of path-CQs over* $\mathbf{S}$ *is polynomial-time evaluable.*

5. Non-Efficient PAC Learnability

We now consider PAC learnability in the non-strong version and show that *no class of unary CQs that includes all path-CQs is efficiently PAC learnable*, cf. Theorem 1.1 from the introduction.

Recall that we cannot use Proposition 2.6 directly to prove non-efficient PAC learnability, for two reasons. First, the polynomial-size fitting property does not hold for path-CQs. And second, the classes that we consider may contain CQs that are not path-CQs, and thus polynomial-time evaluability also fails, despite Theorem 4.3. To circumvent the latter issue, we work with a restricted class of instances.

5.1. Tree-Shaped Instances

Definition 5.1 (Tree-Shaped Instances and CQs). *Let* $\mathbf{S}$ *be a schema that consists of a binary relation symbol* R *and any number of unary relation symbols, and let* I *be an* $\mathbf{S}$*-instance. We say that* I *is* tree-shaped *if the following two conditions hold:*

1. *There is a function level*: $\text{adom}(I) \to \mathbb{N}$ *such that, for each fact* $R(a, b)$ *of* I, $\mathit{level}(b) = \mathit{level}(a) + 1$.
2. I *does not contain two binary facts* $R(a, b), R(a', b)$ *that agree on the second value but not on the first.*

A CQ over $\mathbf{S}$ *is said to be tree-shaped if its canonical instance is tree-shaped.*[5]

Lemma 5.2. *Fix a schema* $\mathbf{S}$ *that consists of one binary relation symbol and any number of unary relation symbols. Given a CQ* q *over* $\mathbf{S}$,

1. *we can test in polynomial time whether there exists a tree-shaped instance* I *such that* $q(I) \neq \emptyset$,
2. *if the answer to the above question is positive, then we can construct in polynomial time a tree-shaped CQ* q' *such that for all tree-shaped instances* I, $q(I) = q'(I)$.

Proof. It suffices to prove the claim for connected CQs (the general case then follows by a component-wise analysis). Therefore, let q be a connected CQ.

Let $\sim$ be the smallest equivalence relation over the variables of q such that, whenever $R(u, v)$ and $R(u', v')$ are conjuncts of q and $v \sim v'$ then also $u \sim u'$. Let q' be the quotient of q w.r.t. $\sim$ (that is, q' is obtained from q by choosing a representative of each $\sim$-equivalence class, and replacing every occurrence of a variable x by the representative of the $\sim$-equivalence class of x). It is easy to see that, for all tree-shaped instances I, $a \in q(I)$ iff $a \in q'(I)$ (here, the left-to-right direction uses the tree-shape of I, while the right-to-left direction holds for every instance I).

If q' contains a directed cycle, then clearly, $q'(I) = \emptyset$ for all tree-shaped instances I, and we are done.

Assume, therefore, that q' does not contain a directed cycle. Since q' is connected, there must then exist a (free or existentially quantified) variable y for which q' does not contain any conjunct of the form $R(\cdot, y)$. Furthermore, any simple path from y to any other variable z must consist entirely of forward edges, otherwise, the path would be of the form

$$y \xrightarrow{R} \cdots \xrightarrow{R} u \xrightarrow{R} v \xleftarrow{R} w \xleftarrow{R} \cdots \xleftarrow{R} z$$

and then u and w would have been identified when we constructed q'. It follows that q' is tree-shaped. Furthermore, let $I_{q'}$ be the canonical instance of q'. Then, clearly, $q'(I_{q'}) \neq \emptyset$. □

Since tree-shaped CQs are α-acyclic and hence can be evaluated in polynomial time (on the class of all instances) [30], Lemma 5.2 immediately implies:

Proposition 5.3. *Fix a schema* $\mathbf{S}$ *that contains one binary relation symbol and any number of unary relation symbols. For every class* C *of CQs over* $\mathbf{S}$, *the concept class* $(C, Ex_{\mathit{tree}}, \models)$, *where* Ex_{tree} *is the set of tree-shaped* $\mathbf{S}$*-instances, is polynomial-time evaluable.*

In what follows, we will therefore only work with tree-shaped instances.

5.2. A reduction from 3CNF satisfiability

Fix a schema $\mathbf{S}$ containing a binary relation symbol R and a unary relation symbol P.

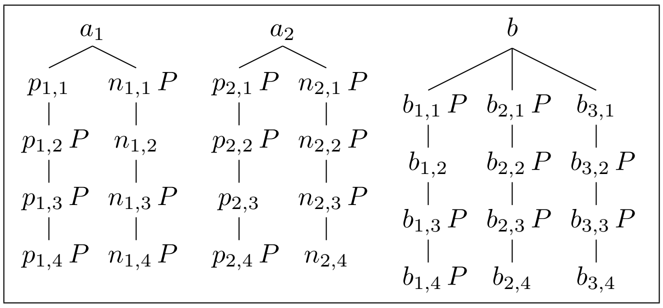
We use a reduction from the satisfiability problem for 3CNF formulas, inspired by [23, 19]. Let $\phi = \phi_1 \wedge \cdots \wedge \phi_k$ be any 3CNF formula over a propositional signature $\mathit{PROP} = \{X_1, \ldots, X_m\}$. We denote by $\mathit{LIT} = \{X_i, \overline{X_i} \mid i \leq m\}$ the set of all literals over PROP. For every $l \in \mathit{LIT}$, set $j_l = 2i$ if l is of the form X_i and $j_l = 2i - 1$ if l is of the form $\overline{X_i}$. Define an $\mathbf{S}$-instance I_ϕ as follows:

- $R(a_i, p_{i,1})$ and $R(a_i, n_{i,1})$ for $i \leq m$
- $R(p_{i,j}, p_{i,j+1})$ and $R(n_{i,j}, n_{i,j+1})$ for $i \leq m$, $j < 2m$
- $P(p_{i,j_l})$ for every literal $l \in \mathit{LIT} \setminus \{\overline{X_i}\}$
- $P(n_{i,j_l})$ for every literal $l \in \mathit{LIT} \setminus \{X_i\}$
- $R(b, b_{i,1})$ for $i \leq k$
- $R(b_{i,j}, b_{i,j+1})$ for $i \leq k$ and $b \leq 2m$
- $P(b_{i,j_l})$ for every $l \in \mathit{LIT}$ and $i \leq k$ with l not occurring in the clause ϕ_i.

Let $E_\phi = \{((I_\phi, a_i), +) \mid i \leq m\} \cup \{((I_\phi, b), -)\}$.

Example 5.4. *Let* $\mathit{PROP} = \{X_1, X_2\}$ *and consider the formula* $\phi = X_1 \wedge X_2 \wedge (\overline{X_1} \vee X_2)$. *Then, the corresponding* $\mathbf{S}$*-instance* I_ϕ *can be depicted as follows (where each edge represents an* R*-edge directed downwards):*

[5] The *canonical instance* of a CQ is the instance whose active domain consists of the variables of the query and whose facts are the conjuncts of the query.



Lemma 5.5. *For all 3CNF formulas ϕ:*

1. *From a satisfying assignment for ϕ, one can construct in polynomial time a path-CQ that fits E_ϕ.*
2. *Conversely, if there is a CQ that fits E_ϕ, then ϕ has a satisfying assignment.*

In particular, whenever there is a CQ that fits E_ϕ, then there is a fitting path-CQ of size polynomial in $|PROP|$.

Proof. 1. Let v be a satisfying assignment for ϕ. Let

$$q(x_0) :- \exists x_1, \dots x_{2m}(R(x_0, x_1) \wedge \cdots \wedge R(x_{2m-1}, x_{2m}) \wedge \bigwedge_{l \in LIT \text{ such that } v \models l} P(x_{j_l})).$$

Clearly, each $a_i \in q(I_\phi)$ and $b \notin q(I_\phi)$.

2. Let $q(x)$ be a unary CQ that fits E_ϕ. By Lemma 5.2, we may assume that q is a tree-shaped CQ. Furthermore, we may assume without loss of generality that q is connected. Let $level_q \colon Vars(q) \to \mathbb{N}$ be as given by Definition 5.1. We may assume $level_q(x) = 0$ (if there was any $y \in Vars(q)$ with $level_q(y) < level_q(x)$, then q would not fit the positive examples of E_ϕ).

Thus, $q(x)$ is a connected tree-shaped CQ, where x is the root of the tree. Since $q(x)$ fits the negative example (I_ϕ, b), we have that $b \notin q(I_\phi)$. This means that either (i) q contains a conjunct of the form $P(x)$, or (ii) for some $y \in Vars(q)$ with $level_q(y) = 1$, the subtree of q rooted at y, does not admit a homomorphism to $(I_\phi, b_{i,1})$ for any $i \leq n$. It is easy to see that (i) cannot happen, because it would imply that q does not fit the positive examples in E_ϕ. Therefore, case (ii) must apply. Let y be the variable in question, and let us denote by $q'(y)$ the subtree of q rooted at y (with y as its free variable).

We know that $q'(I_\phi)$ does not contain $b_{i,1}$ for any $i \leq n$. Furthermore, it is easy to see (from the fact that q fits the positive examples in E_ϕ), that for each $i \leq m$, either $p_{i,1}$ or $n_{i,1}$ belongs to $q'(I_\phi)$.

Now, let L_y be the set

$$\{l \in LIT \mid q' \text{ has a conjunct } P(z) \text{ with } level_q(z) = j_l + 1\}$$

Claim 1: L_y does not contain both $X_i, \overline{X_i}$ for any $i \leq m$.

Claim 1 follows immediately from the fact that $q(x)$ fits the positive examples.

Claim 2: L_y contains a literal from each clause of ϕ.

Suppose, for the sake of a contradiction, that ϕ has a clause ϕ_i, such that no literal occurring in ϕ_i belongs to L_y. Then, $b_{i,1}$ belongs to $q'(I_\phi)$, as witnessed by the variable assignment that maps each variable z to $b_{i,level_q(z)-1}$. However, we know that $b_{i,1} \notin q'(I_\phi)$, a contradiction.

Claim 1 and 2 together imply that ϕ is satisfiable. Indeed, it suffices to take any truth assignment consistent with the literals in L_y. □

From Lemma 5.5, together with the NP-hardness of 3CNF satisfiability, we immediately get:

Theorem 5.6. *Fix any schema* **S** *that contains at least a binary relation symbol and a unary relation symbol, and let C be any class of unary CQs over* **S** *that includes all path-CQs. Then the fitting problem for C is NP-hard.*

Now, putting everything together, we can prove Theorem 1.1, restated here:

Theorem 5.7. *(assuming RP $\neq$ NP) Fix a schema* **S** *containing at least one binary relation symbol R and one unary relation symbol P. Let C be any class of unary CQs over* **S** *that includes all path-CQs. Then C is not efficiently PAC learnable, even w.r.t. single-instance distributions.*

Proof. Assume that the concept class $C = (C, Ex, \models)$ is efficiently PAC learnable. Then, by Proposition 2.8, so is $C' = (C, Ex', \models)$ where $Ex' = \{(I, a) \mid I = I_\phi$ for some 3CNF formula ϕ and $a \in \{a_1, a_2, b\}\}$. It follows from Lemma 5.5 that C' has the polynomial-size fitting property. Furthermore, C' is polynomial-time evaluable since all examples in Ex' are tree-shaped and by Proposition 5.3. By Proposition 2.6, the fitting problem for C' is thus solvable in RP. By Theorem 5.6, this implies that RP = NP.

A careful inspection of the proof of Proposition 2.6 and the construction of our examples reveals that even efficient PAC learnability w.r.t. single-instance distributions already gives us, in the same way as above, an RP-algorithm for the fitting problem for C'. □

Remark 5.8. The above proof involves path-CQs of unbounded depth, over a fixed schema. It is easy to see that if we were to bound both the depth of the path-CQs and keep the schema fixed, we would end up with a finite concept class, trivializing the PAC learning problem.

Remark 5.9. The above non-learnability proof cannot be adapted to UCQs in an obvious way. In fact, we crucially use the fact that the fitting problem for path-CQs is NP-hard whereas the fitting problem for UCQs that are unions of path-CQs can be solved in polynomial time. On the other hand, as mentioned earlier, it follows from results in [6] that UCQs are not efficiently PAC learnable, assuming RP $\neq$ NP.

Remark 5.10. The fact that the above proof involves a reduction from the satisfiability problem for 3CNF formulas is remarkable, given that 3CNF formulas themselves *are* efficiently PAC learnable [22].

Remark 5.11. Efficient PAC learnability as defined in Definition 2.5 (in the non-strong version) is sometimes also known as *strong PAC learnability.* In contrast, *weak PAC learnability* then merely requires the existence of a learner that works for *some* non-trivial choice of δ and ϵ. A well-known result in computational learning theory states that, for polynomial-time evaluable concept classes, weak learnability implies strong learnability (cf. [22]). Since the concept class of CQs is not polynomial-time evaluable, Theorem 1.1, taken at face value, does not imply that the same result holds in the weak PAC model. Nevertheless, inspection of our proof immediately shows that it yields the same result also for the weak PAC model.

6. PAC Learnability with Membership Queries

We prove Theorem 1.2 from the introduction. Formally, a *membership oracle* $MEMB_\phi$, for a concept ϕ, is an oracle that, given any unlabeled example e, returns (in unit time) its label according to ϕ. PAC learning with access to a membership oracle for the target concept can be viewed as a formal model of active learning.

Theorem 6.1. *Fix any schema* $\mathbf{S}$ *and* $k \geq 0$. *There is an algorithm that takes as input a set* E *of examples labeled according to a* k*-ary CQ* q^* *over* $\mathbf{S}$*, has access to a membership oracle for* q^**, and outputs a* k*-ary CQ* q *over* $\mathbf{S}$ *with* $|q| \leq |q^*|$ *that fits* E*. Moreover, the running time of the algorithm is polynomial in* $||E||$ *and* $|q^*|$*.*

Proof. We use ideas similar to the ones used in the proof that CQs are efficiently exactly learnable with membership and equivalence queries [6, 7]. Before we describe the algorithm, we introduce a number of basic concepts.

Let I, J be instances over the same schema. A mapping $h\colon \text{adom}(I) \to \text{adom}(J)$ is called *homomorphism from* I *to* J if $R(h(\mathbf{c})) \in J$ for every $R(\mathbf{c}) \in I$. Given tuples $\mathbf{a}$ and $\mathbf{b}$ of values from I and J, respectively, we write $(I, \mathbf{a}) \to (J, \mathbf{b})$ to denote the existence of a homomorphism h from I to J with $h(\mathbf{a}) = \mathbf{b}$. Homomorphisms compose in the sense that $(I, \mathbf{a}) \to (J, \mathbf{b})$ and $(J, \mathbf{b}) \to (K, \mathbf{c})$ implies $(I, \mathbf{a}) \to (K, \mathbf{c})$.

The *direct product* $I \times J$ of two instances (over the same schema $\mathbf{S}$), is the $\mathbf{S}$-instance that consists of all facts of the form $R(\langle a_1, b_1\rangle, \dots, \langle a_n, b_n\rangle)$, where $R(a_1, \dots, a_n)$ is a fact of I and $R(b_1, \dots, b_n)$ is a fact of J. Note that the active domain of $I \times J$ consists of pairs from $\text{adom}(I) \times \text{adom}(J)$. The direct product $(I, \mathbf{a}) \times (J, \mathbf{b})$ of two examples, where $\mathbf{a} = a_1, \dots, a_k$ and $\mathbf{b} = b_1, \dots b_k$ are of the same length, is given by $(I \times J, (\langle a_1, b_1\rangle, \dots, \langle a_k, b_k\rangle)$. Note that, in general, this may not yield a well-defined example, because there is no guarantee that the distinguished elements $\langle a_1, b_1\rangle, \dots, \langle a_k, b_k\rangle$ belong to $\text{adom}(I \times J)$. When it is well-defined, then the projections to the respective components witness that both $(I, \mathbf{a}) \times (J, \mathbf{b}) \to (I, \mathbf{a})$ and $(I, \mathbf{a}) \times (J, \mathbf{b}) \to (J, \mathbf{b})$.

A *critical positive example* for a CQ q^* is a positive example $(I, \mathbf{a})$ for q^*, such that, for every proper subinstance $I' \subsetneq I$, $(I', \mathbf{a})$ is a negative example for q^*.

The following claim is easy to prove ([7, Lemma 5.4]):

Claim 1: Given a positive example $(I, \mathbf{a})$ for an unknown CQ q^*, we can construct from it in linear time a critical positive example $(I', \mathbf{a})$ for q^*, with $I' \subseteq I$, given access to a membership oracle for q^*.

Claim 2: If $(I, \mathbf{a})$ and $(J, \mathbf{b})$ are positive examples for a CQ q^*, then $(I, \mathbf{a}) \times (J, \mathbf{b})$ is a well-defined example, and it is a positive example for q^*.

Proof of Claim 2: Let $(I, \mathbf{a})$ and $(J, \mathbf{b})$ be positive examples for a CQ q^*. Let h_1 and h_2 be the respective witnessing variable assignments. Then the map h given by $h(x) = (h_1(x), h_2(x))$ is a satisfying variable assignment for q^* in $(I, \mathbf{a}) \times (J, \mathbf{b})$, showing that the latter is a positive example for q^*. It remains to show that it is a well-defined example, i.e., that each distinguished element occurs in a fact. This follows from the fact that each free variable of q^* occurs in a conjunct of q^* (by the definition of CQs), and that each distinguished element of $(I, \mathbf{a}) \times (J, \mathbf{b})$ is the h-image of a free variable of q^* (cf. [7, Lemma 5.5]).

Given a set E of examples labeled according to q^*, the algorithm proceeds as follows. Let $(I_1, \mathbf{a}_1), \dots, (I_n, \mathbf{a}_n)$ be an enumeration of the positive examples in E. We construct, by induction on n, a critical positive example $(J, \mathbf{b})$ for q^* such that there is a homomorphism from $(J, \mathbf{b})$ to each $(I_i, \mathbf{a}_i)$. This is done by applying Claim 1 and Claim 2 in an interleaved fashion. More precisely:

- Start by setting $(J_1, \mathbf{b}_1)$ to be the critical positive example obtained from $(I_1, \mathbf{a}_1)$ via Claim 1.
- For $i = 2, \dots, n$, let $(J'_i, \mathbf{b}'_i)$ be $(J_{i-1}, \mathbf{b}_{i-1}) \times (I_i, \mathbf{a}_i)$ and obtain $(J_i, \mathbf{b}_i)$ as critical positive example from $(J'_i, \mathbf{b}'_i)$ via Claim 1.
- Set $(J, \mathbf{b}) = (J_n, \mathbf{b}_n)$.

Note that, by Claim 2 and the fact that homomorphisms compose, each $(J'_i, \mathbf{b}'_i)$ is a well-defined example that has a homomorphism to all examples $(I_1, \mathbf{a}_1), \dots, (I_i, \mathbf{a}_i)$. Thus, $(J, \mathbf{b})$ has a homomorphism to all positive examples. Let $\mathbf{b} = b_1, \dots, b_k$ and let q be the canonical CQ of $(J, \mathbf{b})$, that is, the CQ $q(x_{b_1}, \dots, x_{b_k})$ that has a conjunct for every fact of J, where each element $b \in \text{adom}(J)$ is replaced by a corresponding variable x_b. Then q fits the positive examples in E since $(J, \mathbf{b})$ has a homomorphism to each positive example. It also fits the negative examples in E: $(J, \mathbf{b})$ is a positive example for q^* by construction and if q fails to fit a negative example $(I, \mathbf{a})$ in E, then $(J, \mathbf{b})$ has a homomorphism to $(I, \mathbf{a})$, which, by composition of homomorphisms, leads to a contradiction with q^* fitting $(I, \mathbf{a})$.

Furthermore, one can easily see that any *critical* positive example $(I, \mathbf{a})$ for q^* satisfies $|I| \leq |q^*|$. Hence, each J_i satisfies $|J_i| \leq |q^*|$. This implies, in particular, that $|q| \leq |q^*|$ as required. Moreover, it implies that $|J'_i| \in O(||E|| \cdot |q^*|)$, for all i. Since J_i is obtained from J'_i in linear time by Claim 1, the running time of this algorithm is $O(||E||^2 \cdot |q^*|)$. □

The algorithm given in Theorem 6.1 is an Occam algorithm (with $\alpha = 0$ and $k = 1$) in the sense of Definition 2.9, except for the fact that it uses a membership oracle. While Theorem 2.10 is stated for the case without membership queries, its proof applies also to Occam algorithms with membership queries, yielding efficient PAC learnability with membership queries (stated as Theorem 1.2 in the introduction):

Corollary 6.2. *Fix any schema* $\mathbf{S}$ *and* $k \geq 0$. *The class of all* k*-ary CQs over* $\mathbf{S}$ *is efficiently PAC learnable with membership queries.*

Remark 6.3. The proof of Theorem 6.1 establishes something stronger, namely that CQs are efficiently PAC learnable with membership queries even when the schema $\mathbf{S}$ and the arity k are not fixed but treated as part of the input of the learning task. This is remarkable, because it follows from results in [13] that CQs are not PAC predictable with membership queries when the arity is treated as part of the input (under suitable cryptographic assumptions). However, note that efficient PAC learnability (with membership queries) implies PAC predictability (with membership queries) only for concept classes that are polynomial-time evaluable, which the class of CQs is not.

Remark 6.4. We expect that, with respect to each of the various notions of "acyclicity" mentioned in the introduction, acyclic CQs are efficiently PAC learnable with membership queries. However, since efficient PAC learnability (with or without membership queries) is not a monotone property of concept classes, this requires a case-by-case analysis. A challenge is posed by the fact that the positive examples $(I_i, \mathbf{a}_i)$ are not guaranteed to correspond to queries from the considered class, and thus neither are the hypotheses that our algorithm generates.

The above proof can also be modified to apply to the concept class of *unions of conjunctive queries (UCQs)*. By a k-ary UCQ over a schema $\mathbf{S}$ we mean a non-empty finite disjunction of k-ary CQs over $\mathbf{S}$.

Theorem 6.5. *Fix any schema* $\mathbf{S}$ *and* $k \geq 0$. *The class of* k*-ary UCQs over* $\mathbf{S}$ *is efficiently PAC learnable with membership queries.*

Proof. We sketch the modified algorithm. Given a set E of labeled examples, it proceeds as follows. Let $(I_1, \mathbf{a}_1), \ldots, (I_n, \mathbf{a}_n)$ be an enumeration of the positive examples in E. We construct sets of critical positive examples $X_0, \ldots, X_n$ such that for all i and all $(I_j, \mathbf{a}_j)$ with $j < i \leq n$, there exists a $(J, \mathbf{b}) \in X_i$ that admits a homomorphism to $(I_j, \mathbf{a}_j)$. As before, this is done by applying Claim 1 and Claim 2 in an interleaved fashion.

More precisely, set $X_0 = \emptyset$; for $i = 1, \ldots, n$, we first test whether there is a $(J, \mathbf{b}) \in X_{i-1}$ such that $(J, \mathbf{b}) \times (I_i, \mathbf{a}_i)$ is a positive example for the target query q^*. We use a membership query for this. If such $(J, \mathbf{b}) \in X_{i-1}$ exists, then we choose an arbitrary one and set $X_i = (X_{i-1} \setminus \{(J, \mathbf{b})\}) \cup \{(J', \mathbf{b}')\}$, where $(J', \mathbf{b}')$ is a subinstance of $(J, \mathbf{b}) \times (I_i, \mathbf{a}_i)$ that is a critical positive example for q^*. Otherwise (if no such $(J, \mathbf{b}) \in X_{i-1}$ exists), we set $X_i = X_{i-1} \cup \{(J', \mathbf{b}')\}$ where $(J', \mathbf{b}')$ is a subinstance of $(I_i, \mathbf{a}_i)$ that is a critical positive example for q^*.

Let q be the UCQ that is the disjunction of the canonical CQs of the examples in X_n. By similar arguments as before, we can show that q fits E and $|q| \leq |q^*|$. In particular, for each $i \leq n$ the sum of the sizes of the structures in X_i is at most the size of q^*. □

Remark 6.6. The problem of learning *GAV schema mappings* closely corresponds to the problem of learning UCQs (cf. [7]). In particular, Theorem 6.5 implies that GAV schema mappings are efficiently PAC learnable with membership queries. This resolves an open question in [6].

7. Conclusion

We established a strong negative result on the efficient PAC learnability of classes of CQs that include all path-CQs. Although our result indicates that interesting classes of CQs tend to not be efficiently PAC learnable, from a theoretical perspective it would be interesting to work towards a complete classification of classes of CQs that are (or are not) efficiently PAC learnable. On the positive side, we showed that CQs and UCQs are efficiently PAC learnable with membership queries.

In the following, we discuss how one could try to overcome the negative result by loosening the running time requirements. A first observation is that while PAC learnability of (the class of all) CQs cannot be attained by a polynomial-time algorithm, PAC learning with *only polynomial sample size* is always possible when more running time is granted. Indeed, this approach has been successfully exploited in [9] for PAC learning unary tree-shaped CQs (over a schema that contains only unary and binary relations) with the help of a SAT solver.

The fact that a PAC learning algorithm for CQs exists with polynomial sample size but super-polynomial running time, is not difficult to establish. One can simply use an Occam algorithm that enumerates candidate CQs q in the order of increasing size, checks for each q whether it fits the input examples E, and returns the first fitting CQ found. If a fitting CQ exists, then there is one of size single exponential in $||E||$ [5]. We may thus terminate (and return an arbitrary CQ) when that bound is reached. The algorithm runs in double exponential time even if we check in a brute-force way whether candidate CQs fit the input examples. The bound on the sample size stated after Theorem 2.9 applies despite the non-polynomial running time. We thus obtain a PAC algorithm with polynomial sample size and double exponential running time.

It is an interesting question whether and when a more modest superpolynomial running time suffices. In particular, one may consider running times that also depend on the target query q rather than only on the input set of examples E. From this perspective, the above algorithm attains running time $||E||^{O(|q|)}$ while time $f(q) \cdot \text{poly}(||E||)$ with f a computable function would clearly be preferable. This resembles fixed-parameter tractability (FPT) in the study of the parameterized complexity of query evaluation (with the size of the query being the parameter), so let us refer to it as *FPT PAC learning*. To make this well-defined, it is convenient to view FPT PAC learning as a promise problem, meaning that the input examples are promised to have a fitting query from the considered class.[6] Alternatives are to treat the non-existing target query as being of size 1 (which is a strong requirement) and to grant unlimited running time in the case that there is no fitting query (declaring that case a corner case).

In the setting of FPT PAC learning, classes of CQs of bounded treewidth and (more generally) bounded submodular width should be expected to play a prominent role because these notions are tightly linked to CQ evaluation in FPT [18, 24]. They generalize all notions of acyclicity mentioned in this paper, such as α-acyclicity. The exact same Occam algorithm described above yields that for every $k \geq 1$, the class C_k of CQs of submodular width at most k is FPT PAC learnable with polynomial sample size. This raises a number of questions: Is the class of all CQs FPT PAC learnable? If not, can we characterize the classes of CQs that are? And how exactly does the running time of the algorithms depend on the parameter?

References

[1] Dana Angluin. Queries and concept learning. *Mach. Learn.*, 2(4):319–342, 1988.

[2] Martin Anthony and Norman L. Biggs. *Computational Learning Theory: An Introduction*. Cambridge University Press, 1992.

[3] Marta Arias and Roni Khardon. Learning closed Horn expressions. *Information and Computation*, 178(1):214–240, 2002.

[4] Anselm Blumer, Andrzej Ehrenfeucht, David Haussler, and Manfred K. Warmuth. Learnability and the Vapnik-Chervonenkis dimension. *J. ACM*, 36(4):929–965, 1989.

[5] Balder ten Cate and Víctor Dalmau. The product homomorphism problem and applications. In *Proc. of ICDT*, pages 161–176. Schloss Dagstuhl - Leibniz-Zentrum für Informatik, 2015.

[6] Balder ten Cate, Víctor Dalmau, and Phokion G. Kolaitis. Learning schema mappings. *ACM Trans. Database Syst.*, 38(4):28:1–28:31, 2013.

[7] Balder ten Cate and Víctor Dalmau. Conjunctive queries: Unique characterizations and exact learnability. *ACM Trans. Database Syst.*, 47(4):14:1–14:41, 2022.

[8] Balder ten Cate, Víctor Dalmau, Maurice Funk, and Carsten Lutz. Extremal fitting problems for conjunctive queries. To appear in Proceedings of PODS 2023. Available at https://arxiv.org/pdf/2206.05080.pdf, 2022.

[9] Balder ten Cate, Maurice Funk, Jean Christoph Jung, and Carsten Lutz. SAT-based PAC learning of description logic concepts. In *Proc. of IJCAI)*, 2023.

[10] Hubie Chen and Matthew Valeriote. Learnability of solutions to conjunctive queries. *J. Mach. Learn. Res.*, 20(1):2422–2449, 2019.

[11] William W. Cohen. Cryptographic limitations on learning one-clause logic programs. In *Proc. of AAAI*, pages 80–85. AAAI Press / The MIT Press, 1993.

[12] William W. Cohen. The dual DFA learning problem: Hardness results for programming by demonstration and learning first-order representations (extended abstract). In *Proc. of COLT*, pages 29–40. ACM, 1996.

[13] Víctor Dalmau. A dichotomy theorem for learning quantified boolean formulas. *Mach. Learn.*, 35(3):207–224, 1999.

[14] Víctor Dalmau and Peter Jeavons. Learnability of quantified formulas. *Theor. Comput. Sci.*, 306(1):485–511, 2003.

[15] Ronald Fagin. Degrees of acyclicity for hypergraphs and relational database schemes. *J. ACM*, 30(3):514–550, 1983.

[16] Maurice Funk. Concept-by-example in $\mathcal{EL}$ knowledge bases. Master's thesis, University of Bremen, 2019.

[17] Maurice Funk, Jean Jung, Carsten Lutz, Hadrien Pulcini, and Frank Wolter. Learning description logic concepts: When can positive and negative examples be separated? In *Proc. of IJCAI*, pages 1682–1688, 08 2019.

[18] Martin Grohe. The complexity of homomorphism and constraint satisfaction problems seen from the other side. *J. ACM*, 54(1):1:1–1:24, 2007.

[19] David Haussler. Learning conjunctive concepts in structural domains. *Mach. Learn.*, 4:7–40, 1989.

[20] David Haussler, Michael J. Kearns, Nick Littlestone, and Manfred K. Warmuth. Equivalence of models for polynomial learnability. *Inf. Comput.*, 95(2):129–161, 1991.

[21] Kouichi Hirata. Prediction-hardness of acyclic conjunctive queries. *Theor. Comput. Sci.*, 348(1):84–94, 2005.

[22] Michael J. Kearns and Umesh V. Vazirani. *An Introduction to Computational Learning Theory*. MIT Press, 1994.

[23] Jörg-Uwe Kietz. Some lower bounds for the computational complexity of inductive logic programming. In *Proc. of ECML*, pages 115–123. Springer, 1993.

[24] Dániel Marx. Tractable hypergraph properties for constraint satisfaction and conjunctive queries. *J. ACM*, 60(6):42:1–42:51, 2013.

[25] Shan-Hwei Nienhuys-Cheng and Roland de Wolf. *Foundations of Inductive Logic Programming*. Springer, 1997.

[26] Leonard Pitt and Leslie G. Valiant. Computational limitations on learning from examples. *J. ACM*, 35(4):965–984, 1988.

[27] Robert E. Schapire. The strength of weak learnability. *Mach. Learn.*, 5:197–227, 1990.

[28] Leslie G. Valiant. A theory of the learnable. *Commun. ACM*, 27:1134–1142, 1984.

[29] Ross Willard. Testing expressibility is hard. In *Proc. of CP*, pages 9–23. Springer, 2010.

[30] Mihalis Yannakakis. Algorithms for acyclic database schemes. In *Proc. of VLDB*, page 82–94. VLDB Endowment, 1981.

[6] The lower bounds proved in this paper then no longer apply.