Concept Learning in Description Logics — Part 3:

Exact and PAC Learning

KR Tutorial on Concept Learning in Description Logics, Rhodes, Sep 03

Exact Learning

developed in 1987 by Dana Angluin in the context of learning finite automata

> our assumption: logic and domain expertise are not in the same hands



Learner and Teacher agree on ontology ${\cal O}$

Question: Does Learner have a **strategy** to efficiently identify q_T ?

Questions



Example



What is known?

Efficient Learnability

=

learning strategy is guaranteed to identify target in time polynomial in signature, ontology, target, largest counterexample

query class	ontology	questions	learnability	today
$\mathscr{EL}/\mathscr{ELI}$ -concepts	no	MQ	efficient	¢
\mathscr{CL} -concepts	\mathcal{EL}	MQ+EQ	efficient	⇐
CQ	no	MQ+EQ	efficient	[×]
CQ/ELJ-concepts	ELJ	MQ+EQ	not efficient	
CQ	DL-Lite/ \mathscr{EL}	MQ+EQ	open	
\mathscr{ELI} -concepts	EL	MQ+EQ	open	

Sources

ten Cate, Dalmau, & Kolaitis, ToDS, 2013 ten Cate & Dalmau, ToDS, 2022 Funk, Jung, & Lutz, IJCAI, 2021/2022

Learning Strategy

All known learning algorithms follow a general scheme: they construct

 $q_0 \subsetneq_{\mathcal{O}} q_1 \subsetneq_{\mathcal{O}} \dots \subsetneq_{\mathcal{O}} q_n = q_T$

Start q_0 : very strong query that is guaranteed to entail q_T

Step $q_i \rightarrow q_{i+1}$: two different strategies for weakening q_i a) based on **frontiers** \approx minimal weakenings of q_i b) based on incorporation of counterexample (usually via **product**)

Key ingredient Using MQs, we can (syntactically) **minimize** the q_i

Lemma Sequence $q_0, ..., q_n$ as above with all q_i minimal is bounded by a polynomial in signature, ontology, and target

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Is there a polynomial time learning algorithm? (polynomial in the size of C_T , \mathfrak{O} , Σ and largest counterexample)?

Learning $\mathcal{EL}\operatorname{-}\!\mathbf{Concepts}$ under Ontologies

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We will look at the polynomial time learnability of \mathcal{EL} -concepts under ontologies. First step: empty ontology ($\mathcal{O} = \emptyset$)

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Especially: $C \sqsubseteq C_T$ if and only if $\mathcal{D}_C \models C_T(a_C)$

If the response to the membership query $\mathcal{D}_C \models C_T(a_C)$ is "Yes", then $C \sqsubseteq C_T$.

We can use a membership query to test $C \sqsubseteq C_T$

If there is a concept *C* such that $C \sqsubseteq C_T$ and $C_T \not\sqsubseteq C$,

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Any such *D* moves us closer to C_T (decreases number of possibilites for C_T)

How can we construct such a *D*?

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Frontiers

We need to check all possible generalizations of C

Definition (Frontier of C)

A set of concepts \mathcal{F} is a *frontier of C* if 1. $C \sqsubseteq D$ and $D \not\sqsubseteq C$ for all $D \in \mathcal{F}$

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Only small part of *C* needed for $C \sqsubseteq C_T (\leqslant |C_T|)$

minimize(C): for each existential restriction, remove if it is unecessary $C \sqsubseteq \text{minimize}(C) \sqsubseteq C_T \text{ and } |\text{minimize}(C)| \leqslant |C_T$

Lemma

A sequence of minimized concepts that approaches C_T has at most polynomial length (in $|C_T|$)

Putting it all together

```
Input An \mathcal{EL}-concept C_0 such that C_0 \sqsubseteq C_T

Output An \mathcal{EL}-concept C_H such that C_H \equiv C_T

C_H \coloneqq C_0

while there is a D in the frontier of C_H with D \sqsubseteq C_T do

C_H \coloneqq \mininimize(D)

end while

return C_H
```

Theorem (ten Cate and Dalmau 2021)

EL-concepts are polynomial time learnable using only membership queries (under the empty ontology)

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(\mathcal{D}, a_1)	Double cycle	C_T
A_{1}, A_{2}, A_{3}	A_1, A_2, A_3	
a_1	a_1	a_1
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- Repeatedly double cycles and minimize (membership queries) to obtain C with $C \sqsubseteq C_T$
- extract-el: from a data instance (\mathcal{D}, a) with $\mathcal{D} \models C_T(a)$, extract an \mathcal{EL} -concept C such that $\mathcal{D} \models C(a)$ and $C \sqsubseteq C_T$

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- Practicality asks a lot of membership queries

Non-empty & C-ontologies

Now we move on to learning \mathcal{EL} -concepts under \mathcal{EL} -ontologies.

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Theorem (F., Jung, Lutz, 2021)

EL-concepts are not polynomial time learnable under EL-ontologies using only membership queries

Using only membership queries

Consider an \mathcal{EL} ontology \mathcal{O} with the CIs:

 $A_i \sqcap B_i \sqsubseteq A_1 \sqcap B_1 \sqcap \cdots \sqcap A_n \sqcap B_n$ for $1 \leq i \leq n$

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and the set of concepts $S = \{\alpha_1 \sqcap \cdots \sqcap \alpha_n \mid \alpha_i \in \{A_i, B_i\}\}$

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Counter examples and Products

- Learner asks equivalence query with hypothesis C_H
- If $\mathfrak{O} \not\models C_H \not\equiv C_T$, then teacher returns counter example (\mathfrak{D}, a) such that
- $\mathcal{O}, \mathcal{D} \models C_H(a) \text{ and } \mathcal{O}, \mathcal{D} \not\models C_T(a), \text{ or }$

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$$\begin{array}{ccc} C_H & (\mathcal{D}, b_1) \\ a_1 & A & b_1 & B \\ \downarrow r & & \circlearrowright \\ a_2 & & r \\ \swarrow s & \swarrow r \\ a_3 & B & a_4 & A \end{array}$$

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- $\mathcal{O}, \mathcal{D} \not\models C_H(a) \text{ and } \mathcal{O}, \mathcal{D} \models C_T(a).$

Need: generalize C_H such that $\mathcal{O}, \mathcal{D} \models C_H(a) \implies \text{direct product} \times$

$$\begin{array}{ccc} C_H & (\mathcal{D}, b_1) \\ a_1 & A & b_1 & B \\ \downarrow r & & \circlearrowright \\ a_2 & & r \\ \swarrow s & \swarrow r \\ a_3 & B & a_4 & A \end{array}$$

Counter examples and Products

Learner asks equivalence query with hypothesis C_H

If $\mathfrak{O} \not\models C_H \not\equiv C_T$, then teacher returns counter example (\mathfrak{D}, a) such that

- $\mathcal{O}, \mathcal{D} \models C_H(a) \text{ and } \mathcal{O}, \mathcal{D} \not\models C_T(a), \text{ or } (\text{Not possible if we ensure that } \mathcal{O} \models C_H \sqsubseteq C_T)$
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Compact Models

 $C_H \times (\mathcal{D}, a)$ does not work under \mathcal{EL} -ontologies. Let $\mathcal{O} = \{A \sqsubseteq \exists r. \top, B \sqsubseteq \exists r. \top\}$

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a_2	b_2		a_2

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In \mathcal{EL} there can be infinite consequences ($A \sqsubseteq \exists r.A$)

Fortunately, for \mathcal{EL} there are compact universal models $\mathcal{G}_{C_{H}, \mathfrak{O}}$ of ontologies (with size polynomial in $|C_{H}|$ and $|\mathfrak{O}|$)

Learning \mathcal{EL} -Concepts under OntologiesAlgorithm with Compact Model

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Theorem (F., Jung, Lutz 2021)

EL-concepts are polynomial time learnable under EL-ontologies

Remarks

• Conjunctive Queries

 \times -based learning algorithm for conjunctive queries (ten Cate, Dalmau, Kolaitis 2013)

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Learning $\mathcal{EL}\operatorname{-}\!\mathbf{Concepts}$ under Ontologies

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Remarks

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PAC Learning

KR Tutorial on Concept Learning in Description Logics, Rhodes, Sep 03

PAC Learning — Motivation

So far concentrated on **fitting/separability problem**: given positive/negative examples, find a concept/query that fits

Neglected the aspect of generalization

we want the fitting concept to generalize well to unseen examples

Leslie Valiant introduced PAC learning in a seminal paper in 1984

Notion of PAC (probably – approximately – correct) tries to capture generalization

Plan

- 1. Definition
- 2. Boundaries
- 3. Occams Razor & Bounded Fitting
- 4. SPELL demo

Statistical Machine Learning



Papayas on some unknown island

random papayas
$$P_1, \ldots, P_n$$

 f^* = "nature" labels with "tasty" (+) or "not tasty (-) $(P_1, +), \dots, (P_n, -)$

rule predicting tastyness e.g.:

"if papaya is yellow and has size 10-13 cm and is not too soft, then it's tasty"

Statistical Machine Learning



No access to all examples \Rightarrow two kinds of errors

- $h \operatorname{approximates} f^* \Rightarrow \operatorname{approximation} parameter \epsilon$
- **A** works only probably \Rightarrow confidence parameter δ

PAC learnability

Class Q is PAC learnable if there are (\mathbf{A}, m_0) s.t.:

- A is learning algorithm
- if given $m_Q(\epsilon, \delta, n)$ examples labeled by q of size n,
 - A outputs with high probability $\geq 1 \delta$ a hypothesis $h \in Q$ with small error $\leq \epsilon$

 $\operatorname{error}_{D,f^*}(h) = Pr_{e \sim D}(f^*(e) \neq h(e))$

No Papayas today

Examples = databases, Q = class of queries

PAC Learnability

PAC learnability Class Q is PAC learnable if there are (\mathbf{A}, m_Q) s.t.: **A** is learning algorithm **i** given $m_Q(\epsilon, \delta, n)$ examples labeled by q of size n, **A** outputs with high probability $\geq 1 - \delta$ a hypothesis $h \in Q$ with small error $\leq \epsilon$

Theorem Every class of queries $Q \subseteq$ FO is PAC learnable.

Proof Every class of queries is union $Q = Q_1 \cup Q_2 \cup Q_3 \cup ...$ where Q_i is the size(*i*)-fragment of Q

Each Q_i is finite and any countable union of finite classes is PAC-learnable \Box

Two notions of Efficiency:

a)	polynomial time	\Rightarrow	efficient PAC learning	Known:
b)	m_O polynomial in $n, 1/\varepsilon, 1/\delta$	\Rightarrow	sample-efficient PAC learning	a) \Rightarrow b)

Failure of Efficient PAC

Q has polynomial size fitting property if

whenever a fitting query exists, there exists one of size polynomial in E^+, E^-

${\it Q}$ has polynomial time evaluation property if

there is a polynomial time algorithm

Theorem (Pitt & Valiant, J. ACM 1984)

Let Q be polynomial time evaluable and have the polynomial size fitting property. **Then:** If Q is efficiently PAC learnable, then the fitting problem for Q is in RP.

Consequence Any class $Q \subseteq CQs$ containing all Path Queries is **not** efficiently PAC learnable (unless NP=RP).

Proof Assume *Q* is efficiently PAC learnable [ten Cate, Funk, J, Lutz 2023] *Q* is also PAC learnable over the instances from the NP-hardness proof
1) Over these instances we have polynomial size fitting property
2) Instances are tree-shaped ⇒ polynomial time evaluation
Apply Pitt & Valiant.

Efficient PAC with Membership Queries

Tight relation between Exact Learnability and PAC Learnability

Efficient exact learnability with EQ \Rightarrow Efficient PAC learnability (very often, converse also true)

Efficient exact learnability with EQ+MQ \Rightarrow Efficient PAC learnability with MQs

Transfer results

query class	ontology	questions	learnability
EL/ELJ-concepts	no	MQ	efficient
\mathscr{CL} -concepts	\mathcal{EL}	MQ+EQ	efficient
CQ	no	MQ+EQ	efficient
CQ/ELJ-concepts	\mathcal{ELI}	MQ+EQ	not efficient
CQ	DL-Lite/ \mathscr{EL}	MQ+EQ	open
\mathscr{ELI} -concepts	\mathcal{EL}	MQ+EQ	open

Sample Efficiency of Product Algorithm

Recall the "product algorithm" for \mathscr{CL} :

- Given concepts C_1, \ldots, C_n and D_1, \ldots, D_k :
- 1. compute product concept $C := C_1 \times \ldots \times C_n$
- 2. if $D_i \not\sqsubseteq C$ for all *i*, return *C*
- 3. otherwise return "no fitting concept"

Product algorithm returns always the most specific fitting concept

Bad News Any fitting algorithm that returns a most specific fitting concept (if it exists), is **not** sample-efficient! [ten Cate, Funk, J, Lutz IJCAI'23]

So the "natural" algorithm does not enjoy generalization abilities

Same holds for algorithms that

- a) return the most general fitting concept
- b) return the fitting concept with minimal quantifier depth

Occam's Razor (William of Ockham, 14th century)

"The simplest explanation is usually the best one"

Original formulation "Entities must not be multiplied beyond necessity" ("multiplied" is here in the sense of "combined")

Computational Learning Theory has poured this intuition into the following definition

Learning algorithm **A** is an **Occam algorithm** if there are a polynomial p and $\alpha \in (0,1)$ such that **A** outputs a concept of size $p(s) \cdot m^{\alpha}$, where s is the size of the target and m is the number of examples.

Theorem Every Occam algorithm **A** is a **sample-efficient** PAC learning algorithm. [Blumer, Ehrenfeucht, Haussler, & Warmuth J. ACM 1989]

 \Rightarrow Occam algorithms are one way to obtain sample-efficient PAC learning algorithms.

(For many hypothesis classes, a converse of this is also true)

Bounded Fitting

Input:	Ontology \mathcal{O} , examples E^+, E^-
Bounded	d Fitting proceeds in rounds:
Round 1 Round 2 :	: search for a fitting concept of size 1 : search for a fitting concept of size 2
Round <i>i</i> :	search for a fitting concept of size i
Return th	ne first fitting concept that is found in this way

Similarity with Bounded Model Checking

[Biere, Cimatti, Clarke, Zhu TACAS 1999]

Bounded fitting is Occam Algorithm (independent of ontology/query language)

sample efficient with complexity:

 $O(\frac{1}{\varepsilon} \cdot \log \frac{1}{\varepsilon} \cdot \frac{1}{\delta} \cdot \log |\Sigma| \cdot ||q_T||)$

Flexibility

- different size measures work
- different sequences such as 1, 2, 4, 8, ... work

SPELL: Bounded Fitting for $\mathscr{E}\mathscr{L}$

Observation Problem in

Round *i*: search for a fitting concept of size *i*

is **NP-complete** for ontology and query language \mathscr{EL}

Our system SPELL (\Rightarrow <u>https://github.com/spell-system/SPELL</u>)

implements Bounded Fitting for \mathscr{CL} leveraging a SAT solver

 \Rightarrow Talk tomorrow @DL with more information and detailed benchmarks

SPELL Demo