

Learning Logically Defined Hypotheses

Martin Grohe RWTH Aachen

Outline

- I. A Declarative Model-Theoretic Framework for ML
- II. First-Order Hypotheses on Low-Degree Structures (joint work with Martin Ritzert)
- III. Monadic Second-Order Hypotheses on Strings (joint work with Christof Löding and Martin Ritzert)
- IV. Concluding Remarks

A Declarative Model-Theoretic Framework for ML

Observations about today's ML practice

 Algorithmic focus: goal is to approximate an unknown function as well as possible (rather than understanding the function)

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Declarative approach

Try to separate model from solver as far as possible.

Background structure

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Parametric model

Model described by formula of a suitable logic, which usually has certain free variables for parameters.

Goal

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Data

A list of applicants, or rather certain pieces of information about the applicants, labelled by the information of whether they succeeded or not.

Scenario 1

Suppose for each person we only have the following information:

p = number of publications, t = years since PhD.

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Representation in our framework

- Background structures: ordered field of the reals
- Model: $\varphi(x_1, x_2; y_1, y_2) := (x_1 \ge y_1 \cdot x_2 + y_2)$

Scenario 2

We have a publication database of a schema that includes relations

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Our model may say something like the following (with parameters $a, b, c_1, \ldots, c_m, d_1, \ldots, d_n$):

- ▶ the candidate has at least *a* publications on average per year
- and at least b single-author publications
- ► and either a joint publication with an author from one of the universities c₁,..., c_m
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This can be expressed by a SQL query $\varphi(x; y_1, \dots, y_{m+n+2})$.

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problems} here.
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    Finite or infinite structure $\red B$ with universe $U
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    \alert{Instance space} is $U(B)^k$ for some $k$.
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1&\text{if } B\models\phi(\bar u\smid\bar v),\\ 9
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Select all positions with letter 'B' in LaTeX math mode.

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Hypotheses

For each parameter tuple $\bar{v} \in U(B)^{\ell}$ a Boolean function $\llbracket \varphi(\bar{x}; \bar{v}) \rrbracket^{B} \colon U(B)^{k} \to \{0, 1\}$ defined by

$$\llbracket \varphi(\bar{x}\,;\,\bar{v})
brace^B(\bar{u}) := egin{cases} 1 & ext{if } B \models \varphi(\bar{u}\,;\,\bar{v}), \ 0 & ext{otherwise.} \end{cases}$$

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- Usually, only a small part of the background structure can be inspected at runtime
- At this point it is wide open what may constitute good logics for specifying models.
- Approach probably best suited for applications where specifications in some kind of logic or formal language are common, such as verification or database systems.

Learning

Input

Learning algorithms have access to background structure B and receive as input a training sequence T of labelled examples:

$$(\overline{u}_1, \lambda_1), \ldots, (\overline{u}_t, \lambda_t) \in U(B)^k \times \{0, 1\}.$$

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Goal

Find hypothesis of the form $\llbracket \varphi(\bar{x}; \bar{v}) \rrbracket^B$ that generalises well, that is, predicts true target values for instances $\bar{u} \in U(B)^k$ well.

The training error $\operatorname{err}_{T}(H)$ (a.k.a. empirical risk) of a hypothesis H on a training sequence T is the fraction of examples in T labelled wrong by H.

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• \mathcal{H} is a set of hypothesis of the form $[\![\varphi(\bar{x};\bar{v})]\!]^B$.

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Often we regard φ or at least its quantifier rank fixed. Then this amounts to empirical risk minimisation (ERM).

Remarks on VC-Dimension and PAC-Learning

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- This implies PAC-learnability (in an information theoretic sense).
- ► However, it comes without any guarantees on efficiency.

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- However, we still assume the structure to be very large, and we want our learning algorithms to run in sublinear time in the size of the structure.
- To be able to do meaningful computations in sublinear time, we usually need some form of local access to the structure. For example, we should be able to access the neighbours of a vertex in a graph.

Complexity Considerations

We strive for algorithms running in time polynomial in the size of the training data, regardless of the size of the background structure (or at most polylogarithmic in the size of the background structure).

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- Then we can simply ignore the regularisation term (only depending on φ) and follow the ERM paradigm: we need to find a formula of quantifier rank at most q and a parameter tuple that minimise the training error.

First-Order Hypotheses on <u>Low-Degree St</u>ructures

Theorem (G., Ritzert 2017) There is a learner for FO running in time

 $(d+t)^{O(1)}$

where

- t = |T| is the length of the training sequence
- ► d is the maximum degree of the background structure B
- the constant hidden in the O(1) depends on q, k, ℓ .







Idea Exploit locality of FO (Gaifman's Theorem).

Key Lemma

Parameters far away from all training examples are irrelevant.



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Algorithm

Search through all local formulas of desired quantifier rank and all parameter settings close to training points and check which hypothesis has the smallest training error.

Monadic Second-Order Hypotheses on Strings

String $a_1 \ldots a_n$ over alphabet Σ viewed as structure with

- ▶ universe {1, . . . , *n*},
- binary order relation \leq on positions,
- for each $a \in \Sigma$ a unary relation R_a that contains all positions i such that $a_i = a$.

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Example

baa<mark>a</mark>acabcaaaaaaaab<mark>a</mark>aaa<mark>a</mark>baacaaa<u>aaab</u>aaaaaaaaaaabbaccc<mark>a</mark>acbcba

Formula

$$\varphi(x; y) = R_a(x) \land \exists z \Big(z < x \land \forall z' \big(z < z' < x \to R_a(z') \big) \\ \land \big((R_b(z) \land z < y) \lor (R_c(z) \land z \ge y) \big) \Big)$$

with parameter v = 35 consistent with training examples.

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Theorem (G., Löding, Ritzert 2017)

- 1. There are learners running in time $t^{O(1)}$ for quantifier-free formulas and 1-dimensional existential formulas over strings.
- 2. There is no sublinear learning algorithm for ∃∀-formulas or 2-dimensional existential formulas over strings.

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Bummer

Previous theorem shows that learning MSO (even full FO) is not possible in sublinear time.

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Example

Solution: Index on Background Structure

We can resolve this by building an index data structure over the background string.

We do this is a pre-processing phase where we only have access to the background structure, but not yet the training examples.





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Simons Factorisation Trees (Simon 1982)

We can construct a factorisation tree of constant height for a given string in linear time (where the constant depends non-elementarily on the quantifier rank q).

Learning MSO

Theorem (G., Löding, Ritzert 2017)

There is a learner for MSO over strings with pre-processing time O(n) and learning time $t^{O(1)}$.

Pre-Processing

In the pre-processing phase, our algorithm builds a Simon factorisation tree for the background string B.



One by one, the training examples are incorporated into the factorisation tree.



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Where do we go from here?

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- What are suitable logics anyway?
- Go beyond Boolean classification.
- Can we design practical learning algorithms for our framework?

Vision

Design an data analysis system much like a databases system, providing an interface to "predictive queries" and for querying complex ML models (like ANNs).

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