Computational learning theory.
PAC learning. VC dimension.

Petr Pošík

Czech Technical University in Prague
Faculty of Electrical Engineering
Dept. of Cybernetics

Computational Learning Theory, COLT

Introduction and basic concepts

Concept

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- even number, four-wheel vehicle, active politician, smart man, correct hypothesis

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Object $x \in X$ is described with values of some features:

- number {value}
- vehicle {manufacturer, engine type, number of doors, ...}
- politician {number of votings in the parliament, number of law proposals, number of law amendment proposals, number of interpellations, ...}

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- politician $\{$number of votings in the parliament, number of law proposals, number of law amendment proposals, number of interpellations, . . . $\}$

Target concept $c \in C$ corresponds to certain subset of X, $c \subseteq X$:

- each instance of $x \in X$ is either an *example* or a *counter-example* of a concept c
- characteristic function $f_c : X \rightarrow \{0, 1\}$
  - if $f_c(x) = 1$, x is a positive example for concept c
  - if $f_c(x) = 0$, x is a negative example (counter-example) of concept c
- Concept c is any boolean function f over X!

Hypothesis

Inductive learning task: find a hypothesis (model) h, which corresponds as much as possible to the target concept c, given

- a subset $D \subset X$ of examples (and counter-examples) of the target concept (training data) and
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The goal of learning:

- find a hypothesis h which is **correct for all examples** from X, i.e.

$$\forall x \in X : h(x) = c(x).$$

COLT: Goals

Computational learning theory (COLT) tries to theoretically characterize

1. the machine learning *problem complexity*, i.e.
   - under what circumstances learning is actually possible,
2. the *abilities of ML algorithms*, i.e.
   - under what circumstances, a learning algorithm is able to learn successfully.

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COLT tries to answer questions like:

- Are there some problem complexity classes independently of the model/algorithm used?
- What type of model (class of hypotheses) should we use? Is there an algorithm which is consistently better then some other algorithm?
- How many training examples do we need so that a model (hypothesis) can be successfully learned?
- If the hypothesis space is large, is it actually possible to find the best hypothesis in a reasonable time?
- How complex should the resulting hypothesis be?
- If we find a hypothesis which is correct for all the training data $D \subset X$, *how can we be sure that the hypothesis is also correct for the rest of the data* $X \setminus D$???
- How many errors will the algorithm make before it learns the target concept successfully?

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Generalization ability:

- The ability of a learning algorithm to build a model which is able to correctly classify also the examples which were not part of the training data set D.
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Notation:

- $P_A(h)$: prior probability that algorithm A generates hypothesis h
- $P_A(h|D)$: probability that algorithm A generates h given the training data D:
  - in case of deterministic algorithms (nearest neighbors, decision trees, etc.), $P_A(h|D)$ is zero almost everywhere with the exception of a single hypothesis
  - in case of stochastic algorithms (e.g. neural network trained from random initial weights), the distribution $P_A(h|D)$ is non-zero for a larger subset of all hypotheses
- $P(c|D)$: the distribution of concepts consistent with training data D

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If we do not know the target concept c, a natural measure of the algorithm generalization ability is the expected error over all concepts given the training data D:

$$E(\mathrm{Err}_A|D) = \sum_{h,c} \sum_{x \in X \setminus D} P(x) \cdot I(c(x) \neq h(x)) \cdot P_A(h|D) \cdot P(c|D)$$

Without knowing $P(c|D)$ we cannot compare 2 algorithms based on their generalization error!!!

Example

Assume that

- objects are described by 3 binary attributes,
- we have a single concept c, and
- 2 deterministic algorithms and their corresponding hypotheses h_1 and h_2: training data are memorized, one algorithm assigns new data to class +1, the other to class -1.

	$\boldsymbol{x}$	c	h_1	h_2
D	000	1	1	1
	001	-1	-1	-1
	010	1	1	1
$X \setminus D$	011	-1	1	-1
	100	1	1	-1
	101	-1	1	-1
	110	1	1	-1
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COLT
- Concept
- Hypothesis
- COLT: Goals
- Generalization
- Example
- NFL
- Bias

PAC learning

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Given a concept c:

- $E(\mathrm{Err}_{A_1}|c, D) = 0.4$, $E(\mathrm{Err}_{A_2}|c, D) = 0.6$,
- algorithm A_1 is clearly better than A_2.

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- algorithm A_1 is clearly better than A_2.

During the hypothesis building, we do not know the target concept c!

- Assuming we have no prior information about concept c, all concepts are equally probable.
- Training set D
  - allows us to eliminate all inconsistent hypotheses (224 in our case), but
  - it does not allow us to choose the right hypothesis among the consistent ones (in our case, there are 32 hypotheses remaining), because
  - averaged over all concepts c consistent with D, both hypotheses are equally successful!

No Free Lunch

"No Free Lunch" theorem: For any 2 algorithms A_1 and A_2 (represented by $P_{A_1}(h|D)$ and $P_{A_2}(h|D)$) the following statements hold independently of the sampling distribution $P(\boldsymbol{x})$ and independently of a particular training data set D:

1. Averaged over all concepts c, $E(\mathrm{Err}_{A_1}|c, D) = E(\mathrm{Err}_{A_2}|c, D)$.
2. Averaged over all distributions $P(c)$, $E(\mathrm{Err}_{A_1}|c, D) = E(\mathrm{Err}_{A_2}|c, D)$.

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NFL corollaries:

- You can try hard to build one super algrithm and one terrible algorithm, but averaged over all concepts, both algorithms are equally good.
- If A_1 is better than A_2 on certain kind of problems, there must be other kind of problems where A_2 is better than A_1.
- All statements like "alg. 1 is better than alg. 2" are not saying anything about the algorithms, but rather about the set of concepts which were used to test the algorithms.
- In practice, for certain application area, we seek an algorithm which
  - works worse on problems we do not expect in the field, while
  - works well on problems which are highly probable.
- *Generalization is not possible without (often implicit) bias of the algorithm!*
- *The more the model assumptions correspond to the data, the better the generalization ability of the model!*

Bias

Inductive bias (předpojatost, zaujetí modelu):

- The sum of all (even implicit) assumptions the model makes about the application area.
- Taking advantage of these assumptions allows the model to generalize, i.e. to provide correct predictions even for unknown data, if the model assumptions correspond to reality.

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Possible sources of model bias:

- Language bias:
  - The language of hypotheses does not need to correspond to the language of concepts.
  - Some concepts cannot be expressed in the hypotheses language.
  - Different language may allow for efficient learning.
- Preference bias:
  - Algorithm prefers some of the hypotheses consistent with D.
  - Algorithm may even choose a slightly inconsistent hypothesis.
  - Occam's razor
- ...

PAC learning

PAC learning

Probably Approximately Correct (PAC) learning:

- Characterizes the concept classes which are/are not learnable by certain class of hypotheses
  - using a “reasonable” number of training examples and
  - using an algorithm with “reasonable” computational complexity,

  for both
  - finite hypotheses spaces and
  - infinite hypotheses spaces (capacity, VC dimension).
- Defines a natural measure of complexity of the hypotheses spaces (VC dimension) which allows us to bound the required size of training data for inductive learning.

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PAC learning assumptions:

- *Independence:* Examples $E_i = (x_i, c_i)$ are sampled independently, i.e. $P(E_i | E_{i-1}, E_{i-2}, \ldots) = P(E_i)$.
- *Identically distributed:* Future examples shall be sampled from a distribution equal to the one used for the previous examples: $P(E_i) = P(E_{i-1}) = \ldots$.
- Both conditions together are often denoted as "i.i.d." (independent and identically distributed).

(In this lecture we also assume that concept c is deterministic and that it is part of the hypotheses space H).

Hypothesis error rate

Real error rate of hypothesis h

- with regard to the target concept c and
- with regard to the distribution of examples $P(X)$ is

$$\mathrm{Err}(h) = \sum_{x \in X} I(h(x) \neq c(x)) \cdot P(x),$$

- i.e. it is the probability that the hypothesis classifies example x incorrectly.

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Is it possible to determine the number of training examples required to learn concept c with 0 error rate?

- If the set of training examples D is only a subset of X, there are still several hypotheses consistent with D (see NFL).
- Training examples are chosen randomly and can be misleading.

PAC framework

PAC framework defines what it actually means to *successfully learn* a concept.

- It does not require the ability to *learn any concept* that can be defined over X:
  - We are interested in certain subsets of all concepts $C \subseteq 2^X$. (Some concepts cannot be learned, e.g. when C is infinite and H is finite.)
  - Similarly, algorithm A will search for an appropriate hypothesis in certain hypotheses class H only.
  - $C = H$ may, but does not have to be fulfilled.
- It does not require zero error of the learned hypothesis h.
  - The hypothesis error rate is bounded with a small constant ϵ.
- It does not require the algorithm to produce the hypothesis with an acceptable error rate each time.
  - The probability of this event is however bounded by a small constant δ.

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A concept class C is **PAC-learnable** using the hypotheses class H if

- for all concepts $c \in C$, all distributions $P(X)$, $X = \{0,1\}^n$, and for any $0 < \epsilon, \delta < 1$
- there is a polynomial algorithm A, which returns a hypothesis with $\mathrm{Err}(h) \leq \epsilon$ with probability at least $1 - \delta$
- using at most polynomial amount of training examples $(x_i, c(x_i))$ sampled from $P(X)$.
- "Polynomial": growing at most at polynomial rate with $\frac{1}{\epsilon}$, $\frac{1}{\delta}$ and n.

Consistent PAC learning

A consistent learning algorithm

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- The size m of the training set D required to PAC-learn the concept c using H.
- It grows with the problem dimensionality (with the number n of object attributes).
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How many training examples do we need to be able to say that *with a sufficiently high probability all consistent hypotheses are approximately correct?*

- Let's denote the set of bad hypotheses $H_B = \{h \in H : \text{Err}(h) > \epsilon\}$, $h_B \in H_B$.
- $\Pr(h_B \text{ is consistent with 1 training example}) \leq 1 - \epsilon$
- $\Pr(h_B \text{ is consistent with all training examples}) \leq (1-\epsilon)^m$ (Examples are independent.)
- $\Pr(H_B \text{ contains a hypothesis consistent with all training examples}) \leq |H_B|(1-\epsilon)^m \leq |H|(1-\epsilon)^m$

  Probability that a consistent hypothesis is not approximately correct.
- Let's bound the probability of this event with a small constant δ: $|H|(1-\epsilon)^m \leq \delta$.
- Using $1 - \epsilon \leq e^{-\epsilon}$:

$$m \geq \frac{1}{\epsilon}(\ln \frac{1}{\delta} + \ln |H|)$$

If h is consistent with m examples, then $\text{Err}(h) \leq \epsilon$ with the probability at least $1-\delta$.

Sample complexity

Sample complexity:

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Let H be the class of all boolean functions over n attributes:

- $|H| = 2^{2^n}$
- Sample complexity m grows like $\ln |H|$, i.e. like 2^n.
- But the maximal training set size grows like 2^n as well.
- PAC-learning in the class of all boolean functions requires training on all (or almost all) possible training examples!
- Reason:
  - H contains enough hypotheses to classify any set of examples in any way.
  - For any training set of m examples, the number of hypotheses consistent with the training data which classify example $\boldsymbol{x}_{m+1}$ as positive is the same as the number of consistent hypotheses which classify this example as negative.
  - See NFL: *to allow for any generalization, we need to constrain the hypotheses space H.*

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  - See NFL: *to allow for any generalization, we need to constrain the hypotheses space H.*

Observation: m is a function of $|H|$:

- If we get an additional information (constraint limiting the class of admissible hypotheses) and embed it in the training algorithm (introduce bias), then a lower number of training examples shall be sufficient!
- **Domain knowledge** plays an important role.

Example: Decision list

Decision list (DL)

- is a sequence of tests (each test is a conjunction of literals).
- If a test succeeds, DL returns the class assigned to that test. Otherwise it continues with another test.
- *Unconstrained* DL can represent any boolean function!

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Let's constrain the hypotheses space H to the language k-DL:

- Set of decision lists where each test is a conjunction of at most k literals.
- The k-DL language contains the language k-DT (set of decision trees with the depth at most k) as its subset.
- The particular instance of the k-DL language depends on the set of attributes (the representation used).
- Let k-DL(n) be the k-DL language over n Boolean attributes.

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How can we show that the hypotheses class k-DL is PAC-learnable?

1. Show that sample complexity is at most polynomial (see next slide).
2. Show that there is a learning algorithm with at most polynomial computational complexity. (Not presented, but e.g. CN2 algorithm will do.)

Example: Decision list (cont.)

Let's show that any hypothesis from k-DL can be accurately approximated by learning from a training set of a reasonable size:

- We need to estimate the number of hypotheses in the language.
- Let $Conj(n, k)$ be the set of tests (conjunctions of at most k literals over n attributes).
- Each test is assigned with an output value "Yes", "No", or it does not have to be present in the list at all, thus there are at most $3^{|Conj(n,k)|}$ different sets of tests.
- Each of these sets of test may be used in an arbitrary order, thus $|k\text{−DL}(n)| \leq 3^{|Conj(n,k)|} \cdot |Conj(n, k)|!$.
- The number of at most k literals with n attributes: $|Conj(n, k)| = \sum_{i=0}^{k} \binom{2n}{i} = \mathcal{O}(n^k)$.
  $2n$, since the conjunction can contain each individual attribute test directly or in negation.
- After simplification: $k\text{−DL}(n) = 2^{\mathcal{O}(n^k \log_2(n^k))}$
- Substituting this result for $|H|$ to the sample complexity equation:
  $m \geq \frac{1}{\epsilon}\left(\ln\frac{1}{\delta} + \mathcal{O}\left(n^k \log_2(n^k)\right)\right)$
- m grows polynomially with n
- Any algorithm that returns a k-DL consistent with training data will PAC-learn a k-DL concept with a reasonable training set size.

Example: DNF Formulas

Disjunctive normal form (DNF):

- Objects described with n Boolean attributes $a_1, \ldots, a_n$.
- DNF formula: a disjunction of conjunctions, e.g. $(a_1 \land \neg a_2 \land a_5) \lor (\neg a_3 \land a_4)$

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What is the size of the hypotheses space H:

- 3^n possible conjunctions.
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PAC-learning of DNF formulas is still an open problem.

Examples of results for PAC learning

1. Conjunctive concepts are PAC-learnable, but
   concepts in the form of a disjunction of 2 conjunctions are not PAC-learnable.
2. Linearly separable concepts (perceptrons) are PAC-learnable in both Boolean and real spaces. But
   a conjunction of 2 perceptrons is not PAC-learnable, similarly to a disjunction of 2 perceptrons and multi-layer perceptrons with 2 hidden units. If we additionally constrain the weights to values 0 and 1, then even perceptrons in Boolean space are not PAC-learnable.
3. The classes k-CNF, k-DNF and k-DL are PAC-learnable for a given k. But
   we do not know if DNF formulas, CNF formulas, or decision trees are PAC-learnable.

VC dimension

Disadvantages of using $|H|$ in the sample complexity formula:

- Results in a worst-case estimate.
- It is often very pessimistic, it overesimates the number of required training examples.
- $|H|$ cannot be used for infinite hypotheses spaces.

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Capacity, Vapnik-Chervonenkis dimension $VC(H)$

- Another measure of the complexity (flexibility) of the hypotheses class H: it quantifies the bias of embodied in ceartain hypotheses class H.
- Applicable even for infnite H.
- Can provide a tighter bound for the sample complexity.

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- Another measure of the complexity (flexibility) of the hypotheses class H: it quantifies the bias of embodied in ceartain hypotheses class H.
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Sample complexity using VC dimension:

- Hypotheses space H, concepts space C, $C \subseteq H$.
- Sample complexity for any consistent algorithm learning $c \in C$ using H is

$$m \geq \frac{1}{\epsilon}\left(4\log_2\frac{2}{\delta} + 8 \cdot VC(H) \cdot \log_2\frac{13}{\epsilon}\right)$$

VC dimension (cont.)

VC dimensions for certain hypotheses classes H:

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  It can be shown that $\sin(\alpha x)$ can in 1D space correctly classify any number of examples.

- VC dimension of SVM with RBF kernel without any constraint on the penalty term: $VC(f_{SVM-RBF}) = \infty$

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Other uses of VC dimension:

- Estimation of a true (testing) error of a classifier on the basis of the training data only.
- "Structural risk minimization", the basic principle of SVM.

Summary

- **Generalization requires bias!!!**
- NFL: All models/algorithms are equally good on average.
  - If a certain class of models works better for certain class of problems, there must be another class of problems, for which it workse worse.
  - Our goal is to find models/algorithms which
    - work well for problem classes often observed in practice, and
    - have below average performace on problem classes which are not practically important.
- Probably Approximately Correct (PAC) learning:
  - specifies what it means to "learn correctly".
  - introduces tolerances for the model error (ϵ) and for the probability (δ) that a learned model has a larger error than ϵ.
  - allows to estimate the required training set size.
- VC dimension:
  - a measure of flexibility of (even infinite) hypotheses class.
  - usually provides tighter estimates of the sample complexity than the formula with $|H|$.