Foundations of Machine Learning
Lecture 2

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PAC Model,
Guarantees for Learning with Finite Hypothesis Sets

Motivation

- Some computational learning questions
  - What can be learned efficiently?
  - What is inherently hard to learn?
  - A general model of learning?
- Complexity
  - Computational complexity: time and space.
  - Sample complexity: amount of training data needed to learn successfully.
  - Mistake bounds: number of mistakes before learning successfully.

This lecture

- PAC Model
- Sample complexity, finite H, consistent case
- Sample complexity, finite H, inconsistent case

Definitions and Notation

- X: set of all possible instances or examples, e.g., the set of all men and women characterized by their height and weight.
- $c\colon X \to \{0,1\}$: the target concept to learn; can be identified with its support $\{x \in X : c(x) = 1\}$.
- C: concept class, a set of target concepts c.
- D: target distribution, a fixed probability distribution over X. Training and test examples are drawn according to D.

Definitions and Notation

- S: training sample.
- H: set of concept hypotheses, e.g., the set of all linear classifiers.
- The learning algorithm receives sample S and selects a hypothesis h_S from H approximating c.

Errors

- **True error or generalization error** of h with respect to the target concept c and distribution D :

$$R(h) = \Pr_{x \sim D}[h(x) \neq c(x)] = \mathop{\mathrm{E}}_{x \sim D}[1_{h(x) \neq c(x)}].$$

- **Empirical error**: average error of h on the training sample S drawn according to distribution D,

$$\widehat{R}_S(h) = \Pr_{x \sim \widehat{D}}[h(x) \neq c(x)] = \mathop{\mathrm{E}}_{x \sim \widehat{D}}[1_{h(x) \neq c(x)}] = \frac{1}{m} \sum_{i=1}^{m} 1_{h(x_i) \neq c(x_i)}.$$

- **Note**: $R(h) = \mathop{\mathrm{E}}_{S \sim D^m}\left[\widehat{R}_S(h)\right].$

PAC Model

(Valiant, 1984)

- PAC learning: Probably Approximately Correct learning.
- Definition: concept class C is PAC-learnable if there exists a learning algorithm L such that:
  - for all $c \in C, \epsilon > 0, \delta > 0$, and all distributions D,

$$\Pr_{S \sim D^m}[R(h_S) \leq \epsilon] \geq 1 - \delta,$$

  - for samples S of size $m = poly(1/\epsilon, 1/\delta)$ for a fixed polynomial.

Remarks

- Concept class C is known to the algorithm.
- Distribution-free model: no assumption on D.
- Both training and test examples drawn $\sim D$.
- Probably: confidence $1-\delta$.
- Approximately correct: accuracy $1-\epsilon$.
- Efficient PAC-learning: L runs in time $poly(1/\epsilon, 1/\delta)$.
- What about the cost of the representation of $c \in C$?

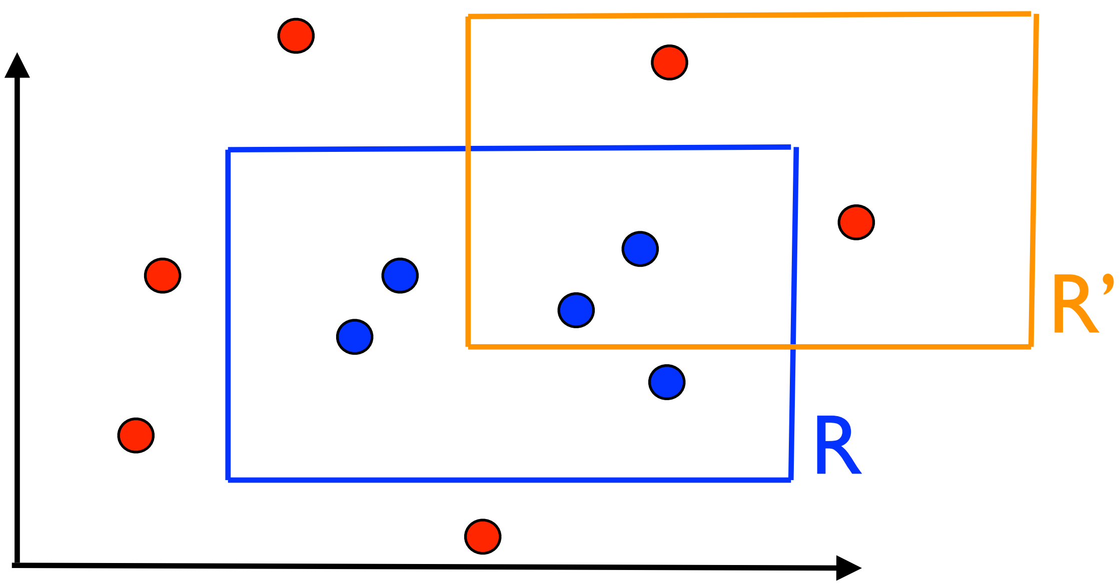
PAC Model - New Definition

- Computational representation:
  - cost for $x \in X$ in $O(n)$.
  - cost for $c \in C$ in $O(size(c))$.
- Extension: running time.

$$O(poly(1/\epsilon, 1/\delta)) \longrightarrow O(poly(1/\epsilon, 1/\delta, n, size(c))).$$

Example - Rectangle Learning

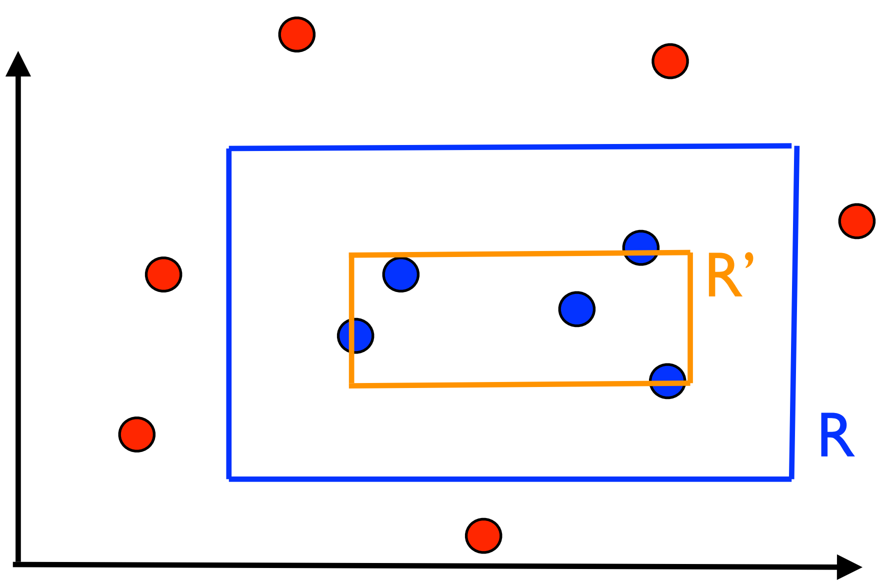
- Problem: learn unknown axis-aligned rectangle R using as small a labeled sample as possible.



- Hypothesis: rectangle R'. In general, there may be false positive and false negative points.

Example - Rectangle Learning

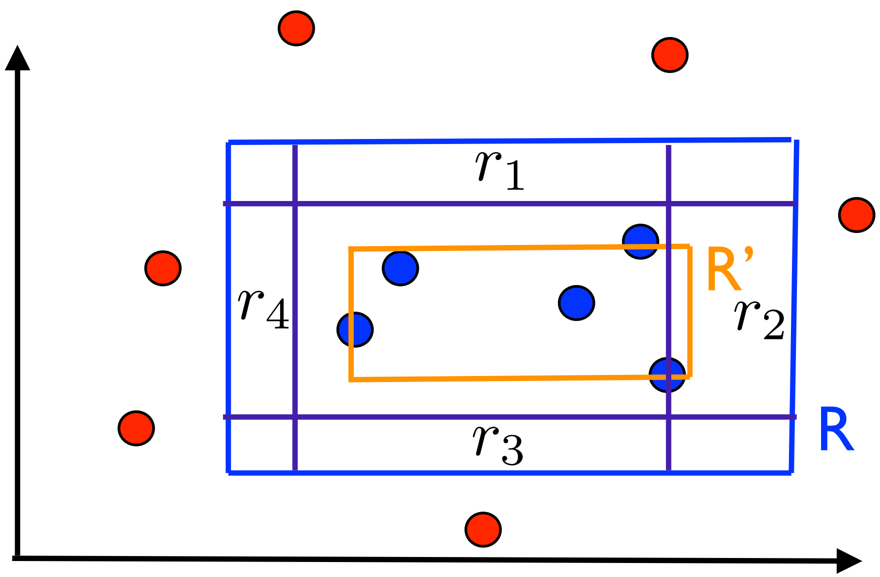
- Simple method: choose tightest consistent rectangle R' for a large enough sample. How large a sample? Is this class PAC-learnable?



- What is the probability that $R(\mathrm{R}') > \epsilon$?

Example - Rectangle Learning

- Fix $\epsilon > 0$ and assume $\Pr_D[\text{R}] > \epsilon$ (otherwise the result is trivial).
- Let r_1, r_2, r_3, r_4 be four smallest rectangles along the sides of R such that $\Pr_D[r_i] \geq \frac{\epsilon}{4}$.



$$\text{R} = [l, r] \times [b, t]$$
$$r_4 = [l, s_4] \times [b, t]$$
$$s_4 = \inf\{s \colon \Pr\left[[l, s] \times [b, t]\right] \geq \tfrac{\epsilon}{4}\}$$
$$\Pr_D\left[[l, s_4[\times [b, t]\right] < \tfrac{\epsilon}{4}$$

Example - Rectangle Learning

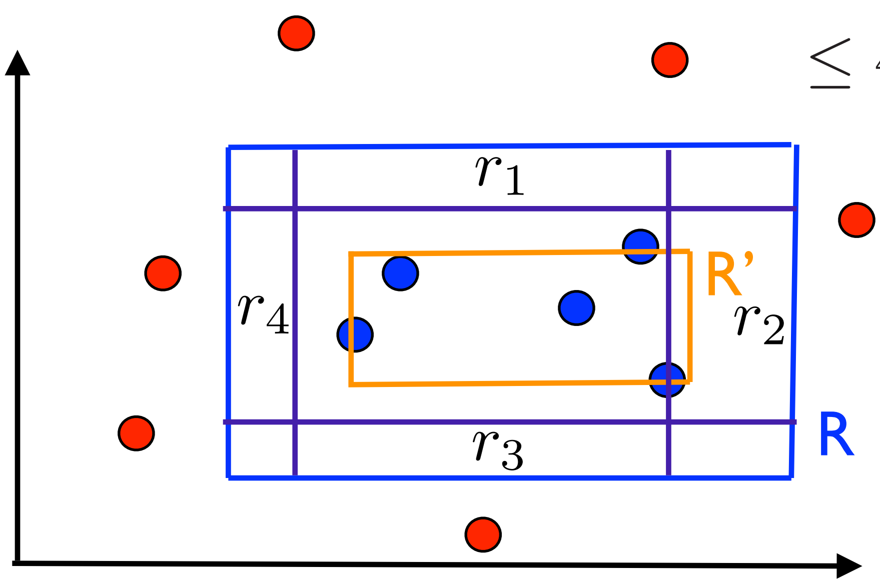
- Errors can only occur in $\mathrm{R}-\mathrm{R}'$. Thus (geometry),

  $R(\mathrm{R}') > \epsilon \Rightarrow \mathrm{R}'$ misses at least one region r_i.

- Therefore, $\Pr[R(\mathrm{R}') > \epsilon] \leq \Pr[\cup_{i=1}^{4} \{\mathrm{R}' \text{ misses } r_i\}]$

$$\leq \sum_{i=1}^{4} \Pr[\{\mathrm{R}' \text{ misses } r_i\}]$$

$$\leq 4(1 - \tfrac{\epsilon}{4})^m \leq 4e^{-\frac{m\epsilon}{4}}.$$



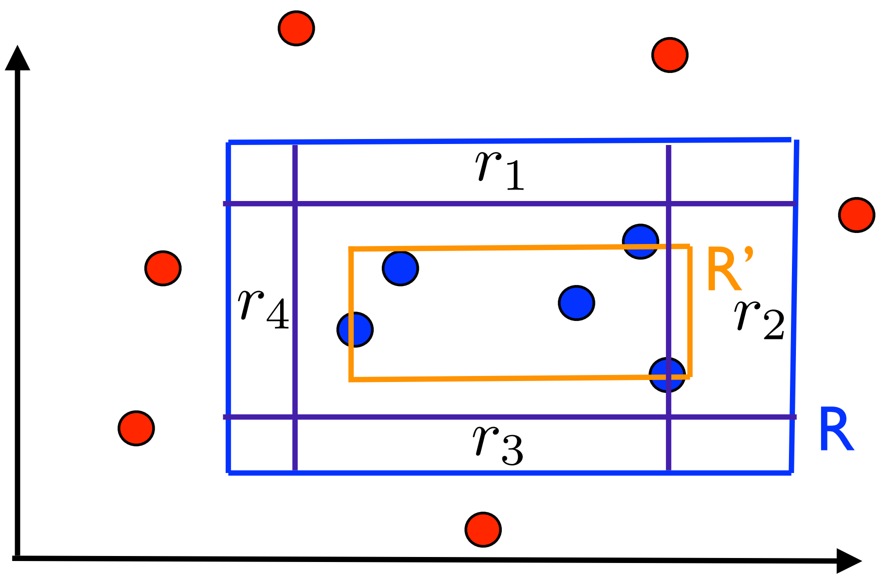
Example - Rectangle Learning

- Set $\delta > 0$ to match the upper bound:

$$4e^{-\frac{m\epsilon}{4}} \leq \delta \Leftrightarrow m \geq \frac{4}{\epsilon} \log \frac{4}{\delta}.$$

- Then, for $m \geq \frac{4}{\epsilon} \log \frac{4}{\delta}$, with probability at least $1-\delta$,

$$R(\mathsf{R}') \leq \epsilon.$$



Notes

- Infinite hypothesis set, but simple proof.
- Does this proof readily apply to other similar concepts classes?
- Geometric properties:
  - key in this proof.
  - in general non-trivial to extend to other classes, e.g., non-concentric circles (see HW2, 2006).

→ Need for more general proof and results.

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Learning Bound for Finite H - Consistent Case

- **Theorem**: let H be a finite set of functions from X to $\{0, 1\}$ and L an algorithm that for any target concept $c \in H$ and sample S returns a consistent hypothesis h_S: $\widehat{R}(h_S) = 0$. Then, for any $\delta > 0$, with probability at least $1 - \delta$,

$$R(h_S) \leq \frac{1}{m}(\log |H| + \log \frac{1}{\delta}).$$

Learning Bound for Finite H - Consistent Case

- **Proof**: Fix $h \in H$, then

$$\Pr[h \text{ consistent} \,|\, R(h) < \epsilon] \leq (1-\epsilon)^m.$$

- Thus,

$$\begin{aligned}
&\Pr[\exists h \in H \colon h \text{ consistent} \wedge R(h) > \epsilon] \\
&\quad = \Pr[(h_1 \in H \text{ consistent} \wedge R(h_1) > e) \vee \cdots \vee (h_{|H|} \in H \text{ consistent} \wedge R(h_{|H|}) > \epsilon)] \\
&\quad \leq \sum_{h \in H} \Pr[h \text{ consistent} \wedge R(h) > \epsilon] \qquad \text{(union bound)} \\
&\quad \leq \sum_{h \in H} \Pr[h \text{ consistent} \mid R(h) > \epsilon] \\
&\quad \leq \sum_{h \in H} (1-\epsilon)^m = |H|(1-\epsilon)^m \leq |H| e^{-m\epsilon}.
\end{aligned}$$

Remarks

- The algorithm can be ERM if problem realizable.
- Error bound linear in $\frac{1}{m}$ and only logarithmic in $\frac{1}{\delta}$.
- $\log_2 |H|$ is the number of bits used for the representation of H.
- Bound is loose for large $|H|$.
- Uninformative for infinite $|H|$.

Conjunctions of Boolean Literals

- Example for $n=6$.
- Algorithm: start with $x_1 \wedge \overline{x}_1 \wedge \cdots \wedge x_n \wedge \overline{x}_n$ and rule out literals incompatible with positive examples.

0	1	1	0	1	1	+
0	1	1	1	1	1	+
0	0	1	1	0	1	-
0	1	1	1	1	1	+
1	0	0	1	1	0	-
0	1	0	0	1	1	+
0	1	?	?	1	1	

$$\longrightarrow \overline{x}_1 \wedge x_2 \wedge x_5 \wedge x_6.$$

Conjunctions of Boolean Literals

- **Problem**: learning class C_n of conjunctions of boolean literals with at most n variables (e.g., for $n=3$, $x_1 \wedge \overline{x_2} \wedge x_3$).
- **Algorithm**: choose h consistent with S.
  - Since $|H|=|C_n|=3^n$, sample complexity:
    $$m \geq \frac{1}{\epsilon}\big((\log 3)\, n + \log \tfrac{1}{\delta}\big).$$
    $\delta=.02, \epsilon=.1, n=10, m \geq 149.$
  - Computational complexity: polynomial, since algorithmic cost per training example is in $O(n)$.

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Inconsistent Case

- No $h \in H$ is a consistent hypothesis.
- The typical case in practice: difficult problems, complex concept class.
- But, inconsistent hypotheses with a small number of errors on the training set can be useful.
- Need a more powerful tool: Hoeffding's inequality.

Hoeffding's Inequality

- Corollary: for any $\epsilon > 0$ and any hypothesis $h : X \to \{0, 1\}$ the following inequalities holds:

$$\Pr[R(h) - \widehat{R}(h) \geq \epsilon] \leq e^{-2m\epsilon^2}$$

$$\Pr[\widehat{R}(h) - R(h) \geq \epsilon] \leq e^{-2m\epsilon^2}.$$

- Combining these one-sided inequalities yields

$$\Pr[|R(h) - \widehat{R}(h)| \geq \epsilon] \leq 2e^{-2m\epsilon^2}.$$

Application to Learning Algorithm?

- Can we apply that bound to the hypothesis h_S returned by our learning algorithm when training on sample S?
- No, because h_S is not a fixed hypothesis, it depends on the training sample. Note also that $\mathrm{E}[\widehat{R}(h_S)]$ is not a simple quantity such as $R(h_S)$.
- Instead, we need a bound that holds simultaneously for all hypotheses $h \in H$, a uniform convergence bound.

Generalization Bound - Finite H

- Theorem: let H be a finite hypothesis set, then, for any $\delta > 0$, with probability at least $1-\delta$,

$$\forall h \in H,\ R(h) \leq \widehat{R}_S(h) + \sqrt{\frac{\log|H| + \log\frac{2}{\delta}}{2m}}.$$

- Proof: By the union bound,

$$\begin{aligned}
&\Pr\left[\max_{h\in H}\left|R(h) - \widehat{R}_S(h)\right| > \epsilon\right] \\
&= \Pr\left[\left|R(h_1) - \widehat{R}_S(h_1)\right| > \epsilon \vee \ldots \vee \left|R(h_{|H|}) - \widehat{R}_S(h_{|H|})\right| > \epsilon\right] \\
&\leq \sum_{h\in H} \Pr\left[\left|R(h) - \widehat{R}_S(h)\right| > \epsilon\right] \\
&\leq 2|H|\exp(-2m\epsilon^2).
\end{aligned}$$

Remarks

- Thus, for a finite hypothesis set, whp,

$$\forall h \in H, R(h) \leq \widehat{R}_S(h) + O\left(\sqrt{\frac{\log |H|}{m}}\right).$$

- Error bound in $O(\frac{1}{\sqrt{m}})$ (quadratically worse).
- $\log_2 |H|$ can be interpreted as the number of bits needed to encode H.
- Occam's Razor principle (theologian William of Occam): "plurality should not be posited without necessity".

Occam's Razor

- Principle formulated by controversial theologian William of Occam: "plurality should not be posited without necessity", rephrased as "the simplest explanation is best";
  - invoked in a variety of contexts, e.g., syntax. Kolmogorov complexity can be viewed as the corresponding framework in information theory.
  - here, to minimize true error, choose the most parsimonious explanation (smallest $|H|$).
  - we will see later other applications of this principle.

Lecture Summary

- C is PAC-learnable if $\exists L, \forall c \in C, \forall \epsilon, \delta > 0, m = P\left(\frac{1}{\epsilon}, \frac{1}{\delta}\right)$,
$$\Pr_{S \sim D^m}[R(h_S) \leq \epsilon] \geq 1 - \delta.$$
- Learning bound, finite H consistent case:
$$R(h) \leq \frac{1}{m}\left(\log |H| + \log \frac{1}{\delta}\right).$$
- Learning bound, finite H inconsistent case:
$$R(h) \leq \widehat{R}_S(h) + \sqrt{\frac{\log |H| + \log \frac{2}{\delta}}{2m}}.$$
- How do we deal with infinite hypothesis sets?

References

- Anselm Blumer, A. Ehrenfeucht, David Haussler, and Manfred K. Warmuth. Learnability and the Vapnik-Chervonenkis dimension. *Journal of the ACM (JACM)*, Volume 36, Issue 4, 1989.

- Michael Kearns and Umesh Vazirani. *An Introduction to Computational Learning Theory*, MIT Press, 1994.

- Leslie G. Valiant. *A Theory of the Learnable*, Communications of the ACM 27(11):1134–1142 (1984).

Appendix

Universal Concept Class

- Problem: each $x \in X$ defined by n boolean features. Let C be the set of all subsets of X.
- Question: is C PAC-learnable?
- Sample complexity: H must contain C. Thus,

$$|H| \geq |C| = 2^{(2^n)}.$$

The bound gives $m = \frac{1}{\epsilon}((\log 2)\, 2^n + \log \frac{1}{\delta}).$

- It can be proved that C is not PAC-learnable, it requires an exponential sample size.

k-Term DNF Formulae

- Definition: expressions of the form $T_1 \vee \cdots \vee T_k$ with each term T_i conjunctions of boolean literals with at most n variables.

- Problem: learning *k*-term DNF formulae.

- Sample complexity: $|H| = |C| = 3^{nk}$. Thus, polynomial sample complexity $\frac{1}{\epsilon}((\log 3)\, nk + \log \frac{1}{\delta})$.

- Time complexity: intractable if $RP \neq NP$: the class is then not efficiently PAC-learnable (proof by reduction from graph 3-coloring). But, a strictly larger class is!

k-CNF Expressions

- Definition: expressions $T_1 \wedge \cdots \wedge T_j$ of arbitrary length j with each term T_i a disjunction of at most k boolean attributes.

- Algorithm: reduce problem to that of learning conjunctions of boolean literals. $(2n)^k$ new variables:

$$(u_1, \ldots, u_k) \rightarrow Y_{u_1, \ldots, u_k}.$$

  - the transformation is a bijection;
  - effect of the transformation on the distribution is not an issue: PAC-learning allows any distribution D.

k-Term DNF Terms and k-CNF Expressions

- Observation: any k-term DNF formula can be written as a k-CNF expression. By associativity,

$$\bigvee_{i=1}^{k} u_{i,1} \wedge \cdots \wedge u_{i,n_i} = \bigwedge_{j_1 \in [1,n_1], \ldots, j_k \in [1,n_k]} u_{1,j_1} \vee \cdots \vee u_{k,j_k}.$$

  - Example: $(u_1 \wedge u_2 \wedge u_3) \vee (v_1 \wedge v_2 \wedge v_3) = \bigwedge_{i,j=1}^{3} (u_i \vee v_j)$.
  - But, in general converting a k-CNF (equiv. to a k-term DNF) to a k-term DNF is intractable.

- Key aspects of PAC-learning definition:
  - cost of representation of concept c.
  - choice of hypothesis set H.