Introduction to Machine Learning

Foundations and Applications

Paul J. Atzberger
University of California Santa
Barbara



Statistical Learning Theory PAC-Learning Generalization Bounds

Framework for characterizing learning problems and algorithms.

Goal: Assess how well a model predicts future input-output relations.

"There is nothing more practical than a good theory."

-- James C. Maxwell.



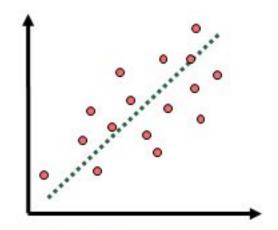
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Mathematical Definitions: Consider c: $X \to Y$, X-input, Y-output. Let c = concept, $C = \{\text{concept class}\}\$, $H = \{\text{hypothesis function space}\}\$, $D_{x,y} \sim X \times Y$ be unknown probability distribution on $X \times Y$, and $V(h(x_i), y_i) = \text{loss function}$.

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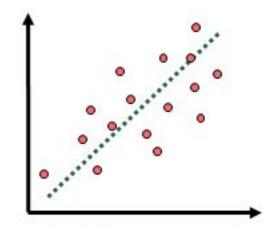
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Regression: $V(h(x), y) = (h(x) - y)^2$, (least-squares L^2 -loss).

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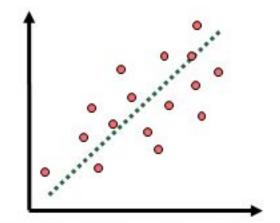


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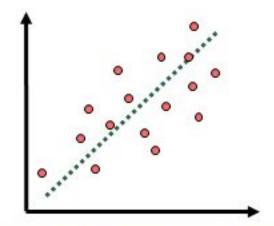
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Practical Challenges: Distribution D usually unknown, optimization is often non-convex and in high-dimensional spaces.

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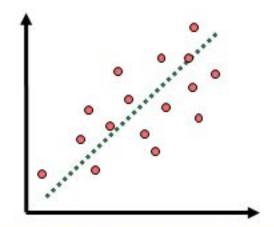
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Notation and definitions:

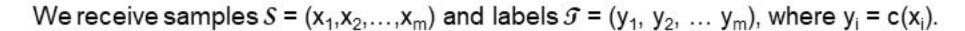
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y output space

 $c(x): \mathcal{X} \to \mathcal{Y}$ concept

C concept class

hypothesis class





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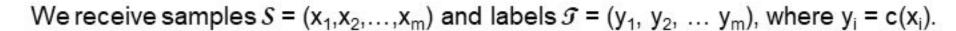
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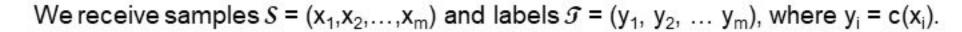
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- (i) fits to explain the training data S, \mathcal{F} well.
- (ii) generalizes to give correct results for new unseen data points drawn from D_x .



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We receive samples $S = (x_1, x_2, ..., x_m)$ and labels $\mathcal{F} = (y_1, y_2, ..., y_m)$, where $y_i = c(x_i)$.

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Definition: The generalization error (risk) for 0-1 classification $y=\{0,1\}$ is

$$R(h) = \Pr\{h_S(x) \neq c(x)\} = E_{x \sim D} \left[1_{h_S(x) \neq c(x)}\right]$$



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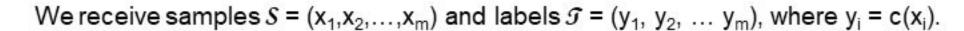
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However, in practice this is NOT computable since we do not known c(x) and D.



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Probability Approximately Correct (PAC) Learning Framework.

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PAC-learning

We say a concept class \mathcal{C} is **PAC-learnable** if there exists an algorithm \mathcal{A} and polynomial bound so that given $\varepsilon > 0$ and $\delta > 0$, the following holds for any distribution $D \in \mathcal{D}$ on \mathcal{X} , target concept c in \mathcal{C} , and sample size $m \ge \text{poly}(1/\varepsilon, 1/\delta, n, \text{size}(c))$

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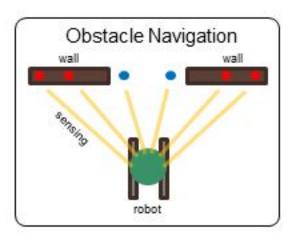
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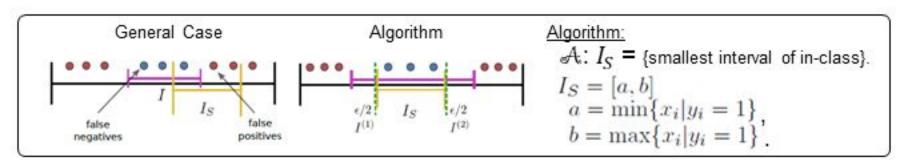
We call \mathcal{A} the PAC-learning algorithm for \mathcal{C} .

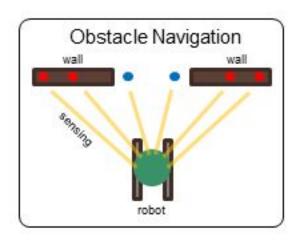
Example: Learning intervals on \mathbb{R} -line.



$$(S, T) = \{(x_i, y_i)\}_{i=1}^m, x_i \in \mathbb{R}, y_i \in \{0, 1\}$$

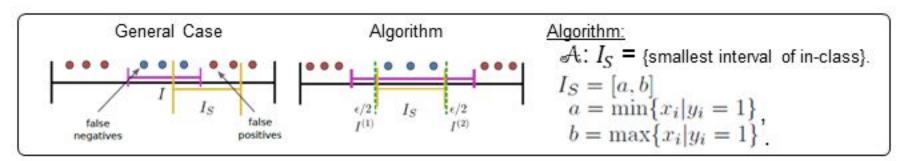
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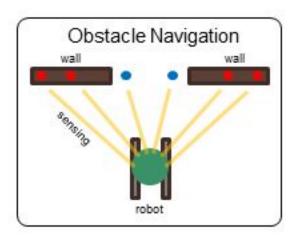




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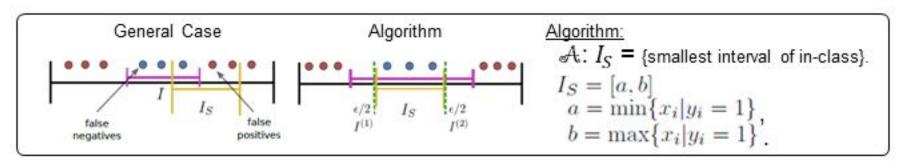
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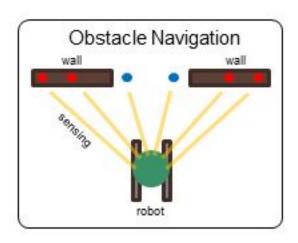




We need to show: Given $\epsilon > 0$, $\delta > 0$ there exists a polynomial bound in samples m with $(\mathcal{S}, \mathcal{T}) = \{(x_i, y_i)\}_{i=1}^m, x_i \in \mathbb{R}, y_i \in \{0, 1\}$ $\Pr_{\mathbf{x} \sim D^m} \left\{ R(I_S) \leq \epsilon \right\} \geq 1 - \delta.$

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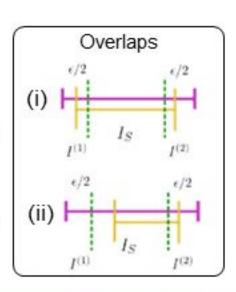


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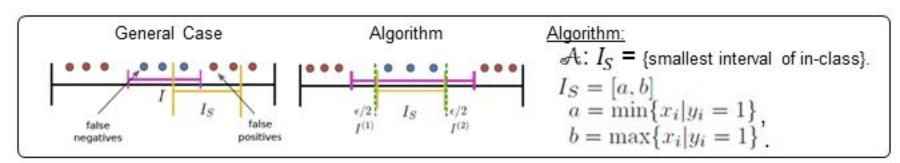
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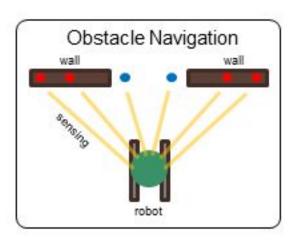
Since $I_S \subset I$, we only need to worry about false negatives. This has

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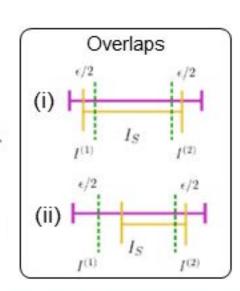
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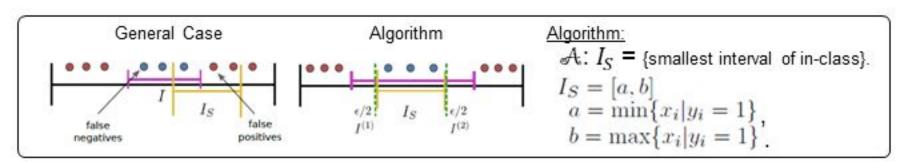
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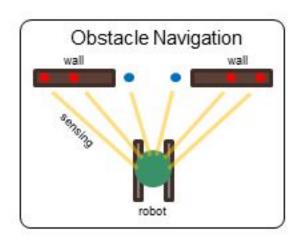
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If $I_S \cap I^{(i)} \neq \emptyset, \forall i=1,2$ then $R(I_S) \leq \epsilon$. By contrapositive $R(I_S) > \epsilon \Rightarrow \exists i \text{ s.t } I_S \cap I^{(i)} = \emptyset.$



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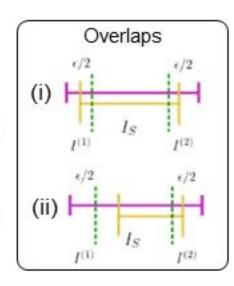
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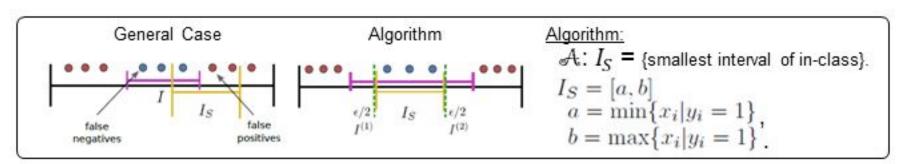
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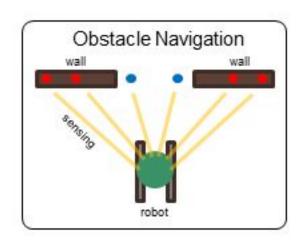
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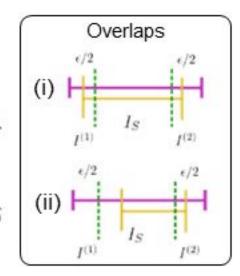
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$$\Rightarrow m > \frac{2}{\epsilon} \ln\left(\frac{2}{\delta}\right). \quad \blacksquare$$

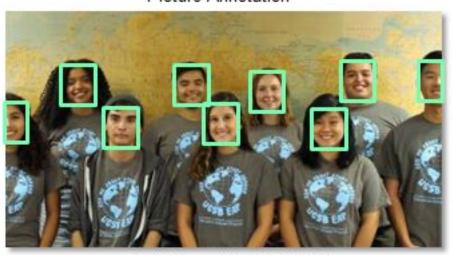


Example: Learning axis-aligned rectangles.

Building Identification

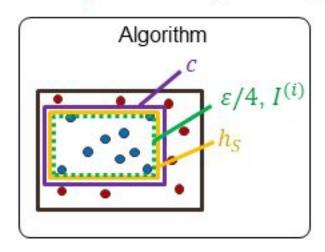


Google Maps: UCSB South Hall



Facial Recognition: UCSB EAP

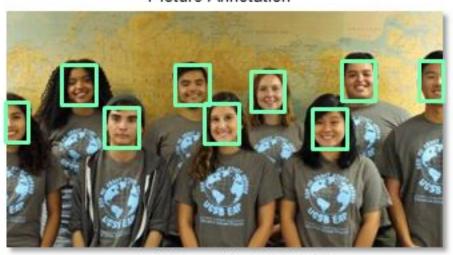
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Building Identification

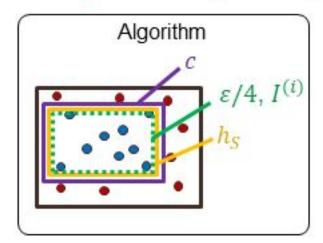


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Facial Recognition: UCSB EAP

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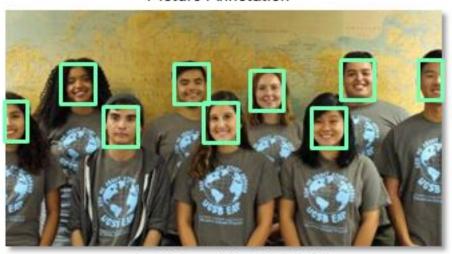
We need to show

$$\Pr\{R(h_S) \le \epsilon\} \ge 1 - \delta$$

Building Identification

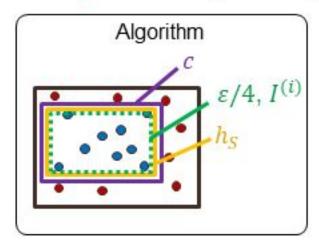


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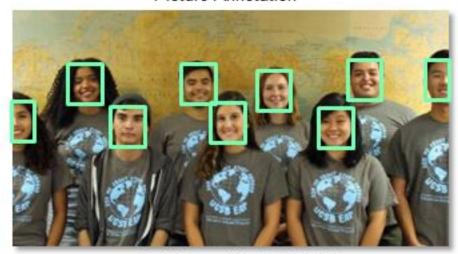
This implies

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Building Identification

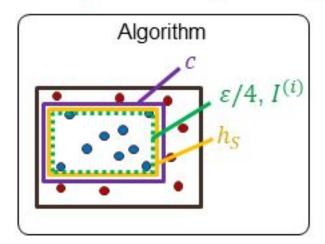


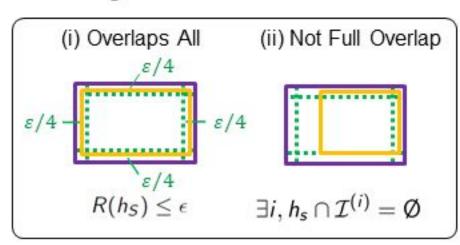
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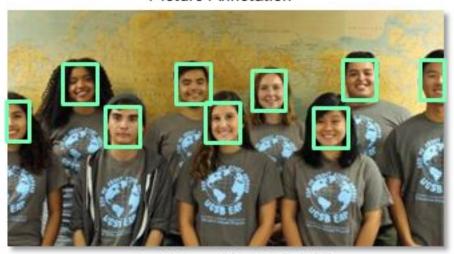
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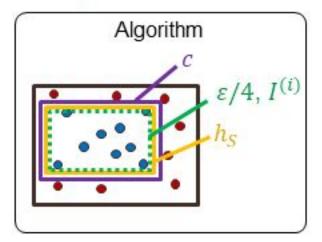


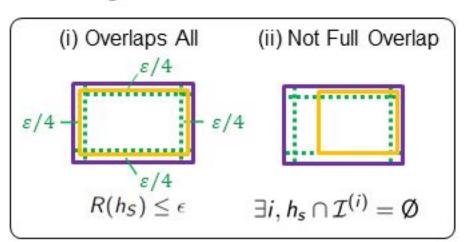
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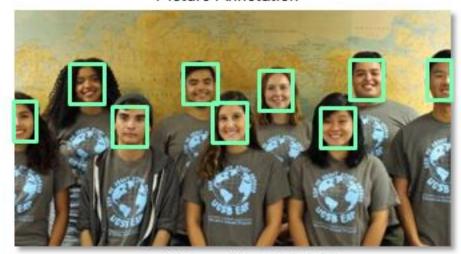
$$R(h_S) > \epsilon \implies \exists i \text{ s.t. } h_S \cap I^{(i)} = \emptyset$$

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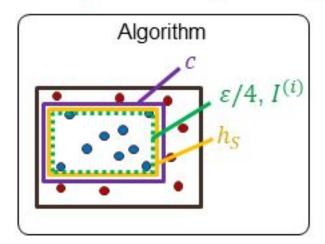


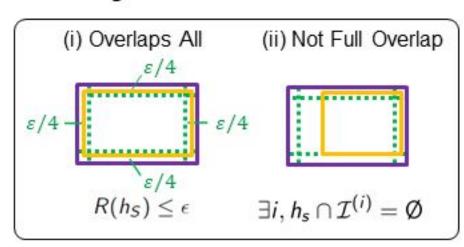
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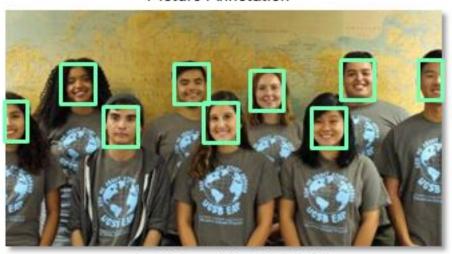
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$$\cdot \leq 4 \left(1 - \epsilon/4 \right)^m \leq 4 \exp\left[-\epsilon m/4 \right] < \delta.$$

Building Identification

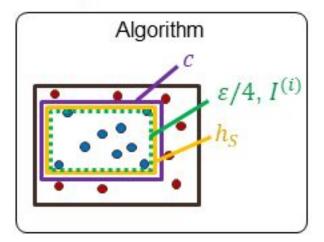


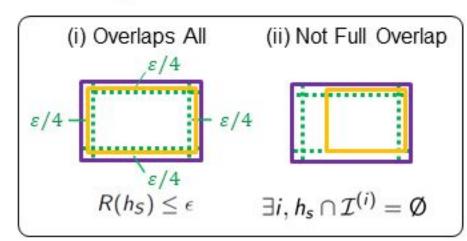
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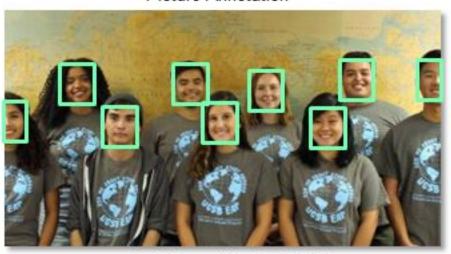
Bound on samples m

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Building Identification

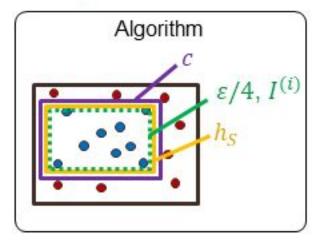


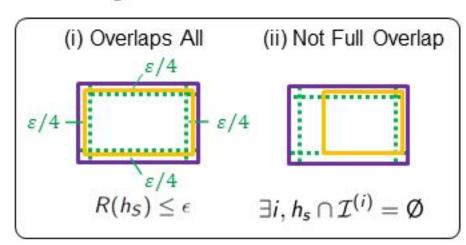
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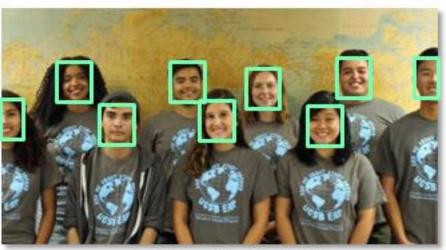
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Building Identification

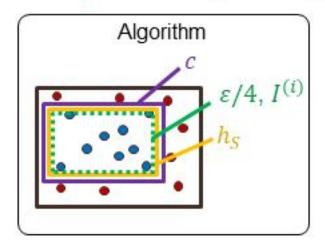


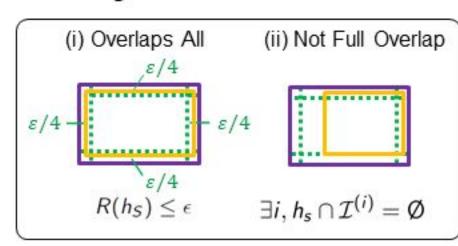
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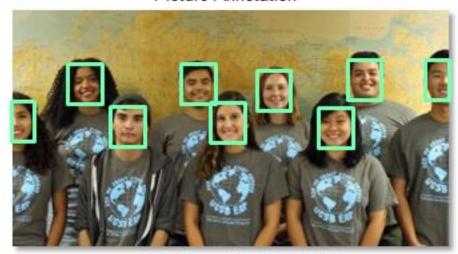
Bound on risk R

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Building Identification

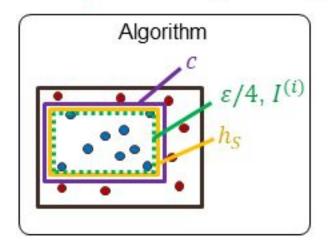


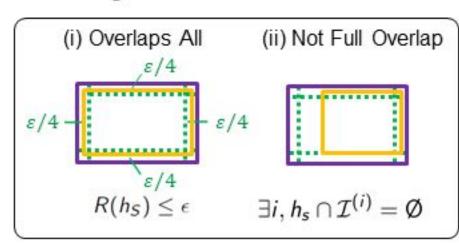
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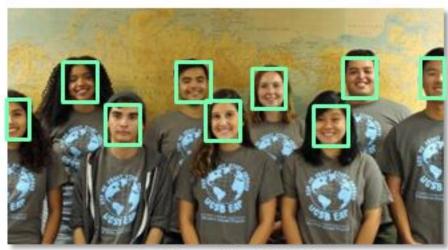
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Building Identification



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Guarantees on Sampling Complexity



How many samples do we need to guarantee a given level of precision ϵ , δ in PAC-learning?

What is bound M so for $m \ge M$ we have $\Pr\{R(h_S) \le \epsilon\} \ge 1 - \delta$?

$$\hat{R}(h) = \frac{1}{m} \sum_{i=1}^{m} 1_{h_S(x_i) \neq c(x_i)}$$

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- (i) consistent case: C ⊂ H, hypotheses include all concepts.
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Theorem: Consistent-Finite Hypothesis Spaces \mathcal{H} . Let \mathcal{A} be any learning algorithm that has zero Empirical Generalization $\operatorname{Error} \hat{R}(h_S) = 0$ then PAC-learning bound $\operatorname{Pr}\{R(h_S) \leq \epsilon\} \geq 1 - \delta$ is guaranteed to hold for m samples satisfying

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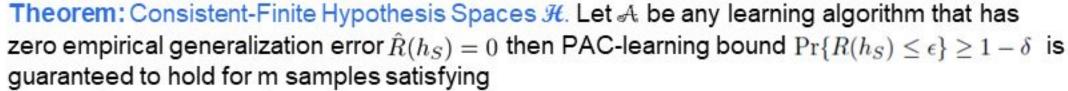
Finite Consistent-Case: Guarantees on Sampling Complexity



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Finite Consistent-Case: Guarantees on Sampling Complexity



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Finite Consistent-Case: Guarantees on Sampling Complexity



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Finite Consistent-Case: Guarantees on Sampling Complexity



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$$\leq |\mathcal{H}| (1 - \epsilon)^{m} \leq |\mathcal{H}| \exp(-\epsilon m) \leq \delta$$

$$\Rightarrow \log(|\mathcal{H}|) - \epsilon m \leq \log(\delta)$$
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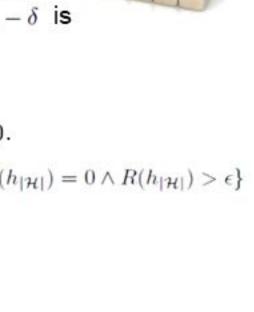
Finite Consistent-Case: Guarantees on Sampling Complexity



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

$$\begin{split} \Pr_{\mathcal{S} \sim D^m} \{ h \in \mathcal{H} \wedge \hat{R}(h) &= 0 \wedge R(h) > \epsilon \} = \Pr_{\mathcal{S} \sim D^m} \{ h_1 \in \mathcal{H} \wedge \hat{R}(h_1) = 0 \wedge R(h_1) > \epsilon \vee \dots \vee h_{|\mathcal{H}|} \in \mathcal{H} \wedge \hat{R}(h_{|\mathcal{H}|}) = 0 \wedge R(h_{|\mathcal{H}|}) > \epsilon \} \\ &\leq \sum_{i=1}^{|\mathcal{H}|} \Pr\{ h_i \in \mathcal{H} \wedge \hat{R}(h_i) = 0 \wedge R(h_i) > \epsilon \} \\ &\leq \sum_{i=1}^{|\mathcal{H}|} \Pr\{ h_i \in \mathcal{H} \wedge \hat{R}(h_i) = 0 | R(h_i) > \epsilon \} \\ &\leq |\mathcal{H}| (1 - \epsilon)^m \leq |\mathcal{H}| \exp\left(-\epsilon m\right) \leq \delta \\ &\Rightarrow \log(|\mathcal{H}|) - \epsilon m \leq \log(\delta) \\ &\Rightarrow m \geq \frac{1}{\epsilon} \left(\log(|\mathcal{H}|) + \log\left(\frac{1}{\delta}\right) \right) \end{split}$$

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Finite-Consistent Case: Guarantees on Sampling Complexity



$$R(h_S) \le \frac{1}{m} \left(\log |H| + \log \frac{1}{\delta} \right)$$

Finite-Consistent Case: Guarantees on Sampling Complexity



$$R(h_S) \le \frac{1}{m} \left(\log |H| + \log \frac{1}{\delta} \right)$$

Proof: Follows setting
$$\epsilon = \frac{1}{m} \left(\log \left(|H| \right) + \log \left(\frac{1}{\delta} \right) \right)$$

Finite-Consistent Case: Guarantees on Sampling Complexity



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- However, consistency e ⊂ H requires "big enough" hypothesis space H to capture target concepts.

Example: Boolean Conjunctions.

Let z_i be Boolean variable, a conjunction is: $c = \overline{z_1} \wedge z_2 \wedge z_5 \wedge z_6$.



0	1	1	0	1	1	+
0	1	1	Ι	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	

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The concept class $|\mathcal{C}_n| = 3^n$, since in n-conjunction either z_i , $\overline{z_i}$, or ϕ .



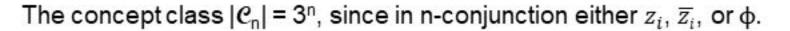
+	1	1	0	1	1	0
+	1	1	1	1	1	0
-	1	0	1	1	0	0
+	1	1	1	1	1	0
-	0	1	1	0	0	1
+	1	1	0	0	1	0
	1	1	?	?	1	0

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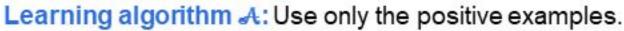
Note could learn directly with as few as 2n examples if special ones chosen.



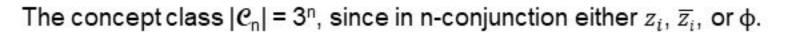
0	1	1	0	1	1	+
0	1	1	1	1	1	+
0	0	1	1	0	1	7.
0	1	1	1	1	1	+
1	0	0	1	1	0	-
0	1	0	0	1	1	+
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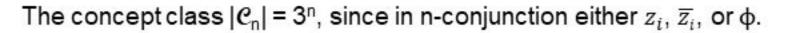
0	1	1	0	1	1	+
0	1	ı	Ι	Τ	1	+
0	0	1	1	0	1	-
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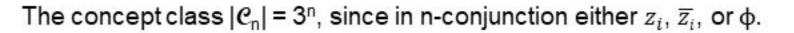
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0	1	ı	Ι	Τ	1	+
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0	1	1	1	1	1	+
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$$C = z_1 \wedge \bar{z}_2 \wedge z_3$$

 $z_1 \sim$ "it is raining"

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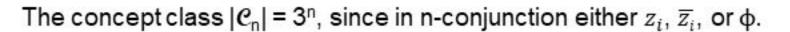
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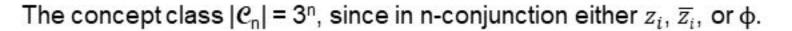
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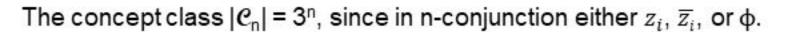
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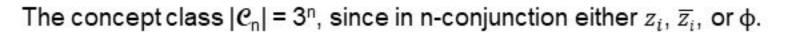
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Note statistical learning might not be as efficient as direct methods when available.



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0	1	1	Ι	1	1	+
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Learning completely generic functions is just too hard to do efficiently (too many possibilities).

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Stochastic vs Deterministic Learning: Above applies also when label y for feature vector x is not unique, as in many real-world data sets. Uncertainty captured by $D \sim \mathcal{X} \times \mathcal{Y}$, allowing for a type of stochastic learning. **Goal:** Find best assignment y = h(x) minimizing generalization error.

Finite-Inconsistent Case: Guarantees on Sampling Complexity

Theorem: Inconsistent-Finite Hypothesis Spaces \mathcal{H} . Let \mathcal{A} be any learning algorithm that has empirical generalization error $\hat{R}(h_S)$ then for any $h \in \mathcal{H}$ we have

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These results show even in the inconsistent case for enough samples m a small training set error is still indicative for obtaining an hypothesis h with best generalization error.

Finite-Inconsistent Case: Guarantees on Sampling Complexity

Theorem: Inconsistent-Finite Hypothesis Spaces \mathcal{H} . Let \mathcal{A} be any learning algorithm that has empirical generalization error $\hat{R}(h_S)$ then for any $h \in \mathcal{H}$ we have



$$R(h) \le \widehat{R}(h) + \sqrt{\frac{\log|H| + \log\frac{2}{\delta}}{2m}}$$

This shows training error is indicative of the generalization error with enough samples

$$\left|\hat{R}(h) - R(h)\right| \le \sqrt{\frac{\log(|H|) + \log(\frac{2}{\delta})}{2m}}$$

This means if we have small training set error $\hat{R}(h_S)$ then "with enough" samples we can obtain small gap in generalization errors.

For Agnostic PAC-Learnable concepts we have $\Pr\{R(h_S) - \min_{h \in \mathcal{H}} R(h) \le \epsilon\} \ge 1 - \delta$

These results show even in the inconsistent case for enough samples m a small training set error is still indicative for obtaining an hypothesis h with best generalization error.

Note, only $m^{-1/2}$ scaling in the bound (compare to the finite-consistent case ~ m^{-1}).

Concentration Inequalities

Lemma: Markov Inequality $\Pr[X \ge \epsilon] = \Pr[e^{tX} \ge e^{t\epsilon}] \le e^{-t\epsilon} \operatorname{E}[e^{tX}]$ for $t \ge 0$.



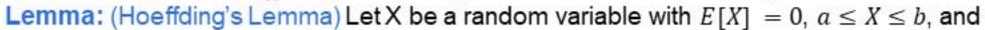
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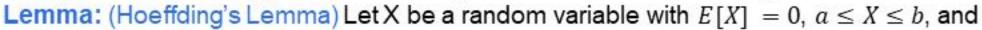


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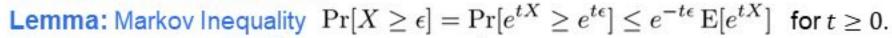


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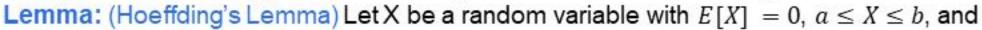
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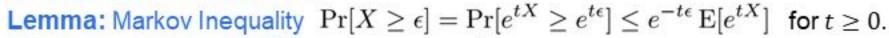


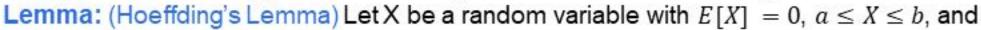
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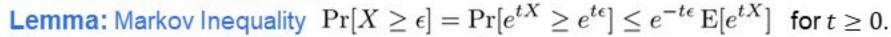
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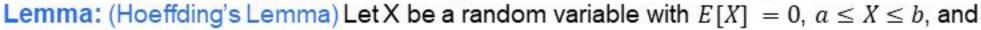
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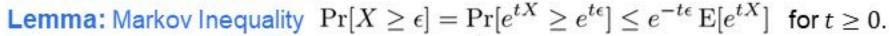
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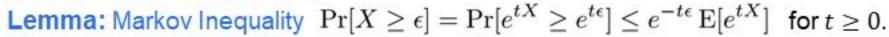
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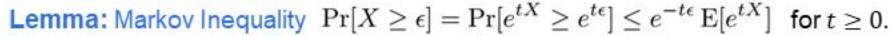
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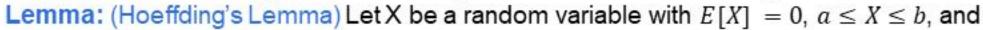
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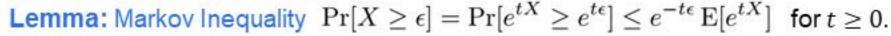
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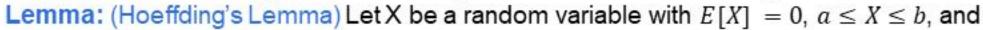
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Lemma: (Hoeffding's Inequality) Let $X_1, X_2, ..., X_m$ be random variables with $a_i \le X_i \le b_i$, $b_i > a_i$ and $S_m = \sum_{i=1}^m X_i$ then we have the bounds

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$$\psi(t) = \frac{-8t\epsilon + t^2Q}{8}$$



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Concentration Inequalities

Lemma: (Hoeffding's Inequality) Let $X_1, X_2, ..., X_m$ be random variables with $a_i \le X_i \le b_i$,

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Probability Theory and Inequalities

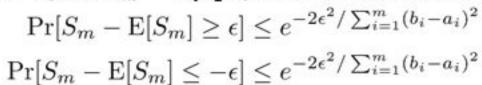
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Similarly, we obtain the other case using $\tilde{Z}_m = -Z_m$.



Finite-Inconsistent Case: Guarantees on Sampling Complexity

Lemma: Let samples $S=\{(x_1,y_1),(x_2,y_2),...,(x_m,y_m)\}$ be chosen i.i.d. on $\{0,1\}$ from $D \sim \mathcal{X} \times \mathcal{Y}$ then

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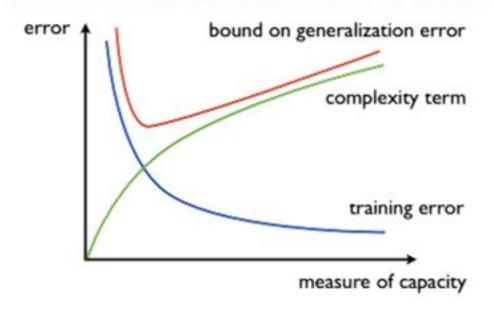
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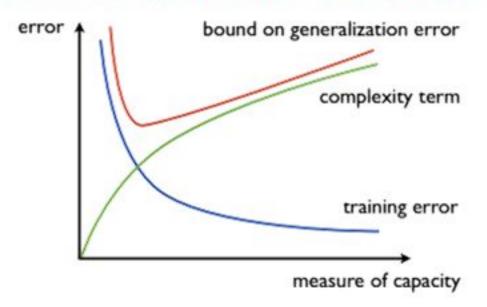
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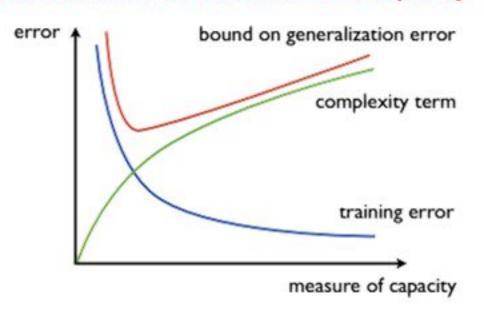








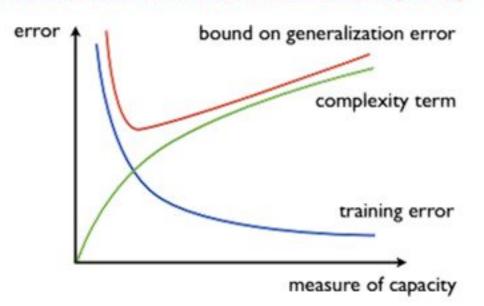
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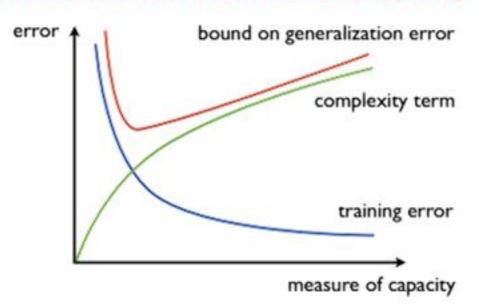
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- Central challenge in machine learning is to find appropriate hypothesis classes for given learning tasks.

Minimax Rate

$$\mathcal{V}_m(\mathcal{C}) = \inf_{h_S = \mathcal{A}(\cdot)} \sup_{D_X, c \in \mathcal{C}} E_{S:|S|=m} \left[R(h_S) \right]$$

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A concept class $\mathcal C$ is PAC-learnable if $\mathcal V_m^{PAC}(\mathcal C) \to 0$.

More precisely, given $\epsilon > 0$, $\exists M = poly(1/\epsilon)$ such that $m \geq M$, we have

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Theorem (PAC Learning $\leftarrow \rightarrow$ Minimax): For a concept class \mathcal{C} the minimax rate converges to zero with polynomial sampling complexity if and only if the concept class \mathcal{C} is PAC-learnable.





Theorem (PAC Learning ←→ Minimax):

Given $\epsilon > 0$, $\mathcal{V}^{PAC}_m(\mathcal{C}) \leq \epsilon$ with $m \geq \operatorname{poly}(1/\epsilon)$ holds if and only if there is an algorithm \mathcal{A} so that given $\epsilon > 0$, $\delta > 0$, $\Pr_{S \sim D^m} \left\{ R(h_S) \leq \epsilon \right\} \geq 1 - \delta$ for $m \geq \operatorname{poly}(1/\epsilon, 1/\delta)$ holds.



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We obtain the bound

$$E_{S:|S|=m}\left[R(\tilde{\tilde{\mathcal{A}}}(S))\right] \leq \Pr_{S \sim \mathcal{D}^m} \{R(\tilde{\tilde{\mathcal{A}}}(S) \leq \epsilon\} \cdot \epsilon + \Pr_{X \sim \mathcal{D}} \{R(\tilde{\tilde{\mathcal{A}}}(S) > \epsilon\} \cdot 1 \leq \epsilon + \delta \leq \epsilon + \frac{1}{2}\epsilon = \frac{3}{2}\epsilon = \tilde{\epsilon}.$$



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Given (ii) we have $\exists \tilde{\mathcal{A}}$ s.t. given $\epsilon > 0$, $\delta = \epsilon/2$, $\exists M = \operatorname{poly}\left(\frac{1}{\epsilon}, \frac{1}{\epsilon}\right)$ s.t. for $D_X \in \mathfrak{D}$, $c \in C$,

$$\Pr_{S \sim \mathcal{D}^m} \{ R(\tilde{\tilde{\mathcal{A}}}(S)) \le \epsilon \} \ge 1 - \delta \Rightarrow \Pr_{S \sim \mathcal{D}^m} \{ R(\tilde{\tilde{\mathcal{A}}}(S)) > \epsilon \} < \delta, \ m \ge M.$$

We obtain the bound

$$\begin{split} E_{S:|S|=m}\left[R(\tilde{\tilde{\mathcal{A}}}(S))\right] &\leq \Pr_{S\sim\mathcal{D}^m}\{R(\tilde{\tilde{\mathcal{A}}}(S)\leq\epsilon\}\cdot\epsilon + \Pr_{X\sim\mathcal{D}}\{R(\tilde{\tilde{\mathcal{A}}}(S)>\epsilon\}\cdot 1\leq\epsilon + \delta\leq\epsilon + \frac{1}{2}\epsilon = \frac{3}{2}\epsilon = \tilde{\epsilon}.\\ &\Rightarrow \begin{cases} \mathcal{V}^{PAC}(\mathcal{C})\leq\tilde{\epsilon}\\ m\geq \operatorname{poly}(1/\tilde{\epsilon}) \end{cases} \end{split}$$



Theorem (PAC Learning ←→ Minimax):

Given $\epsilon > 0$, $\mathcal{V}_m^{PAC}(\mathcal{C}) \leq \epsilon$ with $m \geq \operatorname{poly}(1/\epsilon)$ holds if and only if there is an algorithm \mathcal{A} so that given $\epsilon > 0$, $\delta > 0$, $\Pr_{S \sim D^m} \left\{ R(h_S) \leq \epsilon \right\} \geq 1 - \delta$ for $m \geq \operatorname{poly}(1/\epsilon, 1/\delta)$ holds.

Proof: $(i) \Rightarrow (ii)$ follows readily.

We show $(ii) \Rightarrow (i)$

$$R(h_S) = \Pr_{X \sim \mathcal{D}} \{ h_S(X) \neq c(X) \}$$

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$$\Rightarrow \mathcal{V}_m^{PAC} \to 0$$
 , as $m \to \infty$.

Minimax Rates and Learning Tasks

PAC-Learning Classification

$$\mathcal{V}_{m}^{PAC}(\mathcal{C}) = \inf_{h_{S} = \mathcal{A}(\cdot)} \sup_{D_{X}, c \in \mathcal{C}} E_{S:|S| = m} \left[\Pr_{x \sim D} \left\{ h_{S}(x) \neq c(x) \right\} \right]$$



$$\mathcal{V}_{m}^{NR}(\mathcal{C}) = \inf_{h_{S} = \mathcal{A}(\cdot)} \sup_{D_{X}, c \in \mathcal{C}} E_{S:|S|=m} \left[\left(h_{S}(x) - c(x) \right)^{2} \right]$$

Agnostic PAC-Learning

$$\mathcal{V}_{m}^{A-PAC}(\mathcal{C}) = \inf_{h_{S} = \mathcal{A}(\cdot)} \sup_{D_{X}, c \in \mathcal{C}} E_{S:|S|=m} \left[R(h_{S}) - \inf_{h' \in \mathcal{H}} R(h') \right]$$



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Comparison of learning problems:

Case:
$$\mathcal{C} \subset \{\pm 1\}^{\mathcal{X}}$$

$$4\mathcal{V}_{m}^{PAC}(\mathcal{C}) \leq \mathcal{V}_{m}^{NR}(\mathcal{C}) \leq \mathcal{V}_{m}^{A-PAC}(\mathcal{C})$$



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Case:
$$C \subset R^{\mathcal{X}}$$

$$\mathcal{V}_{m}^{NR}(C) \leq \mathcal{V}_{m}^{A-PAC}(C)$$



Machine Learning Algorithms and Tasks

 Guaranteed performance for unknown distributions D_x requires we have some restriction on the hypothesis class H and concept class C.

Image Classification



Robotics / Controls



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Forecasting



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Machine Learning Algorithms and Tasks

- Guaranteed performance for unknown distributions D_x requires we have some restriction on the hypothesis class H and concept class C.
- There is no general learning algorithm that works for all possible tasks.
- These assertions correspond to so-called "No Free Lunch Theorems."

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- There is no general learning algorithm that works for all possible tasks.
- These assertions correspond to so-called "No Free Lunch Theorems."
- To achieve good performance learning algorithms must make some use of knowledge / mathematical structure of the specific task.

Image Classification



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Therefore, u is **not** PAC-Learnable.

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Theorem: Let concept class be all binary functions, $\mathcal{C} = \mathcal{U} = \{\text{all functions } f(z) : \mathcal{X} \to \{0,1\}\},$ where \mathcal{X} is discrete space of finite binary sequences $\{\{0,1\}^N, N \in \mathbb{N}\} = \{(\mathbf{z}_1, \mathbf{z}_2, \dots, \mathbf{z}_N), \ z_i \in \{0,1\}\}.$ For the universal concept class \mathcal{U} we have $\mathcal{V}_m^{PAC}(\mathcal{C}) \not \to 0$.

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Proof:

For a given sample size, let $\mathcal{X} \subset \Omega$ of binary sequences s.t. $|\mathcal{X}| = 2n$.

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$$\geq \frac{1}{2} \Pr\{X \not\in \mathcal{S}\} \geq \frac{1}{2} \cdot \frac{1}{2} = \frac{1}{4}.$$

$$\mathcal{D} \sim \text{uniform on } \mathcal{X}, \ |\mathcal{X}| = 2n$$

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No Free Lunch Theorem

<u>Significance:</u> If the hypothesis class \$\mathcal{H}\$, target concept class \$\mathcal{C}\$ are too general and the distribution \$D_{\mathcal{X}}\$ is unknown then there is no guarantees on algorithmic performance on the tasks.

Image Classification



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- Must utilize some knowledge or structure of the tasks to be solved.
- Central goal of this course is to consider wide variety of specific tasks and develop associated well-suited learning algorithms.

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- This means no generic all purpose learning algorithms exist.
- Must utilize some knowledge or structure of the tasks to be solved.
- Central goal of this course is to consider wide variety of specific tasks and develop associated well-suited learning algorithms.

Support Vector Machines

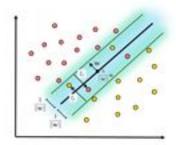


Image Classification



Robotics Controllers



New Scientist Delta, MIT and Cornell (Steven Collins)

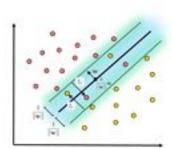


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Support Vector Machines



Neural Networks

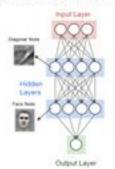


Image Classification



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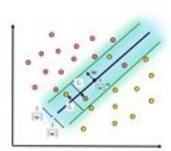


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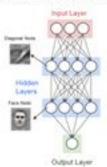
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Neural Networks



Clustering Methods

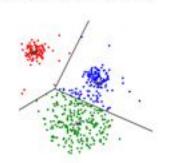


Image Classification



Robotics Controllers



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