#### Introduction to Learning Theory

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Machine Learning (CS771A)

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#### "Theory is the first term in the Taylor series expansion of Practice" - T. Cover, Cove

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$$L_{\mathcal{D}}(h) = \frac{1}{N} \sum_{n=1}^{N} \mathbb{I}(h(\boldsymbol{x}_n) \neq y_n)$$

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  - We want to know how much worse it is..
  - .. without doing experiments

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- Consider K hyp.  $\{h_1, \ldots, h_K\}$ . Prob. that **at least one** of these is bad

 $P_{\mathcal{D}\sim P^N}(``h_1 \text{ is bad}" \cup \ldots \cup ``h_K \text{ is bad}") \leq K(1-\epsilon)^N \quad (using union bound)$ 

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• Since  $K \leq |\mathcal{H}|$ , K can be replaced by the size of set  $\mathcal{H}$ 

 $P_{\mathcal{D}\sim P^N}(\exists h: "h \text{ is bad"}) \leq |\mathcal{H}|(1-\epsilon)^N \quad (\text{Uniform Convergence})$ 

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$$L_P(h) \leq rac{\log |\mathcal{H}| + \log rac{1}{\delta}}{N}$$

## PAC Learnability and Efficient PAC Learnability

Definition: An algorithm A is an (ε, δ)-PAC learning algorithm if, for all distributions D: given samples from D, the probability that it returns a "bad hypothesis" h is at most δ, where a "bad" hypothesis is one with test error rate more than ε on D.

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  - Note: a similar notion of an efficient (ε, δ)-PAC learning algorithm holds in terms of the number of training examples required (polynomial in <sup>1</sup>/<sub>ε</sub> and <sup>1</sup>/<sub>δ</sub>)

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• Using the union bound, we have:

$$P(\exists h: L_P(h) - L_D(h) \ge \epsilon) \le |\mathcal{H}|e^{-2N\epsilon^2}$$

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• Suppose  $|\mathcal{H}|e^{-2N\epsilon^2} = \delta$ . Then for a given  $\epsilon$  and  $\delta$ 

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.. gives the min. number of training ex. required to ensure that  $L_P(h) - L_D(h) \le \epsilon$  with probability at least  $1 - \delta$ 

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- Note: Number of examples grows as square of  $1/\epsilon$  (note:  $\epsilon < 1$ )
  - ullet In zero training error case, it grows linearly with  $1/\epsilon$
  - For given  $\epsilon, \delta$ , the non-zero training error case requires more examples

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$$L_{\mathcal{P}}(h) \leq L_{\mathcal{D}}(h) + \sqrt{\frac{\log |\mathcal{H}| + \log \frac{1}{\delta}}{2N}}$$

- Let's consider the hypothesis class of DTs with k leaves
- Suppose data has D binary features/attributes

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$$\begin{split} & \mathsf{H}_{1} = \mathsf{A} \operatorname{unber} of decision trees with k leaves \\ & \mathsf{H}_{1} = 2 \\ & \mathsf{H}_{2} = (\operatorname{Rhockes} of root attribute)^{+} \\ & (If of to subtrees with 1 isal?)^{(r)} (right subtrees with k-2 leaves) \\ & \circ (If a subtrees with 2 leaves)^{+} (if right subtrees with k-2 leaves) \\ & \cdots \\ & \circ (If subtrees with k-1 leaves)^{+} (if right subtrees with 1 leav)) \\ & H_{k} = n \sum_{i=1}^{k-1} H_{i} H_{k-i} = \vartheta^{k-1} \mathbf{C}_{k-1} \qquad (\mathbf{C}_{k-1}: \mathsf{Catalan Number}) \end{split}$$

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• A loose bound (using Sterling's approximation):  $H_k \leq D^{k-1}2^{2k-1}$ 

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- A loose bound (using Sterling's approximation):  $H_k \leq D^{k-1}2^{2k-1}$
- Thus  $\log_2 H_k \le (k-1) \log_2 D + 2k 1$  (linear in k)

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 $\bullet\,$  For the finite sized hypothesis class  ${\cal H}\,$ 

$$L_P(h) \leq L_{\mathcal{D}}(h) + \sqrt{rac{\log |\mathcal{H}| + \log rac{1}{\delta}}{2N}}$$

- What happens when the hypothesis class size  $|\mathcal{H}|$  is infinite?
  - Example: the set of all linear classifiers

-

 $\bullet$  For the finite sized hypothesis class  ${\cal H}$ 

$$L_P(h) \leq L_{\mathcal{D}}(h) + \sqrt{rac{\log |\mathcal{H}| + \log rac{1}{\delta}}{2N}}$$

- What happens when the hypothesis class size  $|\mathcal{H}|$  is infinite?
  - Example: the set of all linear classifiers
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  - .. enters the Vapnik-Chervonenkis dimension (VC dimension)
  - VC dimension: a measure of the complexity of a hypothesis class

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# Shattering

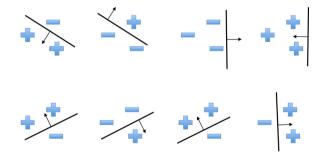
• A set of points is shattered by a hypothesis class *H* if, no matter how the points are labeled, there exists some *h* ∈ *H* that can separate the points

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• Figure above: 3 points in 2D,  $\mathcal{H}$ : set of linear classifiers

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The concept of shattering is used to define the VC dimension of hypothesis classes

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Consider the following shattering game between us and an adversary

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The VC dimension of  $\mathcal{H}$ , in that input space, is the maximum *d* we can choose so that we always succeed in the game

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VC dimension of linear classifiers in  $\mathbb{R}^2 = 3$ ?

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VC dimension intuition: How many points the hypothesis class can "memorize"

Recall the PAC based Generalization Bound

$$\mathsf{ExpectedLoss}(h) \leq \mathsf{TrainingLoss}(h) + \sqrt{rac{\log |\mathcal{H}| + \log rac{1}{\delta}}{2N}}$$

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For hypothesis classes with infinite size ( $|\mathcal{H}| = \infty$ ), but VC dimension *d*:

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For linear classifiers, what does it imply?

Having fewer features is better (since it means smaller VC dimension)

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Recall: VC dimension of an SVM with RBF kernel is infinite. Is it a bad thing?

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Recall: VC dimension of an SVM with RBF kernel is infinite. Is it a bad thing? Not really. SVM's large margin property ensures good generalization

Theorem (Vapnik, 1982):

- Given N data points in  $\mathbb{R}^D$ :  $\boldsymbol{X} = \{\boldsymbol{x}_1, \dots, \boldsymbol{x}_N\}$  with  $||\boldsymbol{x}_n|| \leq R$
- Define  $\mathcal{H}_{\gamma}$ : set of classifiers in  $\mathbb{R}^D$  having margin  $\gamma$  on  $\boldsymbol{X}$

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The VC dimension of  $\mathcal{H}_{\gamma}$  is bounded by:

$$VC(\mathcal{H}_{\gamma}) \leq \min\left\{D, \left\lceil \frac{4R^2}{\gamma^2} \right\rceil
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Large  $\gamma \Rightarrow$  small VC dim.  $\Rightarrow$  small complexity of  $\mathcal{H}_{\gamma} \Rightarrow$  good generalization

Machine Learning (CS771A)

• We care about the expected error, not the training error

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- Generalization bounds quantify the difference between these two errors
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  - But even loose bounds are often useful for understanding the basic properties of learning models/algorithms