10-301/601: Introduction to Machine Learning Lecture 16 – Learning Theory (Infinite Case)

Henry Chai

10/26/22

Why is the answer C?

• Let \mathcal{H} be the set of all conjunctions over M Boolean variables, $\mathbf{x} \in \{0,1\}^M$; examples of conjunctions are • $h(\mathbf{x}) = x_1(1-x_2)x_4x_{10}$ $|\mathcal{H}| = 3^{\circ}$ • $h(\mathbf{x}) = (1-x_3)(1-x_4)x_8$ $\neq 10^3$

• Assuming $c^* \in \mathcal{H}$, if $\underline{M = 10}$, $\epsilon = 0.1$, and $\delta = 0.01$, at least how many labelled examples do we need to satisfy the PAC criterion using Theorem 1?

A. 1 (TOXIC)

B. $10(2 \ln 10 + \ln 100) \approx 92$ F. $100(2 \ln 10 + \ln 10) \approx 691$ C. $10(3 \ln 10 + \ln 100) \approx 116$ G. $100(3 \ln 10 + \ln 10) \approx 922$ D. $10(10 \ln 2 + \ln 100) \approx 116$ H. $100(10 \ln 2 + \ln 10) \approx 924$ E. $10(10 \ln 3 + \ln 100) \approx 156$ I. $100(10 \ln 3 + \ln 10) \approx 1329$

How does the statistical learning theory corollary follow from this theorem? • For a finite hypothesis set \mathcal{H} s.t. $c^* \in \mathcal{H}$ and arbitrary distribution p^* , if the number of labelled training data points satisfies

$$M \ge \frac{1}{\epsilon} \left(\ln(|\mathcal{H}|) + \ln\left(\frac{1}{\delta}\right) \right)$$

then with probability at least $1 - \delta$, all $h \in \mathcal{H}$ with $\widehat{R}(h) = 0$ have $R(h) \leq \epsilon$

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• Solving for *e* gives...

How does the statistical learning theory corollary follow from this theorem? • For a finite hypothesis set \mathcal{H} s.t. $c^* \in \mathcal{H}$ and arbitrary distribution p^* , given a training data set S s.t. |S| = M, all $h \in \mathcal{H}$ with $\hat{R}(h) = 0$ have

$$R(h) \leq \frac{1}{M} \left(\ln(|\mathcal{H}|) + \ln\left(\frac{1}{\delta}\right) \right)$$

with probability at least $1 - \delta$.

Front Matter

- Announcements
 - HW5 released 10/13, due 10/27 (tomorrow) at 11:59 PM
 - HW6 released 10/27 (tomorrow), due 11/4 at 11:59 PM
 - Only two late days allowed on HW6
- Exam 2 on 11/10, two weeks from tomorrow (more details to follow)
 - All topics between Lecture 8 and Lecture 17 (next Monday's lecture) are in-scope
 - Exam 1 content may be referenced but will not be
 - the primary focus of any question
 - Exam 3 scheduled
 - Thursday, December 15th from 9:30 AM to 11:30 AM
 - Sign up for peer tutoring! See <u>Piazza</u> for more details

Recall -Theorem 1: Finite, Realizable Case • For a finite hypothesis set \mathcal{H} s.t. $c^* \in \mathcal{H}$ and arbitrary distribution p^* , if the number of labelled training data points satisfies

$$M \ge \frac{1}{\epsilon} \left(\ln(|\mathcal{H}|) + \ln\left(\frac{1}{\delta}\right) \right)$$

then with probability at least $1 - \delta$, all $h \in \mathcal{H}$ with $\widehat{R}(h) = 0$ have $R(h) \le \epsilon$

Recall -Theorem 2: Finite, Agnostic Case • For a finite hypothesis set ${\cal H}$ and arbitrary distribution p^* , if the number of labelled training data points satisfies

$$M \ge \frac{1}{2\epsilon^2} \left(\frac{\ln(|\mathcal{H}|) + \ln\left(\frac{2}{\delta}\right)}{\delta} \right)$$

then with probability at least $1 - \delta$, all $h \in \mathcal{H}$ satisfy $|R(h) - \hat{R}(h)| \leq \epsilon$

• Bound is inversely quadratic in ϵ , e.g., halving ϵ means we need four times as many labelled training data points

What happens when $|\mathcal{H}| = \infty$?

• For a finite hypothesis set $\mathcal H$ and arbitrary distribution p^* , if the number of labelled training data points satisfies

$$M \ge \frac{1}{2\epsilon^2} \left(\ln(|\mathcal{H}|) + \ln\left(\frac{2}{\delta}\right) \right)$$

then with probability at least $1 - \delta$, all $h \in \mathcal{H}$ satisfy $|R(h) - \hat{R}(h)| \leq \epsilon$

- Insight: $|\mathcal{H}|$ measures how complex our hypothesis set is
- Idea: define a different measure of hypothesis set complexity

Labellings

• Given some finite set of data points $S = (x^{(1)}, ..., x^{(M)})$ and some hypothesis $h \in \mathcal{H}$, applying h to each point in S results in a <u>labelling</u>

• $\left(h(\boldsymbol{x}^{(1)}), \dots, h(\boldsymbol{x}^{(M)})\right)$ is a vector of M +1's and -1's

• Important note: our discussion of PAC learning assumes binary classification

• Given $S = (x^{(1)}, ..., x^{(M)})$, each hypothesis in \mathcal{H}

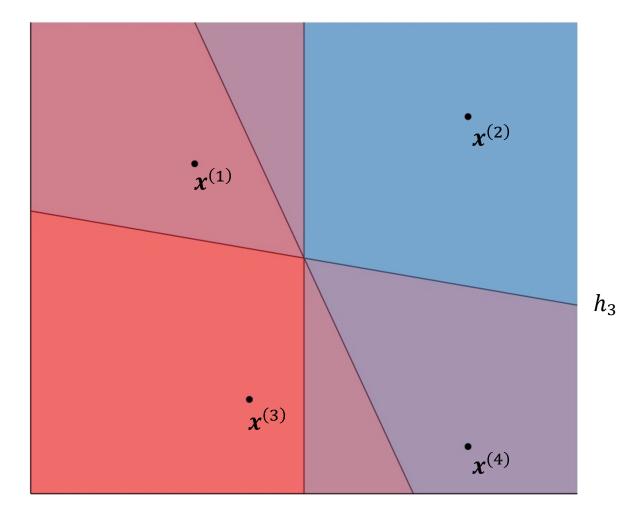
induces a labelling but not necessarily a unique labelling

• The set of labellings induced by \mathcal{H} on S is

$$\mathcal{H}(S) = \left\{ \left(h(\boldsymbol{x}^{(1)}), \dots, h(\boldsymbol{x}^{(M)}) \right) \mid h \in \mathcal{H} \right\}$$

Example: Labellings

 $\mathcal{H} = \{h_1, h_2, h_3\}$

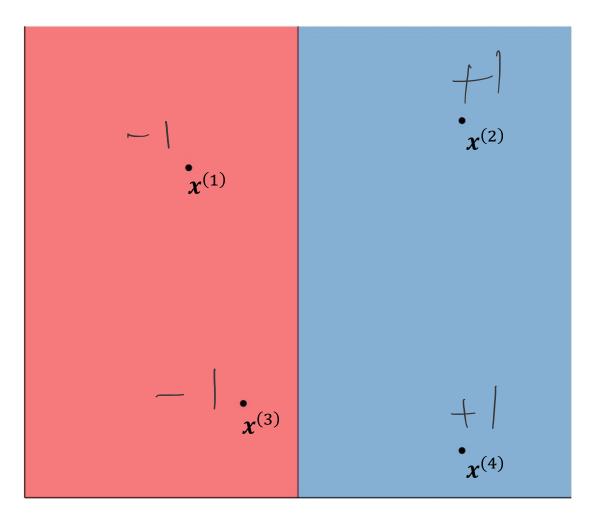


 h_1 h_2



 $\mathcal{H} = \{h_1, h_2, h_3\}$

 $\begin{pmatrix} h_1(x^{(1)}), h_1(x^{(2)}), h_1(x^{(3)}), h_1(x^{(4)}) \end{pmatrix}$ = (-1, +1, -1, +1)

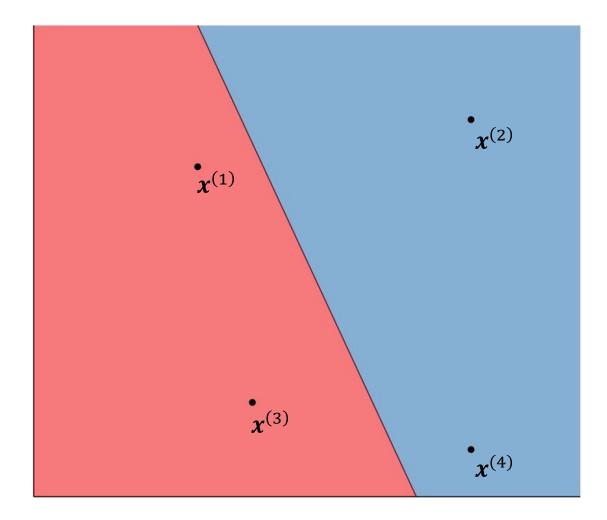


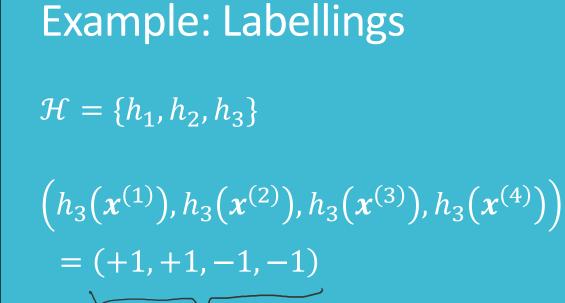
 h_1

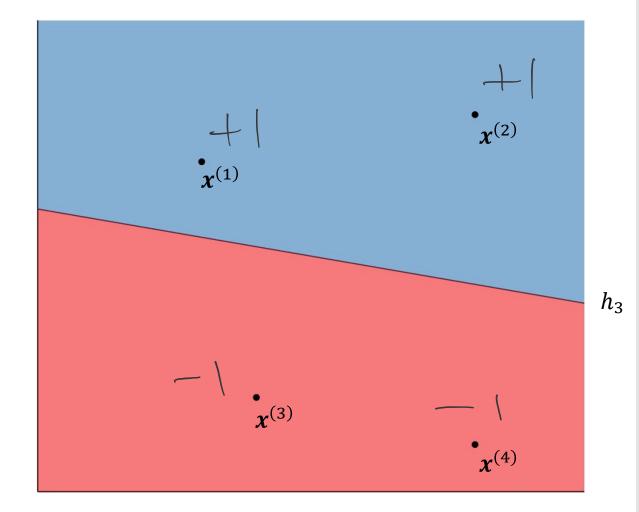


 $\mathcal{H} = \{h_1, h_2, h_3\}$

 $(h_2(\mathbf{x}^{(1)}), h_2(\mathbf{x}^{(2)}), h_2(\mathbf{x}^{(3)}), h_2(\mathbf{x}^{(4)}))$ = (-1, +1, -1, +1)





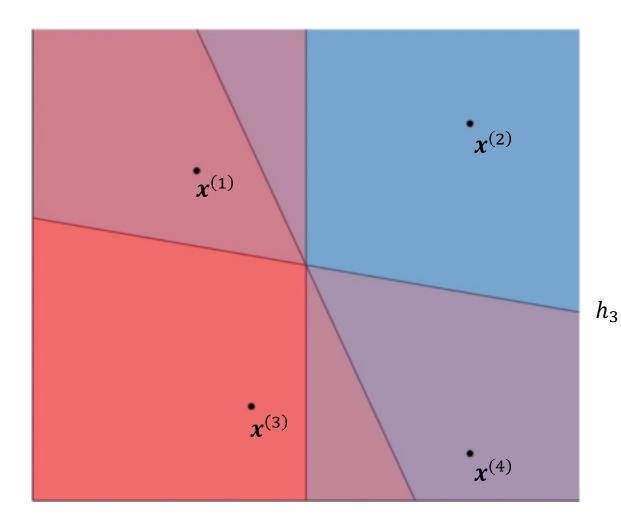


Example: Labellings

 $\mathcal{H} = \{h_1, h_2, h_3\}$

 $\mathcal{H}(S) \\ = \{(+1, +1, -1, -1), (-1, +1, -1, +1)\}$

 $|\mathcal{H}(S)| = 2$



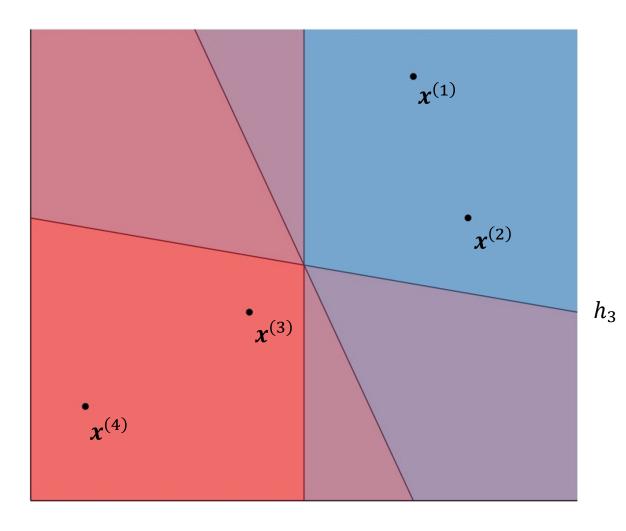
 h_1 h_2

Example: Labellings

 $\mathcal{H} = \{h_1, h_2, h_3\}$

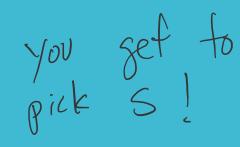
 $\mathcal{H}(S) = \{(+1, +1, -1, -1)\}$

 $|\mathcal{H}(S)| = 1$



 h_1 h_2

VC-Dimension



- $\mathcal{H}(S)$ is the set of all labellings induced by \mathcal{H} on S
 - If |S| = M, then $|\mathcal{H}(S)| \le 2^M$
 - \mathcal{H} shatters *S* if $|\mathcal{H}(S)| = 2^M$
- The <u>VC-dimension</u> of \mathcal{H} , $VC(\mathcal{H})$, is the size of the largest set S that can be shattered by \mathcal{H} .
 - If \mathcal{H} can shatter arbitrarily large finite sets, then $VC(\mathcal{H}) = \infty$
- To prove that $VC(\mathcal{H}) = d$, you need to show
- \longrightarrow 1. \exists some set of d data points that \mathcal{H} can shatter and

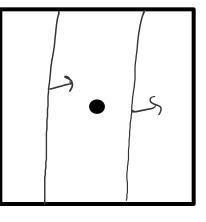
earrow a a set of d+1 data points that ${\mathcal H}$ can shatter

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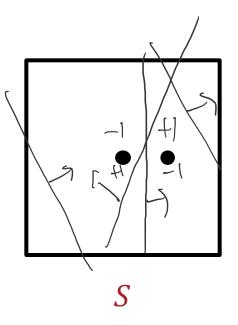
• $x \in \mathbb{R}^2$ and $\mathcal{H} =$ all 2-dimensional linear separators

• What is $VC(\mathcal{H})$?

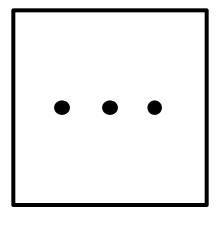
• Can $\mathcal H$ shatter some set of 1 point?



- $x \in \mathbb{R}^2$ and $\mathcal{H} =$ all 2-dimensional linear separators
- What is $VC(\mathcal{H})$?
 - Can ${\cal H}$ shatter some set of 1 point? \checkmark
 - Can $\mathcal H$ shatter some set of 2 points?



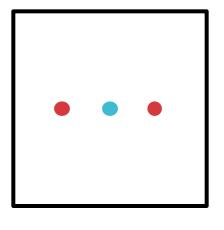
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 - Can ${\cal H}$ shatter some set of 1 point? \checkmark
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• $x \in \mathbb{R}^2$ and $\mathcal{H} =$ all 2-dimensional linear separators

• What is $VC(\mathcal{H})$?

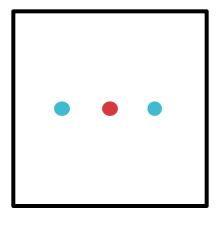
- Can $\mathcal H$ shatter some set of 1 point?
- Can \mathcal{H} shatter some set of 2 points?
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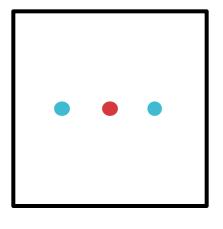
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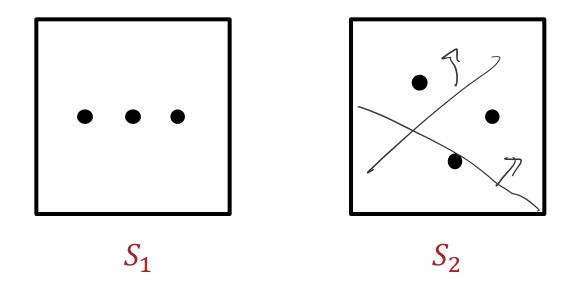
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• What is $VC(\mathcal{H})$?

- Can $\mathcal H$ shatter some set of 1 point?
- Can $\mathcal H$ shatter some set of 2 points?
- Can \mathcal{H} shatter **some** set of 3 points?



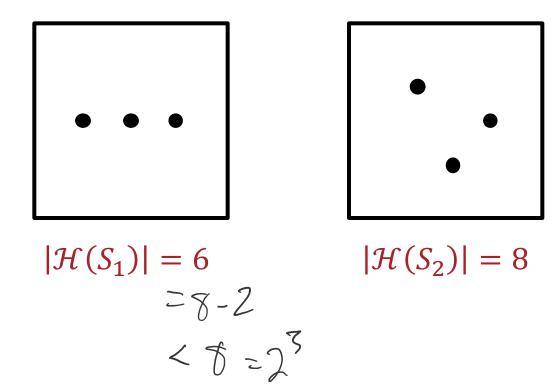
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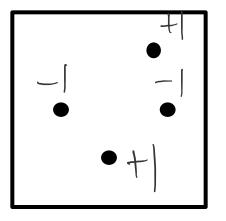
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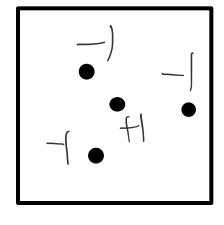
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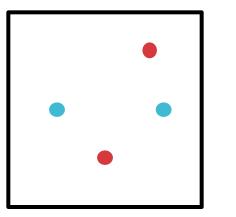
S₁ All points on the convex hull

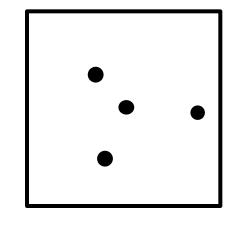
At least one point inside the convex hull

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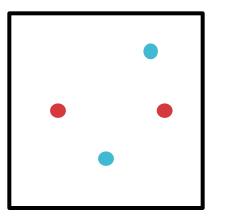
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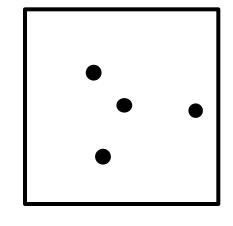
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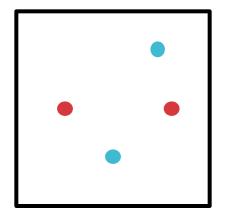
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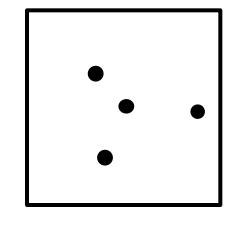
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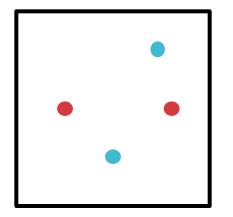
 $|\mathcal{H}(S_1)| = 14$ All points on the convex hull

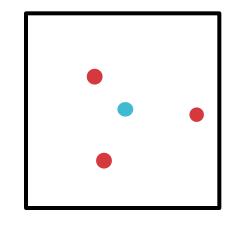
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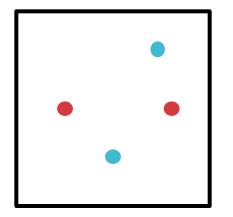
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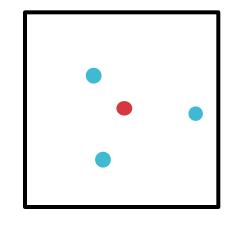
At least one point inside the convex hull

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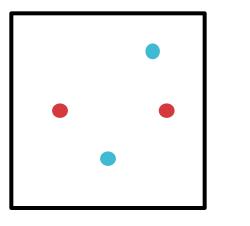


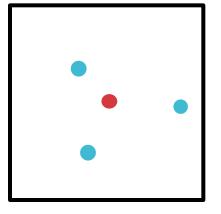
 $|\mathcal{H}(S_1)| = 14$ All points on the convex hull

At least one point inside the convex hull

• $x \in \mathbb{R}^2$ and $\mathcal{H} =$ all 2-dimensional linear separators

- What is $VC(\mathcal{H})$?
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 - Can ${\mathcal H}$ shatter some set of 4 points? imes





 $|\mathcal{H}(S_1)| = 14 \leq 2^{\mathsf{H}}$

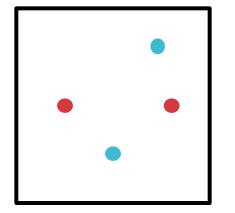
All points on the At least one point convex hull inside the convex hull

 $|\mathcal{H}(S_2)| = 14$

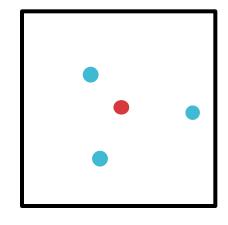
• $x \in \mathbb{R}^2$ and $\mathcal{H} =$ all 2-dimensional linear separators

• Can \mathcal{H} shatter some set of 1 point?

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• $VC(\mathcal{H}) = 3$



 $|\mathcal{H}(S_1)| = 14$ All points on the convex hull

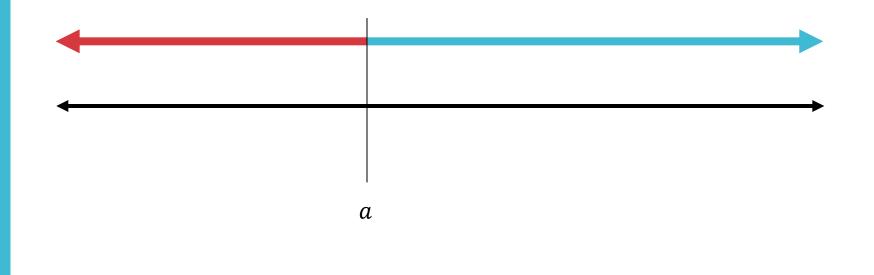
At least one point inside the convex hull

 $|\mathcal{H}(S_2)| = 14$

• $x \in \mathbb{R}^2$ and $\mathcal{H} =$ all d-dimensional linear separators

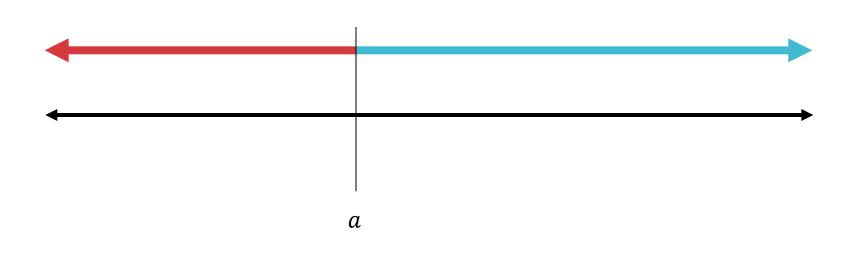
• $VC(\mathcal{H}) = d + 1$

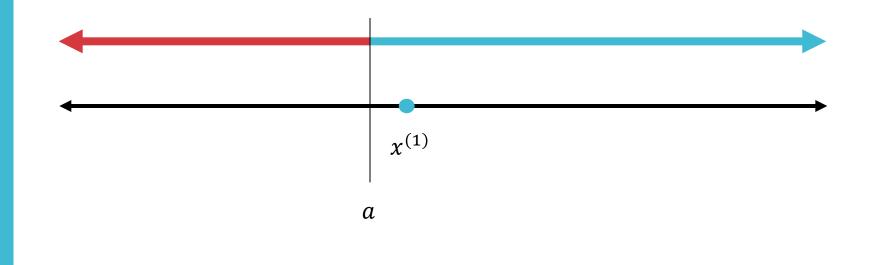
• $x \in \mathbb{R}$ and $\mathcal{H} =$ all 1-dimensional positive rays, i.e., all hypotheses of the form $h(x; a) = \operatorname{sign}(x - a)$

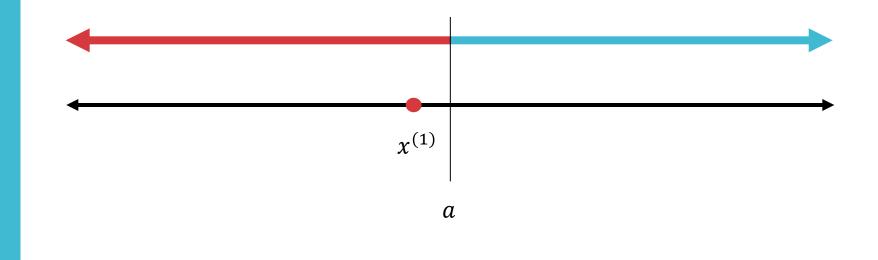


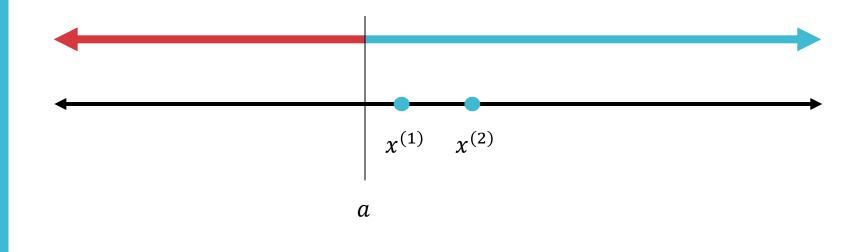
Poll Question 1: What is $VC(\mathcal{H})$? A. -1 (TOXIC) B. 0 C. 1 D. 2 E. 3

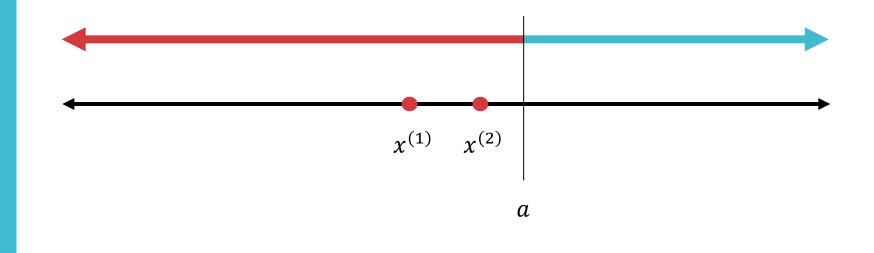
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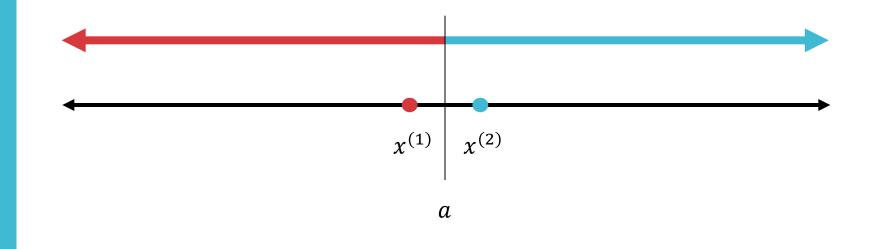


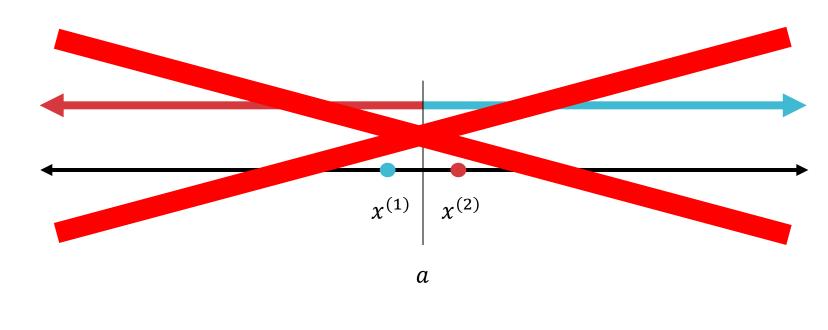




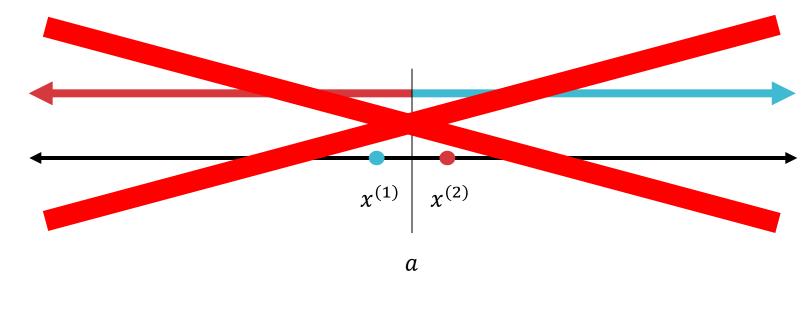






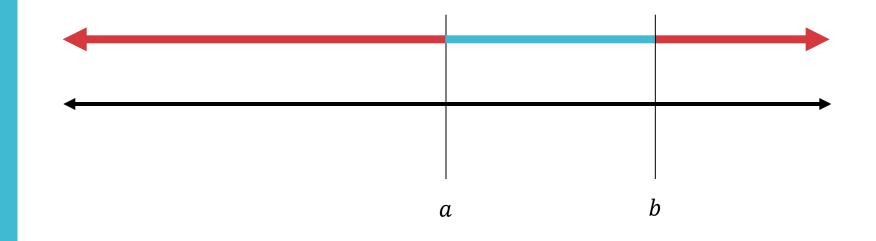


• $x \in \mathbb{R}$ and \mathcal{H} = all 1-dimensional positive rays, i.e., all hypotheses of the form $h(x; a) = \operatorname{sign}(x - a)$



• $VC(\mathcal{H}) = 1$

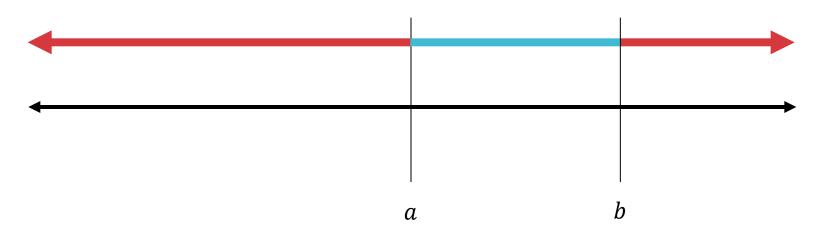
• $x \in \mathbb{R}$ and $\mathcal{H} =$ all 1-dimensional positive intervals



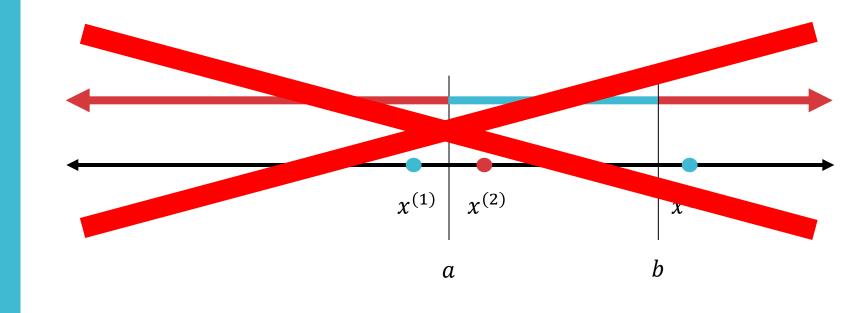
What is $VC(\mathcal{H})$? A. 0 **B.** 1 C. 1.5 (TOXIC) D. 2 E. 3

Poll Question 2:

• $x \in \mathbb{R}$ and $\mathcal{H} =$ all 1-dimensional positive intervals



• $x \in \mathbb{R}$ and $\mathcal{H} =$ all 1-dimensional positive intervals



• $VC(\mathcal{H}) = 2$

VC-Dimension: Example

Theorem 3: Vapnik-Chervonenkis (VC)-Bound where C*EH

• Infinite, realizable case: for any hypothesis set \mathcal{H} and distribution p^* , if the number of labelled training data points satisfies

$$M = \mathcal{O}\left(\frac{1}{\epsilon}\left(VC(\mathcal{H})\log\left(\frac{1}{\epsilon}\right) + \log\left(\frac{1}{\delta}\right)\right)\right)$$

then with probability at least $1 - \delta$, all $h \in \mathcal{H}$ with $\widehat{R}(h) = 0$ have $R(h) \le \epsilon$

Statistical Learning Theory Corollary 3 Infinite, realizable case: for any hypothesis set *H* and distribution p^{*}, given a training data set S s.t. |S| = M, all h ∈ *H* with *R*(h) = 0 have

$$R(h) \le O\left(\frac{1}{M}\left(VC(\mathcal{H})\log\left(\frac{M}{VC(\mathcal{H})}\right) + \log\left(\frac{1}{\delta}\right)\right)\right)$$

with probability at least $1 - \delta$.

Theorem 4: Vapnik-Chervonenkis (VC)-Bound • Infinite, agnostic case: for any hypothesis set \mathcal{H} and distribution p^* , if the number of labelled training data points satisfies

$$M = O\left(\frac{1}{\epsilon^2} \left(VC(\mathcal{H}) + \log\left(\frac{1}{\delta}\right)\right)\right)$$

then with probability at least $1 - \delta$, all $h \in \mathcal{H}$ have $|R(h) - \hat{R}(h)| \le \epsilon$

Statistical Learning Theory Corollary 4 Infinite, agnostic case: for any hypothesis set *H* and distribution p^{*}, given a training data set S s.t. |S| = M, all h ∈ H have

$$R(h) \le \widehat{R}(h) + O\left(\sqrt{\frac{1}{M}\left(VC(\mathcal{H}) + \log\left(\frac{1}{\delta}\right)\right)}\right)$$

with probability at least $1 - \delta$.

Approximation Generalization Tradeoff

How well does *h* generalize? $R(h) \leq \hat{R}(h) + O\left(\sqrt{\frac{1}{M}\left(VC(\mathcal{H}) + \log\left(\frac{1}{\delta}\right)\right)}\right)$ How well does *h* approximate *c**?

Approximation Generalization Tradeoff

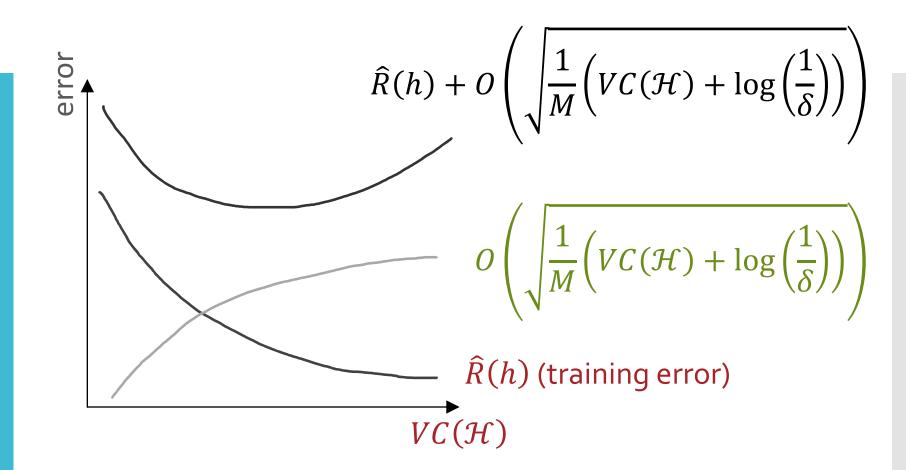
Increases as $VC(\mathcal{H})$ increases $R(h) \leq \widehat{R}(h) + O\left(\sqrt{\frac{1}{M}\left(VC(\mathcal{H}) + \log\left(\frac{1}{\delta}\right)\right)}\right)$ Decreases as $VC(\mathcal{H})$ increases

Can we use this corollary to guide model selection? Infinite, agnostic case: for any hypothesis set H and distribution p^{*}, given a training data set S s.t. |S| = M, all h ∈ H have

$$R(h) \le \widehat{R}(h) + O\left(\sqrt{\frac{1}{M}\left(VC(\mathcal{H}) + \log\left(\frac{1}{\delta}\right)\right)}\right)$$

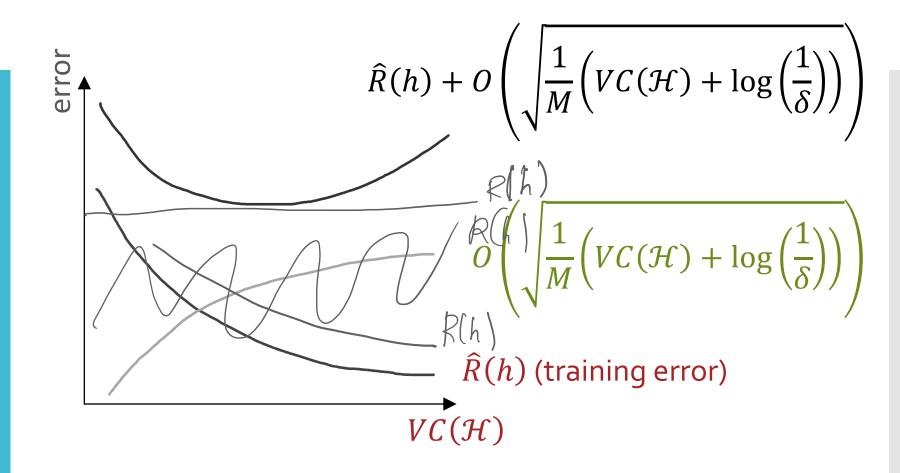
with probability at least $1 - \delta$.

Learning Theory and Model Selection

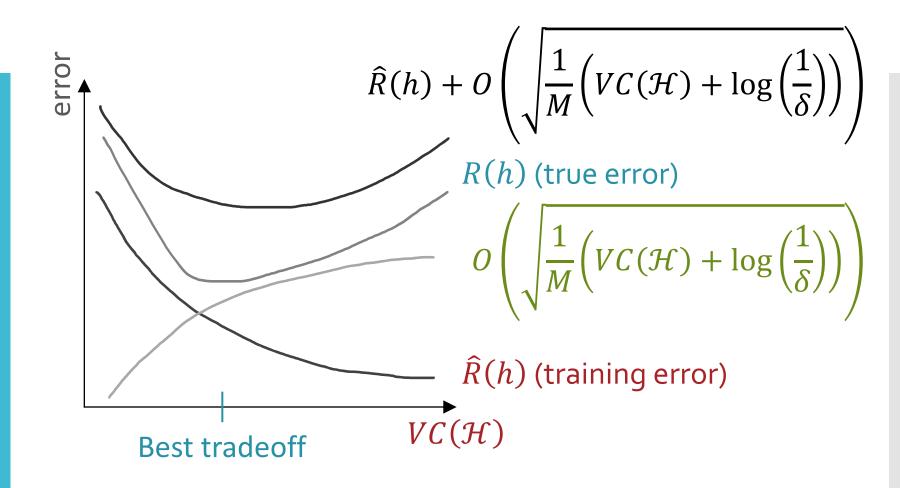


- How can we find this "best tradeoff" for linear separators?
- Use a regularizer! By (effectively) reducing the number of features our model considers, we reduce its VC-dimension.

Learning Theory and Model Selection



Learning Theory and Model Selection



- How can we find this "best tradeoff" for linear separators?
- Use a regularizer! By (effectively) reducing the number of features our model considers, we reduce its VC-dimension.

Learning Theory Learning Objectives You should be able to...

- Identify the properties of a learning setting and assumptions required to ensure low generalization error
- Distinguish true error, train error, test error
- Define PAC and explain what it means to be approximately correct and what occurs with high probability
- Apply sample complexity bounds to real-world machine learning examples
- Theoretically motivate regularization

Poll Question 3:

What questions do you have?

You should be able to...

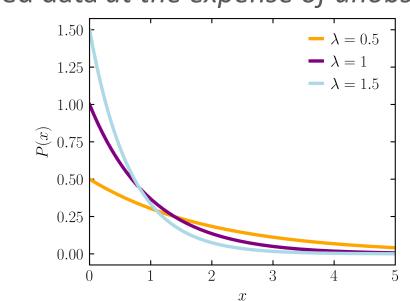
- Identify the properties of a learning setting and assumptions required to ensure low generalization error
- Distinguish true error, train error, test error
- Define PAC and explain what it means to be approximately correct and what occurs with high probability
- Apply sample complexity bounds to real-world machine learning examples
- Theoretically motivate regularization

Recall: Probabilistic Learning

- Previously:
 - (Unknown) Target function, $c^*: \mathcal{X} \to \mathcal{Y}$
 - Classifier, $h: \mathcal{X} \to \mathcal{Y}$
 - Goal: find a classifier, h, that best approximates c*
- Now:
 - (Unknown) Target *distribution*, $y \sim p^*(Y|\mathbf{x})$
 - Distribution, $p(Y|\mathbf{x})$
 - Goal: find a distribution, p, that best approximates p^*

Recall: Maximum Likelihood Estimation (MLE)

- Insight: every valid probability distribution has a finite amount of probability mass as it must sum/integrate to 1
- Idea: set the parameter(s) so that the likelihood of the samples is maximized
- Intuition: assign as much of the (finite) probability mass to the observed data *at the expense of unobserved data*
- Example: the exponential distribution



Bernoulli Distribution MLE

- A Bernoulli random variable takes value 1 with probability ϕ and value 0 with probability 1ϕ
- The pmf of the Bernoulli distribution is

 $p(x|\phi) = \phi^x (1-\phi)^{1-x}$

Coin Flipping MLE

- A Bernoulli random variable takes value 1 (or heads) with probability ϕ and value 0 (or tails) with probability 1ϕ
- The pmf of the Bernoulli distribution is $p(x|\phi) = \phi^{x}(1-\phi)^{1-x} \quad \checkmark$
- Given *N* iid samples $\{x^{(1)}, \dots, x^{(N)}\}$, the log-likelihood is $l(\phi) = \{\phi, (f), \dots, f^{(N)}\}, f(\phi)\}$ $= \sum_{i=1}^{N} \log \left(p(x^{(i)}; \emptyset) \right)$ $= \sum_{i=1}^{N} \log \left(\phi^{x^{(i)}} (1-\phi)^{1-x^{(i)}} \right)$ $= \sum_{i=1}^{N} x^{(i)} lg(\phi) + (1 - x^{(i)}) log(1 - \phi)$ = $N_{1} \log(\phi) + N_{0} \log(1-\phi)$

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where

Coin Flipping MLE

- A Bernoulli random variable takes value 1 (or heads) with probability ϕ and value 0 (or tails) with probability 1ϕ
- The pmf of the Bernoulli distribution is $p(x|\phi) = \phi^x (1-\phi)^{1-x}$
- The partial derivative of the log-likelihood is + $N_{o}\log((-\beta))$ $(\phi) = N_1 \log($ N. (1-8)

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Coin Flipping MLE

- A Bernoulli random variable takes value 1 (or heads) with probability ϕ and value 0 (or tails) with probability 1ϕ
- The pmf of the Bernoulli distribution is $p(x|\phi) = \phi^x (1-\phi)^{1-x}$
- The partial derivative of the log-likelihood is

$$\frac{N_1}{\hat{\phi}} - \frac{N_0}{1 - \hat{\phi}} = 0 \rightarrow \frac{N_1}{\hat{\phi}} = \frac{N_0}{1 - \hat{\phi}}$$

$$\rightarrow N_1 (1 - \hat{\phi}) = N_0 \hat{\phi} \rightarrow N_1 = \hat{\phi} (N_0 + N_1)$$

$$\rightarrow \hat{\phi} = \frac{N_1}{N_0 + N_1}$$

• where N_1 is the number of 1's in $\{x^{(1)}, \dots, x^{(N)}\}$ and N_0 is the number of 0's