

10-301/601: Introduction to Machine Learning Lecture 15 – Learning Theory (Infinite Case)

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10/23/23

Front Matter

- Announcements
 - HW5 released 10/9, due 10/27 (Friday) at 11:59 PM
 - Exam 3 scheduled
 - Tuesday, December 12th from 5:30 PM to 8:30 PM
 - Sign up for peer tutoring! See [Piazza](#) for more details
 - Exam 1 exit poll also on Piazza

Recall - Theorem 1: Finite, Realizable Case

- For a *finite* hypothesis set \mathcal{H} such that $c^* \in \mathcal{H}$ (*realizable*) and arbitrary distribution p^* , if the number of labelled training data points satisfies

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

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

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- Making the bound tight and solving for ϵ gives...

Statistical Learning Theory Corollary

- For a *finite* hypothesis set \mathcal{H} such that $c^* \in \mathcal{H}$ (*realizable*) and arbitrary distribution p^* , given a training dataset S where $|S| = M$, 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 $1 - \delta$.

Recall - Theorem 2: Finite, Agnostic Case

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

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

then with probability at least $1 - \delta$, all $h \in \mathcal{H}$ satisfy

$$|R(h) - \hat{R}(h)| \leq \epsilon$$

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

Statistical Learning Theory Corollary

- For a *finite* hypothesis set \mathcal{H} and arbitrary distribution p^* , given a training dataset S where $|S| = M$, all $h \in \mathcal{H}$ have

$$R(h) \leq \hat{R}(h) + \sqrt{\frac{1}{2M} \left(\ln(|\mathcal{H}|) + \ln\left(\frac{2}{\delta}\right) \right)}$$

with probability at least $1 - \delta$.

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

- For a *finite* hypothesis set \mathcal{H} and arbitrary distribution p^* , given a training data set S where $|S| = M$, all $h \in \mathcal{H}$ have

$$R(h) \leq \hat{R}(h) + \sqrt{\frac{1}{2M} \left(\ln(|\mathcal{H}|) + \ln\left(\frac{2}{\delta}\right) \right)}$$

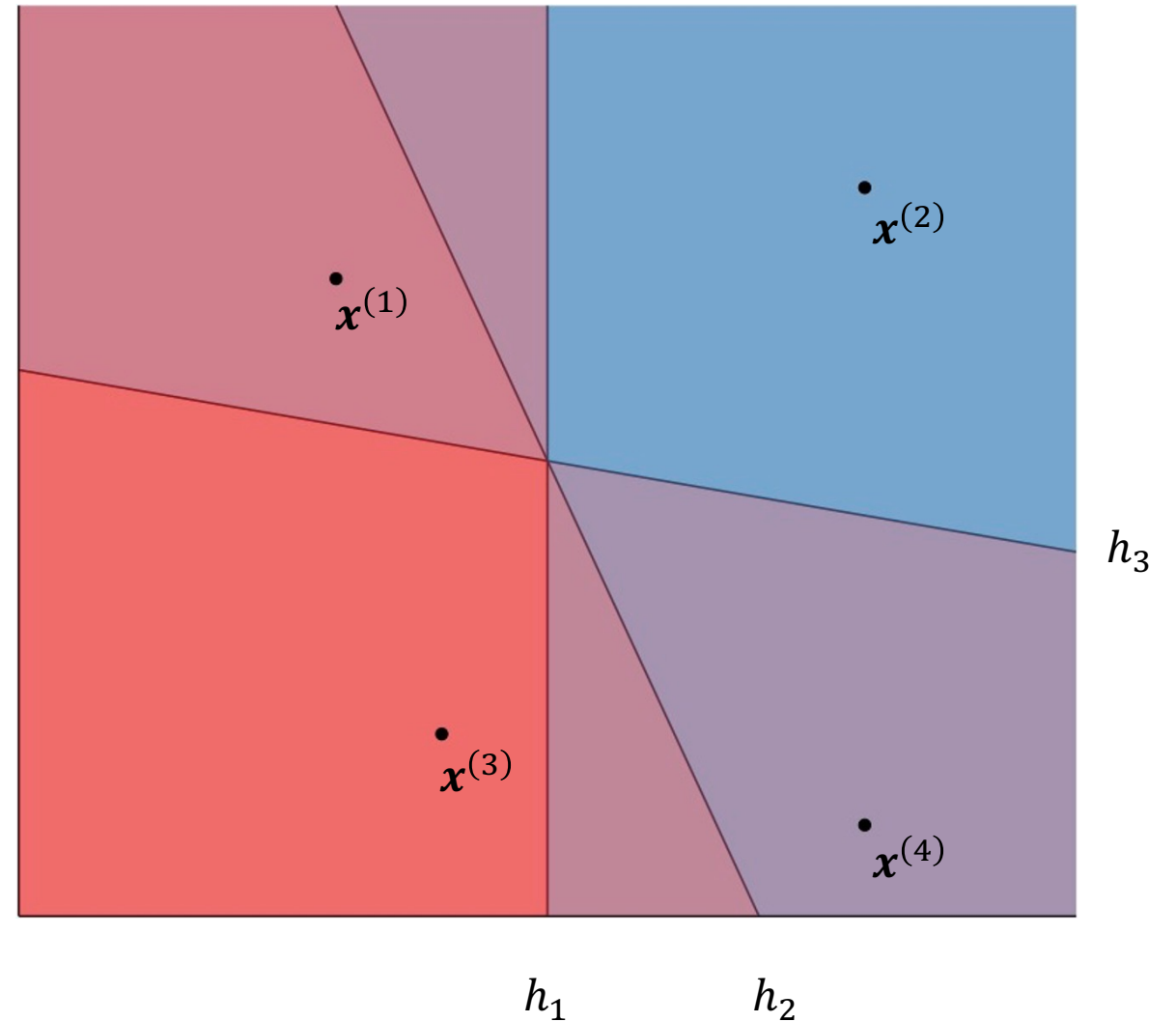
with probability at least $1 - \delta$.

Labellings

- Given some finite set of data points $S = \{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(M)}\}$ and some hypothesis $h \in \mathcal{H}$, applying h to each point in S results in a **labelling**
 - $[h(\mathbf{x}^{(1)}), \dots, h(\mathbf{x}^{(M)})]$ is a vector of M +1's and -1's (recall: our discussion of PAC learning assumes binary classification)
- Given $S = \{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(M)}\}$, 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
$$\mathcal{H}(S) = \{[h(\mathbf{x}^{(1)}), \dots, h(\mathbf{x}^{(M)})] \mid h \in \mathcal{H}\}$$

Example: Labellings

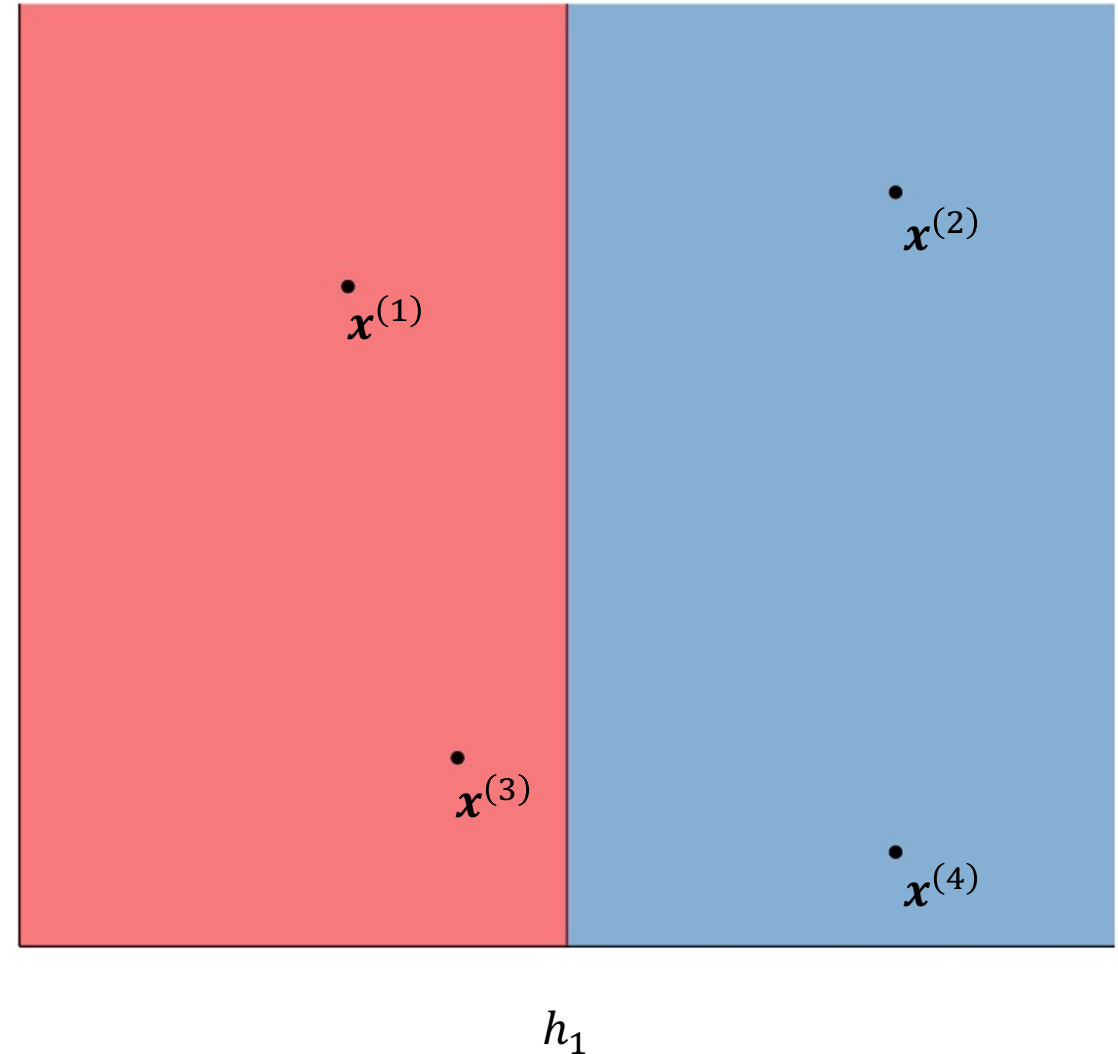
$$\mathcal{H} = \{h_1, h_2, h_3\}$$



Example: Labellings

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

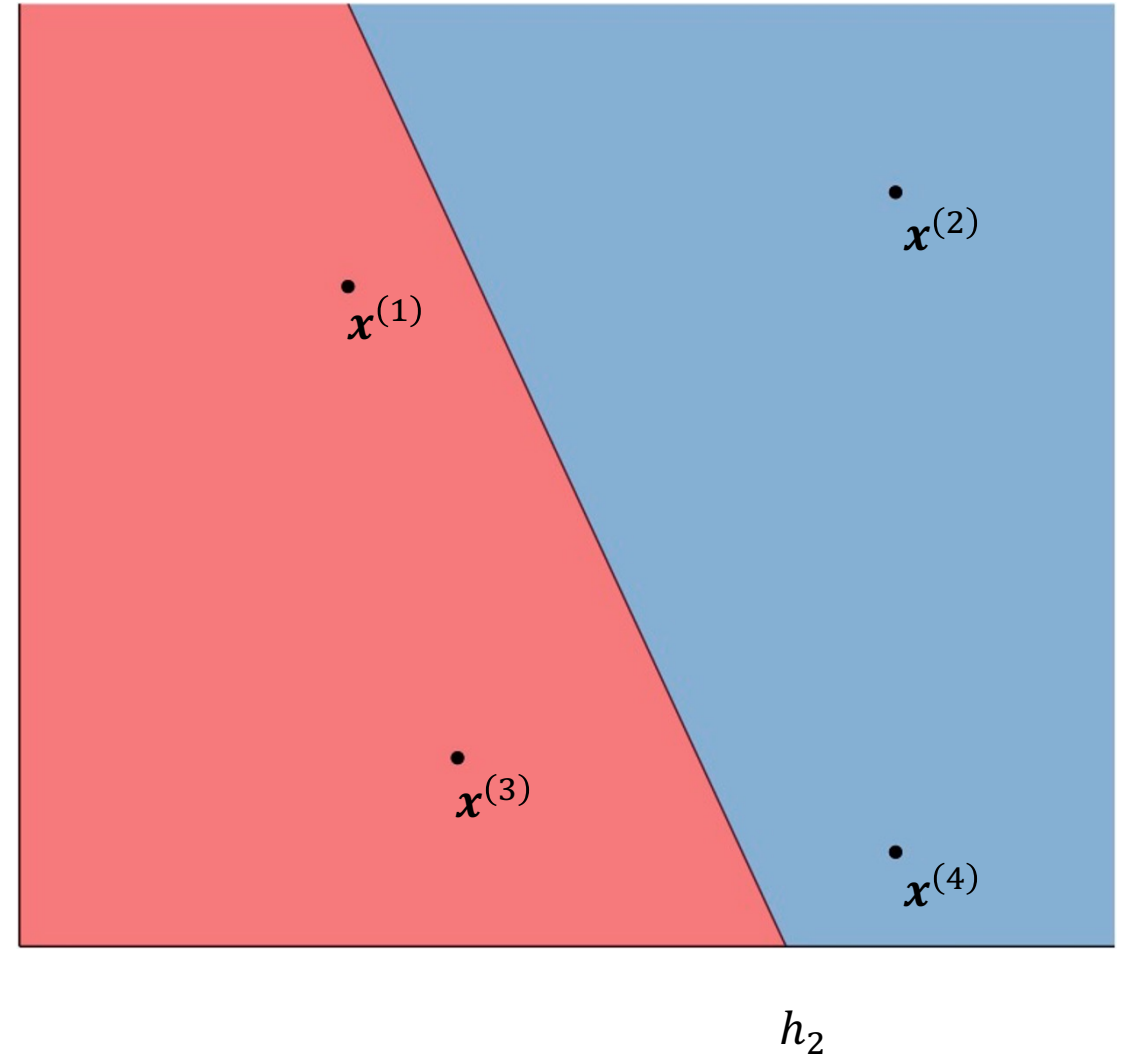
$$\begin{aligned} & [h_1(\mathbf{x}^{(1)}), h_1(\mathbf{x}^{(2)}), h_1(\mathbf{x}^{(3)}), h_1(\mathbf{x}^{(4)})] \\ & = (-1, +1, -1, +1) \end{aligned}$$



Example: Labellings

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

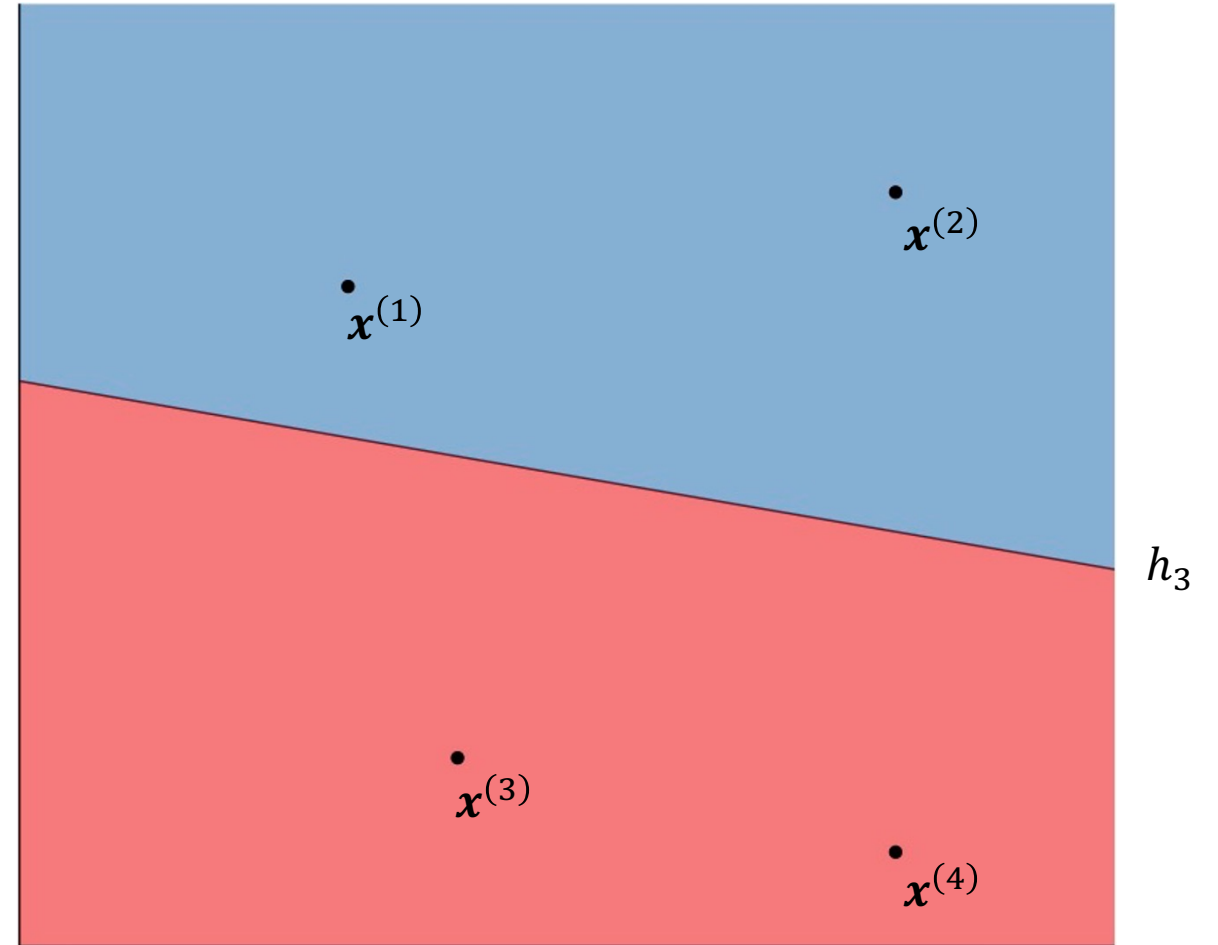
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Example: Labellings

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

$$\begin{aligned} & [h_1(\mathbf{x}^{(1)}), h_1(\mathbf{x}^{(2)}), h_1(\mathbf{x}^{(3)}), h_1(\mathbf{x}^{(4)})] \\ & = (+1, +1, -1, -1) \end{aligned}$$



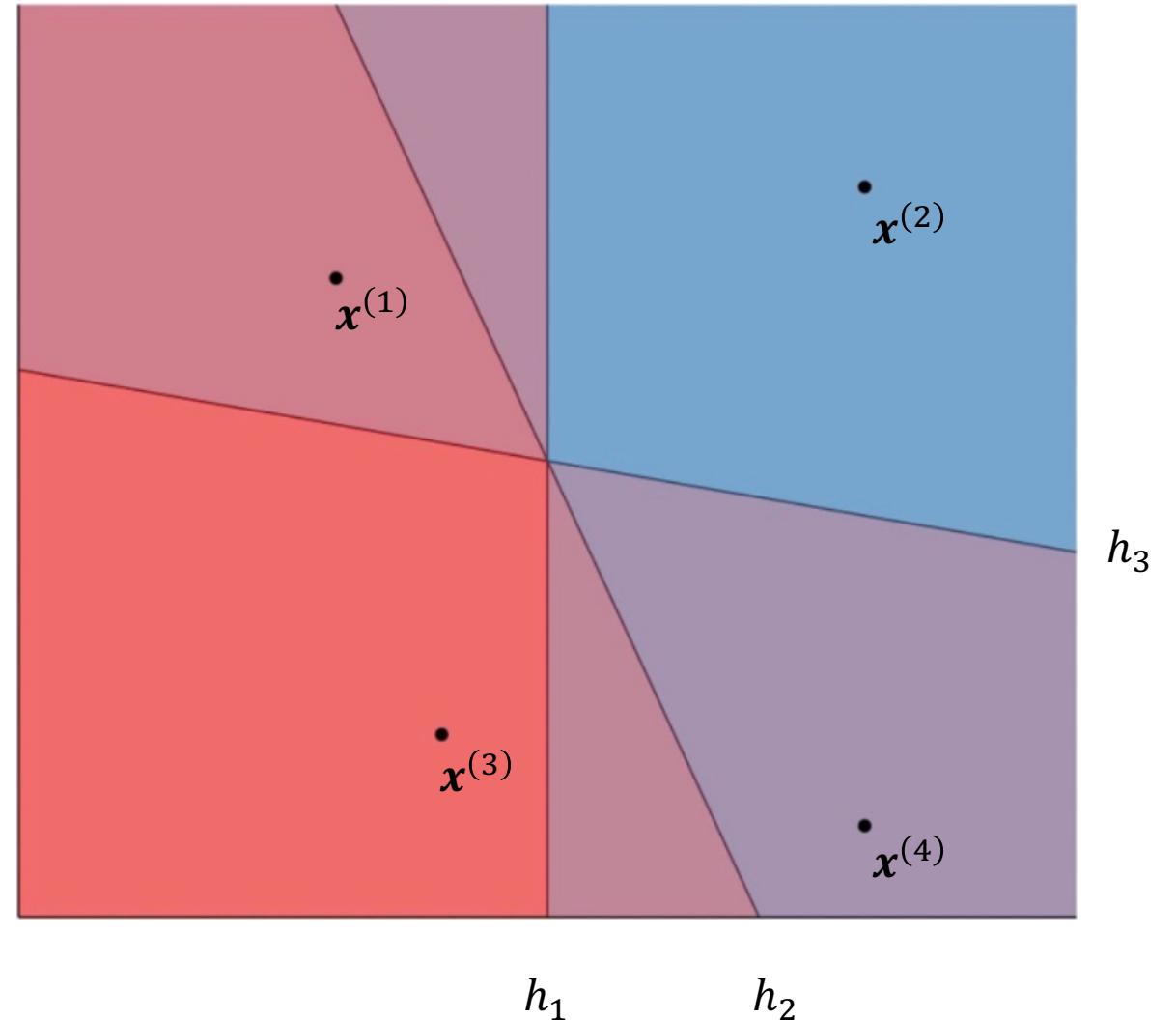
Example: Labellings

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

$$\mathcal{H}(S)$$

$$= \{[+1, +1, -1, -1], [-1, +1, -1, +1]\}$$

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

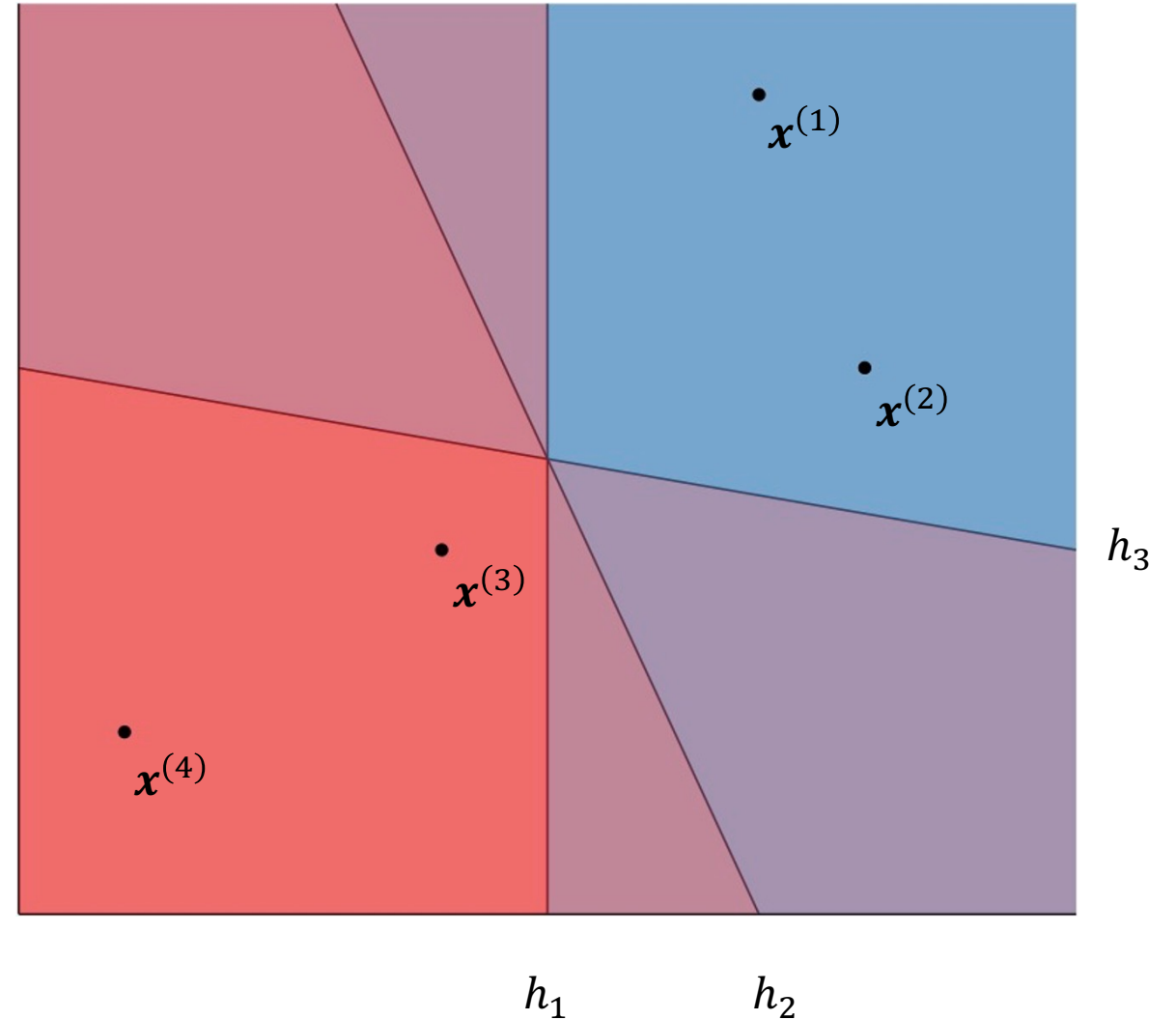


Example: Labellings

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

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

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

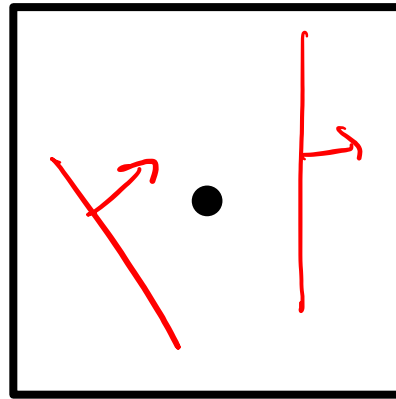


VC-Dimension

- $\mathcal{H}(S)$ is the set of all labellings induced by \mathcal{H} on S
 - If $|S| = M$, then $|\mathcal{H}(S)| \leq 2^M$
 - \mathcal{H} shatters S if $|\mathcal{H}(S)| = 2^M$
- The VC-dimension 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
 1. \exists some set of d data points that \mathcal{H} can shatter and
 2. \nexists a set of $d + 1$ data points that \mathcal{H} can shatter

VC-Dimension: Example

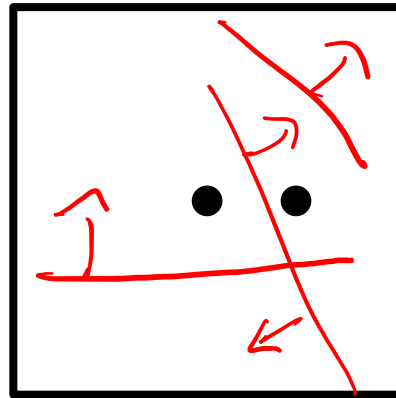
- $x \in \mathbb{R}^2$ and $\mathcal{H} =$ all 2-dimensional linear separators
- What is $VC(\mathcal{H})$?
 - Can \mathcal{H} shatter some set of 1 point? ✓



S

VC-Dimension: Example

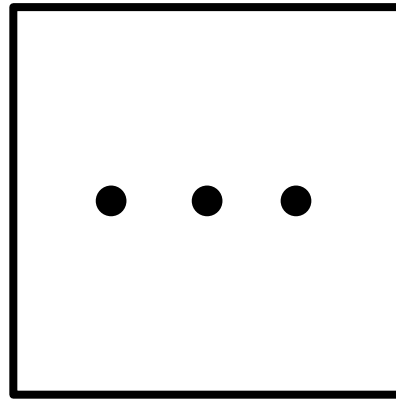
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S

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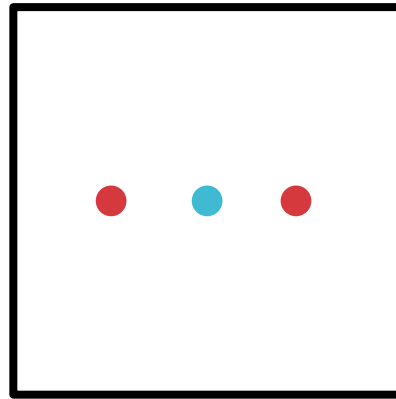
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S

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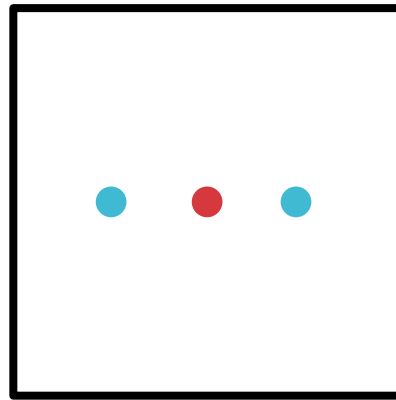
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S

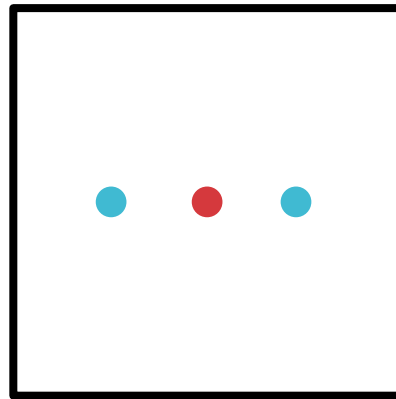
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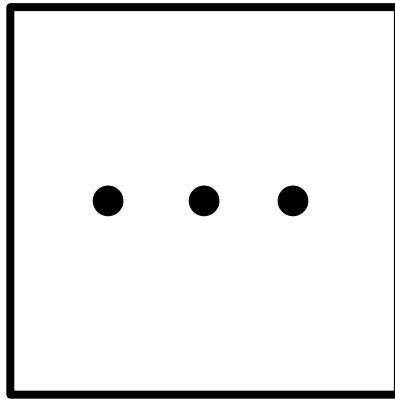
VC-Dimension: Example

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

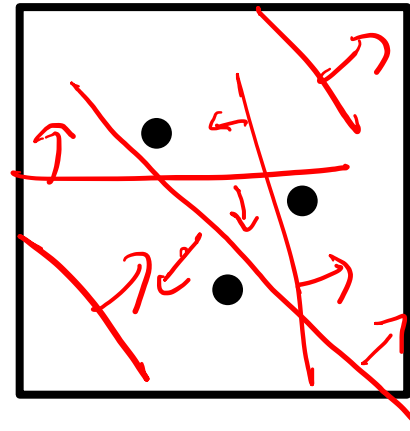


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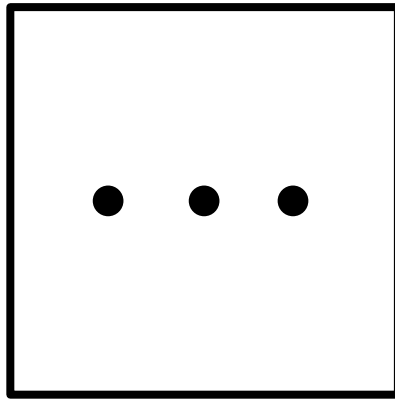
S_1



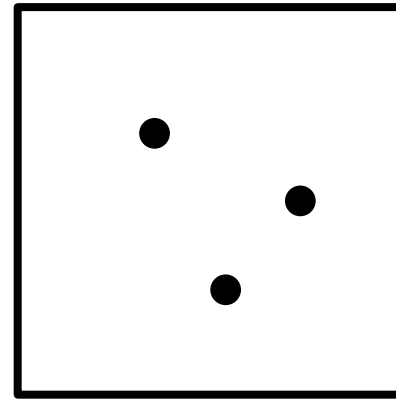
S_2

VC-Dimension: Example

- $\mathbf{x} \in \mathbb{R}^2$ and $\mathcal{H} =$ all 2-dimensional linear separators
- What is $VC(\mathcal{H})$?
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 - Can \mathcal{H} shatter some set of 2 points?
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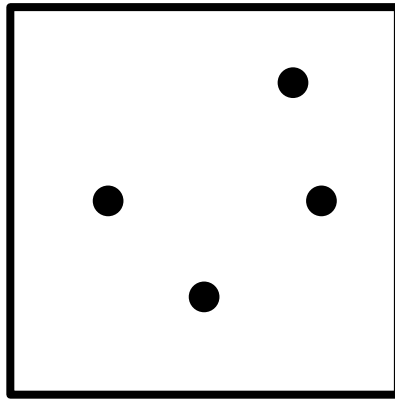
$$|\mathcal{H}(S_1)| = 6$$



$$|\mathcal{H}(S_2)| = 8$$

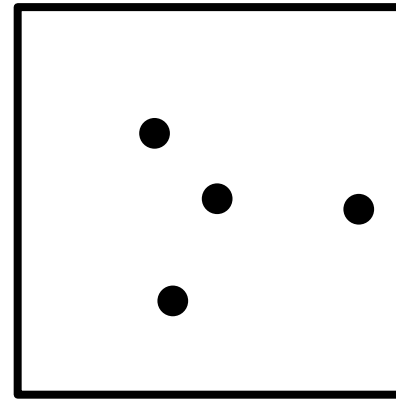
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S_1

All points on the
convex hull

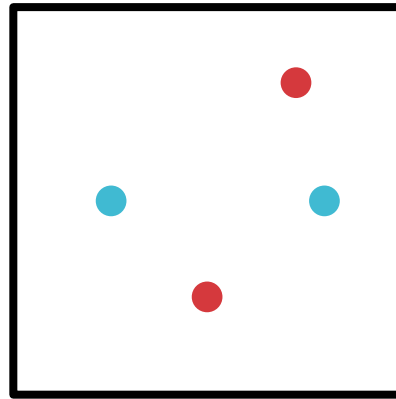


S_2

At least one point
inside the convex hull

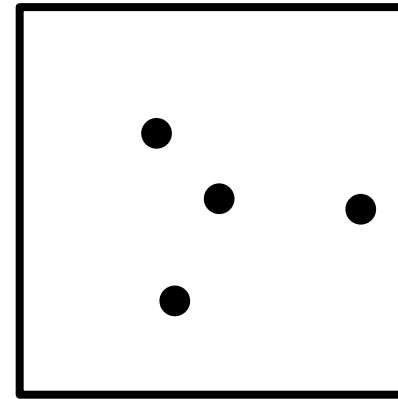
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S_1

All points on the
convex hull

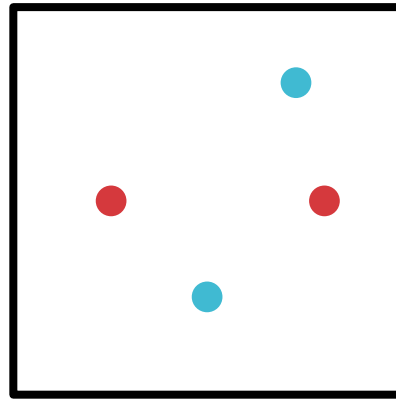


S_2

At least one point
inside the convex hull

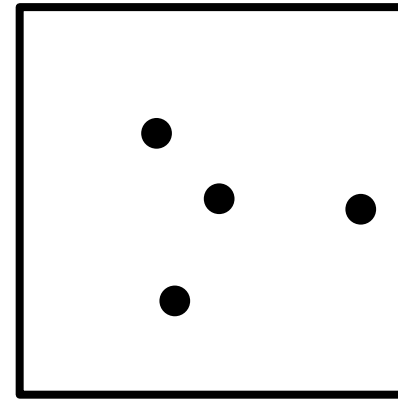
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convex hull

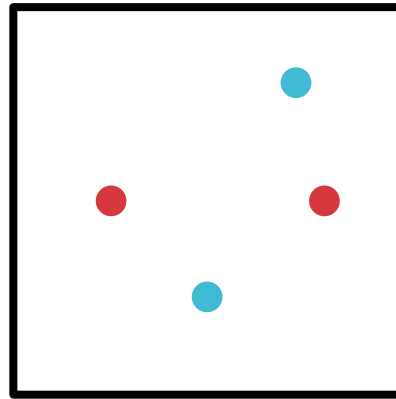


S_2

At least one point
inside the convex hull

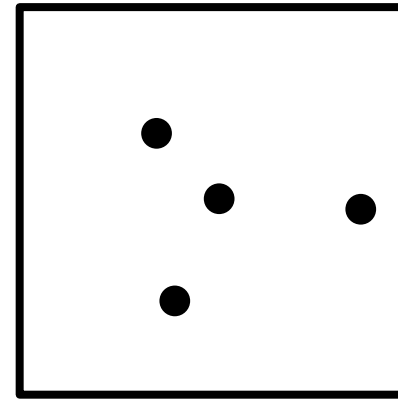
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$$|\mathcal{H}(S_1)| = 14$$

All points on the
convex hull

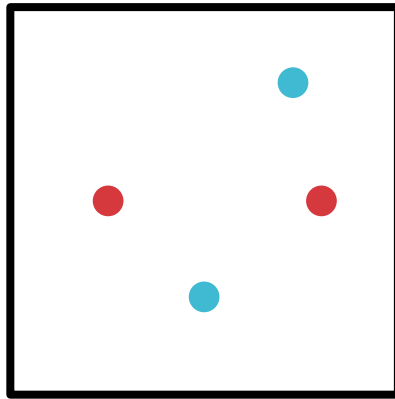


S_2

At least one point
inside the convex hull

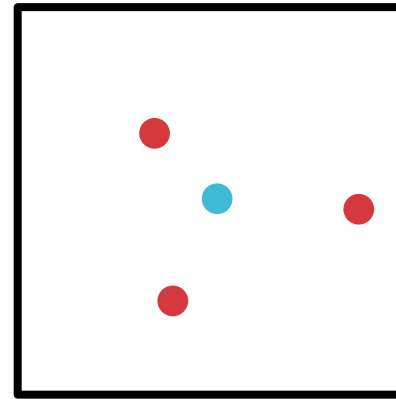
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All points on the
convex hull

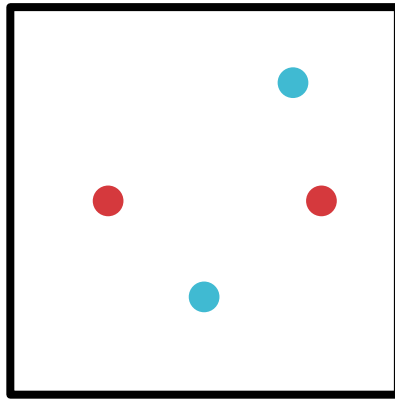


S_2

At least one point
inside the convex hull

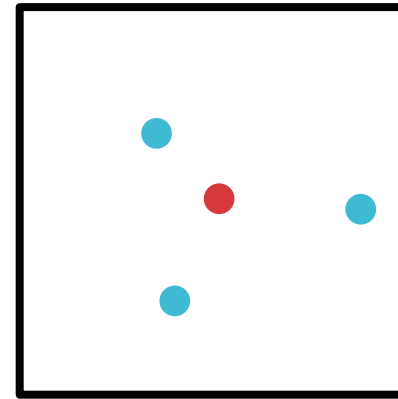
VC-Dimension: Example

- $\mathbf{x} \in \mathbb{R}^2$ 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?
 - Can \mathcal{H} shatter some set of 3 points?
 - Can \mathcal{H} shatter some set of 4 points?



$$|\mathcal{H}(S_1)| = 14$$

All points on the
convex hull



S_2

At least one point
inside the convex hull

VC-Dimension: Example

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

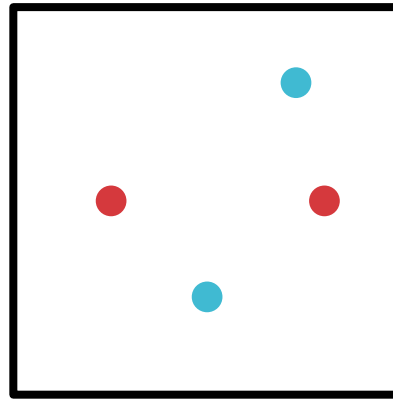
- What is $VC(\mathcal{H})$?

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

- Can \mathcal{H} shatter some set of 2 points? ✓

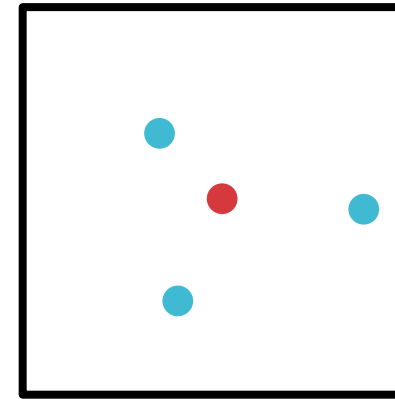
- Can \mathcal{H} shatter some set of 3 points? ✓

- Can \mathcal{H} shatter some set of 4 points? ✗



$$|\mathcal{H}(S_1)| = 14$$

All points on the
convex hull

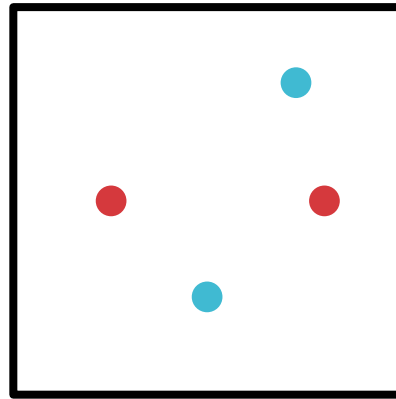


$$|\mathcal{H}(S_2)| = 14$$

At least one point
inside the convex hull

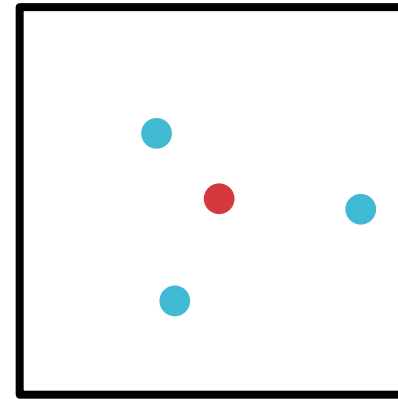
VC-Dimension: Example

- $\mathbf{x} \in \mathbb{R}^2$ and $\mathcal{H} =$ all 2-dimensional linear separators
- $VC(\mathcal{H}) = 3$
 - 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?
 - Can \mathcal{H} shatter some set of 4 points?



$$|\mathcal{H}(S_1)| = 14$$

All points on the
convex hull



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

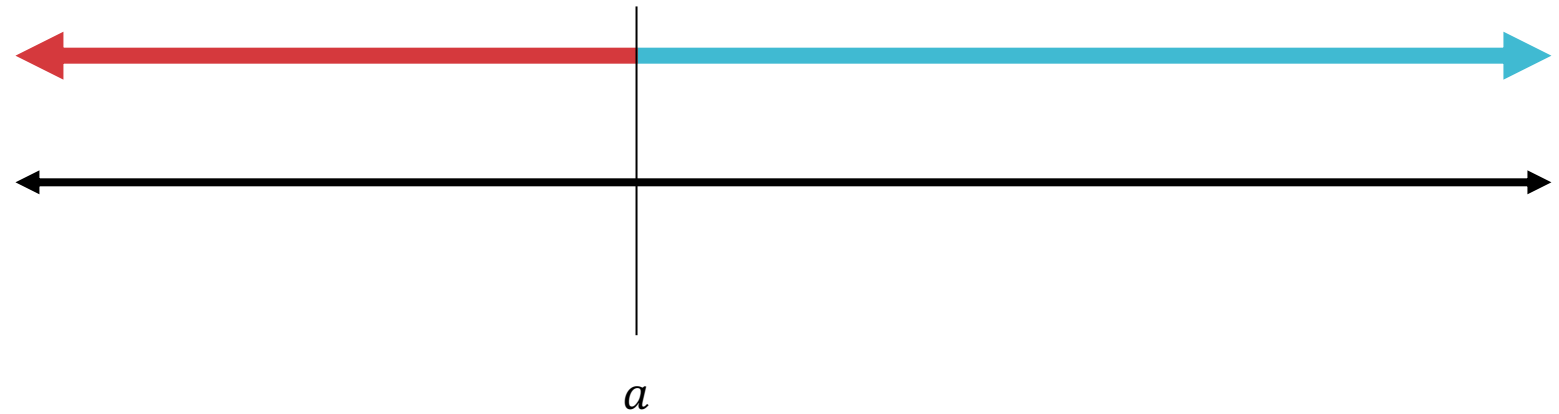
At least one point
inside the convex hull

VC-Dimension: Example

- $x \in \mathbb{R}^d$ and $\mathcal{H} =$ all d -dimensional linear separators
- $VC(\mathcal{H}) = d + 1$

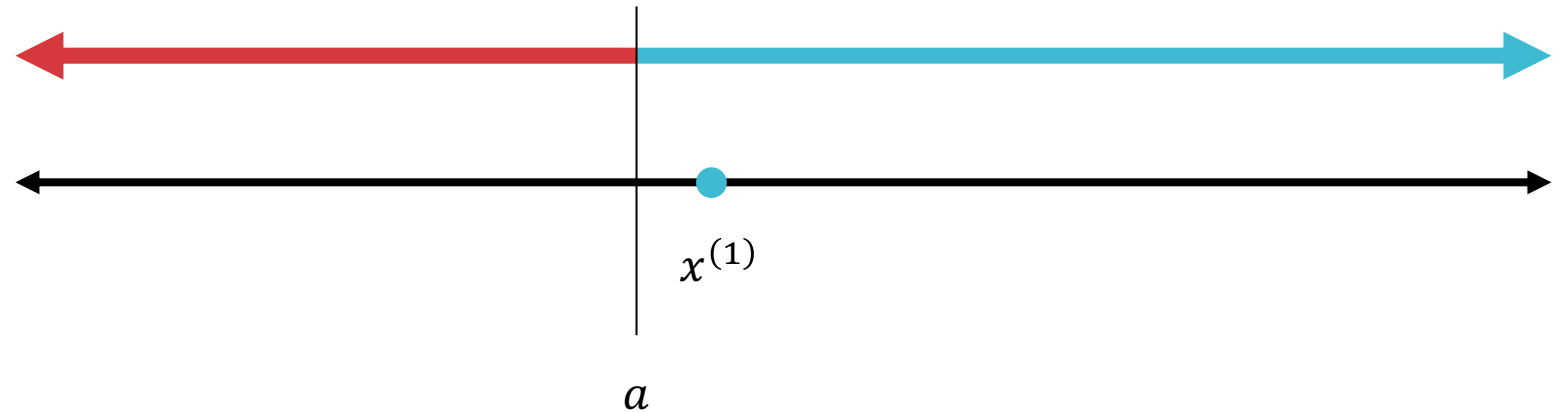
VC-Dimension: Example

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



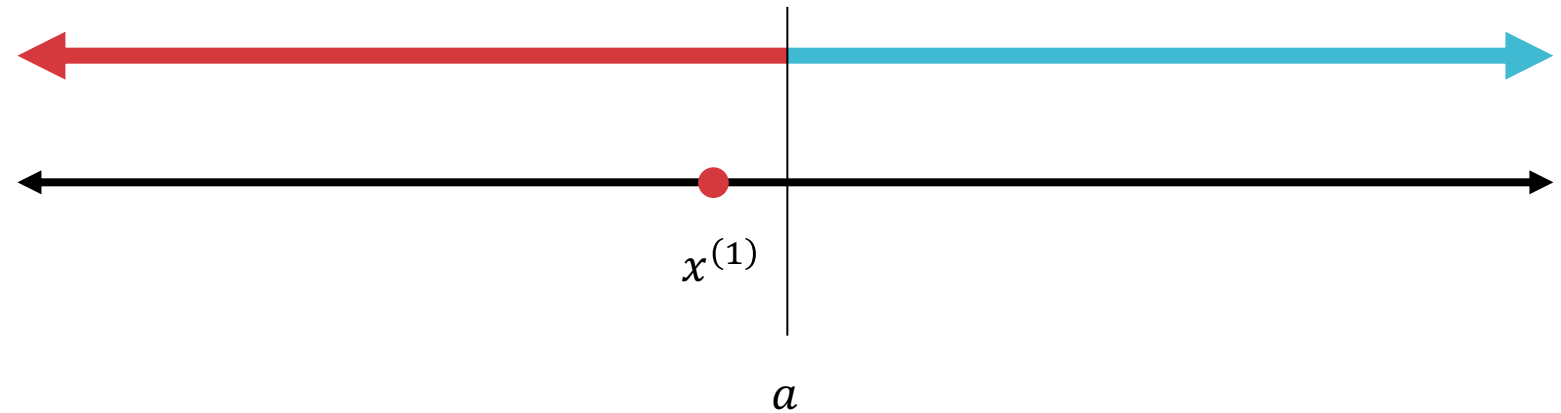
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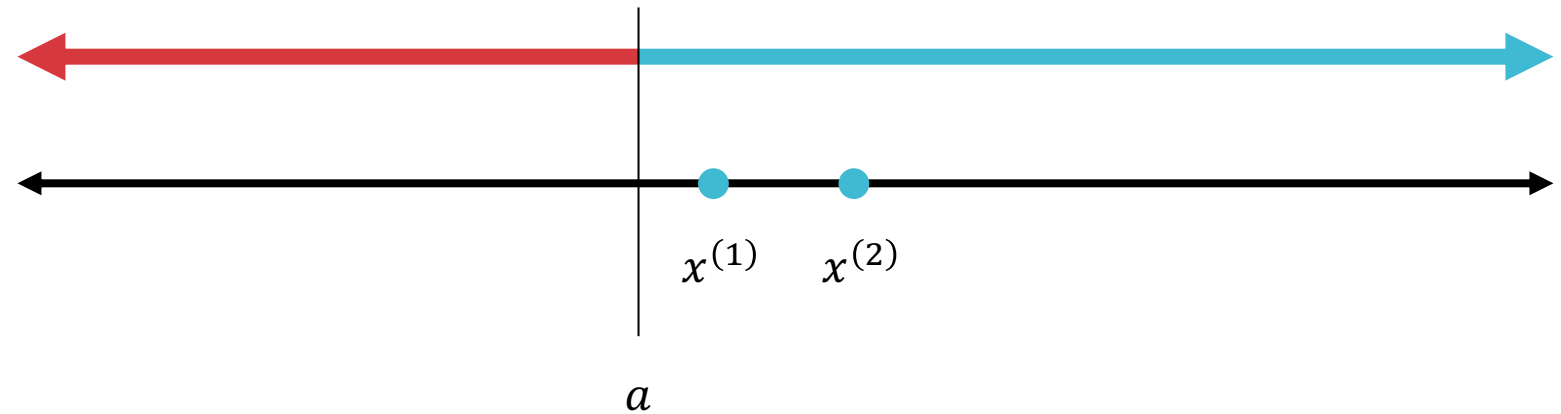
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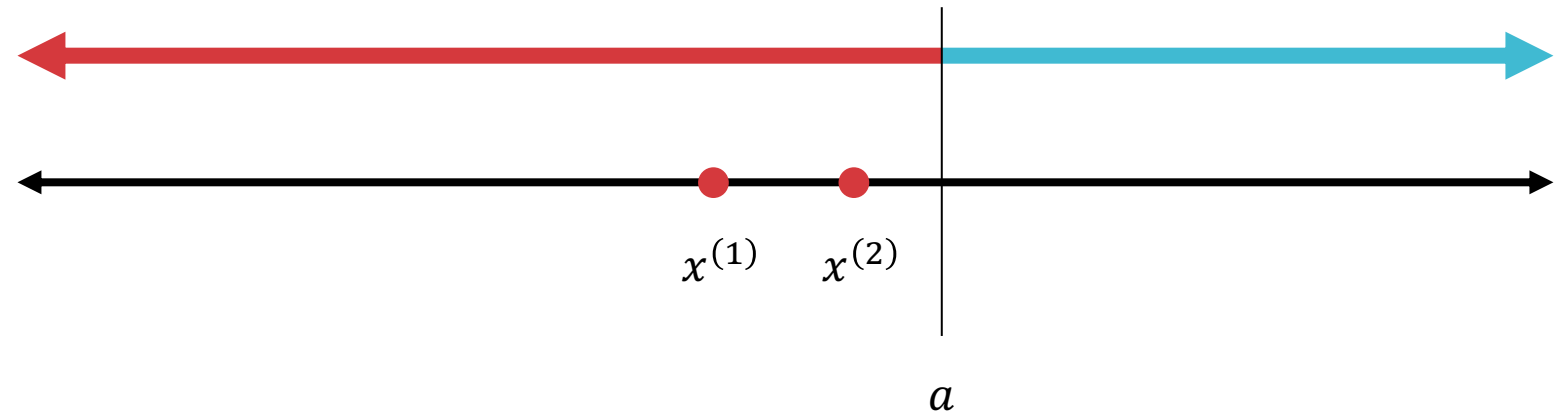
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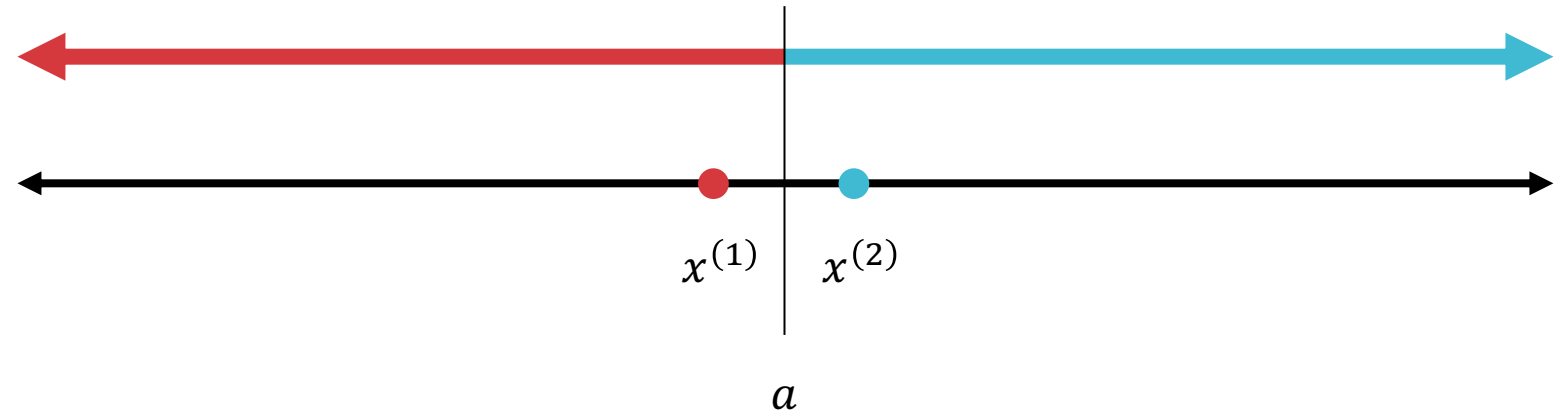
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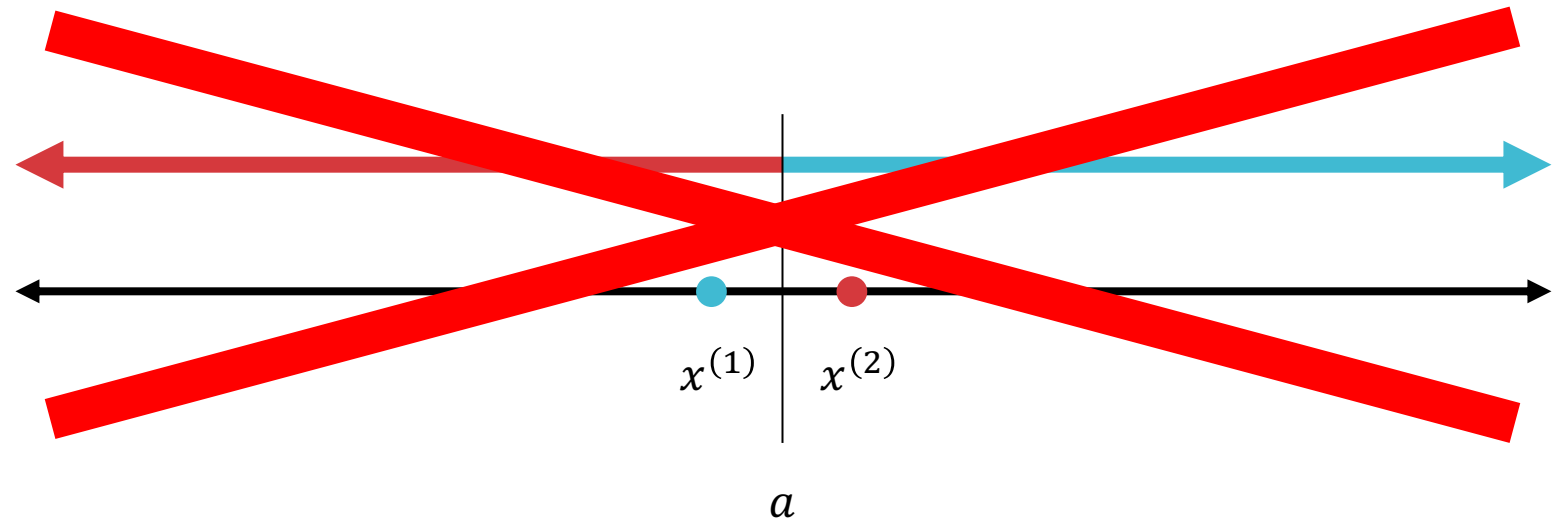
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VC-Dimension: Example

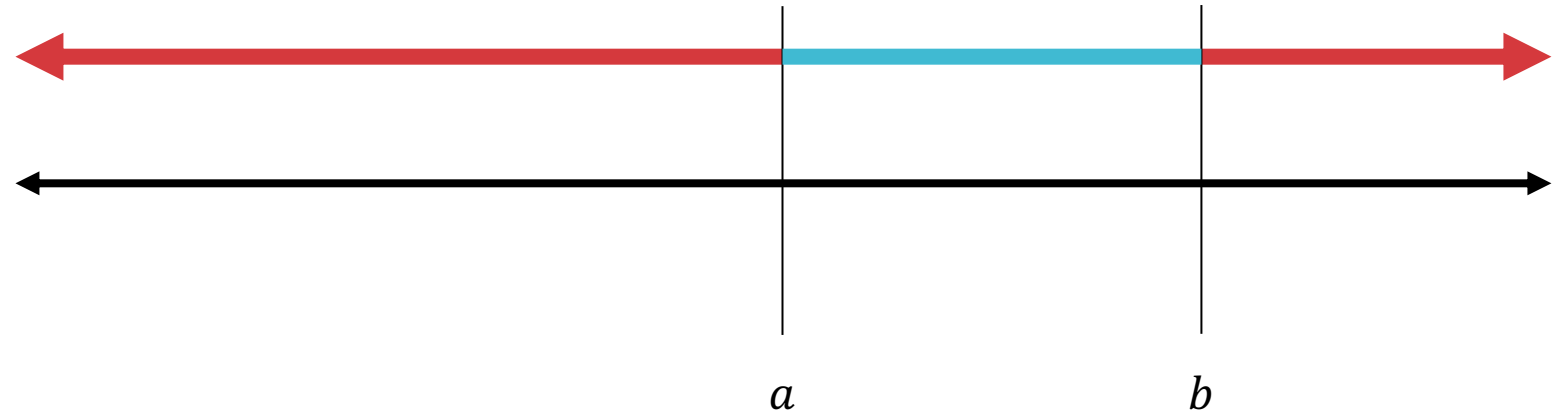
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- $VC(\mathcal{H}) = 1$

VC-Dimension: Example

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



Poll Question 1:

What is $VC(\mathcal{H})$?

A. 0

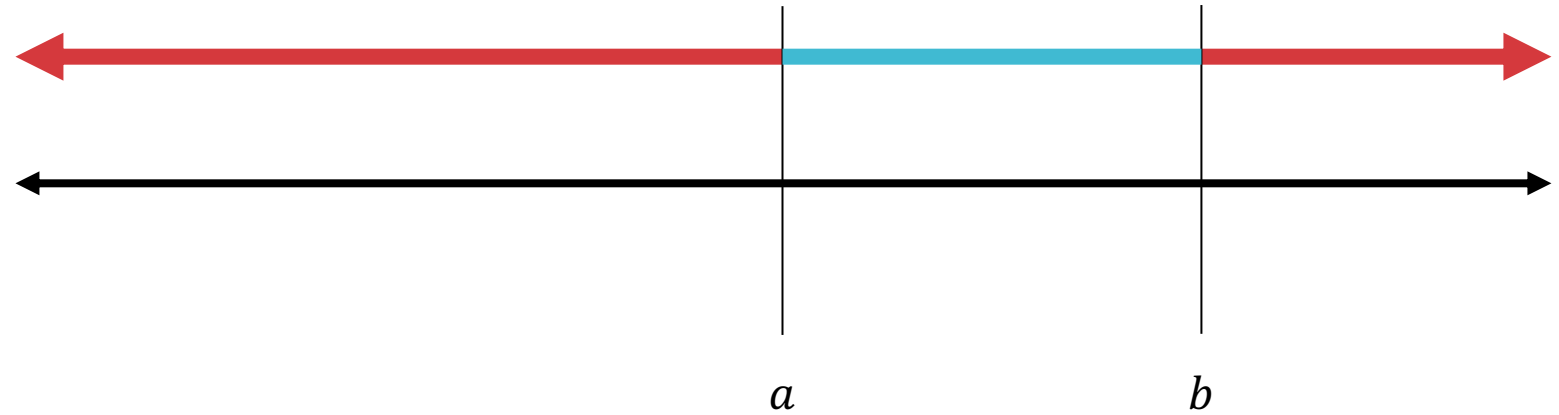
B. 1

C. 1.5 (TOXIC)

D. 2

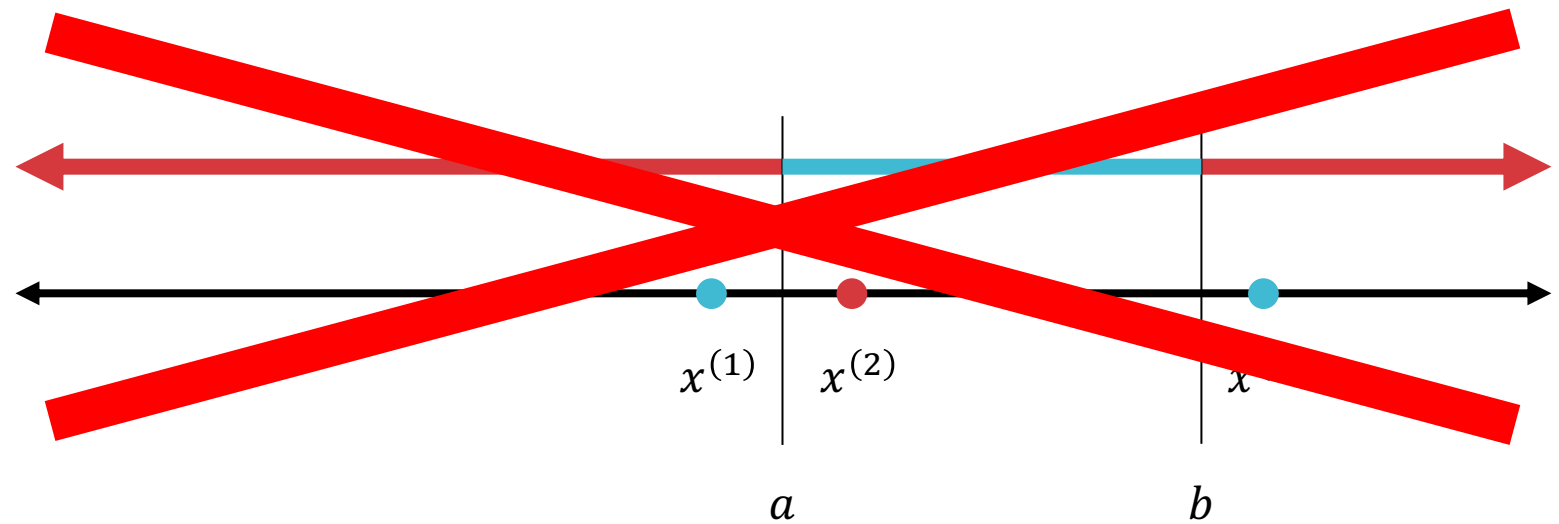
E. 3

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



VC-Dimension: Example

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



- $VC(\mathcal{H}) = 2$

Theorem 3: Vapnik- Chervonenkis (VC)-Bound

- Infinite, realizable case: for any hypothesis set \mathcal{H} such that $c^* \in \mathcal{H}$ and arbitrary distribution p^* , if the number of labelled training data points satisfies

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

(Handwritten red annotations: arrows point from \ln to $\log(\frac{1}{\epsilon})$ and $\log(\frac{1}{\delta})$; a red underline is under $VC(\mathcal{H})$)

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



Statistical Learning Theory Corollary 3

- Infinite, realizable case: for any hypothesis set \mathcal{H} such that $c^* \in \mathcal{H}$ and arbitrary distribution p^* , given a training dataset S where $|S| = M$, all $h \in \mathcal{H}$ with $\hat{R}(h) = 0$ have

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

with probability at least $1 - \delta$.

Theorem 4: Vapnik- Chervonenkis (VC)-Bound

- Infinite, agnostic case: for any hypothesis set \mathcal{H} and arbitrary 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

$$|R(h) - \hat{R}(h)| \leq \epsilon$$

Statistical Learning Theory Corollary 4

- Infinite, agnostic case: for any hypothesis set \mathcal{H} and arbitrary distribution p^* , given a training dataset S where $|S| = M$, all $h \in \mathcal{H}$ have

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

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

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

Increases as $VC(\mathcal{H})$ increases

Decreases as $VC(\mathcal{H})$ increases

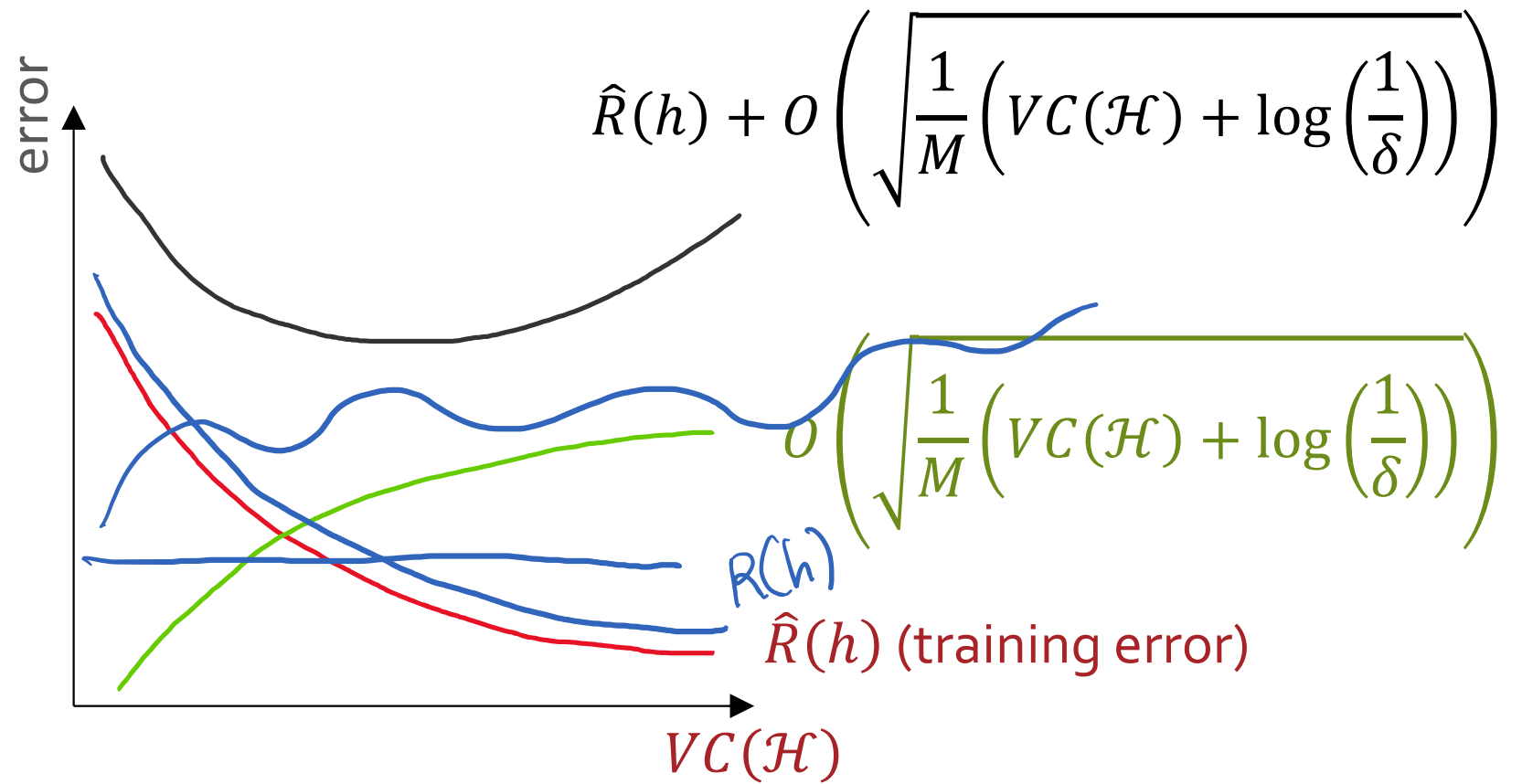
Can we use
this corollary to
guide model
selection?

- Infinite, agnostic case: for any hypothesis set \mathcal{H} and arbitrary distribution p^* , given a training dataset S where $|S| = M$, all $h \in \mathcal{H}$ have

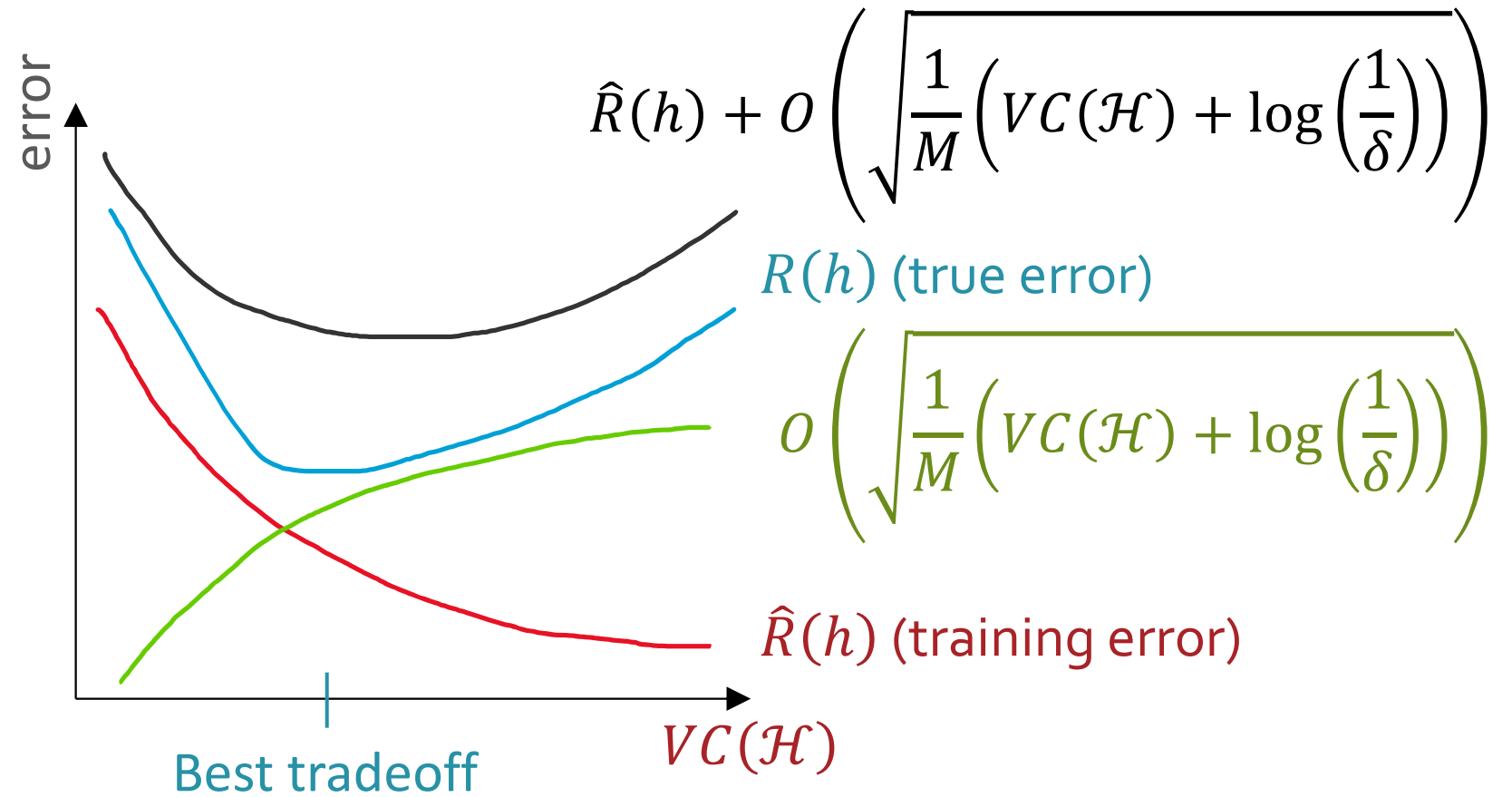
$$R(h) \leq \hat{R}(h) + O\left(\sqrt{\frac{1}{M} \left(VC(\mathcal{H}) + \log\left(\frac{1}{\delta}\right)\right)}\right)$$

with probability at least $1 - \delta$.

Learning Theory and Model Selection



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...

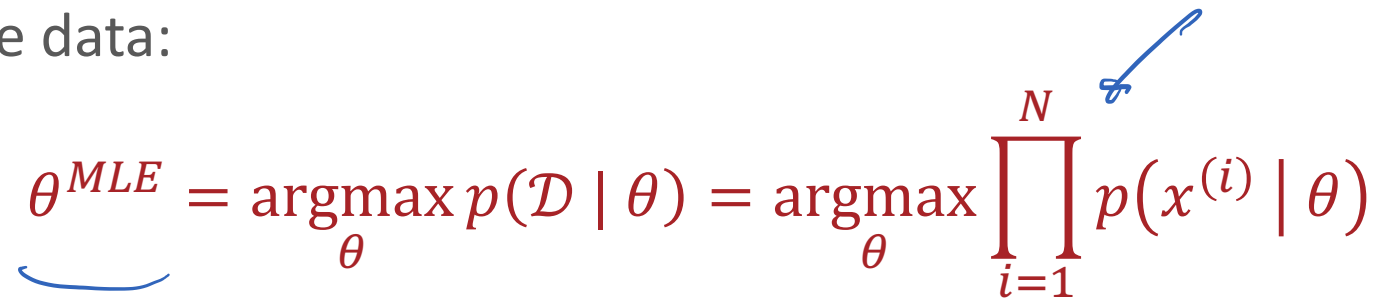
- Identify the properties of a learning setting and assumptions required to ensure low generalization error
- Distinguish true error, train error, test error
- Define PAC and explain what it means to be approximately correct and what occurs with high probability
- Apply sample complexity bounds to real-world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

Recall: Probabilistic Learning

- Previously:
 - (Unknown) Target function, $c^*: \mathcal{X} \rightarrow \mathcal{Y}$
 - Classifier, $h: \mathcal{X} \rightarrow \mathcal{Y}$
 - 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)

- Given independent, identically distributed observations (iid) $\mathcal{D} = \{x^{(i)}\}_{i=1}^N$ from a parametrized probability distribution, MLE sets the parameters by maximizing the likelihood of the data:

$$\theta^{MLE} = \underset{\theta}{\operatorname{argmax}} p(\mathcal{D} | \theta) = \underset{\theta}{\operatorname{argmax}} \prod_{i=1}^N p(x^{(i)} | \theta)$$


- Intuition: assign as much of the (finite) probability mass to the observed data *at the expense of unobserved data*

Recall: Maximum Likelihood Estimation (MLE)

- Given independent, identically distributed observations (iid) $\mathcal{D} = \{x^{(i)}\}_{i=1}^N$ from a parametrized probability distribution, MLE sets the parameters by maximizing the *log*-likelihood of the data:

$$\theta^{MLE} = \operatorname{argmax}_{\theta} \log p(\mathcal{D} | \theta) = \operatorname{argmax}_{\theta} \underbrace{\sum_{i=1}^N \log p(x^{(i)} | \theta)}$$

- Intuition: assign as much of the (finite) probability mass to the observed data *at the expense of unobserved data*

Bernoulli Distribution MLE

- A Bernoulli random variable takes value **1** with probability ϕ and value **0** with probability $1 - \phi$

- The pmf of the Bernoulli distribution is

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

Coin Flipping MLE

$$\log(a^b) = b \log a$$

- A Bernoulli random variable takes value **1** (or heads) with probability ϕ and value **0** (or tails) with probability $1 - \phi$
- The pmf of the Bernoulli distribution is
$$\rightarrow p(x|\phi) = \phi^x (1 - \phi)^{1-x}$$
- Given N iid samples $\{x^{(1)}, \dots, x^{(N)}\}$, the log-likelihood is

$$\begin{aligned} l(\phi) &= \sum_{i=1}^N \log(\phi^{x^{(i)}} (1-\phi)^{1-x^{(i)}}) \\ &= \sum_{i=1}^N x^{(i)} \log \phi + (1-x^{(i)}) \log(1-\phi) \\ &= \sum_{i=1}^N x^{(i)} \log \phi + \sum_{i=1}^N (1-x^{(i)}) \log(1-\phi) \\ &\rightarrow N_1 \log \phi + N_0 \log(1-\phi) \\ &\text{where } N_i = \# \text{ of } i\text{'s in } \mathcal{D} \end{aligned}$$

Coin Flipping MLE

- A Bernoulli random variable takes value **1** (or heads) with probability ϕ and value **0** (or tails) with probability $1 - \phi$
- The pmf of the Bernoulli distribution is

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

- The partial derivative of the log-likelihood is

$$\ell(\phi) = N_1 \log \phi + N_0 \log (1 - \phi)$$

$$\frac{\partial \ell}{\partial \phi} = \frac{N_1}{\phi} + \frac{N_0}{1 - \phi} (-1)$$

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

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

$$\Rightarrow \hat{\phi} = N_1 / (N_0 + N_1) \quad 59$$

Poll Question 2:

After flipping your coin 5 times, what is the MLE of your coin?

- A. 0/5
- B. 1/5
- C. 2/5
- D. 3/5
- E. $\pi/5$ (TOXIC)
- F. 4/5
- G. 5/5

- A Bernoulli random variable takes value **1** (or heads) with probability ϕ and value **0** (or tails) with probability $1 - \phi$

- 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

Maximum a Posteriori (MAP) Estimation

- Insight: sometimes we have *prior* information we want to incorporate into parameter estimation
- Idea: use Bayes rule to reason about the *posterior* distribution over the parameters

$$\begin{aligned} \text{MLE finds } \hat{\theta} &= \operatorname{argmax}_{\theta} P(D|\theta) \\ \text{MAP finds } \hat{\theta} &= \operatorname{argmax}_{\theta} P(\theta|D) \\ &= \operatorname{argmax}_{\theta} \frac{P(D|\theta)P(\theta)}{\rightarrow P(D)} \\ &\Rightarrow \operatorname{argmax}_{\theta} \underbrace{P(D|\theta)}_{\text{likelihood}} \underbrace{P(\theta)}_{\text{prior}} \end{aligned}$$

Maximum a Posteriori (MAP) Estimation

1. Specify the *generative story*, i.e., the data generating distribution, including a *prior distribution*

2. Maximize the log-posterior of $\mathcal{D} = \{x^{(1)}, \dots, x^{(N)}\}$

$$\ell_{MAP}(\theta) = \log p(\theta) + \sum_{i=1}^N \log p(x^{(i)} | \theta)$$

3. Solve in *closed form*: take partial derivatives, set to 0 and solve