Learning Theory

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Lectures 14 and 15

Generalization

Suppose a learning algorithm returns a hypothesis with low training error.

When can we guarantee that the hypothesis's true error is also low?

Main question: How can we use the training error of a learning algorithm to estimate the algorithm's true error?

Generalization

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We will focus on *binary classification*

Recall:

Training error: $\hat{R}(\hat{h}, D) = \frac{1}{n} \sum_{i=1}^{n} 1 \left[\hat{h}(X_i) \neq Y_i \right]$

True error: (Risk)

$$R(\hat{h}) = \mathrm{E}_{(X,Y)\sim P} \left[1 \left[\hat{h}(X) \neq Y \right] \right]$$
$$= \Pr_{(X,Y)\sim P} \left(\hat{h}(X) \neq Y \right)$$

Realizable setting

Suppose that each example is in input space $\mathcal{X}$

In the *realizable setting*:

There is a known *concept class* $\mathcal{C}$, a set of concepts, where each concept c is a rule mapping from $\mathcal{X}$ to $\{0, 1\}$

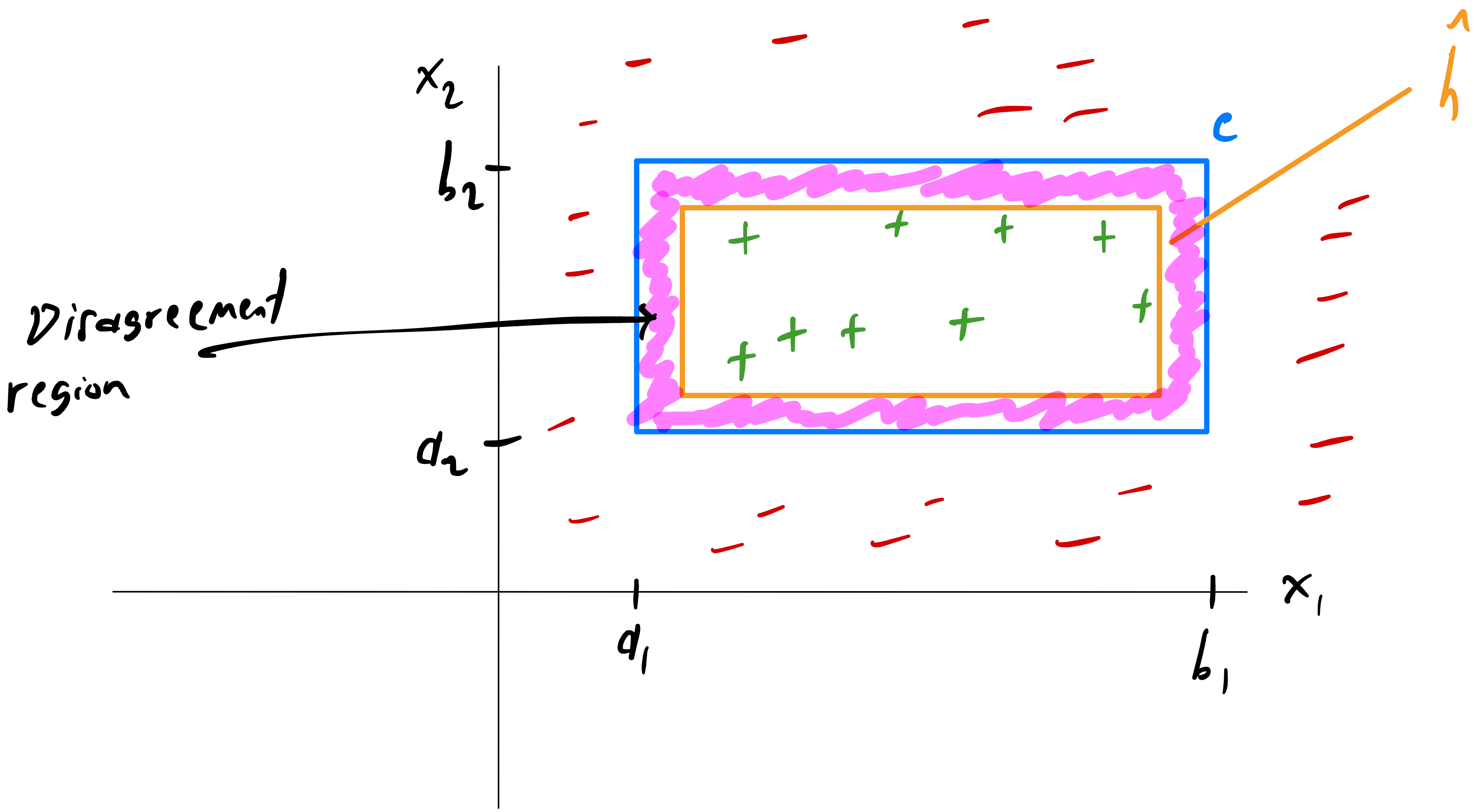
There is a concept $c \in \mathcal{C}$ such that, for any input X, the label is $Y = c(X)$

Given training data, learning algorithm selects hypothesis $\hat{h} \in \mathcal{H}$

$$\underbrace{((x_1, y_1), \ldots, (x_n, y_n))}_{D} \longrightarrow \underset{\text{algorithm}}{\boxed{\mathcal{A}}} \longrightarrow \mathcal{A}(D) = \hat{h}$$

Realizable setting: Example 1

Learning rectangles $\mathcal{X} = \mathbb{R}^2$



$R(\hat{h})$

$= P_r(X \in$ disagreement region $)$

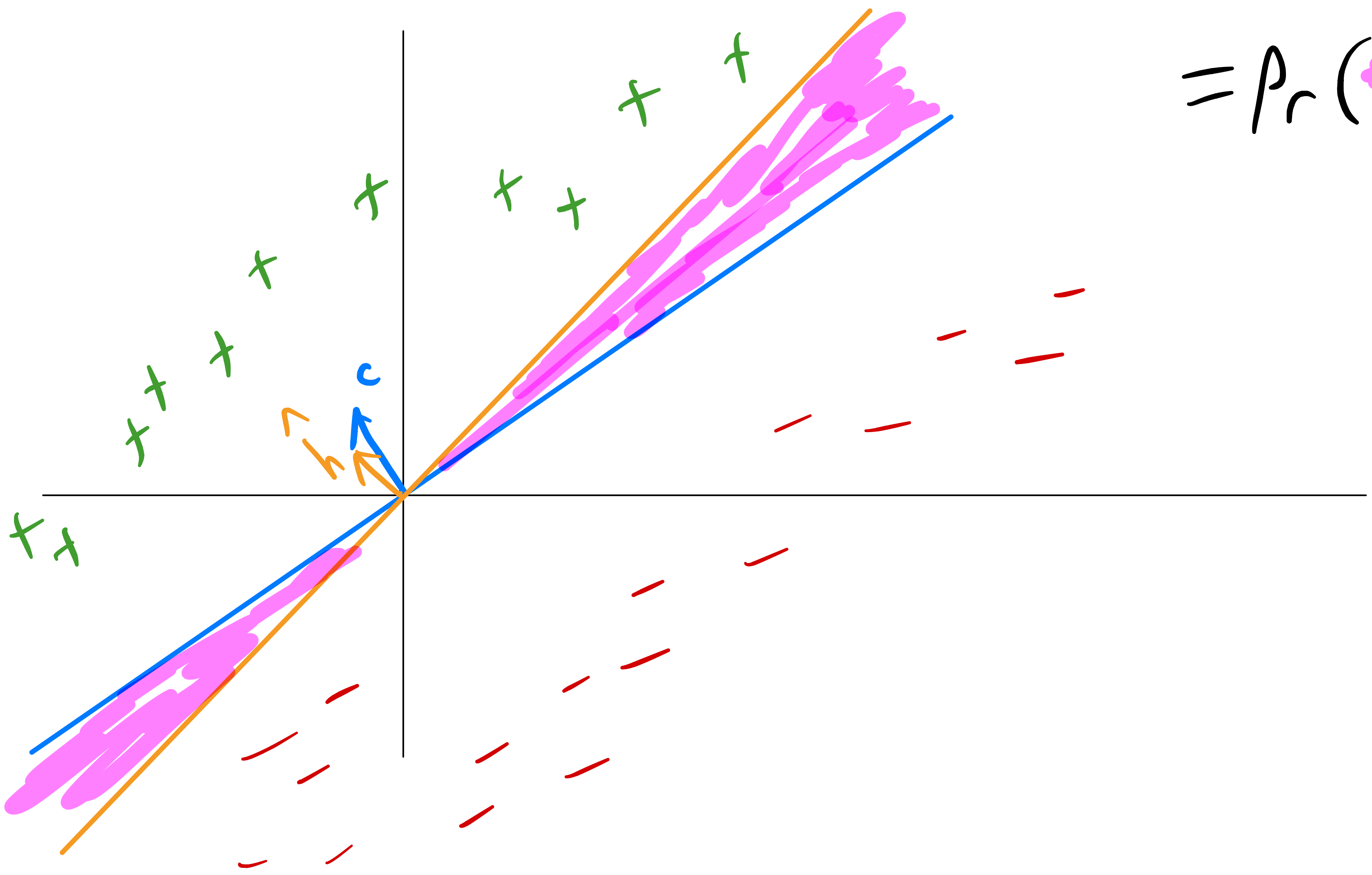
$$c(x) = \mathbb{1}[a_1 \le x_1 \le b_1] \cdot \mathbb{1}[a_2 \le x_2 \le b_2]$$

Realizable setting: Example 2

Homogeneous linear separators in $\mathbb{R}^2$

$R(\hat{h})$

$= Pr($ $)$



Back to generalization

In the realizable setting, we have:

Training error: $\hat{R}(\hat{h}, D) = \frac{1}{n} \sum_{i=1}^{n} 1\left[\hat{h}(X_i) \neq c(X_i)\right]$

Risk: $R(\hat{h}) = \Pr_{X \sim P}\left(\hat{h}(X) \neq c(X)\right)$

Main question:

How can we use training error $\hat{R}(\hat{h}, D)$ to upper bound risk $R(\hat{h})$, ***no matter what distribution the data comes from?***

A bad learning algorithm

memorization algorithm

$$\hat{h}(x) = \begin{cases} y_i & \text{if } \exists\, i \in [n] \;\; x = x_i \\ 0 & \text{otherwise} \end{cases}$$

$$R(\hat{h}) = \Pr_{(x,y)\sim P}(y = 1)$$

Can we guarantee zero risk?

What type of guarantee can we hope to achieve?

What if we try to seek a hypothesis which gets zero risk? Is this possible?

No!

Example: linear separators

But we will try to guarantee

that $n \to \infty$, $R(\hat{h}) \to 0$

PAC Learning

A *Probably approximately correct (PAC) guarantee* is one of the form:

Suppose a learning algorithm outputs a hypothesis $\hat{h}$.

[Then with probability at least $1 - \delta$ (over the training sample),] "Probably"

[the risk $R(\hat{h})$ is at most ε.]

"Approximately correct"

Towards achieving a PAC guarantee

In the realizable setting, we assume $\mathcal{C}$ contains a perfect classifier.

So, let's ensure that any hypothesis we select is consistent with the training sample.

We say that hypothesis $h \in \mathcal{H}$ is *consistent* (with training sample ***D***) if it correctly classifies all the training examples, so $\hat{R}(h, D) = 0$

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Version space: $\hat{V} = \left\{ h \in \mathcal{H} : \hat{R}(h, D) = 0 \right\}$

(set of hypotheses in $\mathcal{H}$ that are consistent with the training sample)

A PAC guarantee

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<u>Theorem</u>

If $|\mathcal{H}| < \infty$, the probability that there is a hypothesis $h \in \hat{V}$ with risk $\underbrace{R(h) > \varepsilon}_{\text{“}\varepsilon\text{-bad”}}$ is at most $|\mathcal{H}| e^{-n\varepsilon}$.

$n = 1000$

$\mathcal{H}$ is a set of recognizers for some virus

$|\mathcal{H}| = 100$

$\varepsilon = 2\% = 0.02$

$100 \cdot e^{-20} \approx 0$

A PAC guarantee

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(set of hypotheses in $\mathcal{H}$ that are consistent with the training sample)

<u>Theorem</u>

If $|\mathcal{H}| < \infty$, the probability that there is a hypothesis $h \in \hat{V}$ with risk $R(h) > \varepsilon$ is at most $|\mathcal{H}| e^{-n\varepsilon}$. $= \delta$

<u>Inversion</u>

$|\mathcal{H}| e^{-n\varepsilon} = \delta$

$\Leftrightarrow \frac{|\mathcal{H}|}{\delta} = e^{n\varepsilon} \Leftrightarrow \frac{\log|\mathcal{H}| + \log\frac{1}{\delta}}{n} = \cancel{n}\varepsilon$

w.p. at least $1-\delta$, all hypotheses h with $R(h) > \varepsilon$ satisfy $\hat{R}(h, D) > 0$.

Proof

Lemma

Let $h \in \mathcal{H}$ be fixed hypothesis s.t. $R(h) > \varepsilon$.

n examples

$$\Pr(\hat{R}(h, D) = 0) \le (1-\varepsilon)^n \le e^{-n\varepsilon}$$

$$1 - x \le e^{-x}$$

Proof

Let $M_i = \begin{cases} 1 & \text{if } h(x_i) \ne y_i \\ 0 & \text{if } h(x_i) = y_i \end{cases}$

$$\Pr(M_i = 1) = R(h)$$

Bernoulli$(R(h))$

$$\Pr(\hat{R}(h, D) = 0) = \Pr(M_1 = 0, M_2 = 0, \dots, M_n = 0)$$

$$= \prod_{i=1}^{n} \Pr(M_i = 0)$$

$$= (1 - R(h))^n$$

$$< (1 - \varepsilon)^n$$

Proof of Theorem

$$\Pr\left(\exists h \in \mathcal{H} : \hat{R}(h, D) = 0 \text{ and } R(h) > \varepsilon\right)$$

$$= \Pr\left(\bigcup_{h \in \mathcal{H}} \{(x_1, \dots, x_n) \in \mathcal{X}^n : \hat{R}(h, D) = 0 \text{ and } R(h) > \varepsilon\}\right)$$

$$\leq \sum_{h \in \mathcal{H}} \Pr\left(\hat{R}(h, D) = 0 \text{ and } R(h) > \varepsilon\right)$$

$$= \sum_{\substack{h \in \mathcal{H} \\ h : R(h) > \varepsilon}} \underbrace{\Pr\left(\hat{R}(h, D) = 0\right)}_{\leq e^{-n\varepsilon}}$$

$$\leq |\mathcal{H}| e^{-n\varepsilon}$$

PAC Learnability

We say that $\mathcal{C}$ is *PAC learnable* if there exists an algorithm $\mathcal{A}$ which, for all concepts $c \in \mathcal{C}$, for all distributions P over an input space $\mathcal{X}$ of dimension d, and for all $\varepsilon > 0$ and $\delta \in (0, 1)$, satisfies:

> If $\mathcal{A}$ is given access to examples drawn from P and labeled according to c, then with probability at least $1 - \delta$, we have that the risk $\Pr\big(\hat{h}(X) \neq c(X)\big) \leq \varepsilon$.

We say $\mathcal{C}$ is *efficiently PAC learnable* if, in addition, $\mathcal{A}$ uses a number of examples polynomial in d, $1/\varepsilon$, and $1/\delta$.

Agnostic Learning

joint distribution over labeled examples (X, Y)

Assume $(X_1, Y_1), \ldots, (X_n, Y_n) \overset{\text{iid}}{\sim} P$

What if no hypothesis in $\mathcal{H}$ has zero risk?

What if no hypotheses (among all rules!) have zero risk?

Let's give up on learning $h \in \mathcal{H}$ with zero training error.

Instead, try to show that $R(h)$ isn't much larger than $\hat{R}(h, D)$

risk

empirical risk

Bounding the risk for a fixed hypothesis h

Hoeffding's inequality

Let $Z, Z_1, Z_2, \ldots, Z_n \overset{\text{iid}}{\sim} P$, where $\begin{array}{l} 0 \leq Z \leq 1 \\ 0 \leq Z_i \leq 1 \text{ for } i = 1, \ldots, n \end{array}$

Then $$\Pr\left(\underbrace{\mathbb{E}[Z]}_{R(h)} \geq \underbrace{\frac{1}{n}\sum_{i=1}^{n} Z_i}_{\hat{R}(h,D)} + \varepsilon\right) \leq e^{-2n\varepsilon^2}$$

Lemma. Let h be a fixed hypothesis. Then

$$\Pr\left(R(h) \geq \hat{R}(h, D) + \varepsilon\right) \leq e^{-2n\varepsilon^2}$$

set $= \delta$ and solve for ε

Equivalently, with probability at least $1 - \delta$

$$R(h) \leq \hat{R}(h, D) + \sqrt{\frac{\log \frac{1}{\delta}}{2n}}$$

$Z = \begin{cases} 1 & \text{if } h(X) \neq Y \\ 0 & \text{o.w} \end{cases}$

$Z_i = \begin{cases} 1 & \text{if } h(X_i) \neq Y_i \\ 0 & \text{o.w.} \end{cases}$

$\mathbb{E}[Z] = R(h)$

Bounding the risk of $\hat{h}$ selected from finite class $\mathcal{H}$

Suppose, given training data $(X_1, Y_1), \ldots, (X_n, Y_n) \overset{\text{iid}}{\sim} P$,

we learn a rule $\hat{h} \in \mathcal{H}$.

Then with probability at least $1 - \delta$,

$$R(\hat{h}) \leq \hat{R}(\hat{h}, D) + \sqrt{\frac{\log |\mathcal{H}| + \log \frac{1}{\delta}}{2n}}$$

Effective size

When $|\mathcal{H}|$ is finite, our notion of size was $|\mathcal{H}|$

What if $|\mathcal{H}|$ is infinite?

New measure of the size of $\mathcal{H}$: "effective size of $\mathcal{H}$"

Effective size of $\mathcal{H}$ relative to training sample $S = \underbrace{(x_1, x_2, \dots, x_n)}_{\text{unlabeled sample}}$ is defined as:

$$|\mathcal{H}_{|S}| = \left| \left\{ h \in \mathcal{H} : \begin{pmatrix} h(X_1) \\ h(X_2) \\ \dots \\ h(X_n) \end{pmatrix} \right\} \right|$$

# of distinct ways we can label sample S using hypotheses in $\mathcal{H}$

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Example

	h_1	h_2	h_3	h_4	h_5
x_1	1	1	1	1	0
x_2	0	0	0	0	0
x_3	0	1	1	0	1

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Example

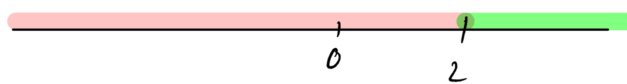
	h_1	h_2	h_3	h_4	h_5
x_1	1	1	1	1	0
x_2	0	0	0	0	0
x_3	0	1	1	0	1

effective size = 3

$|\mathcal{H}_{|S}|$ = "# of distinct ways that we can label S (label $x_1, x_2, \dots, x_n$) using hypotheses in $\mathcal{H}$"

Example (threshold functions)

$\mathcal{X} = \mathbb{R}$ $\quad \mathcal{H} = \{h_t : t \in \mathbb{R}\}$ $\quad h_t(x) = \begin{cases} 1 & \text{if } x \ge t \\ 0 & \text{if } x < t \end{cases}$



$h_2(x)$

For any sample of size n,

$|\mathcal{H}_{|S}| \le n+1$

5 different labelings

+	+	+	+	← very negative t
−	−	−	−	← very positive t
−	+	+	+	
−	−	+	+	
−	−	−	+	

In general, how can we upper bound $|\mathcal{H}_{|S}|$ — "effective size of $\mathcal{H}$ W.R.T. S

^ examples"

Key Tool: VC dimension

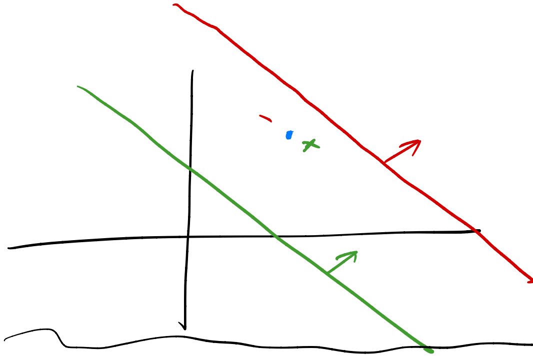
Definition: Shattering

finite unlabeled training sample ($|S| = k$)

We say that $\mathcal{H}$ shatters a set $S \subseteq \mathcal{X}$ if, for every possible labeling of S (2^k of these!), there is $h \in \mathcal{H}$ that is consistent with labeling.

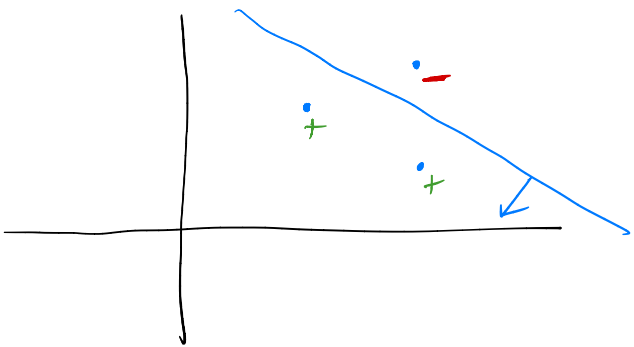
(implication: $|\mathcal{H}_{|S}| = 2^k$)

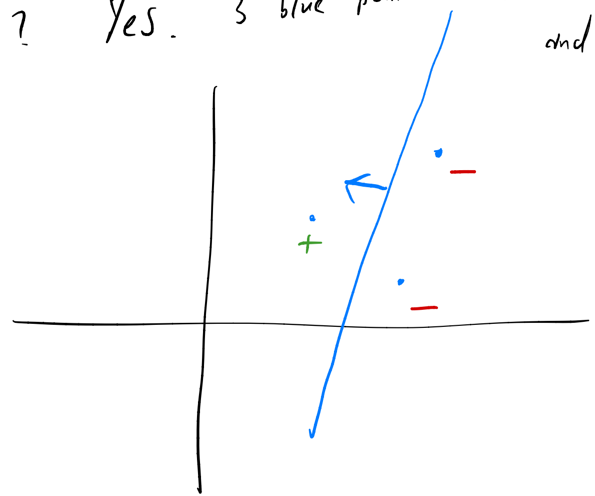
Example (Linear separators in $\mathbb{R}^2$) $\leftarrow \mathcal{H}$



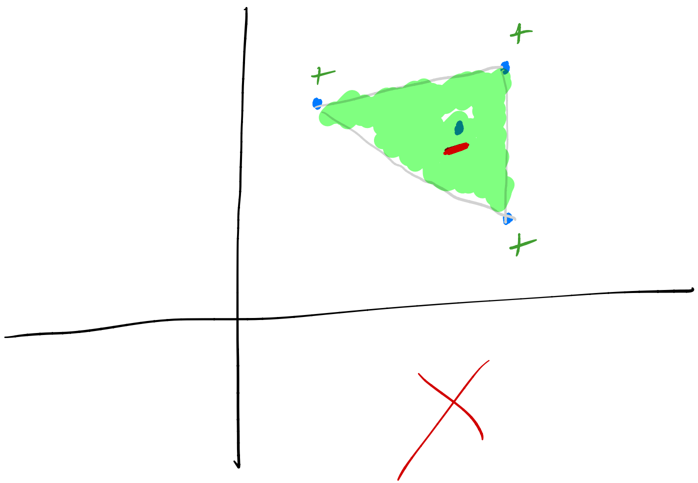
we can shatter an S with one example

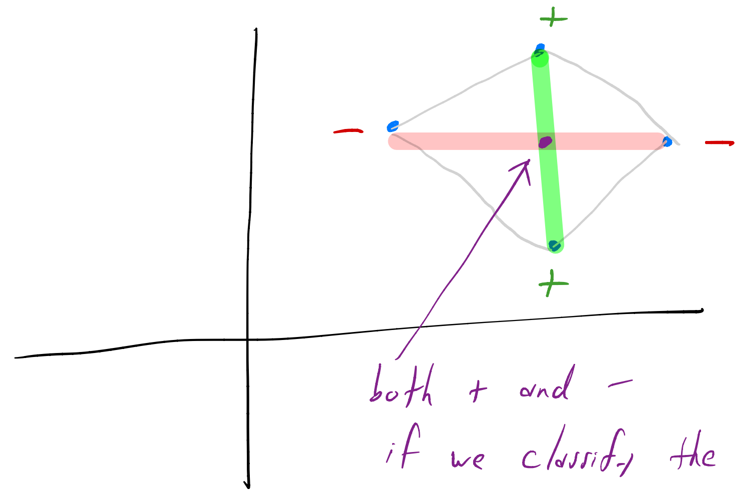
Can we shatter some S with 3 examples? Yes. 3 blue points represent a set s.t. $|S|=3$ and $\mathcal{H}$ shatters S.





Question: Does there exist S with $|S|=4$ s.t. $\mathcal{H}$ shatters S? No!





The largest S that we can shatter is of cardinality 3.

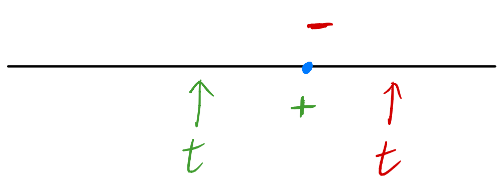
Definition (Vapnik – Chervonenkis Dimension) (V–C)

The VC dimension of $\mathcal{H}$, $VC(\mathcal{H})$, is the cardinality of the largest finite $S \subseteq \mathcal{X}$ that is shattered by $\mathcal{H}$.

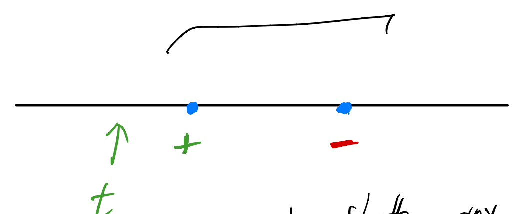
If $\mathcal{H}$ can shatter arbitrarily large sets S, then $VC(\mathcal{H}) = \infty$

Example (Threshold functions)

can shatter an S with $|S|=1$



we cannot achieve this labeling



cannot shatter any S with $|S|=2$

$\Downarrow$

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

Bounding the risk when $\mathcal{H}$ has finite VC dimension

Suppose, given training data $(X_1, Y_1), \ldots, (X_n, Y_n) \stackrel{\text{iid}}{\sim} P$,

we learn a rule $\hat{h} \in \mathcal{H}$.

Then with probability at least $1 - \delta$,

$$R(\hat{h}) \leq \hat{R}(\hat{h}, D) + O\left(\sqrt{\frac{\mathrm{VC}(H) + \log\frac{1}{\delta}}{n}}\right)$$