LEARNING THEORY

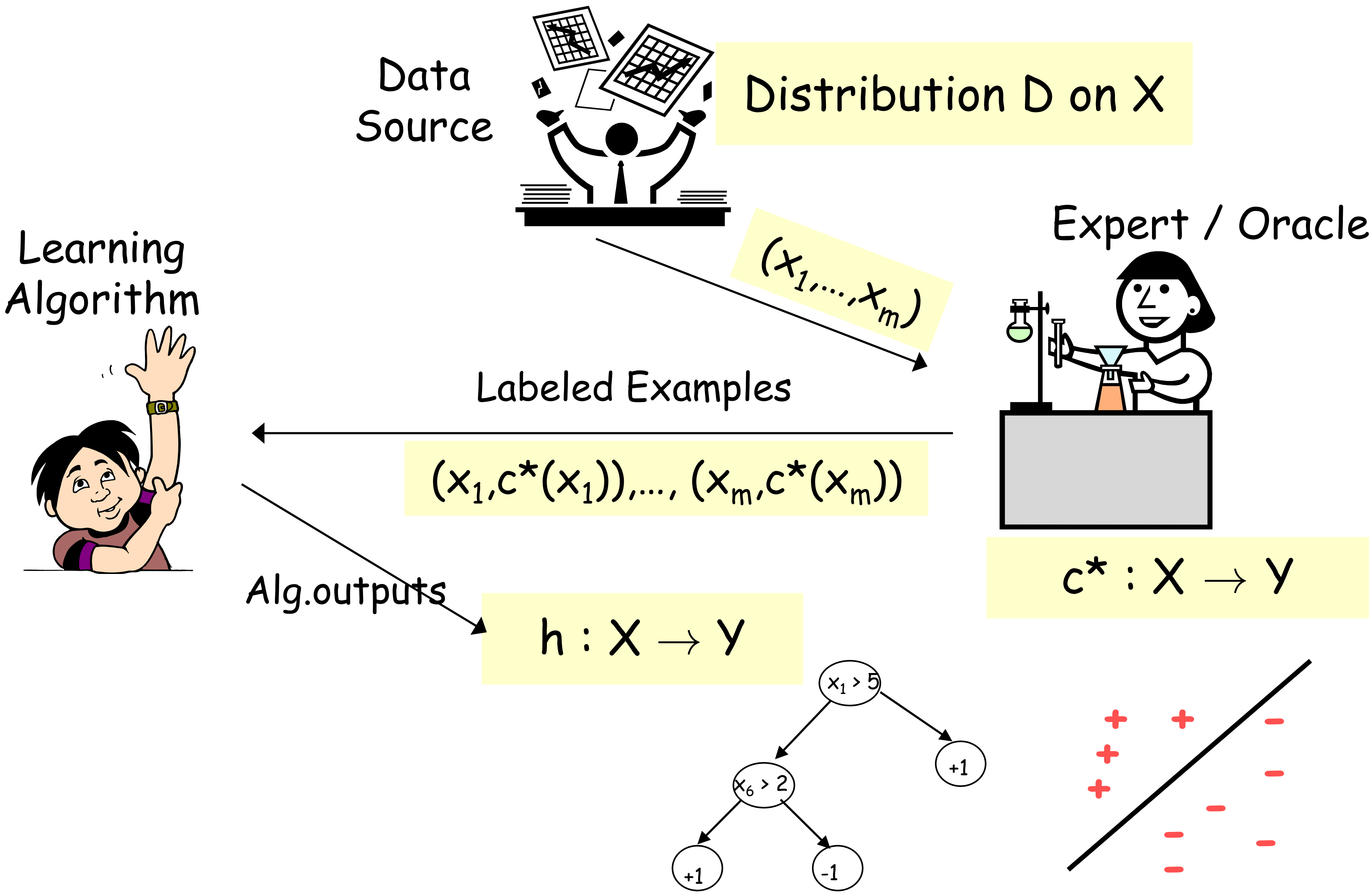
Questions For Today

1. Given a classifier with zero training error, what can we say about generalization error?
(Sample Complexity, Realizable Case)

2. Given a classifier with low training error, what can we say about generalization error?
(Sample Complexity, Agnostic Case)

3. Is there a theoretical justification for regularization to avoid overfitting?
(Structural Risk Minimization)

PAC/SLT models for Supervised Learning



Slide from Nina Balcan

Two Types of Error

True Error (aka. **expected risk**)

$$R(h) = P_{\mathbf{x} \sim p^*(\mathbf{x})}(c^*(\mathbf{x}) \neq h(\mathbf{x}))$$

This quantity is always **unknown**

Train Error (aka. **empirical risk**)

$$\hat{R}(h) = P_{\mathbf{x} \sim \mathcal{S}}(c^*(\mathbf{x}) \neq h(\mathbf{x}))$$

$$= \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}(c^*(\mathbf{x}^{(i)}) \neq h(\mathbf{x}^{(i)}))$$

$$= \frac{1}{N} \sum_{i=1}^{N} \mathbb{1}(y^{(i)} \neq h(\mathbf{x}^{(i)}))$$

We can **measure** this on the training data

where $\mathcal{S} = \{\mathbf{x}^{(1)}, \ldots, \mathbf{x}^{(N)})\}_{i=1}^{N}$ is the training data set, and $\mathbf{x} \sim \mathcal{S}$ denotes that $\mathbf{x}$ is sampled from the empirical distribution.

PAC / SLT Model

We've also referred to this as the "Function Approximation View"

1. Generate instances from *unknown* distribution p^*

$$\mathbf{x}^{(i)} \sim p^*(\mathbf{x}), \ \forall i \tag{1}$$

2. Oracle labels each instance with *unknown* function c^*

$$y^{(i)} = c^*(\mathbf{x}^{(i)}), \ \forall i \tag{2}$$

3. Learning algorithm chooses hypothesis $h \in \mathcal{H}$ with low(est) training error, $\hat{R}(h)$

$$\hat{h} = \underset{h}{\text{argmin}} \, \hat{R}(h) \tag{3}$$

4. Goal: Choose an h with low generalization error $R(h)$

Three Hypotheses of Interest

The **true function** c^* is the one we are trying to learn and that labeled the training data:

$$y^{(i)} = c^*(\mathbf{x}^{(i)}), \; \forall i \tag{1}$$

The **expected risk minimizer** has lowest true error:

$$h^* = \operatorname*{argmin}_{h \in \mathcal{H}} R(h) \tag{2}$$

The **empirical risk minimizer** has lowest training error:

$$\hat{h} = \operatorname*{argmin}_{h \in \mathcal{H}} \hat{R}(h) \tag{3}$$

PAC LEARNING

Probably Approximately Correct (PAC) Learning

Whiteboard:

- PAC Criterion
- Meaning of "Probably Approximately Correct"
- PAC Learnable
- Consistent Learner
- Sample Complexity

Generalization and Overfitting

Whiteboard:

- Realizable vs. Agnostic Cases
- Finite vs. Infinite Hypothesis Spaces

PAC Learning

The **PAC criterion** is that our learner produces a high accuracy learner with high probability:

$$P(|R(h) - \hat{R}(h)| \leq \epsilon) \geq 1 - \delta \tag{1}$$

Suppose we have a learner that produces a hypothesis $h \in \mathcal{H}$ given a sample of N training examples. The algorithm is called **consistent** if for every ϵ and δ, there exists a positive number of training examples N such that for any distribution p^*, we have that:

$$P(|R(h) - \hat{R}(h)| > \epsilon) < \delta \tag{2}$$

The **sample complexity** is the minimum value of N for which this statement holds. If N is finite for some learning algorithm, then $\mathcal{H}$ is said to be **learnable.** If N is a polynomial function of $\frac{1}{\epsilon}$ and $\frac{1}{\delta}$ for some learning algorithm, then $\mathcal{H}$ is said to be **PAC learnable.**

SAMPLE COMPLEXITY RESULTS

Sample Complexity Results

Definition 0.1. The **sample complexity** of a learning algorithm is the number of examples required to achieve arbitrarily small error (with respect to the optimal hypothesis) with high probability (i.e. close to 1).

Four Cases we care about…

We'll start with the finite case…

	Realizable	Agnostic
Finite $\vert\mathcal{H}\vert$		
Infinite $\vert\mathcal{H}\vert$		

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Four Cases we care about…

	Realizable	Agnostic
Finite $\|\mathcal{H}\|$	$N \geq \frac{1}{\epsilon}\left[\log(\|\mathcal{H}\|) + \log(\frac{1}{\delta})\right]$ labeled examples are sufficient so that with probability $(1-\delta)$ all $h \in \mathcal{H}$ with $R(h) \geq \epsilon$ have $\hat{R}(h) > 0$.	
Infinite $\|\mathcal{H}\|$		

Example: Conjunctions

In-Class Quiz:

Suppose H = class of conjunctions over **x** in $\{0,1\}^M$

If M = 10, ε = 0.1, δ = 0.01, how many examples suffice?

	Realizable	Agnostic
Finite $\|\mathcal{H}\|$	$N \geq \frac{1}{\epsilon}\left[\log(\|\mathcal{H}\|) + \log(\frac{1}{\delta})\right]$ labeled examples are sufficient so that with probability $(1-\delta)$ all $h \in \mathcal{H}$ with $R(h) \geq \epsilon$ have $\hat{R}(h) > 0$.	
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Infinite $\|\mathcal{H}\|$		

1. Bound is **inversely linear in epsilon** (e.g. halving the error requires double the examples)
2. Bound is **only logarithmic in |H|** (e.g. quadrupling the hypothesis space only requires double the examples)

1. Bound is **inversely quadratic in epsilon** (e.g. halving the error requires 4x the examples)
2. Bound is **only logarithmic in |H|** (i.e. same as Realizable case)

	Realizable	Agnostic
Finite $\|\mathcal{H}\|$	$N \geq \frac{1}{\epsilon}\left[\log(\|\mathcal{H}\|) + \log(\frac{1}{\delta})\right]$ labeled examples are sufficient so that with probability $(1-\delta)$ all $h \in \mathcal{H}$ with $R(h) \geq \epsilon$ have $\hat{R}(h) > 0$.	$N \geq \frac{1}{2\epsilon^2}\left[\log(\|\mathcal{H}\|) + \log(\frac{2}{\delta})\right]$ labeled examples are sufficient so that with probability $(1-\delta)$ for all $h \in \mathcal{H}$ we have that $\|R(h) - \hat{R}(h)\| < \epsilon$.
Infinite $\|\mathcal{H}\|$		

Generalization and Overfitting

Whiteboard:

- Sample Complexity Bounds (Agnostic Case)
- Corollary (Agnostic Case)
- Empirical Risk Minimization
- Structural Risk Minimization
- Motivation for Regularization

Sample Complexity Results

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Four Cases we care about…

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Finite $\lvert\mathcal{H}\rvert$	$N \geq \frac{1}{\epsilon}\left[\log(\lvert\mathcal{H}\rvert) + \log(\frac{1}{\delta})\right]$ labeled examples are sufficient so that with prob- ability $(1-\delta)$ all $h \in \mathcal{H}$ with have $\hat{R}(h) > 0$.	$N \geq \frac{1}{2\epsilon^2}\left[\log(\lvert\mathcal{H}\rvert) + \log(\frac{2}{\delta})\right]$ la- beled examples are sufficient so $-\ \delta)$ for t $\lvert R(h) -$
Infinite $\lvert\mathcal{H}\rvert$		

We need a new definition of "complexity" for a Hypothesis space for these results (see *VC Dimension*)

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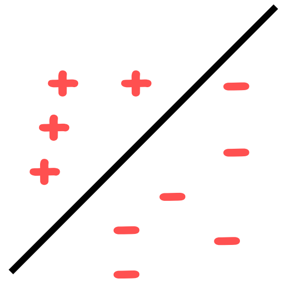
Infinite $\lvert\mathcal{H}\rvert$	$N = O(\frac{1}{\epsilon}\left[\text{VC}(\mathcal{H})\log(\frac{1}{\epsilon}) + \log(\frac{1}{\delta})\right])$ labeled examples are sufficient so that with probability $(1-\delta)$ all $h \in \mathcal{H}$ with $R(h) \geq \epsilon$ have $\hat{R}(h) > 0$.	$N = O(\frac{1}{\epsilon^2}\left[\text{VC}(\mathcal{H}) + \log(\frac{1}{\delta})\right])$ labeled examples are sufficient so that with probability $(1-\delta)$ for all $h \in \mathcal{H}$ we have that $\lvert R(h) - \hat{R}(h)\rvert \leq \epsilon$.

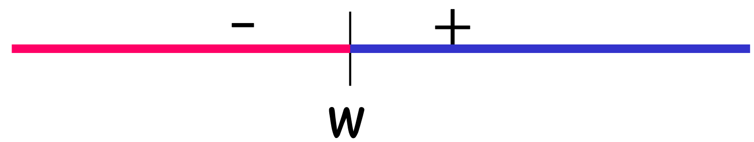
VC DIMENSION

What if H is infinite?

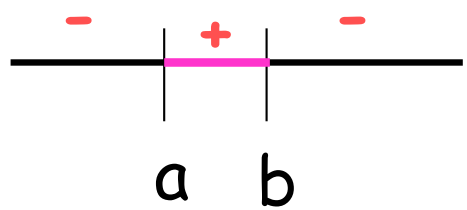
E.g., linear separators in R^d



E.g., thresholds on the real line



E.g., intervals on the real line



Shattering, VC-dimension

Definition:

H[S] – the set of splittings of dataset S using concepts from H.

H shatters S if $|\mathrm{H[S]}| = 2^{|S|}$.

A set of points S is shattered by H is there are hypotheses in H that split S in all of the $2^{|S|}$ possible ways; i.e., all possible ways of classifying points in S are achievable using concepts in H.

Definition: VC-dimension (Vapnik-Chervonenkis dimension)

The VC-dimension of a hypothesis space H is the cardinality of the largest set S that can be shattered by H.

If arbitrarily large finite sets can be shattered by H, then $\mathrm{VCdim(H)} = \infty$

Slide from Nina Balcan

Shattering, VC-dimension

Definition: VC-dimension (Vapnik-Chervonenkis dimension)

The VC-dimension of a hypothesis space H is the cardinality of the largest set S that can be shattered by H.

If arbitrarily large finite sets can be shattered by H, then $\mathrm{VCdim}(H) = \infty$

To show that VC-dimension is d:

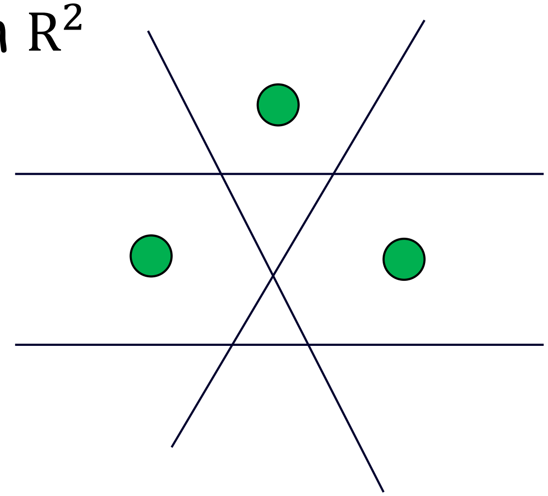
- there exists a set of d points that can be shattered
- there is no set of d+1 points that can be shattered.

Fact: If H is finite, then $\mathrm{VCdim}(H) \leq \log(|H|)$.

Shattering, VC-dimension

E.g., **H=** linear separators in R^2

$\mathrm{VCdim(H)} \geq 3$

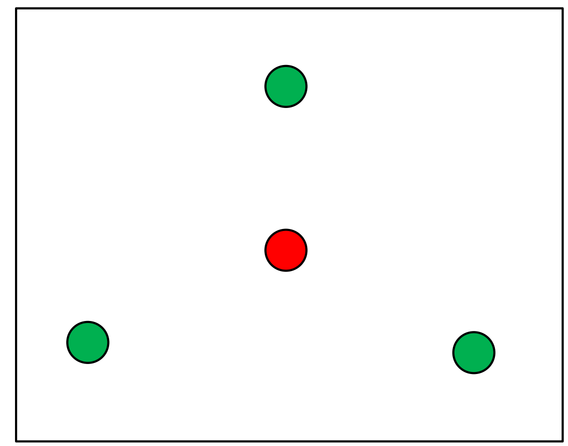


Shattering, VC-dimension

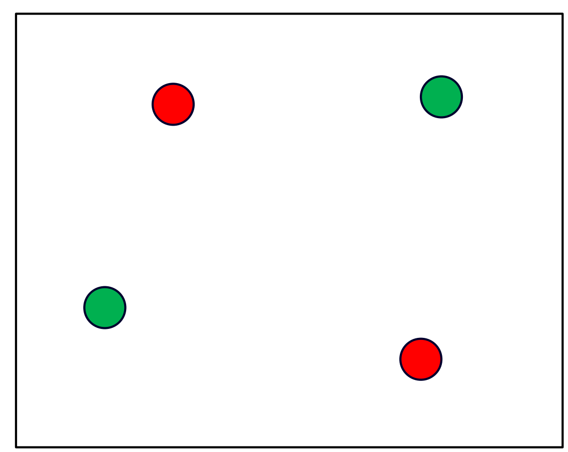
E.g., **H=** linear separators in R^2

$\mathrm{VCdim(H)} < 4$

Case 1: one point inside the triangle formed by the others. Cannot label inside point as positive and outside points as negative.



Case 2: all points on the boundary (convex hull). Cannot label two diagonally as positive and other two as negative.



Fact: VCdim of linear separators in R^d is d+1

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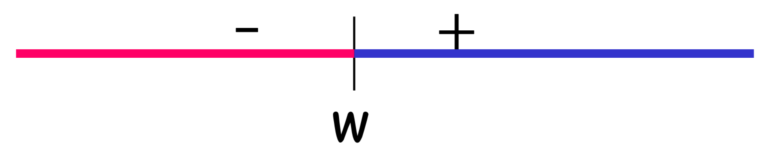
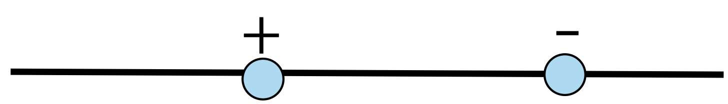
Shattering, VC-dimension

If the VC-dimension is d, that means there exists a set of d points that can be shattered, but there is no set of d+1 points that can be shattered.

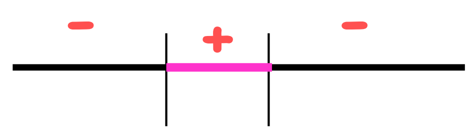
E.g., H= Thresholds on the real line



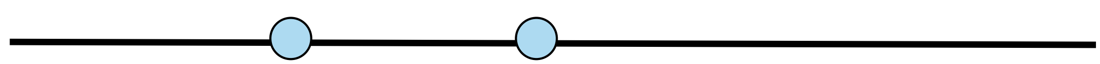
$\mathrm{VCdim(H)} = 1$

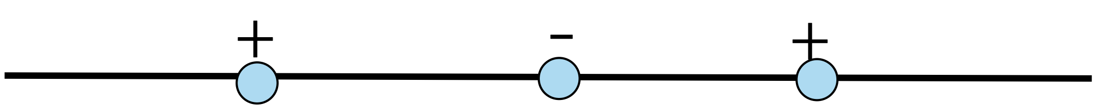


E.g., H= Intervals on the real line



$\mathrm{VCdim(H)} = 2$





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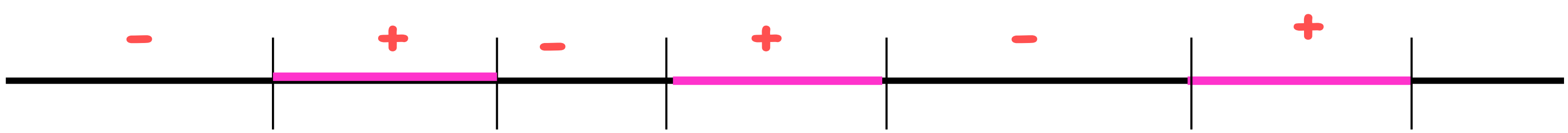
Shattering, VC-dimension

If the VC-dimension is d, that means there exists a set of d points that can be shattered, but there is no set of d+1 points that can be shattered.

E.g., H= Union of k intervals on the real line $\mathrm{VCdim}(\mathrm{H}) = 2\mathrm{k}$



$\mathrm{VCdim}(\mathrm{H}) \geq 2\mathrm{k}$

A sample of size 2k shatters (treat each pair of points as a separate case of intervals)

$\mathrm{VCdim}(\mathrm{H}) < 2\mathrm{k} + 1$

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SLT-style Corollaries

Corollary 3 (Realizable, Infinite $|\mathcal{H}|$). For some $\delta > 0$, with probability at least $(1 - \delta)$, for any hypothesis h in $\mathcal{H}$ consistent with the data (i.e. with $\hat{R}(h) = 0$),

$$R(h) \leq O\left(\frac{1}{N}\left[\text{VC}(\mathcal{H}) \ln\left(\frac{N}{\text{VC}(\mathcal{H})}\right) + \ln\left(\frac{1}{\delta}\right)\right]\right) \tag{1}$$

Corollary 4 (Agnostic, Infinite $|\mathcal{H}|$). For some $\delta > 0$, with probability at least $(1 - \delta)$, for all hypotheses h in $\mathcal{H}$,

$$R(h) \leq \hat{R}(h) + O\left(\sqrt{\frac{1}{N}\left[\text{VC}(\mathcal{H}) + \ln\left(\frac{1}{\delta}\right)\right]}\right) \tag{2}$$

Generalization and Overfitting

Whiteboard:

- Empirical Risk Minimization
- Structural Risk Minimization
- Motivation for Regularization

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   (Sample Complexity, Realizable Case)

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   (Structural Risk Minimization)

Learning Theory 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 learning examples
- Distinguish between a large sample and a finite sample analysis
- Theoretically motivate regularization