CS 760: Machine Learning
PAC Learning

University of Wisconsin-Madison

Outline

- **PAC Learning**
  - definition, sample complexity bounds
- **VC-dimension**
  - motivation, definition, other complexity measures

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Recall: **Generalization error decomposition**

Last time, we were interested in the quantity

$$err(\hat{h}) = \widehat{err}(\hat{h}) + [err(\hat{h}) - \widehat{err}(\hat{h})]$$

$err(\hat{h})$: true risk (test error)

$\widehat{err}(\hat{h})$: empirical risk (training error)

$[err(\hat{h}) - \widehat{err}(\hat{h})]$: generalization gap

If the generalization gap is small and our learning algorithm is empirical risk minimization then the true risk is also small

Today: a framework for bounding the generalization error and gap in terms of the number of samples

PAC Learning: Setup

- input space X (images, documents, feature vectors in $\mathbb{R}^2$, …)

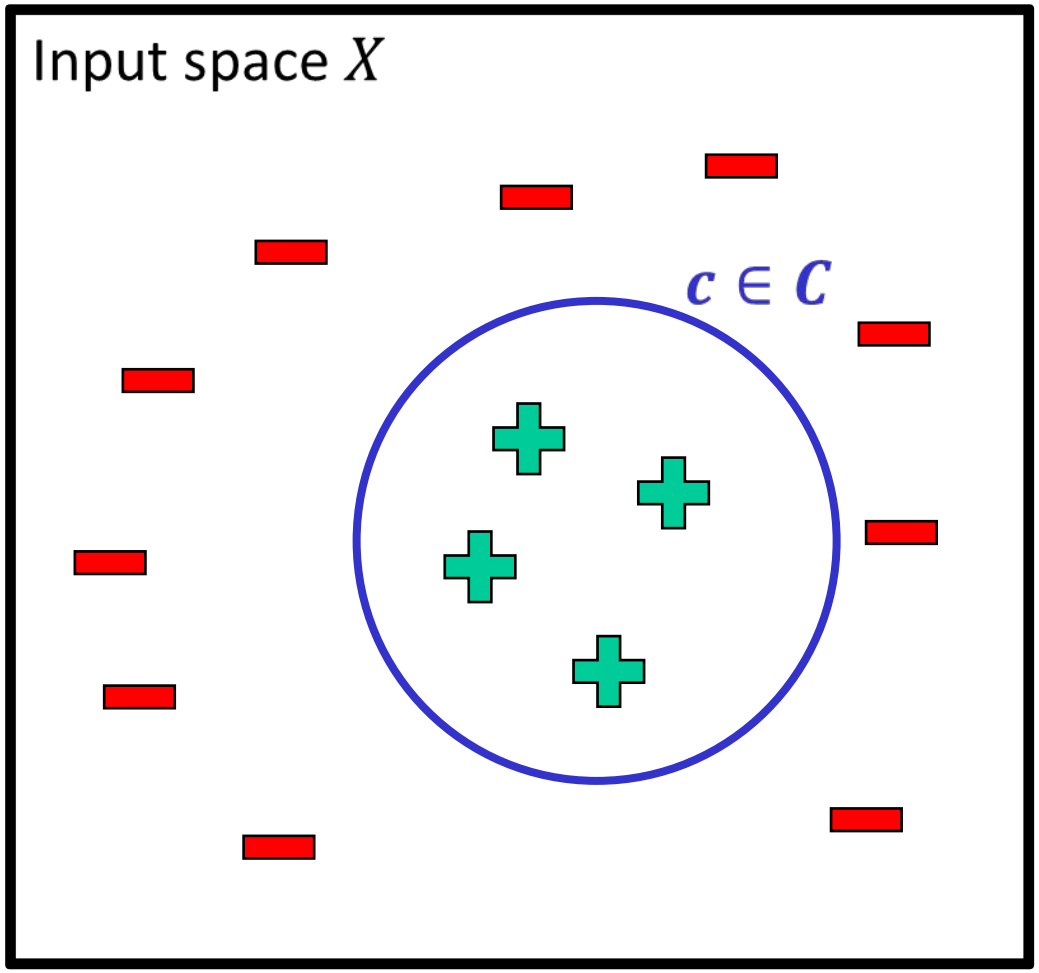
- output space $Y = \{0,1\}$
  - just binary classification in this class
  - extendable to regression / multi-class classification

- hypothesis class H
  - set of functions $f: X \mapsto Y$ that the learning algorithm can output

PAC Learning: Data

- concept class C
  - set of labeling functions $c: X \mapsto Y$
  - represents set of possible true labeling functions
  - example: circles in $\mathbb{R}^2$
  - NOT (always) the same thing as the hypothesis class H
  - ideally $H \supset C$

- data distribution D over $X \times Y$
  - unknown
  - get m samples (x_i, y_i), $i = 1, \ldots, m$ i.i.d. from D
  - $y_i = c(x_i)$ for some $c \in C$

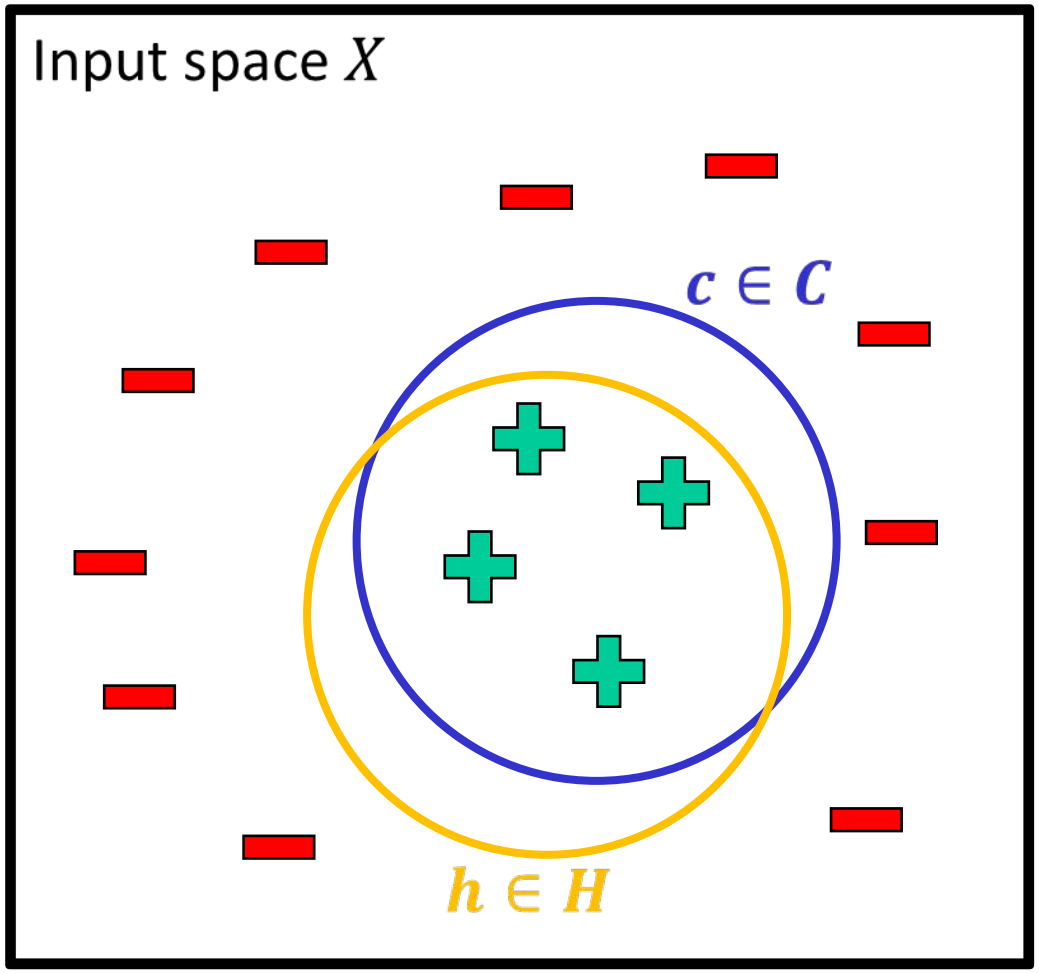


PAC Learning: Goal

Use the training data to **approximate** the unknown target concept $c \in C$ using a hypothesis $h \in H$

Evaluate using **true risk**

$$err(h) = P_{x\sim D}\{h(x) \neq c(x)\} = \mathbb{E}1_{\{h(x)\neq c(x)\}}$$



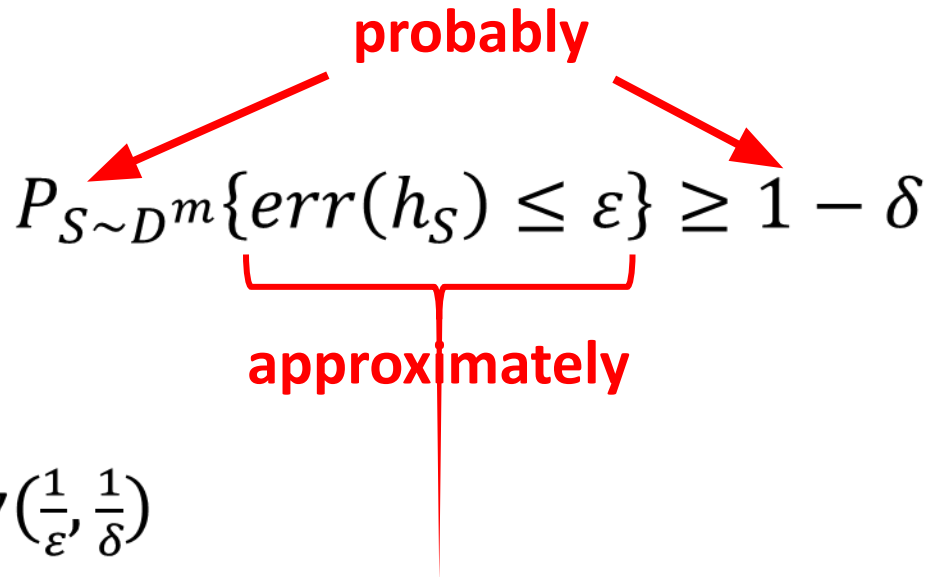
But we only have access to the **empirical risk** $\widehat{err}(h) = \frac{1}{m}\sum_{i=1}^{m} 1_{\{h(x)\neq c(x)\}}$

Thus any approximation must be **probabilistic**

PAC Learning: Definition

PAC = Probably Approximately Correct

A concept class C is **PAC-learnable** if there exists a learning algorithm that takes any dataset S of size m and outputs a hypothesis $h_S: X \mapsto Y$ that for any $\varepsilon, \delta > 0$ has the property



so long as $m \geq poly(\frac{1}{\varepsilon}, \frac{1}{\delta})$

PAC Learning: Definition

In words: C is PAC-learnable **if**

- there is a learning algorithm **and**
- a polynomial function $poly$: $(0,1)^2 \mapsto \mathbb{Z}_+$ **such that**
- the probability the algorithm outputs a model that is wrong on more than ε-fraction of samples from D is at most δ, **so long as**
- the number of samples m is $\geq poly(1/\varepsilon, 1/\delta)$

The polynomial function is called the **sample complexity**

Compare to **computational complexity**: a problem is **tractable** (i.e. in P) if there exists a polynomial time algorithm to solve it

Consistent case guarantee

Suppose there exists a **consistent** learning algorithm:

- always returns h_S with empirical risk $\widehat{err}(h_S) = 0$
- for example: empirical risk minimization on $H \supset C$

Then C is PAC-learnable with sample complexity $\frac{1}{\varepsilon}\log\frac{|H|}{\delta}$

In other words, given m samples, with probability $\geq 1 - \delta$,

$$err(h_S) = err(h_S) - \widehat{err}(h_S) \leq \frac{1}{m}\log\frac{|H|}{\delta}$$

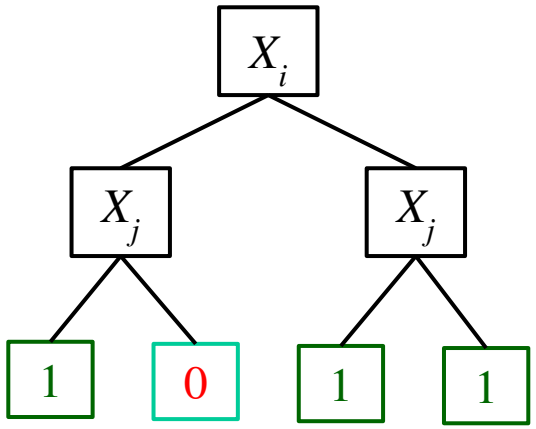
Consistent case: Example

Suppose we have n-dimensional binary data that is perfectly classified by a depth 2 decision tree:

- $|H| = \#\ of\ pairs \times \#\ of\ leaf\ labelings = \binom{n}{2} \times 2^4 = 16\binom{n}{2}$
- If we want success probability ≥ 0.99 and error rate ≤ 0.05 then

$$m \geq \frac{1}{0.05}\left(\log \frac{16n(n-1)}{2 \times 0.01}\right)$$

- If $n = 100$ then we $m \geq 318$ samples suffices.



Inconsistent case

Want to drop the consistency requirement $err(h_S) = 0$

Inconsistent case guarantee:

- w.p. $\geq 1 - \delta$, $err(h) \leq \widehat{err}(h) + \sqrt{\frac{1}{2m} \log \frac{2|H|}{\delta}}$ $\forall\, h \in H$

- quadratically worse error than consistent case

- uniform convergence bounds holds **simultaneously for all h**

PAC learning so far…

Formalizes learning task while allowing for imperfect learning due to randomness / approximation (parameterized via δ and ε)

Can also define **efficient** PAC learnability by requiring the learning algorithm to take polynomial-time compute

Shows how many samples are needed to learn over a finite hypothesis class

What if the hypothesis space is infinite? Can we still learn?

- linear models
- neural networks
- …

$$err(h) \leq \widehat{err}(h) + \sqrt{\frac{1}{2m}\log\frac{2|H|}{\delta}}$$

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Infinite hypothesis classes

Most practical learning algorithms operate over infinite hypothesis classes

Basic PAC results give infinite sample complexity for $|H| = \infty$

Need a different way to quantify the capacity of the class

The **Vapnik-Chervonenkis (VC) dimension** does this by measuring how easy it is for function in H to fit arbitrary labels

Getting started: **Shattering**

Hypothesis space H **shatters** a set of points $S = \{x_1, \dots, x_k\} \in X$ if for every possible labeling $\{y_1, \dots, y_k\} \in \{0,1\}$ of S there exists a function $h \in H$ such that produces that labeling, i.e.

$$h(x_1) = y_1, \dots, h(x_k) = y_k$$

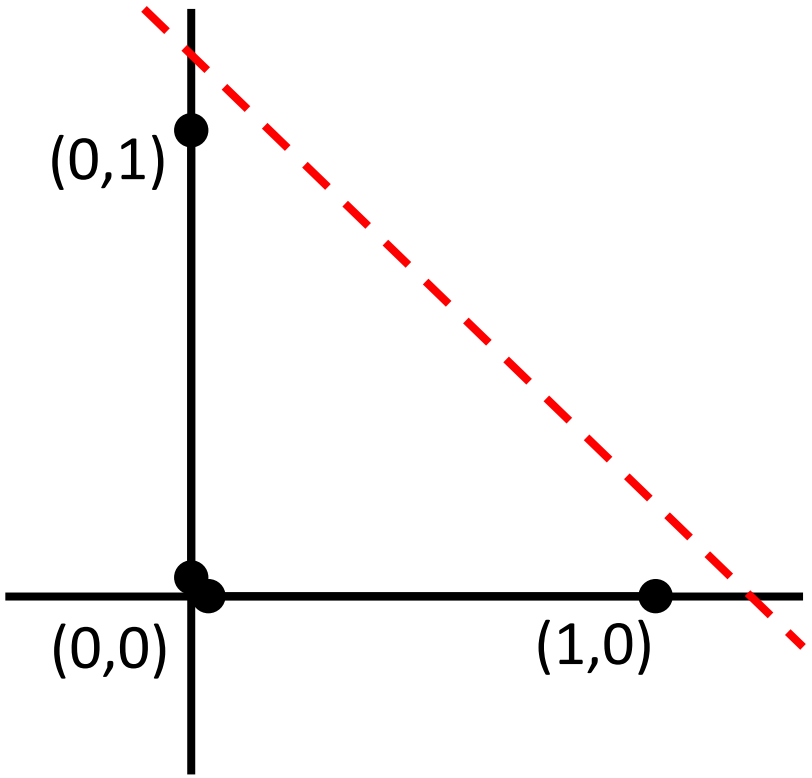
Demonstrates that H is expressive enough to make arbitrary distinctions between these a set of k points.

Shattering example: Lines in 2D

Hypotheses: $H = \{\text{sign}(w_1 x_1 + w_2 x_2 + b) : w_1, w_2, b \in \mathbb{R}\}$
Set of points: $S = \{(0,0), (1,0), (0,1)\}$

2^3 possible labelings:

- (0,0,0)
- (0,0,1)
- (0,1,0)
- (0,1,1)
- (1,0,0)
- (1,0,1)
- (1,1,0)
- (1,1,1)



VC dimension

The **VC dimension of a hypothesis class H** is the size of the largest set of points in X that can be shattered by H

Two step procedure to show $VC(H) = d$:

1. find a set of points $S \subset X$ of size $|S| = d$ that is shattered by H
   - i.e. find d points that can be labeled arbitrarily by functions $h \in H$
   - easier step: only need to find one set of shattered points, NOT all

2. show that no set of $d + 1$ points can be shattered

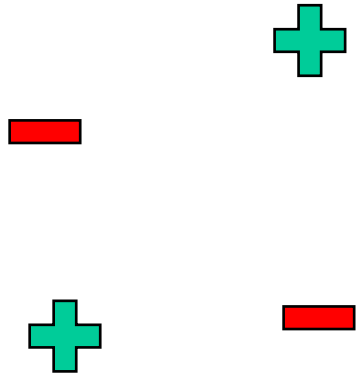
VC dimension example: Lines in 2D

Already demonstrated a set of three points that is shattered by H, so $VC(H) \geq 3$

Is there a set of four points shattered by H?

Case 1: collinear points

Case 2: one point inside convex hull



Case 3: quadrilateral

No! Thus $VC(H) < 4$, and so $VC(H) = 3$

What does the VC-dimension get us?

If H has VC dimension d and we draw m samples i.i.d. from D then with probability at least $1 - \delta$ the following is true for all $h \in H$:

$$err(h) \leq \widehat{err}(h) + \sqrt{\frac{2d}{m}\log\frac{em}{d}} + \sqrt{\frac{1}{m}\log\frac{1}{\delta}}$$

VC-dimension roughly takes the place of $\log|H|$ as a measure of the capacity of the hypothesis class.

VC dimensions of other classes

Linear classifiers in $\mathbb{R}^d$: $d + 1$

Finite hypothesis spaces: $\leq \log |H|$

L-layer ReLU networks with W weights: $O(WL \log W)$

Implications of VC-dimension

Bound suggests roughly $m \approx d = VC(H)$ examples suffice to start getting meaningful generalization

$$err(h) \leq \widehat{err}(h) + \sqrt{\frac{2d}{m}\log\frac{em}{d}} + \sqrt{\frac{1}{m}\log\frac{1}{\delta}}$$

- sometimes okay for linear models over sufficiently large data
- vacuous for modern deep nets (CNNs with millions of weights do well on CIFAR-10, a dataset with <100K examples)

Other measures of hypothesis class capacity

Rademacher complexity: how easily do functions $h \in H$ fit **random** labels?

Covering number: how many functions $h \in H$ are needed so that **the rest are close** to one of them?

Achievements of learning theory

PAC theory provides a way of thinking about the relationship between learning performance, sample size, and model capacity

- works for any data distribution
- capacity measures can be computed for most classes of interest
- many extensions to noisy labels, hypothesis classes that do not contain the target concept, etc.
- bounds generalization error in interpretable ways

Caveats

Drawbacks of most PAC guarantees:

- do not adapt to easy data (worst-case)
- does not consider the effect of optimization
- capacity measures might be misleading for modern deep nets

Thanks Everyone!

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