Learning Theory Part 1: PAC Model

CS 760@UW-Madison

Goals for the lecture

you should understand the following concepts

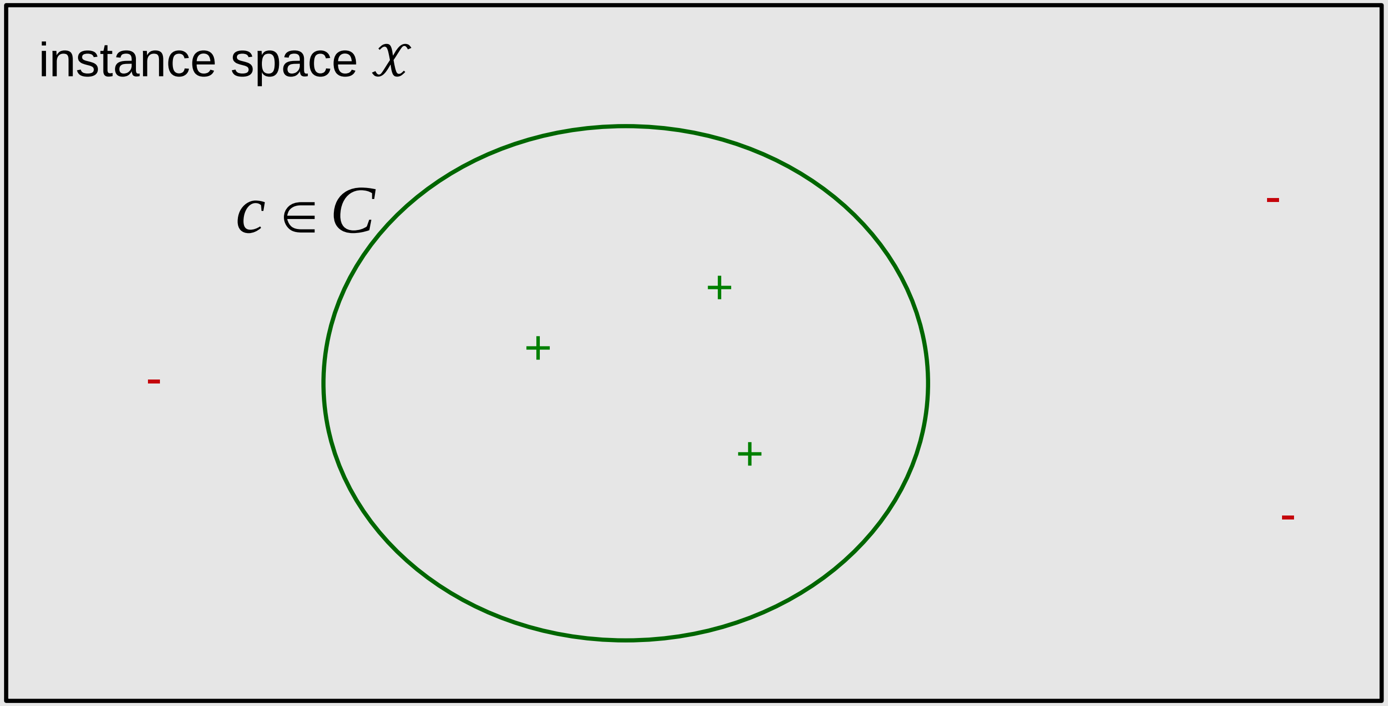
- PAC learnability
- consistent learners and version spaces
- sample complexity
- PAC learnability in the agnostic setting
- the VC dimension
- sample complexity using the VC dimension

PAC learning

- Overfitting happens because training error is a poor estimate of generalization error
  → Can we infer something about generalization error from training error?

- Overfitting happens when the learner doesn't see enough training instances
  → Can we estimate how many instances are enough?

Learning setting #1



- set of instances $\mathcal{X}$
- set of hypotheses (models) H
- set of possible target concepts C
- unknown probability distribution $\mathcal{D}$ over instances

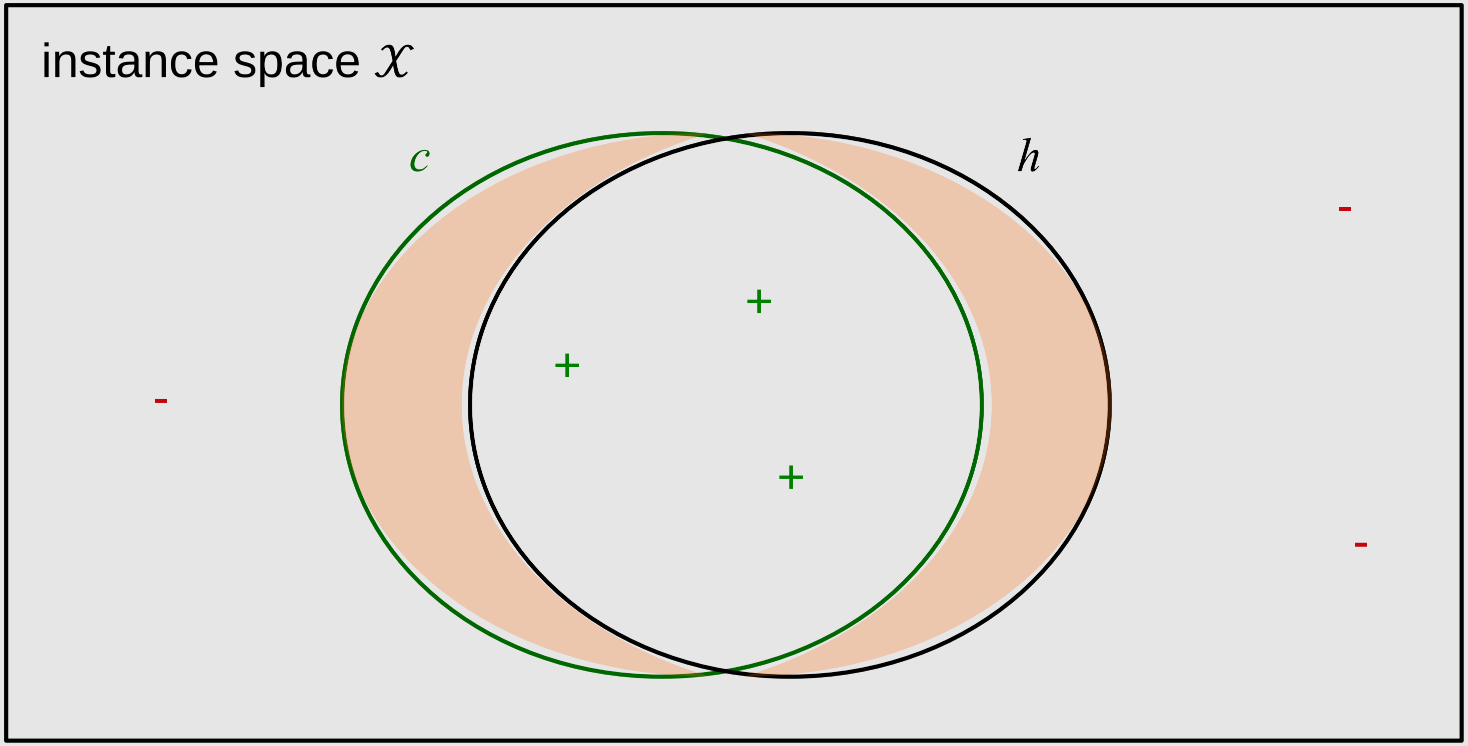
Learning setting #1

- learner is given a set D of training instances $\langle \boldsymbol{x}, c(\boldsymbol{x}) \rangle$ for some target concept c in C
  - each instance $\boldsymbol{x}$ is drawn from distribution $\mathcal{D}$
  - class label $c(\boldsymbol{x})$ is provided for each $\boldsymbol{x}$
- learner outputs hypothesis h modeling c

True error of a hypothesis

the *true error* of hypothesis h refers to how often h is wrong on future instances drawn from $\mathcal{D}$

$$error_{\mathcal{D}}(h) \equiv P_{x \in \mathcal{D}}\left[c(\boldsymbol{x}) \neq h(\boldsymbol{x})\right]$$



Training error of a hypothesis

the *training error* of hypothesis h refers to how often h is wrong on instances in the training set D

$$error_D(h) \equiv P_{x \in D}[c(x) \neq h(x)] = \frac{\sum_{x \in D} \delta(c(x) \neq h(x))}{|D|}$$

Can we bound $error_{\mathcal{D}}(h)$ in terms of $error_{D}(h)$?

Is approximately correct good enough?

To say that our learner L has learned a concept, should we require $error_{\mathcal{D}}(h) = 0$?

this is not realistic:

- unless we've seen every possible instance, there may be multiple hypotheses that are consistent with the training set
- there is some chance our training sample will be unrepresentative

Probably approximately correct learning?

Instead, we'll require that

- the error of a learned hypothesis h is bounded by some constant ε
- the probability of the learner failing to learn an accurate hypothesis is bounded by a constant δ

Probably Approximately Correct (PAC) learning [Valiant, *CACM* 1984]

- Consider a class C of possible target concepts defined over a set of instances $\mathcal{X}$ of length n, and a learner L using hypothesis space H

- C is PAC learnable by L using H if, for all

  $c \in C$

  distributions $\mathcal{D}$ over $\mathcal{X}$

  ε such that $0 < \varepsilon < 0.5$

  δ such that $0 < \delta < 0.5$

- learner L will, with probability at least $(1-\delta)$, output a hypothesis $h \in H$ such that $error_{\mathcal{D}}(h) \leq \varepsilon$ in time that is polynomial in

  $1/\varepsilon$

  $1/\delta$

  n

  size(c)

PAC learning and consistency

- Suppose we can find hypotheses that are consistent with m training instances.
- We can analyze PAC learnability by determining whether
  1. m grows polynomially in the relevant parameters
  2. the processing time per training example is polynomial

Version spaces

- A hypothesis h is *consistent* with a set of training examples D of target concept if and only if $h(\mathbf{x}) = c(\mathbf{x})$ for each training example $\langle \mathbf{x}, c(\mathbf{x}) \rangle$ in D

$$consistent(h, D) \equiv (\forall \langle x, c(x) \rangle \in D)\ \ h(x) = c(x)$$

- The version space $VS_{H,D}$ with respect to hypothesis space H and training set D, is the subset of hypotheses from H consistent with all training examples in D

$$VS_{H,D} \equiv \{h \in H \mid consistent(h, D)\}$$

Exhausting the version space

- The version space $VS_{H,D}$ is ε-exhausted with respect to c and *D* if every hypothesis $h \in VS_{H,D}$ has true error $< \varepsilon$

$$\left(\forall h \in VS_{H,D}\right) error_{\mathcal{D}}(h) < \varepsilon$$

Exhausting the version space

- Suppose that every h in our version space $VS_{H,D}$ is consistent with m training examples
- The probability that $VS_{H,D}$ is <u>not</u> ε-exhausted (i.e. that it contains some hypotheses that are not accurate enough)

$$\le |H| e^{-\varepsilon m}$$

Proof:

$$(1-\varepsilon)^m$$

probability that some hypothesis with error > ε is consistent with m training instances

$$k(1-\varepsilon)^m$$

there might be k such hypotheses

$$|H|(1-\varepsilon)^m$$

k is bounded by $|H|$

$$\le |H| e^{-\varepsilon m}$$

$(1-\varepsilon) \le e^{-\varepsilon}$ when $0 \le \varepsilon \le 1$

Sample complexity for finite hypothesis spaces

[Blumer et al., *Information Processing Letters* 1987]

- we want to reduce this probability below δ

$$|H| e^{-\varepsilon m} \le \delta$$

- solving for m we get

$$m \geq \frac{1}{\varepsilon}\left(\ln|H| + \ln\left(\frac{1}{\delta}\right)\right)$$

log dependence on H

ε has stronger influence than δ

PAC analysis example: learning conjunctions of Boolean literals

- each instance has n Boolean features
- learned hypotheses are of the form $Y = X_1 \wedge X_2 \wedge \neg X_5$

How many training examples suffice to ensure that with prob ≥ 0.99, a consistent learner will return a hypothesis with error ≤ 0.05 ?

there are 3^n hypotheses (each variable can be present and unnegated, present and negated, or absent) in H

$$m \geq \frac{1}{.05}\left(\ln\left(3^n\right) + \ln\left(\frac{1}{.01}\right)\right)$$

for n=10, $m \geq 312$ for n=100, $m \geq 2290$

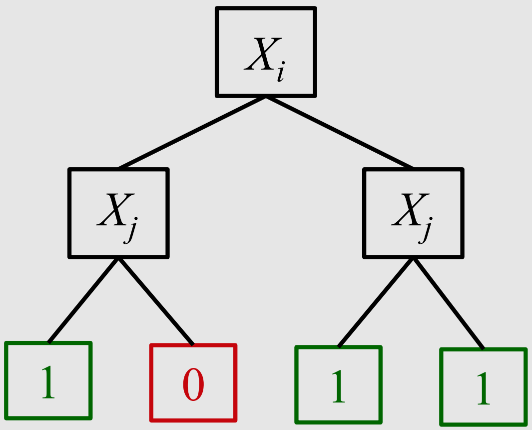
PAC analysis example: learning conjunctions of Boolean literals

- we've shown that the sample complexity is polynomial in relevant parameters: $1/\varepsilon$, $1/\delta$, n
- to prove that Boolean conjunctions are PAC learnable, need to also show that we can find a consistent hypothesis in polynomial time (the FIND-S algorithm in Mitchell, Chapter 2 does this)

FIND-S:
initialize h to the most specific hypothesis $x_1 \wedge \neg x_1 \wedge x_2 \wedge \neg x_2 \ldots\ x_n \wedge \neg x_n$
for each positive training instance $\boldsymbol{x}$
remove from h any literal that is not satisfied by $\boldsymbol{x}$
output hypothesis h

PAC analysis example: learning decision trees of depth 2

- each instance has n Boolean features
- learned hypotheses are DTs of depth 2 using only 2 variables



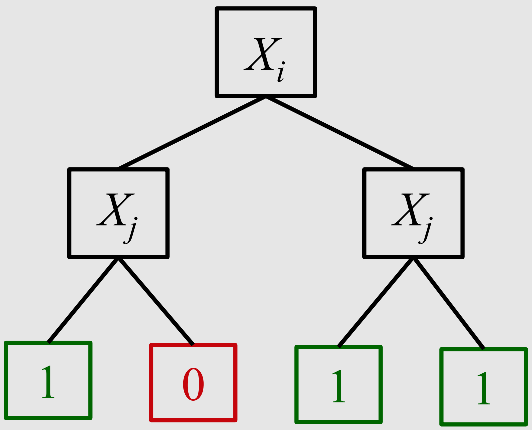
$$|H| = \binom{n}{2} \times 16 = \frac{n(n-1)}{2} \times 16 = 8n(n-1)$$

\# possible split choices

\# possible leaf labelings

PAC analysis example:
learning decision trees of depth 2

- each instance has n Boolean features
- learned hypotheses are DTs of depth 2 using only 2 variables



How many training examples suffice to ensure that with prob ≥ 0.99, a consistent learner will return a hypothesis with error ≤ 0.05 ?

$$m \geq \frac{1}{.05}\left(\ln\left(8n^2 - 8n\right) + \ln\left(\frac{1}{.01}\right)\right)$$

for n=10, $m \geq 224$ for n=100, $m \geq 318$

PAC analysis example: K-term DNF is not PAC learnable

- each instance has n Boolean features
- learned hypotheses are of the form $Y = T_1 \vee T_2 \vee \ldots \vee T_k$ where each T_i is a conjunction of n Boolean features or their negations

$|H| \leq 3^{nk}$, so sample complexity is polynomial in the relevant parameters

$$m \geq \frac{1}{e}\left(nk \ln(3) + \ln\left(\frac{1}{d}\right)\right)$$

however, the computational complexity (time to find consistent h) is not polynomial in m (e.g. graph 3-coloring, an NP-complete problem, can be reduced to learning 3-term DNF)

What if the target concept is not in our hypothesis space?

- so far, we've been assuming that the target concept c is in our hypothesis space; this is not a very realistic assumption

- *agnostic learning* setting
  - don't assume $c \in H$
  - learner returns hypothesis h that makes fewest errors on training data

Hoeffding bound

- we can approach the agnostic setting by using the Hoeffding bound
- let $Z_1 \ldots Z_m$ be a sequence of m independent Bernoulli trials (e.g. coin flips), each with probability of success $E[Z_i] = p$
- let $S = Z_1 + \cdots + Z_m$

$$P[S < (p - \varepsilon)m] \leq e^{-2m\varepsilon^2}$$

Agnostic PAC learning

- applying the Hoeffding bound to characterize the error rate of a given hypothesis

$$P\left[error_{\mathcal{D}}(h) > error_{D}(h) + \varepsilon\right] \leq e^{-2m\varepsilon^2}$$

- but our learner searches hypothesis space to find h_{best}

$$P\left[error_{\mathcal{D}}(h_{best}) > error_{D}(h_{best}) + \varepsilon\right] \leq |H|e^{-2m\varepsilon^2}$$

- solving for the sample complexity when this probability is limited to δ

$$m \geq \frac{1}{2\varepsilon^2}\left(ln|H| + ln\left(\frac{1}{\delta}\right)\right)$$

What if the hypothesis space is not finite?

- **Q:** If H is infinite (e.g. the class of perceptrons), what measure of hypothesis-space complexity can we use in place of $|H|$?

- **A:** the largest subset of $\mathcal{X}$ for which H can guarantee zero training error, regardless of the target function.

this is known as the *Vapnik-Chervonenkis dimension* (VC-dimension)

Shattering and the VC dimension

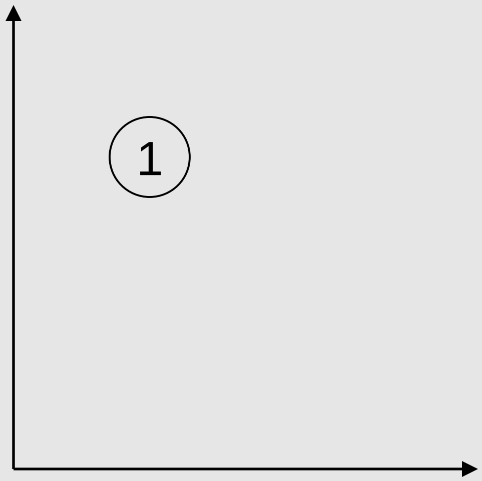
- a set of instances D is *shattered* by a hypothesis space H iff for every dichotomy of D there is a hypothesis in H consistent with this dichotomy

- the *VC dimension* of H is the size of the largest set of instances that is shattered by H

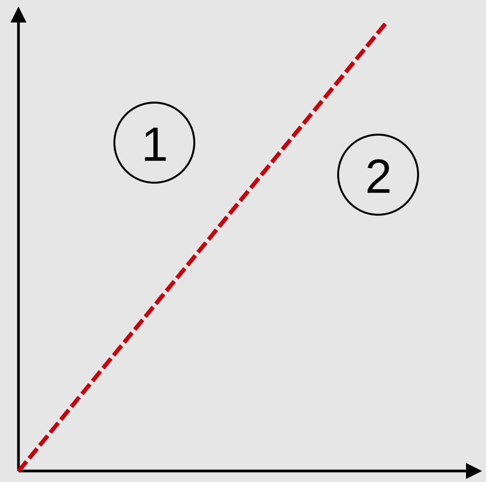
Infinite hypothesis space with a finite VC dimension

consider: H is set of lines in 2D (i.e. perceptrons in 2D feature space)

can find an h consistent with 1 instance no matter how it's labeled



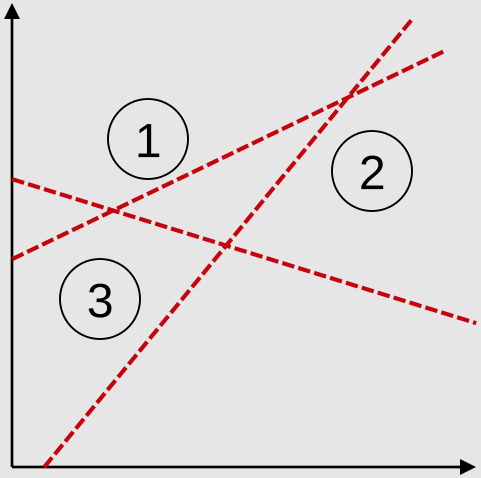
can find an h consistent with 2 instances no matter labeling



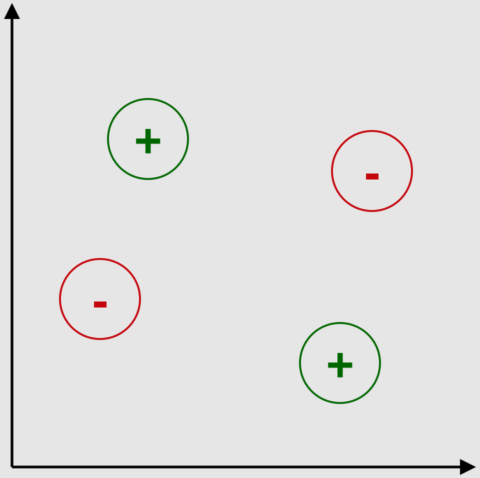
Infinite hypothesis space with a finite VC dimension

consider: H is set of lines in 2D

can find an h consistent with 3 instances no matter labeling (assuming they're not colinear)



cannot find an h consistent with 4 instances for some labelings



can shatter 3 instances, but not 4, so the VC-dim(H) = 3

more generally, the VC-dim of hyperplanes in n dimensions $= n+1$

VC dimension for finite hypothesis spaces

for finite H, VC-dim$(H) \leq \log_2|H|$

Proof:

suppose VC-dim$(H) = d$

for d instances, 2^d different labelings possible

therefore H must be able to represent 2^d hypotheses

$2^d \leq |H|$

$d =$ VC-dim$(H) \leq \log_2|H|$

Sample complexity and the VC dimension

- using VC-dim(H) as a measure of complexity of H, we can derive the following bound [Blumer et al., *JACM* 1989]

$$m \geq \frac{1}{e}\left(4\log_2\left(\frac{2}{d}\right) + 8\text{VC-dim}(H)\log_2\left(\frac{13}{e}\right)\right)$$

m grows log × linear in ε (better than earlier bound)

can be used for both finite and infinite hypothesis spaces

Lower bound on sample complexity

[Ehrenfeucht et al., *Information & Computation* 1989]

- there exists a distribution $\mathcal{D}$ and target concept in C such that if the number of training instances given to L

$$m < \max\left[\frac{1}{e}\log\left(\frac{1}{d}\right), \frac{\text{VC-dim}(C) - 1}{32e}\right]$$

then with probability at least δ, L outputs h such that $error_{\mathrm{D}}(h) > \varepsilon$

Comments on PAC learning

- PAC analysis formalizes the learning task and allows for non-perfect learning (indicated by ε and δ)
- finding a consistent hypothesis is sometimes easier for larger concept classes
  - e.g. although k-term DNF is not PAC learnable, the more general class k-CNF is
- PAC analysis has been extended to explore a wide range of cases
  - noisy training data
  - learner allowed to ask queries
  - restricted distributions (e.g. uniform) over $\mathcal{D}$
  - etc.
- most analyses are worst case
- sample complexity bounds are generally not tight

THANK YOU

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