Learning Theory Part 1: PAC Model

Yingyu Liang
Computer Sciences 760
Fall 2017

http://pages.cs.wisc.edu/~yliang/cs760/

Some of the slides in these lectures have been adapted/borrowed from materials developed by Mark Craven, David Page, Jude Shavlik, Tom Mitchell, Nina Balcan, Matt Gormley, Elad Hazan, Tom Dietterich, and Pedro Domingos.

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

the ONION®
America's Finest News Source

NEWS IN PHOTOS

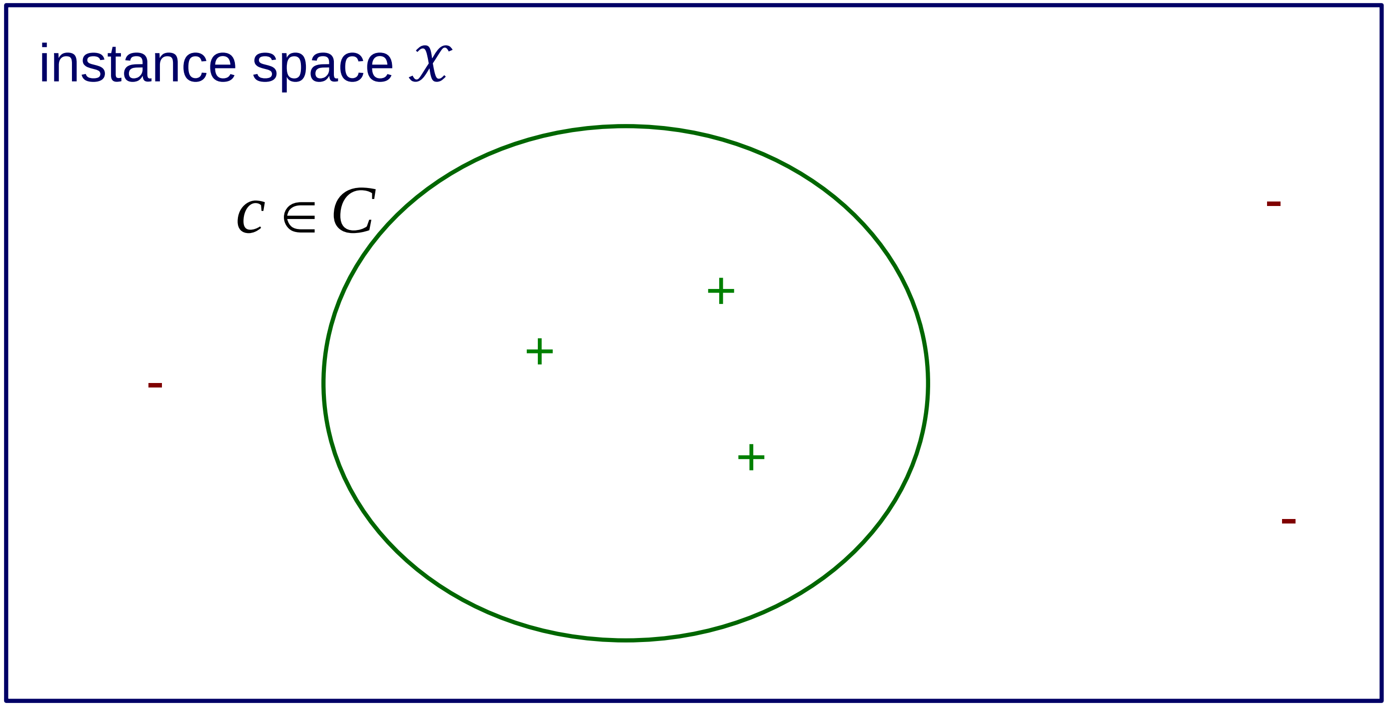
Experimental Band Theoretically Good

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

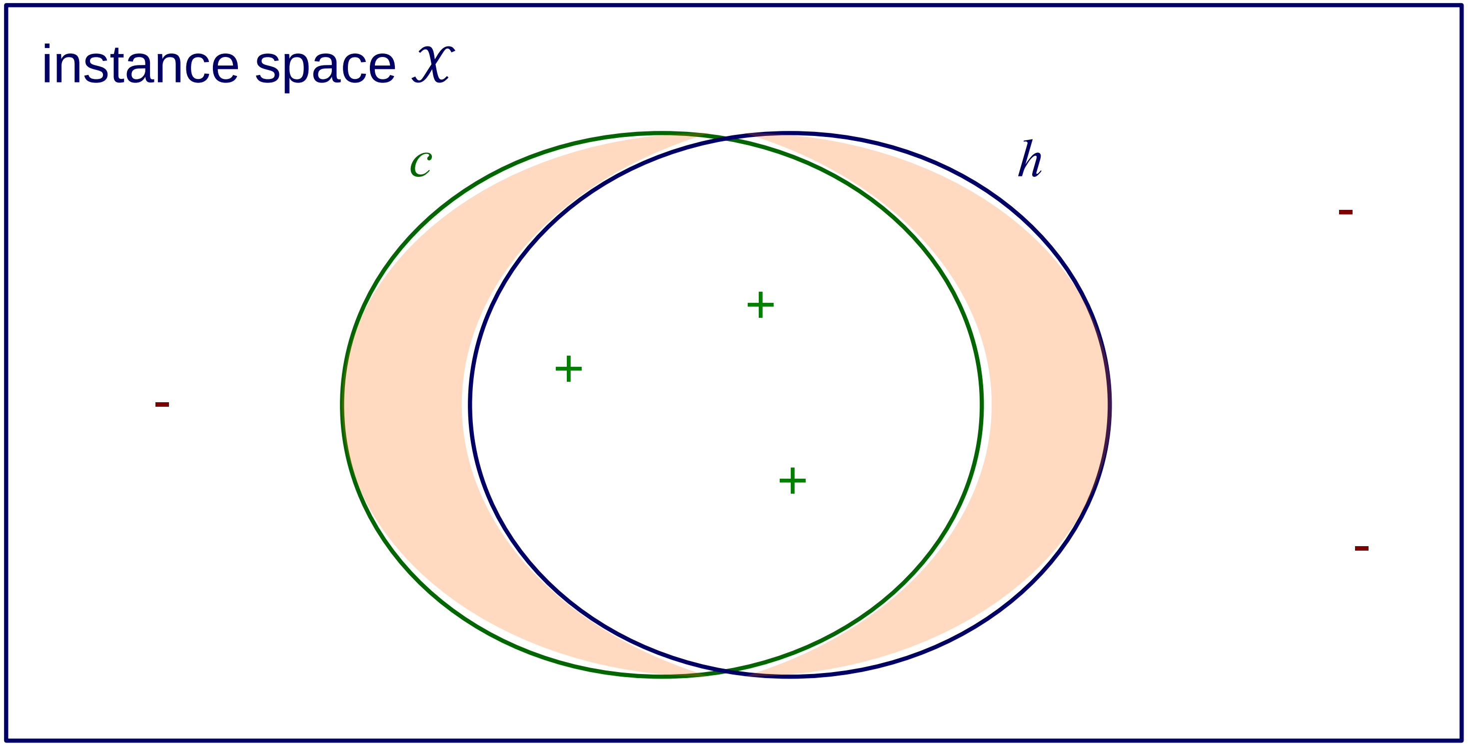
- learner is given a set D of training instances $\langle\, \boldsymbol{x}, c(\boldsymbol{x})\, \rangle$ for some target concept c in C
  - each instance $\boldsymbol{x}$ is drawn from distribution $\mathcal{D}$
  - class label $c(\boldsymbol{x})$ is provided for each $\boldsymbol{x}$

- 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 $error_{\mathrm{D}}(h)$?

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 $(1\text{-}\delta)$, 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 $h(\boldsymbol{x}) = c(\boldsymbol{x})$ for each training example $\langle \boldsymbol{x}, c(\boldsymbol{x}) \rangle$ 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 $VS_{H,\mathrm{D}}$ is ε-exhausted with respect to c and *D* if every hypothesis $h \in VS_{H,\mathrm{D}}$ has true error $< \varepsilon$

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

Exhausting the version space

- Suppose that every h in our version space $VS_{H,\mathrm{D}}$ is consistent with m training examples
- The probability that $VS_{H,\mathrm{D}}$ 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

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

- solving for m we get

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

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

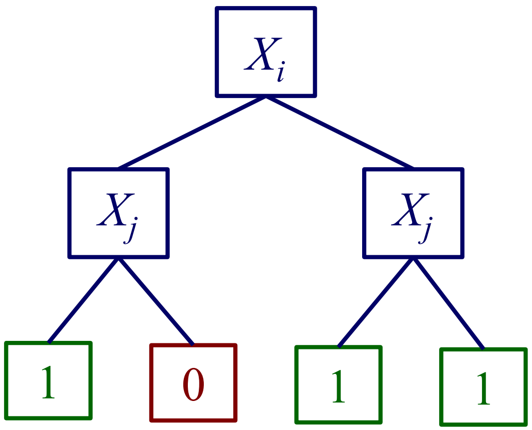
- to prove that Boolean conjunctions are PAC learnable, need to also show that we can find a consistent hypothesis in polynomial time (the FIND-S algorithm in Mitchell, Chapter 2 does this)

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



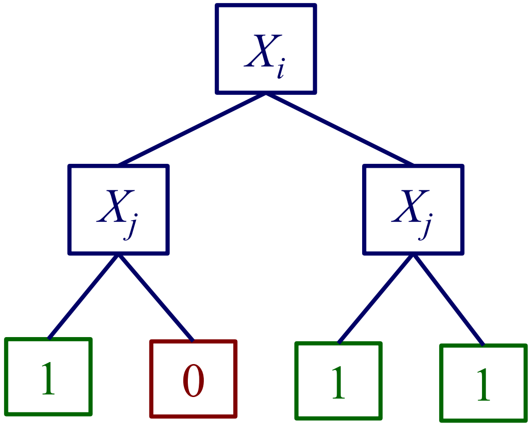
$$|H| = \binom{n}{2} \times 16 = \frac{n(n-1)}{2} \times 16 = 8n(n-1)$$

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

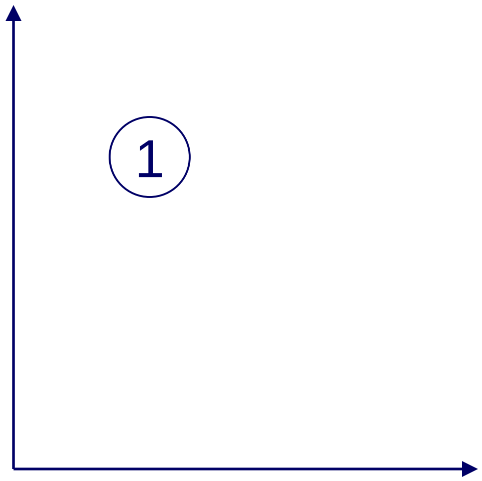
- a set of instances D is *shattered* by a hypothesis space H iff for every dichotomy of D there is a hypothesis in H consistent with this dichotomy

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

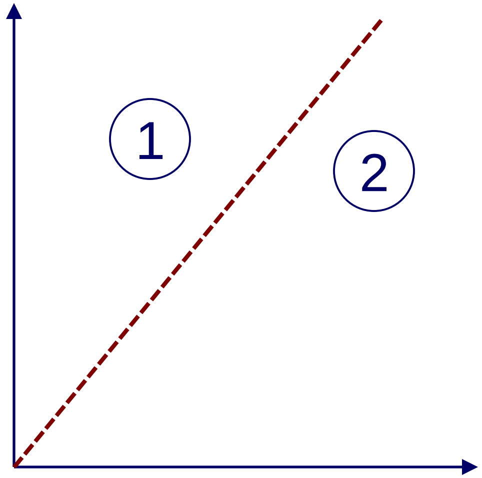
An infinite hypothesis space with a finite VC dimension

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



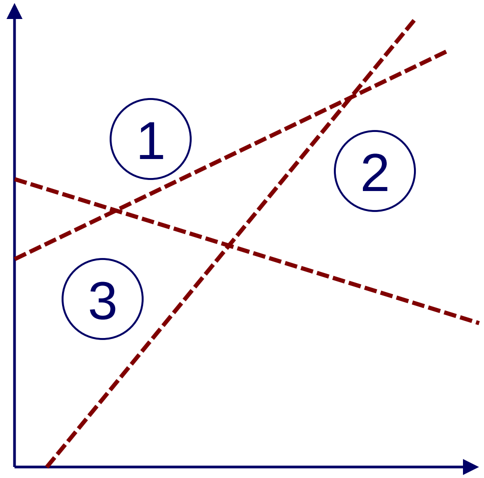
can find an h consistent with 2 instances no matter labeling



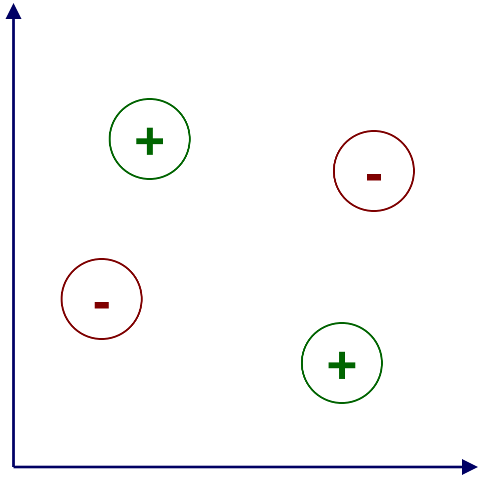
An infinite hypothesis space with a finite VC dimension

consider: H is set of lines in 2D

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



<u>cannot</u> 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 $\times$ 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