Computational Learning Theory

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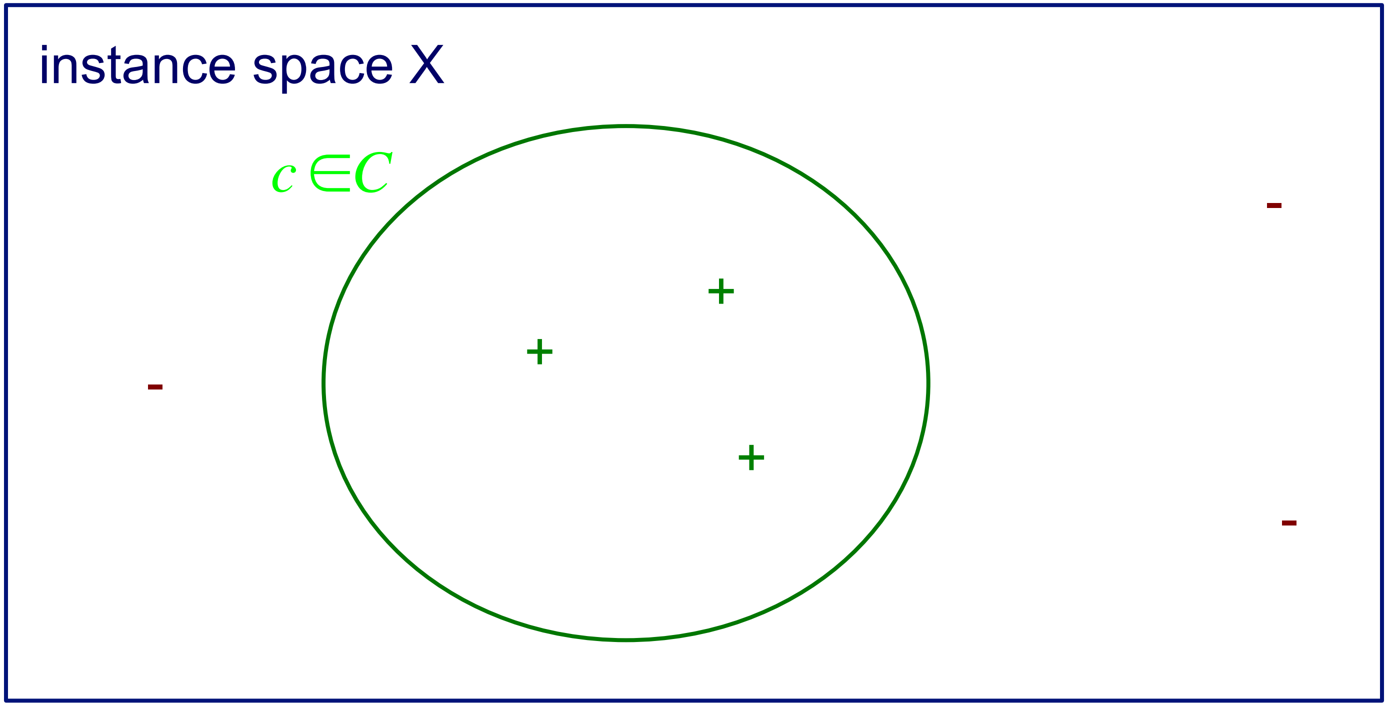
Goals for the lecture

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 on-line learning setting
- the mistake bound model of learnability
- the Halving algorithm
- the Weighted Majority algorithm

Learning setting #1



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

Learning setting #1

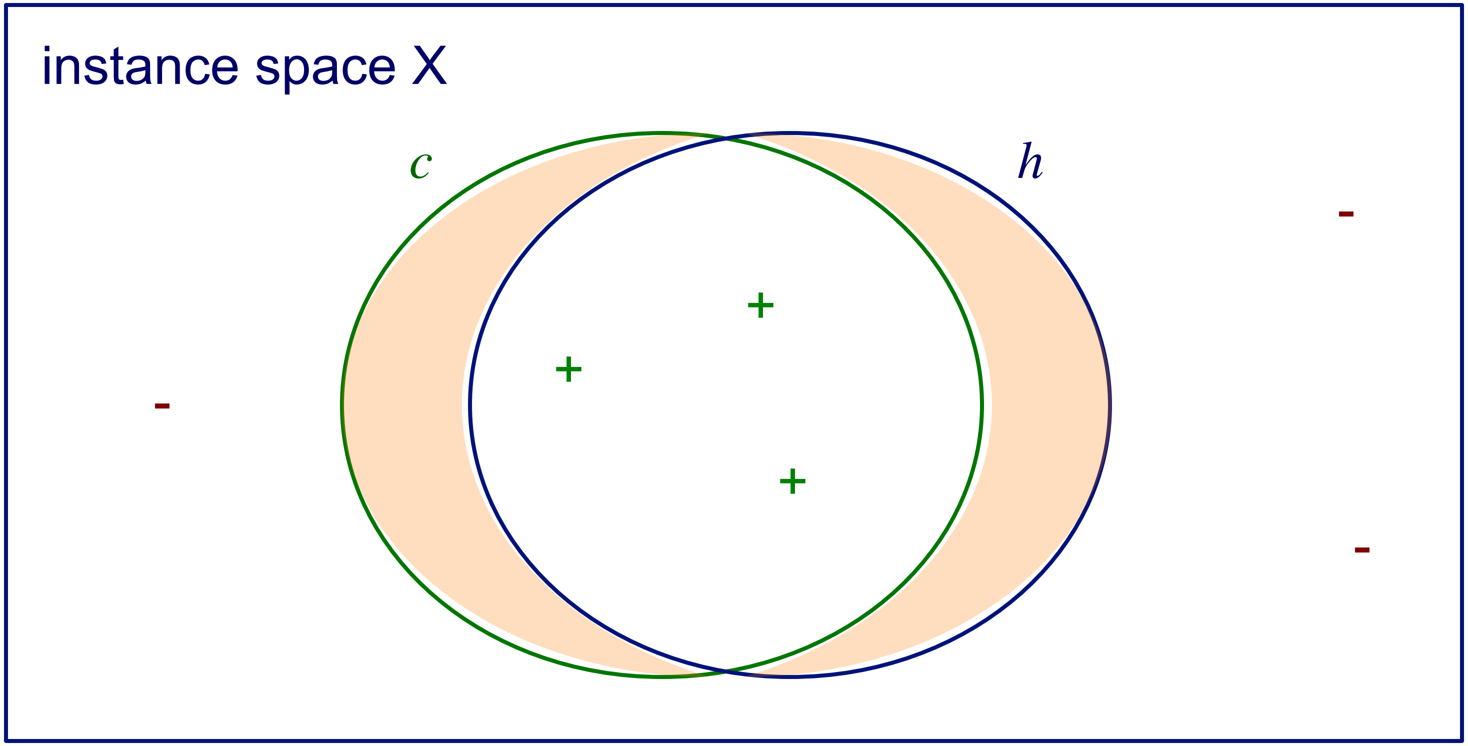
- learner is given a set D of training instances $\langle \boldsymbol{x}, c(\boldsymbol{x}) \rangle$ for some target concept c in C
  - each instance $\boldsymbol{x}$ is drawn from distribution $\mathcal{D}$
  - class label $c(\boldsymbol{x})$ is provided for each $\boldsymbol{x}$

- 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 probability distribution $\mathcal{D}$

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



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

$$error_{\mathrm{D}}(h) \equiv P_{x \in \mathrm{D}}\left[c(\boldsymbol{x}) \neq h(\boldsymbol{x})\right] = \frac{\sum_{x \in \mathrm{D}} \delta(c(\boldsymbol{x}) \neq h(\boldsymbol{x}))}{|\mathrm{D}|}$$

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 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 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 $error_{\mathcal{D}}(h) \leq \varepsilon$, provided time and sample size (from $\mathcal{D}$) 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 *c* if and only if $h(\boldsymbol{x}) = c(\boldsymbol{x})$ for each training example $\langle \boldsymbol{x}, c(\boldsymbol{x}) \rangle$ in D

$$consistent(h,\mathrm{D}) \equiv \left(\forall \langle \boldsymbol{x}, c(\boldsymbol{x})\rangle \in \mathrm{D}\right)\ h(\boldsymbol{x}) = c(\boldsymbol{x})$$

- 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

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

Exhausting the version space

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

$$(\forall h \in VS_{H,D})\ error_D(h) < \varepsilon$$

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)

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

Proof: $(1-\varepsilon)^m$ — probability a particular 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 $|H|$

$\leq |H| e^{-\varepsilon m}$ — $(1-\varepsilon) \leq e^{-\varepsilon}$ when $0 \leq \varepsilon \leq 1$

Sample complexity for finite hypothesis spaces

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

- choose *m* big enough to reduce this probability below δ

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

- solving for m we get desired result as long as:

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

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: $1/\varepsilon,\ 1/\delta, n$

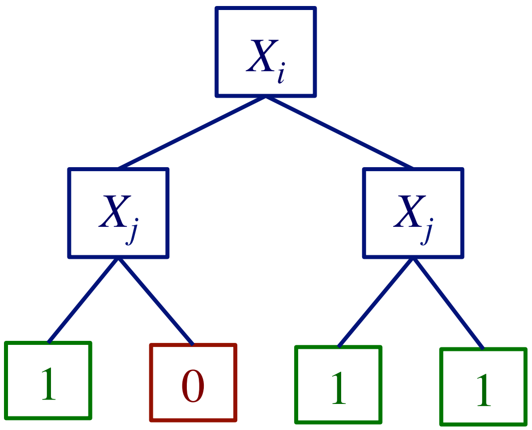
- to prove that Boolean conjunctions are PAC learnable, need to also show that we can find a consistent hypothesis in polynomial time (the FIND-S algorithm in Mitchell, Chapter 2 does this)

FIND-S:

initialize h to the most specific hypothesis $l_1 \wedge \neg l_1 \wedge l_2 \wedge \neg l_2 \ldots\ l_n \wedge \neg l_n$
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



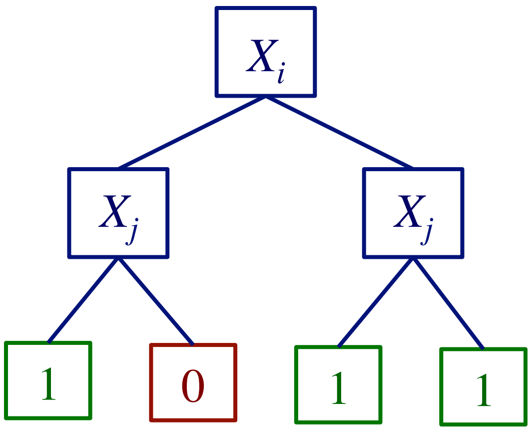
$$|H| = \binom{n}{2} \times 16 = \frac{n(n-1)}{2} \times 16 = 8n(n-1)$$

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

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

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)

Extensions, Results, Questions

- k-term DNF not properly PAC-learnable, but *PAC-predictable*, or PAC learnable in terms of kCNF
- negative results for PAC-predictability more robust
- results not based on NP-hardness of consistency problem, but on hard crytographic problems (Kearns & Valiant, 1994)
  - can’t PAC-learn Boolean formulae (unless can crack RSA)
  - can’t PAC-learn deterministic finite state machines (same)
- open PAC-learning questions include
  - DNF formulae
  - decision trees

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
- even if it is, might want to learn using another class (e.g., kCNF)
- *agnostic learning* setting
  - don't assume $c \in H$
  - learner returns hypothesis h that makes fewest errors on training data

- how many training instances suffice to ensure that $error_{\mathcal{D}}(h) \leq error_D(h) + \varepsilon$?

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

What if the hypothesis space is not finite?

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

- **A:** the largest subset of 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

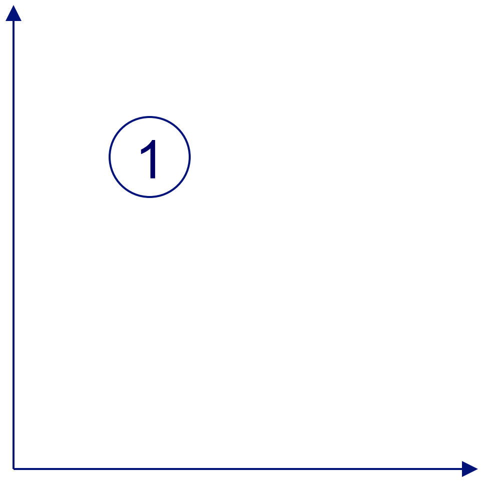
- a set of instances D is *shattered* by a hypothesis space H iff for every dichotomy of D there is a hypothesis in H consistent with this dichotomy

- the *VC dimension* of H defined over instance space X is the size of the largest finite subset of X shattered by H

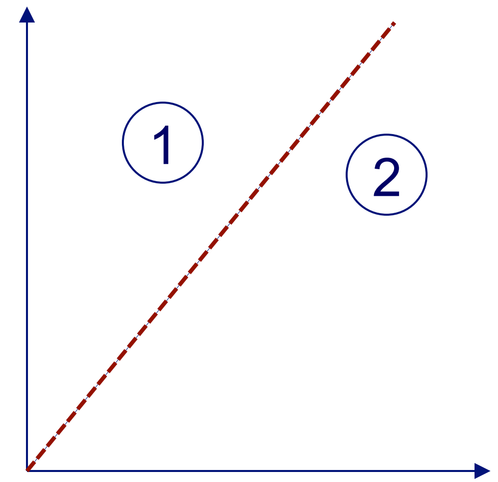
An infinite hypothesis space with a finite VC dimension

consider: H is set of lines (linear separators) in 2D

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



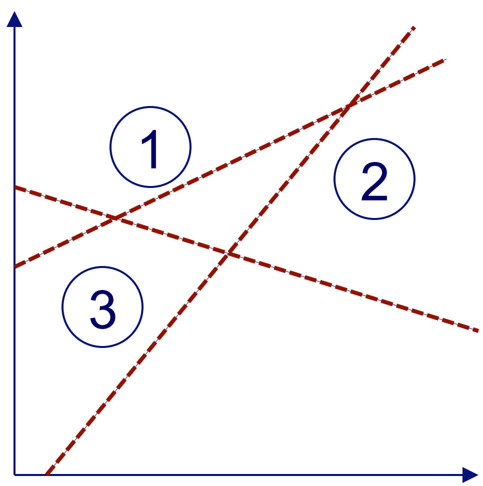
can find an h consistent with 2 instances no matter labeling



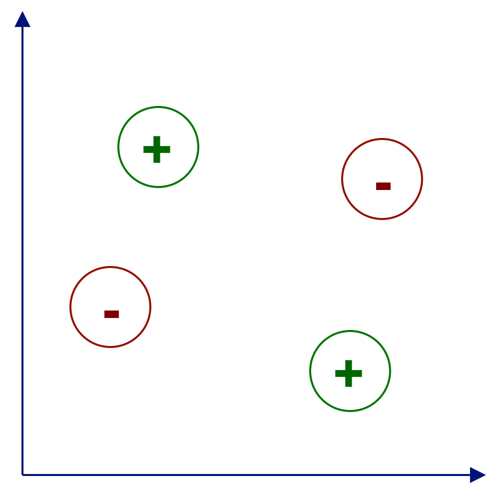
An infinite hypothesis space with a finite VC dimension

consider: H is set of lines in 2D

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



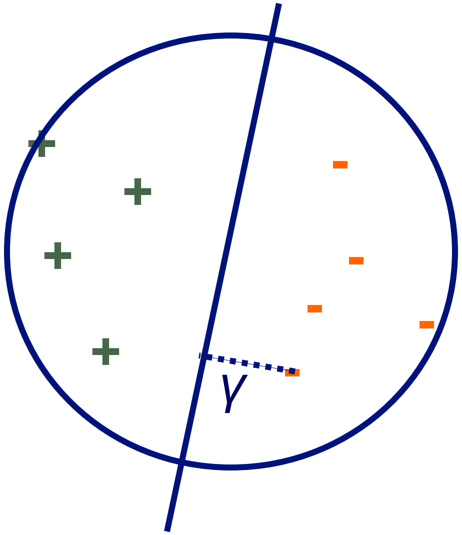
<u>cannot</u> find an h consistent with 4 instances for some labelings



can shatter 3 instances, but not 4 ➔ the VC-dim(H) = 3
more generally, the VC-dim of hyperplanes in n dimensions = $n+1$

Interesting aside

- VC-dim of hyperplane in n dimension is *n+1*
- Let *R* be radius of smallest hypersphere circumscribing the data, and let γ (margin) be smallest distance of any data point to hyperplane
- Can replace *n* in VC-dim with $(R/\gamma)^2$ if smaller



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]

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

m grows log × linear in ε

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 is

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

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

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 (PAC-*prediction)*
  - 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 (active learning)
  - restricted distributions (e.g. uniform) $\mathcal{D}$
- most analyses are worst case -> negative results, very restricted concept classes for positive results
- sample complexity bounds are generally not tight
- contributed major insights to ensembles, active learning, SVMs, …

Learning setting #2: on-line learning

Now let’s consider learning in the *on-line* learning setting:

for $t = 1 \ldots$

learner receives instance $\boldsymbol{x}_t$

learner predicts $h(\boldsymbol{x}_t)$

learner receives label $c(\boldsymbol{x}_t)$ and updates model h

The *mistake bound* model of learning

How many mistakes will an on-line learner make in its predictions before it learns the target concept?

the *mistake bound model* of learning addresses this question

Mistake bound example: learning conjunctions with FIND-S

consider the learning task

- training instances are represented by n Boolean features
- target concept is conjunction of up to n Boolean literals (variable or its negation)

FIND-S:

initialize h to the most specific hypothesis $l_1 \wedge \neg l_1 \wedge l_2 \wedge \neg l_2 \ldots\ l_n \wedge \neg l_n$
for each positive training instance $\boldsymbol{x}$
remove from h any literal that is not satisfied by $\boldsymbol{x}$
output hypothesis h

Example: using FIND-S to learn conjunctions

- suppose we're learning a concept representing the sports someone likes
- instances are represented using Boolean feature that characterize the sport

Snow	(is it done on snow?)
Water	
Road	
Mountain	
Skis	
Board	
Ball	(does it involve a ball?)

Example: using FIND-S to learn conjunctions

$t = 0$ $\quad h$: $snow \wedge \neg snow \wedge water \wedge \neg water \wedge road \wedge \neg road \wedge mountain \wedge \neg mountain \wedge skis \wedge \neg skis \wedge board \wedge \neg board \wedge ball \wedge \neg ball$

$t = 1$ $\quad \boldsymbol{x}$: $snow, \neg water, \neg road, mountain, skis, \neg board, \neg ball$

$h(\boldsymbol{x}) =$ false $\qquad c(\boldsymbol{x}) =$ true

h: $snow \wedge \neg water \wedge \neg road \wedge mountain \wedge skis \wedge \neg board \wedge \neg ball$

$t = 2$ $\quad \boldsymbol{x}$: $snow, \neg water, \neg road, \neg mountain, skis, \neg board, \neg ball$

$h(\boldsymbol{x}) =$ false $\qquad c(\boldsymbol{x}) =$ false

$t = 3$ $\quad \boldsymbol{x}$: $snow, \neg water, \neg road, mountain, \neg skis, board, \neg ball$

$h(\boldsymbol{x}) =$ false $\qquad c(\boldsymbol{x}) =$ true

h: $snow \wedge \neg water \wedge \neg road \wedge mountain \wedge \neg ball$

⋮

Mistake bound example: learning conjunctions with FIND-S

the maximum # of mistakes FIND-S will make = $n + 1$

Proof:

- FIND-S will never mistakenly classify a negative (h is always at least as specific as the target concept)
- initial h has $2n$ literals
- the first mistake on a positive instance will reduce the initial hypothesis to n literals
- each successive mistake will remove at least one literal from h

Halving algorithm

// initialize the version space to contain all $h \in H$

$VS_1 \leftarrow H$

for $t \leftarrow 1$ to T do

given training instance $\langle \boldsymbol{x}_t, c(\boldsymbol{x}_t) \rangle$

$h'(\boldsymbol{x}_t)$ = MajorityVote($VS_t, \boldsymbol{x}_t$)

// eliminate all wrong h from version space (reduce the size of the VS by at least half on mistakes)

$VS_{t+1} \leftarrow \{h \in VS_t : h(\boldsymbol{x}_t) = c(\boldsymbol{x}_t)\}$

return VS_{t+1}

Mistake bound for the Halving algorithm

the maximum # of mistakes the Halving algorithm will make = $\lfloor \log_2 |H| \rfloor$

Proof:

- initial version space contains $|H|$ hypotheses
- each mistake reduces version space by at least half

$\lfloor a \rfloor$ is the largest integer not greater than a

Optimal mistake bound

[Littlestone, *Machine Learning* 1987]

let C be an arbitrary concept class

$$VC(C) \leq M_{opt}(C) \leq M_{Halving}(C) \leq \log_2(|C|)$$

$M_{opt}(C)$: # mistakes by best algorithm (for hardest $c \in C$, and hardest training sequence)

$M_{Halving}(C)$: # mistakes by Halving algorithm

The Weighted Majority algorithm

given: a set of predictors $A = \{a_1 \; \ldots a_n\}$, learning rate $0 \leq \beta < 1$

for all i initialize $w_i \leftarrow 1$
for each training instance $\langle \, \boldsymbol{x}, c(\boldsymbol{x}) \, \rangle$
    initialize q_0 and q_1 to 0
    for each predictor a_i
        if $a_i(\boldsymbol{x}) = 0$ then $q_0 \leftarrow q_0 + w_i$
        if $a_i(\boldsymbol{x}) = 1$ then $q_1 \leftarrow q_1 + w_i$
    if $q_1 > q_0$ then $h(\boldsymbol{x}) = 1$
    else if $q_0 > q_1$ then $h(\boldsymbol{x}) = 0$
    else if $q_0 = q_1$ then $h(\boldsymbol{x}) = 0$ or 1 randomly chosen

    for each predictor a_i do
        if $a_i(\boldsymbol{x}) \neq c(\boldsymbol{x})$ then $w_i \leftarrow \beta \, w_i$

The Weighted Majority algorithm

- predictors can be individual features or hypotheses or learning algorithms
- if the predictors are all of the $h \in H$, then WM is like a weighted voting version of the Halving algorithm
- WM learns a linear separator, like a perceptron
- weight updates are multiplicative instead of additive (as in perceptron/neural net training)
  - multiplicative is better when there are many features (predictors) but few are relevant
  - additive is better when many features are relevant
- approach can handle noisy training data

Notes

- Halving algorithm eliminates inconsistent predictors on *every* round
- Two versions of weighted majority
  - Original only down-weights predictors on rounds where overall prediction is wrong
  - Also a version that down-weights wrong predictors on every round
  - Following bound applies to both versions

Relative mistake bound for Weighted Majority

Let

- D be any sequence of training instances
- A be any set of n predictors
- k be minimum number of mistakes made by best predictor in A for training sequence D

- the number of mistakes over D made by Weighted Majority using $\beta = 1/2$ is at most

$$2.4(k + \log_2 n)$$

Comments on mistake bound learning

- we've considered mistake bounds for learning the target concept exactly
- Learning with polynomial mistake bound and polynomial update time implies PAC learning (can turn any such mistake bounded learner into a PAC learner)
- some of the algorithms developed in this line of research have had practical impact (e.g. Weighted Majority, Winnow)
  [Blum, *Machine Learning* 1997]