Machine Learning 10-601

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Today:

- Computational Learning Theory
- Probably Approximately Coorrect (PAC) learning theorem
- Vapnik-Chervonenkis (VC) dimension

Recommended reading:

- Mitchell: Ch. 7
- suggested exercises: 7.1, 7.2, 7.7

Computational Learning Theory

- What general laws constrain inductive learning?
- Want theory to relate
  - Number of training examples
  - Complexity of hypothesis space
  - Accuracy to which target function is approximated
  - Manner in which training examples are presented
  - Probability of successful learning

* See annual Conference on Computational Learning Theory

Sample Complexity $f: X \to Y$

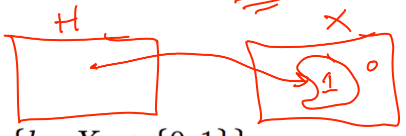
How many training examples suffice to learn target concept

1. If learner proposes instances as queries to teacher?
   - learner proposes x, teacher provides f(x)

2. If teacher (who knows f(x)) proposes training examples?
   - teacher proposes sequence {<x^1, f(x^1)>, … <x^n, f(x^n)>

3. If some random process (e.g., nature) proposes instances, and teacher labels them?
   - instances drawn according to $P(X)$

Sample Complexity 3



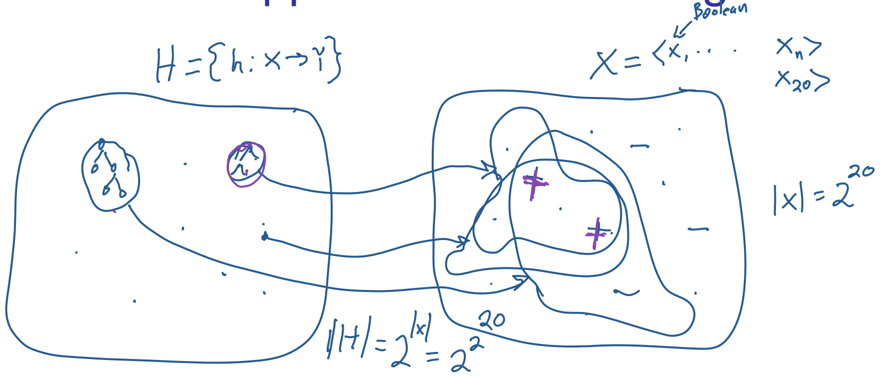
Problem setting:

- Set of instances X
- Set of hypotheses $H = \{h : X \to \{0,1\}\}$
- Set of possible target functions $C = \{c : X \to \{0,1\}\}$
- Sequence of training instances drawn at random from $P(X)$ teacher provides noise-free label $c(x)$

Learner outputs a hypothesis $h \in H$ such that

$$h = \arg\min_{h \in H} \; error_{train}(h)$$

Function Approximation: The Big Picture



$H = \{h : X \to Y\}$
Boolean
$X = \langle x_1, \dots x_n \rangle$
$x_{20} \rangle$
$|X| = 2^{20}$
$|H| = 2^{|X|} = 2^{2^{20}}$

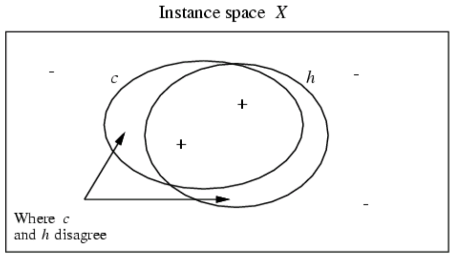
How many labeled examples are needed in order to determine which of the $2^{2^{20}}$ hypotheses is the correct one?

<u>All</u> 2^{20} instances in X must be labeled!

There is no free lunch!

Inductive inference - generalizing beyond the training data is impossible unless we add more assumptions (eg. priors over H)

True Error of a Hypothesis



The *true error* of h is the probability that it will misclassify an example drawn at random from $P(X)$

$$error_{true}(h) \equiv \Pr_{x \sim P(X)}[h(x) \neq c(x)]$$

Two Notions of Error

Training error of hypothesis h with respect to target concept c

- How often $h(x) \neq c(x)$ over training instances D

1 iff arg is true

$$\underbrace{error_{train}} \equiv \Pr_{x \in D}[hx \neq c(x)] = \frac{1}{|D|} \sum_{x \in D} \frac{\delta(h(x) \neq c(x))}{|D|}$$

training examples D

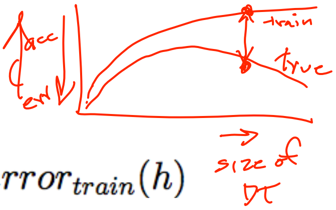
True error of hypothesis h with respect to c

- How often $h(x) \neq c(x)$ over future instances drawn at random from $\mathcal{D}$

$$\underbrace{error_{true}(h)} \equiv \Pr_{x \sim P(X)}[h(x) \neq c(x)]$$

Probability distribution P(X)

Overfitting



Consider a hypothesis h and its

- Error rate over training data: $error_{train}(h)$
- True error rate over all data: $error_{true}(h)$

We say h overfits the training data if

$$error_{true}(h) > error_{train}(h)$$

Amount of overfitting =

$$\boxed{error_{true}(h) - error_{train}(h)}$$

Overfitting

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Can we bound $error_{true}(h)$ in terms of $error_{train}(h)$??

$$error_{train} \equiv \Pr_{x \in D}[h(x) \neq c(x)] = \frac{1}{|D|} \sum_{x \in D} \frac{\delta(h(x) \neq c(x))}{|D|}$$

training examples

$$error_{true}(h) \equiv \Pr_{x \sim P(X)}[h(x) \neq c(x)]$$

Probability distribution P(x)

if D was a set of examples drawn from $P(X)$ and ***independent*** of h, then we could use standard statistical confidence intervals to determine that with 95% probability $error_{true}(h)$ lies in the interval:

$$error_D(h) \pm 1.96 \sqrt{\frac{error_D(h)\,(1 - error_D(h))}{n}}$$

but D is the ***training data*** for h ….

Version Spaces

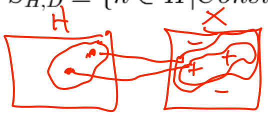
c: X → {0,1}

A hypothesis h is **consistent** with a set of training examples D of target concept c if and only if $h(x) = c(x)$ for each training example $\langle x, c(x)\rangle$ 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 examples D, is the subset of hypotheses from H consistent with all training examples in D.

$$VS_{H,D} \equiv \{h \in H | Consistent(h, D)\} = \{h \in H \mid error_{train}(h) = 0\}$$



Function Approximation: The Big Picture

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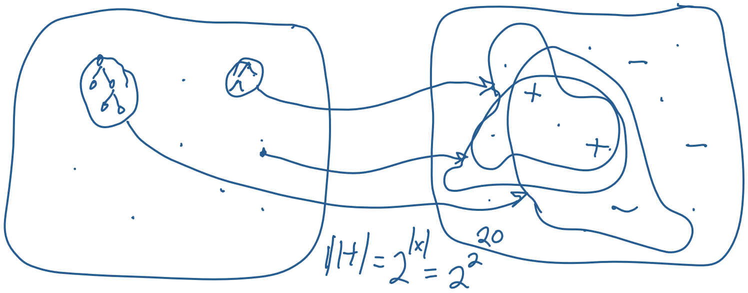
$X = \langle x_1, \ldots x_n \rangle$ Boolean

$x_{20}\rangle$



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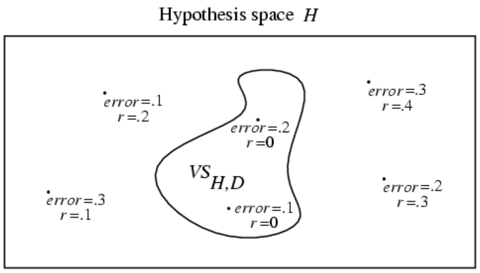
Exhausting the Version Space



(r = training error, $error$ = true error)

Definition: The version space $VS_{H,D}$ with respect to training data D is said to be **ϵ-exhausted** if every hypothesis h in $VS_{H,D}$ has true error less than ϵ.

$$(\forall h \in VS_{H,D})\ error_{true}(h) < \epsilon$$

How many examples will ϵ-exhaust the VS?

Theorem: [Haussler, 1988].

If the hypothesis space H is finite, and D is a sequence of $m \geq 1$ independent random examples of some target concept c, then for any $0 \leq \epsilon \leq 1$, the probability that the version space with respect to H and D is not ϵ-exhausted (with respect to c) is less than

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

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Interesting! This bounds the probability that any consistent learner will output a hypothesis h with $error(h) \geq \epsilon$

outputs h such that $error_{train}(h) = 0$

Any(!) learner that outputs a hypothesis consistent with all training examples (i.e., an h contained in $VS_{H,D}$)

hyp space H

target fn $c: X \to \{0,1\}$

Let $h_1 \dots h_k$ be all of the $h \in H$ s.t. $error_{true}(h) \geq \epsilon$

present m train examps.

Prob that h_1 will be consistent with 1st train example

$< (1-\epsilon)$

Prob that h_1 will be consistent with first m examples

$< (1-\epsilon)^m$ $P(A \vee B) \leq P(A) + P(B)$

Prob that a least one of $h_1 \dots h_k$ survives first m examps

$\leq k(1-\epsilon)^m$

$\leq |H|(1-\epsilon)^m$

$(1-\epsilon) \leq e^{-\epsilon}$
when $0 \leq \epsilon \leq 1$

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

Example: H is Conjunction of up to N Boolean Literals

$$m \geq \frac{1}{\epsilon}(\ln|H| + \ln(1/\delta))$$

Consider classification problem f:X→Y:

- instances: $X = <X_1\ X_2\ X_3\ \overset{n}{X_4}>$ where each X_i is boolean
- Each hypothesis in H is a rule of the form:
  - IF $<X_1\ X_2\ X_3\ X_4> = <0,?,1,?>$, THEN Y=1, ELSE Y=0
  - i.e., rules constrain any subset of the X_i

How many training examples *m* suffice to assure that with probability at least 0.99, *any* consistent learner using H will output a hypothesis with true error at most 0.05?

$$\geq \frac{1}{0.05}\left(\ln 3^{\cancel{4}\,n} + \ln\left(\frac{1}{.01}\right)\right) \geq 180$$

$$m \geq \frac{1}{0.05}\left(n \ln 3 + \ln\left(\frac{1}{.01}\right)\right)$$

What it means

[Haussler, 1988]: probability that the version space is not ε-exhausted after *m* training examples is at most $|H|e^{-\epsilon m}$

$$\Pr[(\exists h \in H) s.t. (error_{train}(h) = 0) \wedge (error_{true}(h) > \epsilon)] \leq |H|e^{-\epsilon m}$$

↑ over diff samples of m training examples

Suppose we want this probability to be at most δ

1. How many training examples suffice?

$$m \geq \frac{1}{\epsilon}(\ln|H| + \ln(1/\delta))$$

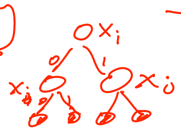
2. If $error_{train}(h) = 0$ then with probability at least (1-δ):

$$error_{true}(h) \leq \frac{1}{m}(\ln|H| + \ln(1/\delta))$$

Example: H is Decision Tree with depth=2

Consider classification problem f:X→Y:

- instances: $X = \langle X_1 \ldots X_N \rangle$ where each X_i is boolean
- learned hypotheses are decision trees of depth 2, using only two variables



How many training examples *m* suffice to assure that with probability at least 0.99, *any* consistent learner will output a hypothesis with true error at most 0.05?

$$\binom{n}{2}\ 16$$

$$m \geq \frac{1}{.05}\left(\ln |H| + \ln \frac{1}{0.01}\right)$$

2 bpsn

$$\left(\frac{n(n-1)}{2} \cdot 16\right)$$

PAC Learning

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.

> *Definition:* C is **PAC-learnable** by L using H if for all $c \in C$, distributions $\mathcal{D}$ over X, ϵ such that $0 < \epsilon < 1/2$, and δ such that $0 < \delta < 1/2$,
> learner L will with probability at least $(1-\delta)$ output a hypothesis $h \in H$ such that $error_{\mathcal{D}}(h) \leq \epsilon$, in time that is polynomial in $1/\epsilon$, $1/\delta$, n and $size(c)$.

PAC Learning

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Sufficient condition:

Holds if learner L requires only a polynomial number of training examples, and processing per example is polynomial

Agnostic Learning

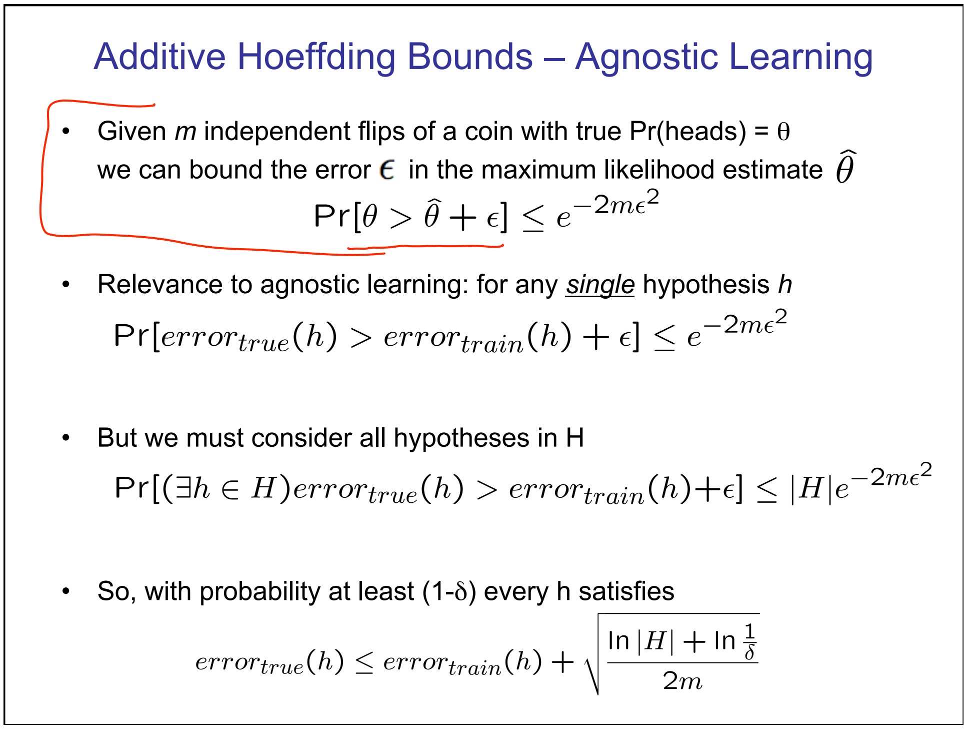
So far, assumed $c \in H$

Agnostic learning setting: don't assume $c \in H$

- What do we want then?
  - The hypothesis h that makes fewest errors on training data
- What is sample complexity in this case?

$$m \geq \frac{1}{2\epsilon^2}(\ln |H| + \ln(1/\delta))$$

Here ε is the difference between the training error and true error of the output hypothesis (the one with lowest training error)



Additive Hoeffding Bounds – Agnostic Learning

- Given *m* independent flips of a coin with true Pr(heads) = θ we can bound the error ϵ in the maximum likelihood estimate $\widehat{\theta}$

$$\Pr[\theta > \underline{\widehat{\theta} + \epsilon]} \leq e^{-2m\epsilon^2}$$

- Relevance to agnostic learning: for any *single* hypothesis *h*

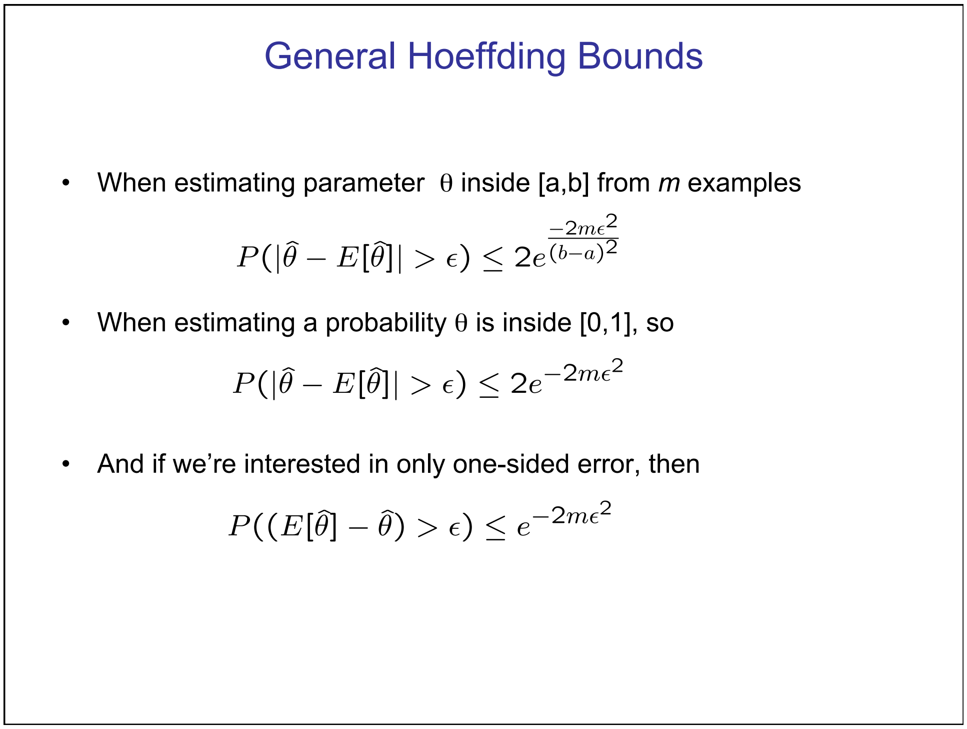
$$\Pr[error_{true}(h) > error_{train}(h) + \epsilon] \leq e^{-2m\epsilon^2}$$

- But we must consider all hypotheses in H

$$\Pr[(\exists h \in H) error_{true}(h) > error_{train}(h) + \epsilon] \leq |H| e^{-2m\epsilon^2}$$

- So, with probability at least (1-δ) every h satisfies

$$error_{true}(h) \leq error_{train}(h) + \sqrt{\frac{\ln |H| + \ln \frac{1}{\delta}}{2m}}$$



General Hoeffding Bounds

- When estimating parameter θ inside [a,b] from *m* examples

$$P(|\widehat{\theta} - E[\widehat{\theta}]| > \epsilon) \leq 2e^{\frac{-2m\epsilon^2}{(b-a)^2}}$$

- When estimating a probability θ is inside [0,1], so

$$P(|\widehat{\theta} - E[\widehat{\theta}]| > \epsilon) \leq 2e^{-2m\epsilon^2}$$

- And if we're interested in only one-sided error, then

$$P((E[\widehat{\theta}] - \widehat{\theta}) > \epsilon) \leq e^{-2m\epsilon^2}$$

$$m \geq \frac{1}{\epsilon}(\ln \underbrace{|H|}_{\infty} + \ln(1/\delta))$$

Question: If H = {h | h: X → Y} is infinite, what measure of complexity should we use in place of |H| ?

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Question: If H = {h | h: X → Y} is infinite, what measure of complexity should we use in place of |H| ?

Answer: The largest subset of X for which H can guarantee zero training error (regardless of the target function c)

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VC dimension of H is the size of this subset

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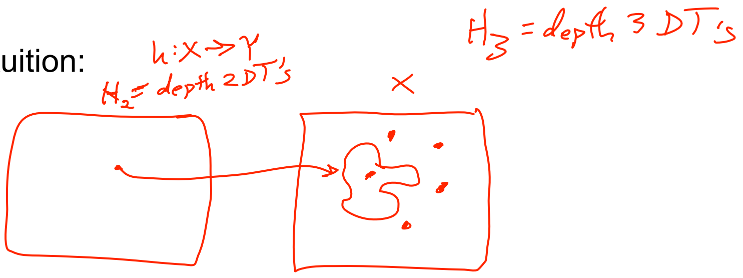
Informal intuition:



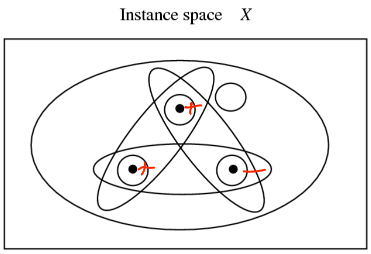
Shattering a Set of Instances

Definition: a **dichotomy** of a set S is a partition of S into two disjoint subsets.

a labeling of each member of S as positive or negative

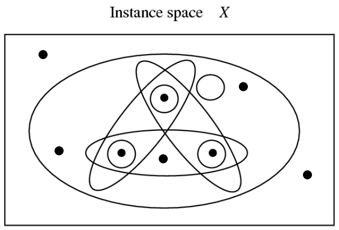
Definition: a set of instances S is **shattered** by hypothesis space H if and only if for every dichotomy of S there exists some hypothesis in H consistent with this dichotomy.

= H can guarantee zero training error over S



The Vapnik-Chervonenkis Dimension

Definition: The **Vapnik-Chervonenkis dimension**, $VC(H)$, of hypothesis space H defined over instance space X is the size of the largest finite subset of X shattered by H. If arbitrarily large finite sets of X can be shattered by H, then $VC(H) \equiv \infty$.



VC(H)=3

Sample Complexity based on VC dimension

How many randomly drawn examples suffice to ε-exhaust $VS_{H,D}$ with probability at least (1-δ)?

ie., to guarantee that any hypothesis that perfectly fits the training data is probably (1-δ) approximately (ε) correct

$$\boxed{m \geq \frac{1}{\epsilon}(4 \log_2(2/\delta) + 8VC(H) \log_2(13/\epsilon))}$$

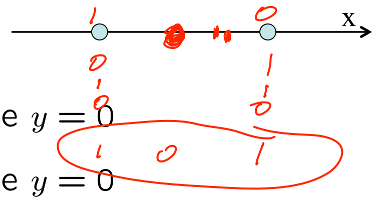
Compare to our earlier results based on |*H*|:

$$m \geq \frac{1}{\epsilon}(\ln(1/\delta) + \ln |H|)$$

VC dimension: examples

Consider X = <, want to learn c:X→{0,1}

What is VC dimension of



- Open intervals:

  H1: if $x > a$ then $y = 1$ else $y = 0$

  VC(H1)=1

  VC(H2)=2

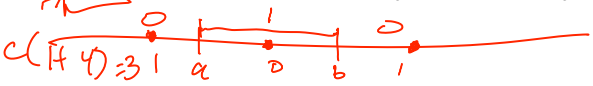
  H2: if $x > a$ then $y = 1$ else $y = 0$
  or, if $x > a$ then $y = 0$ else $y = 1$

- Closed intervals:

  H3: if $a < x < b$ then $y = 1$ else $y = 0$

  H4: if $a < x < b$ then $y = 1$ else $y = 0$
  or, if $a < x < b$ then $y = 0$ else $y = 1$ ✓

VC(H4)=3



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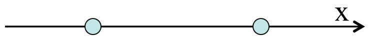


- Open intervals:

  H1: if $x > a$ then $y = 1$ else $y = 0$ VC(H1)=1

  H2: if $x > a$ then $y = 1$ else $y = 0$
  or, if $x > a$ then $y = 0$ else $y = 1$ VC(H2)=2

- Closed intervals:

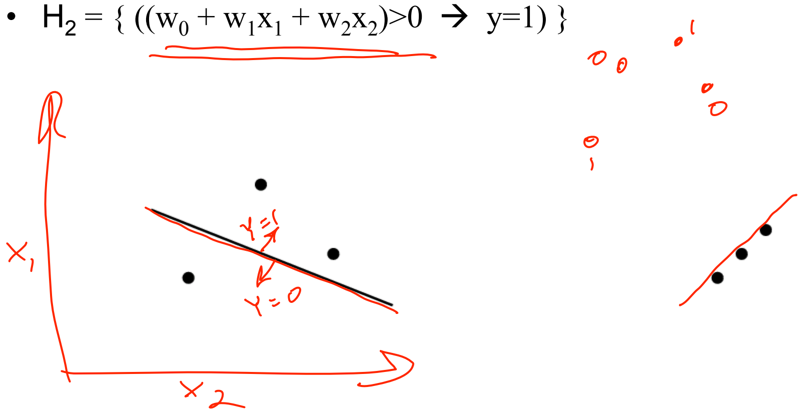
  H3: if $a < x < b$ then $y = 1$ else $y = 0$ VC(H3)=2

  H4: if $a < x < b$ then $y = 1$ else $y = 0$ VC(H4)=3
  or, if $a < x < b$ then $y = 0$ else $y = 1$

VC dimension: examples

What is VC dimension of lines in a plane?

- $H_2 = \{ \underline{((w_0 + w_1x_1 + w_2x_2)>0} \rightarrow y=1) \}$



VC dimension: examples

What is VC dimension of

- $H_2 = \{ ((w_0 + w_1x_1 + w_2x_2)>0 \rightarrow y=1) \}$
  - $VC(H_2)=3$
- For H_n = linear separating hyperplanes in n dimensions, VC $(H_n)=n+1$

For any finite hypothesis space H, can you give an upper bound on VC(H) in terms of |H| ? (hint: yes)

More VC Dimension Examples to Think About

- Logistic regression over n continuous features
  - Over n boolean features?
- Linear SVM over n continuous features
- Decision trees defined over n boolean features

  F: $<X_1, \ldots X_n> \rightarrow Y$
- Decision trees of depth 2 defined over n features
- How about 1-nearest neighbor?

Tightness of Bounds on Sample Complexity

How many examples *m* suffice to assure that any hypothesis that fits the training data perfectly is probably (1-δ) approximately (ε) correct?

$$m \geq \frac{1}{\epsilon}(4\log_2(2/\delta) + 8VC(H)\log_2(13/\epsilon))$$

How tight is this bound?

Tightness of Bounds on Sample Complexity

How many examples *m* suffice to assure that any hypothesis that fits the training data perfectly is probably (1-δ) approximately (ε) correct?

$$m \geq \frac{1}{\epsilon}(4\log_2(2/\delta) + 8VC(H)\log_2(13/\epsilon))$$

How tight is this bound?

Lower bound on sample complexity (Ehrenfeucht et al., 1989):

Consider any class C of concepts such that VC(C) > 1, any learner L, any 0 < ε < 1/8, and any 0 < δ < 0.01. Then there exists a distribution $\mathcal{D}$ P(x) and a target concept in C, such that if L observes fewer examples than

$$\max\left[\frac{1}{\epsilon}\log(1/\delta), \frac{VC(C)-1}{32\epsilon}\right]$$

Then with probability at least δ, L outputs a hypothesis with $error_{\underset{true}{\mathcal{D}}}(h) > \epsilon$

Agnostic Learning: VC Bounds

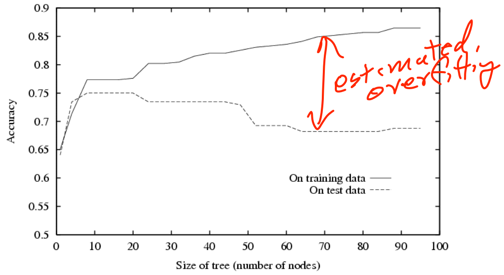
[Schölkopf and Smola, 2002]

With probability at least (1-δ) every $h \in H$ satisfies

$$error_{true}(h) < error_{train}(h) + \sqrt{\frac{VC(H)(\ln \frac{2m}{VC(H)} + 1) + \ln \frac{4}{\delta}}{m}}$$

$Overfitting(h) < \sqrt{}$

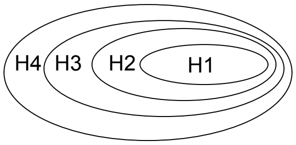
$Overfitting = error_{true}(h) - error_{train}(h)$



Structural Risk Minimization [Vapnik]

Which hypothesis space should we choose?

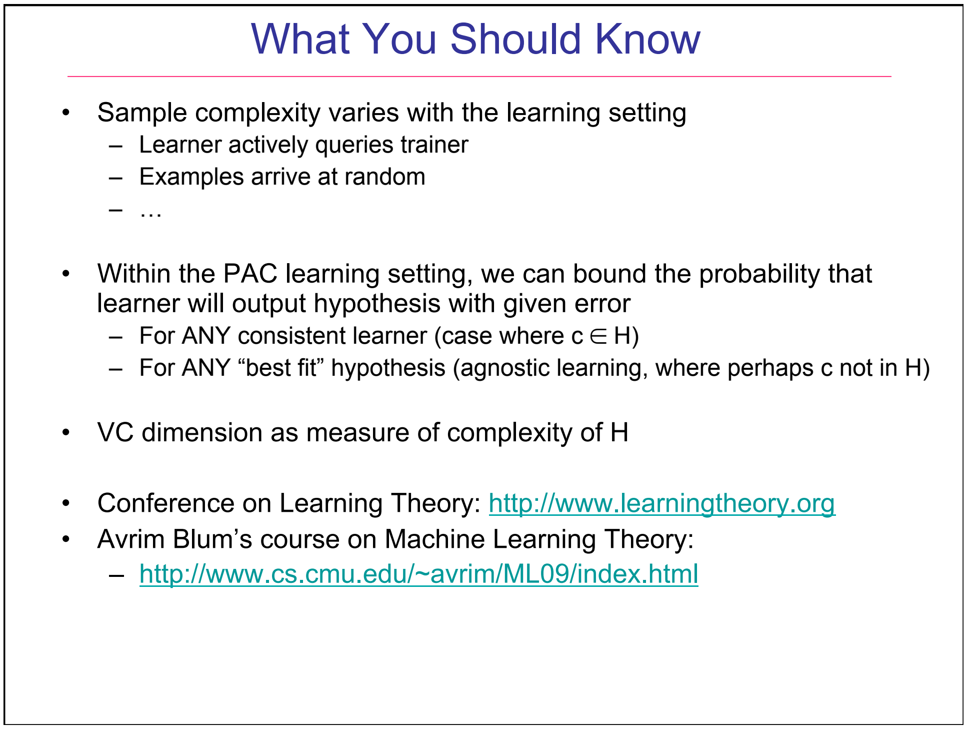
- Bias / variance tradeoff



SRM: choose H to minimize bound on expected true error!

$$error_{true}(h) < error_{train}(h) + \sqrt{\frac{VC(H)(\ln \frac{2m}{VC(H)} + 1) + \ln \frac{4}{\delta}}{m}}$$

* unfortunately a somewhat loose bound...



What You Should Know

- Sample complexity varies with the learning setting
  - Learner actively queries trainer
  - Examples arrive at random
  - …

- Within the PAC learning setting, we can bound the probability that learner will output hypothesis with given error
  - For ANY consistent learner (case where c ∈ H)
  - For ANY “best fit” hypothesis (agnostic learning, where perhaps c not in H)

- VC dimension as measure of complexity of H

- Conference on Learning Theory: http://www.learningtheory.org
- Avrim Blum’s course on Machine Learning Theory:
  - http://www.cs.cmu.edu/~avrim/ML09/index.html