Computational Learning Theory

VC dimension, Sample Complexity, Mistake bounds

Required reading:

- Mitchell chapter 7

Optional advanced reading:

- Kearns & Vazirani, ‘Introduction to Computational Learning Theory’

Machine Learning 10-701

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October 25, 2005

Last time: PAC Learning

1. Finite H, assume target function c $\in$ H

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

Suppose we want this to be at most δ. Then *m* examples suffice:

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

2. Finite H, agnostic learning: perhaps c *not* in H

with probability at least (1-δ) every h in H satisfies

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

What if H is not finite?

- Can't use our result for finite H

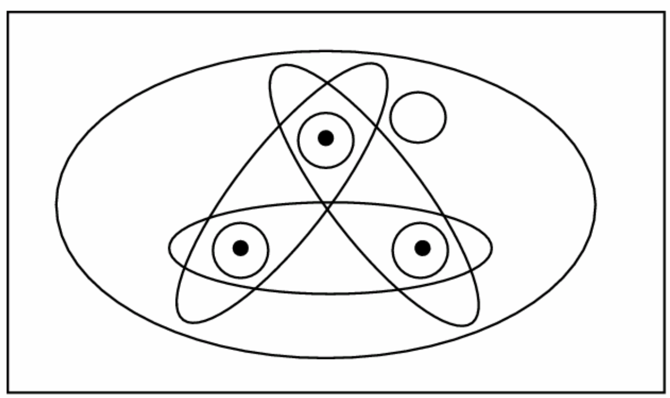
- Need some other measure of complexity for H
  - Vapnik-Chervonenkis (VC) dimension!

Shattering a Set of Instances

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

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.

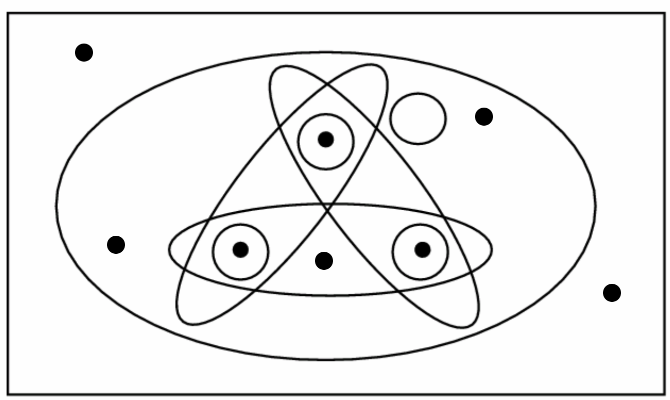
Instance space X



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 $VC(H) \equiv \infty$.

Instance space X



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

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

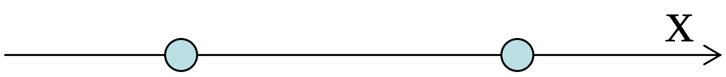
Compare to our earlier results based on |*H*|:

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

VC dimension: examples

Consider X = $\Re$, want to learn c:X→{0,1}

What is VC dimension of



- Open intervals:

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

  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 dimension: examples

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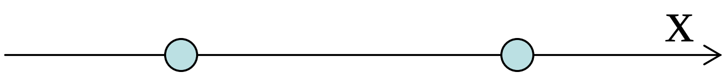


- Open intervals:

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

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

- Closed intervals:

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

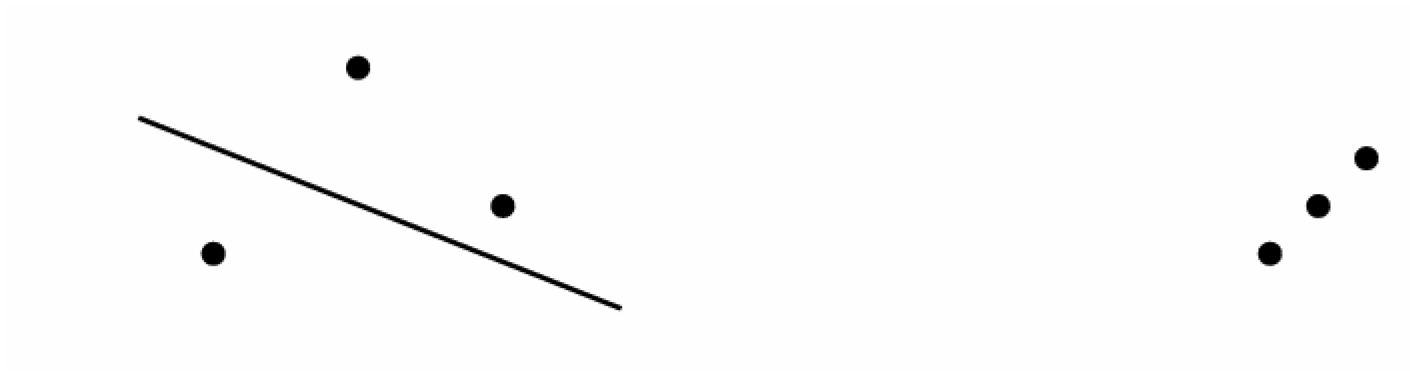
H4: if $a < x < b$ then $y = 1$ else $y = 0$ VC(H4)=3
or, if $a < x < b$ then $y = 0$ else $y = 1$

VC dimension: examples

Consider $X = \Re^2$, want to learn $c: X \rightarrow \{0,1\}$

What is VC dimension of lines in a plane?

- $H = \{ ((w \cdot x+b)>0 \rightarrow y=1) \mid w \in \Re^2, b \in \Re \}$



VC dimension: examples

Consider X = $\Re^2$, want to learn c:X→{0,1}

What is VC dimension of

- H = { ((w·x+b)>0 → y=1) | w ∈$\Re^2$, b ∈ $\Re$}
  - VC(H1)=3
  - For linear separating hyperplanes in n dimensions, VC(H)=n+1

For any finite hypothesis space H,
give an upper bound on VC(H) in terms of |H|

More VC Dimension Examples

- Decision trees defined over n boolean features

  F: $<X_1, \ldots X_n> \rightarrow Y$

- Decision trees defined over n continuous features

  Where each internal tree node involves a threshold test $(X_i > c)$

- Decision trees of depth 2 defined over n features

- Logistic regression over n continuous features? Over n boolean 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?

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

Consider any class C of concepts such that VC(C) ≥ 2, any learner L, any 0 < ε < 1/8, and any 0 < δ < 0.01. Then there exists a distribution $\mathcal{D}$ and target concept in C, such that if L observes fewer examples than

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

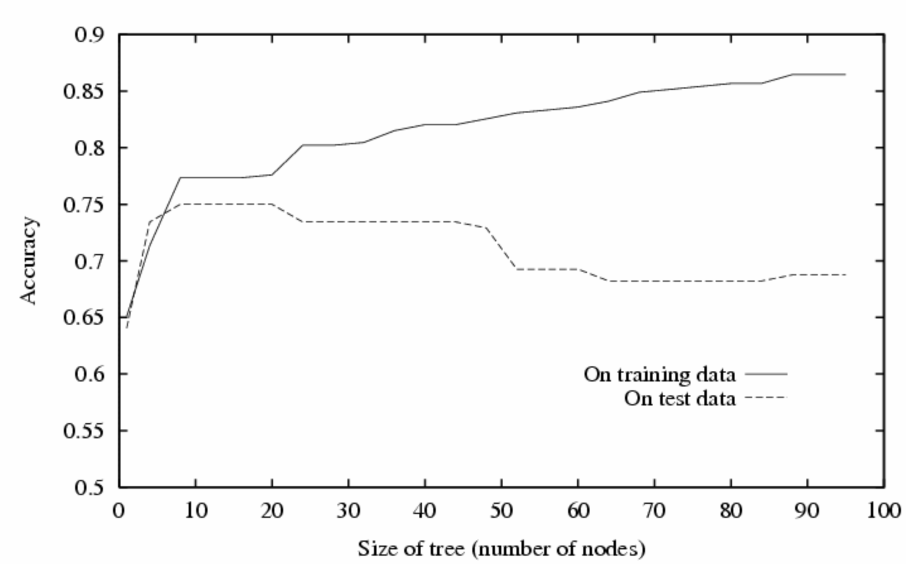
Then with probability at least δ, L outputs a hypothesis with $error_{\mathcal{D}}(h) > \epsilon$

Agnostic Learning: VC Bounds

[Schölkopf and Smola, 2002]

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

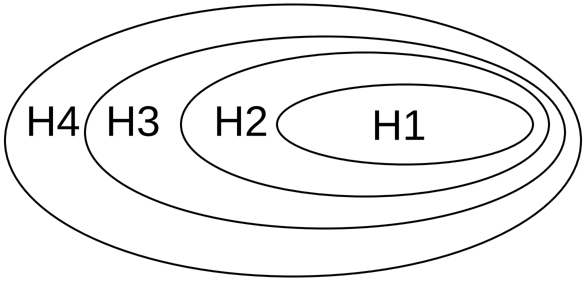
$$error_{true}(h) < error_{train}(h) + \sqrt{\frac{VC(H)(\ln \frac{2m}{VC(H)} + 1) + \ln \frac{4}{\delta}}{m}}$$



Structural Risk Minimization [Vapnik]

Which hypothesis space should we choose?

- Bias / variance tradeoff



SRM: choose H to minimize bound on 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...

Mistake Bounds

So far: how many examples needed to learn?

What about: how many mistakes before convergence?

Let's consider similar setting to PAC learning:

- Instances drawn at random from X according to distribution $\mathcal{D}$
- Learner must classify each instance before receiving correct classification from teacher
- Can we bound the number of mistakes learner makes before converging?

Mistake Bounds: Find-S

Consider Find-S when H = conjunction of boolean literals

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 x
  - Remove from h any literal that is not satisfied by x
- Output hypothesis h.

How many mistakes before converging to correct h?

Mistake Bounds: Halving Algorithm

1. Initialize VS ← H
2. For each training example,
   - remove from VS every hypothesis that misclassifies this example

Consider the Halving Algorithm:

- Learn concept using version space CANDIDATE-ELIMINATION algorithm
- Classify new instances by majority vote of version space members

How many mistakes before converging to correct h?

- ... in worst case?
- ... in best case?

Optimal Mistake Bounds

Let $M_A(C)$ be the max number of mistakes made by algorithm A to learn concepts in C. (maximum over all possible $c \in C$, and all possible training sequences)

$$M_A(C) \equiv \max_{c \in C} M_A(c)$$

Definition: Let C be an arbitrary non-empty concept class. The **optimal mistake bound** for C, denoted $Opt(C)$, is the minimum over all possible learning algorithms A of $M_A(C)$.

$$Opt(C) \equiv \min_{A \in learning\ algorithms} M_A(C)$$

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

Weighted Majority Algorithm

a_i denotes the i^{th} prediction algorithm in the pool A of algorithms. w_i denotes the weight associated with a_i.

- For all i initialize $w_i \leftarrow 1$
- For each training example $\langle x, c(x) \rangle$
  - * Initialize q_0 and q_1 to 0
  - * For each prediction algorithm a_i
    - · If $a_i(x) = 0$ then $q_0 \leftarrow q_0 + w_i$
      If $a_i(x) = 1$ then $q_1 \leftarrow q_1 + w_i$
  - * If $q_1 > q_0$ then predict $c(x) = 1$
    If $q_0 > q_1$ then predict $c(x) = 0$
    If $q_1 = q_0$ then predict 0 or 1 at random for $c(x)$
  - * For each prediction algorithm a_i in A do
    If $a_i(x) \neq c(x)$ then $w_i \leftarrow \beta w_i$

when β=0, equivalent to the Halving algorithm…

Weighted Majority

Even algorithms that learn or change over time…

[Relative mistake bound for WEIGHTED-MAJORITY] Let D be any sequence of training examples, let A be any set of n prediction algorithms, and let k be the minimum number of mistakes made by any algorithm in A for the training sequence D. Then the number of mistakes over D made by the WEIGHTED-MAJORITY algorithm using $\beta = \frac{1}{2}$ is at most

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

What You Should Know

- Sample complexity varies with the learning setting
  - Learner actively queries trainer
  - Examples provided 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 $c \in H$)
  - For ANY "best fit" hypothesis (agnostic learning, where perhaps c not in H)

- VC dimension as measure of complexity of H

- Quantitative bounds characterizing bias/variance in choice of H
  - but the bounds are quite loose...

- Mistake bounds in learning

- Conference on Learning Theory: http://www.learningtheory.org

General Hoeffding Bounds

- When estimating parameter $\theta \in [a,b]$ from *m* examples

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

- When estimating a probability $\theta \in [0,1]$, so

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

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

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