Computational Learning Theory – Part 2

Reading:

• Mitchell chapter 7

Suggested exercises:

• 7.1, 7.2, 7.5, 7.7

Machine Learning 10-701

Tom M. Mitchell
Machine Learning Department
Carnegie Mellon University

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What it means

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

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

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):

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

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 $size(c)$.

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learner L will with probability at least $(1 - \delta)$ output a hypothesis $h \in H$ such that $error_{\mathcal{D}}(h) \leq \epsilon$, in <u>time that is polynomial</u> in $1/\epsilon$, $1/\delta$, n and $size(c)$.

Sufficient condition:

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

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

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

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VC dimension of H is the size of this subset

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

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

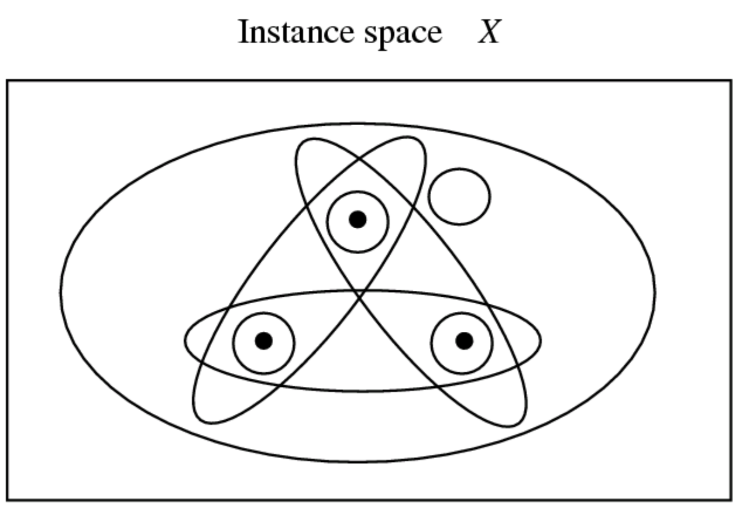
Informal intuition:

Shattering a Set of Instances

a labeling of each member of S as positive or negative

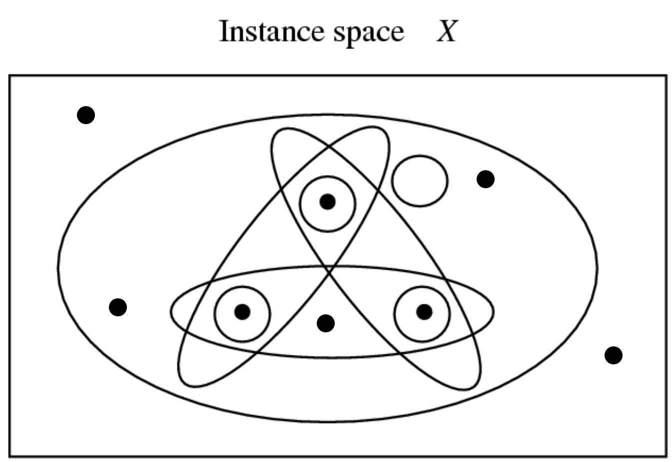
Definition: a **dichotomy** of a set S is a partition of S into two disjoint subsets.

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.



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

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

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 $y = 0$

  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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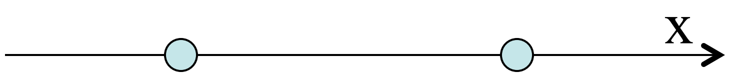


- Open intervals:

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

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

- Closed intervals:

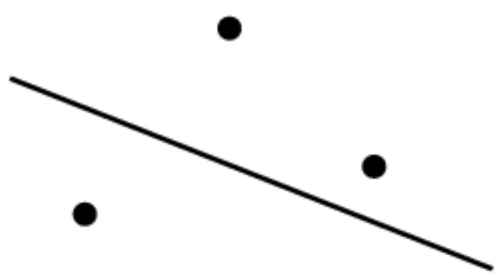
  H3: if $a < x < b$ then $y = 1$ else $y = 0$ VC(H3)=2

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

VC dimension: examples

What is VC dimension of lines in a plane?

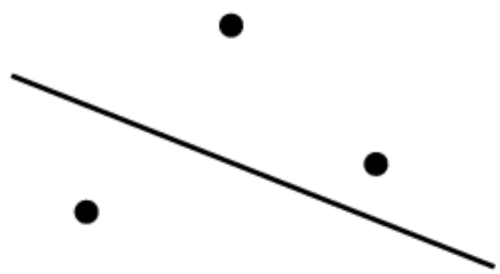
- $H_2 = \{ ((w_0 + w_1x_1 + w_2x_2)>0 \rightarrow y=1) \}$



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 $\mathcal{D}$ and a target concept in C, such that if L observes fewer examples than

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

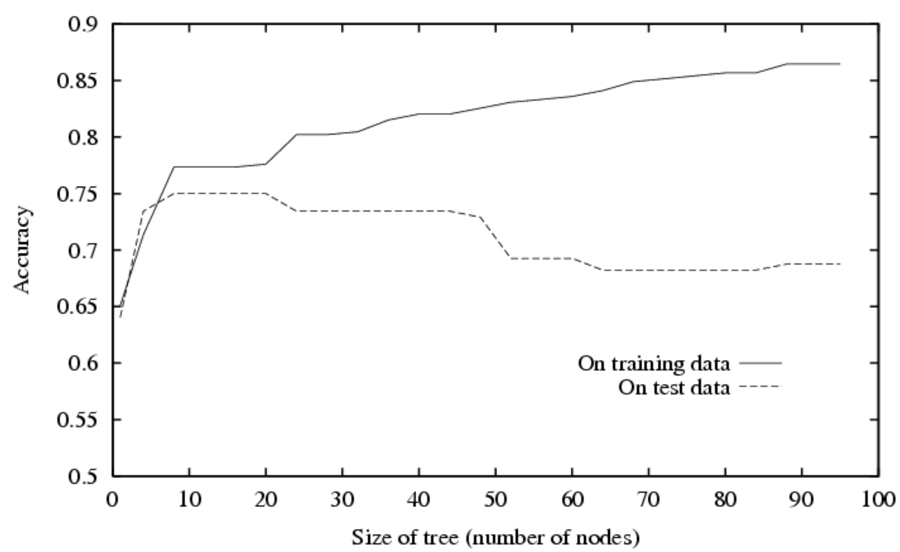
Then with probability at least δ, L outputs a hypothesis with $error_{\mathcal{D}}(h) > \epsilon$

Agnostic Learning: VC Bounds

[Schölkopf and Smola, 2002]

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

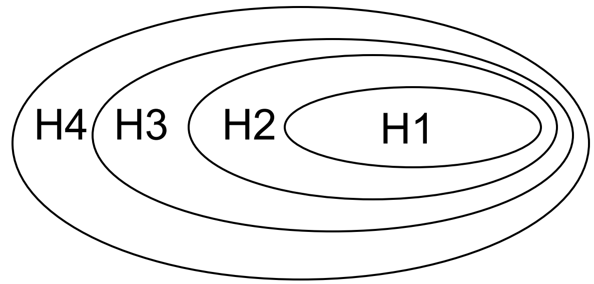
$$error_{true}(h) < error_{train}(h) + \sqrt{\frac{VC(H)(\ln \frac{2m}{VC(H)} + 1) + \ln \frac{4}{\delta}}{m}}$$



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 $M_A(C)$.

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

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

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 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 $c \in H$)
  - For ANY "best fit" hypothesis (agnostic learning, where perhaps c not in H)
- VC dimension as measure of complexity of H
- Mistake bounds
- 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