Computational Learning Theory

Reading:
- Mitchell chapter 7

Suggested exercises:
- 7.1, 7.2, 7.5, 7.7

Machine Learning 10-701

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March 17, 2010

Computational Learning Theory

What general laws constrain inductive learning?

We seek theory to relate:

- Probability of successful learning
- Number of training examples
- Complexity of hypothesis space
- Accuracy to which target function is approximated
- Manner in which training examples presented

Sample Complexity

Want to learn $F : X \to Y$
$C : X \to Y$

How many training examples are sufficient to learn the target concept?

1. If learner proposes instances, as queries to teacher
   - Learner proposes instance x, teacher provides $c(x)$
2. If teacher (who knows c) provides training examples
   - teacher provides sequence of examples of form $\langle x, c(x) \rangle$
3. If some random process (e.g., nature) proposes instances $P(X)$
   - instance x generated randomly, teacher provides $c(x)$

Sample Complexity: 3

Given:

- set of instances X
- set of hypotheses H
- set of possible target concepts C $\quad c : X \to \{0,1\}$ $\quad c \in C$
- training instances generated by a fixed, unknown probability distribution $\mathcal{D}$ over X $\quad \mathcal{D} = P(X)$

Learner observes a sequence D of training examples of form $\langle x, c(x) \rangle$, for some target concept $c \in C$

- instances x are drawn from distribution $\mathcal{D}$
- teacher provides target value $c(x)$ for each

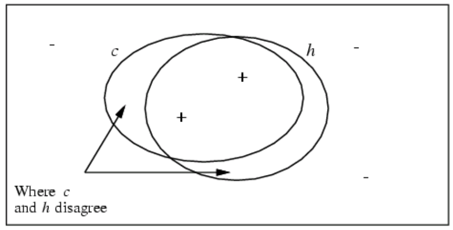
Learner must output a hypothesis h estimating c

- h is evaluated by its performance on subsequent instances drawn according to $\mathcal{D}$

Note: randomly drawn instances, noise-free classifications

True Error of a Hypothesis

Instance space X $\quad P(X) = \mathcal{D}$



Definition: The **true error** (denoted $error_{\mathcal{D}}(h)$) of hypothesis h with respect to target concept c and distribution $\mathcal{D}$ is the probability that h will misclassify an instance drawn at random according to $\mathcal{D}$.

$$error_{\mathcal{D}}(h) \equiv \Pr_{x \in \mathcal{D}}[c(x) \neq h(x)]$$

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

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

training examples

True error of hypothesis h with respect to c

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

$$error_{\mathcal{D}}(h) \equiv \Pr_{x \in \mathcal{D}}[c(x) \neq h(x)]$$

Probability distribution P(x)

Two Notions of Error

Can we bound $error_{\mathcal{D}}(h)$ in terms of $error_{\mathrm{D}}(h)$??

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Probability distribution P(x)

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

$$error_{\mathrm{D}}(h) \pm 1.96 \sqrt{\frac{error_{\mathrm{D}}(h)\,(1 - error_{\mathrm{D}}(h))}{n}}$$

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

Version Spaces

Target concept is the (usually unknown) boolean fn to be learned

c: X → {0,1}

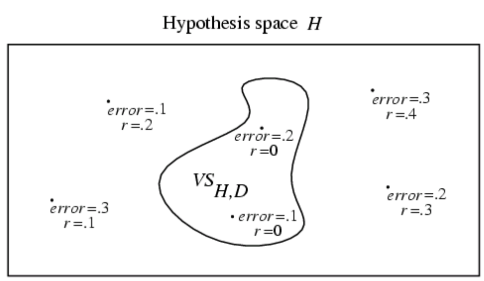
A hypothesis h is **consistent** with a set of training examples D of target concept c if and only if $h(x) = c(x)$ for each training example $\langle x, c(x) \rangle$ in D.

$$Consistent(h, D) \equiv (\forall \langle x, c(x) \rangle \in D)\ h(x) = c(x)$$

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.

$$VS_{H,D} \equiv \{h \in H | Consistent(h, D)\}$$

Exhausting the Version Space



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

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

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

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 $error(h) \geq \epsilon$

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

hyp space H, let $h_1, h_2 \cdots h_k$ be the k hyps in $\underline{H}$ with true error $> \epsilon$

pick h_2

prob h_2 consist with one train example $\leq 1-\epsilon$

" m iid train examps $(1-\epsilon)^m$

$\boxed{\text{prob that at least one of } h_1 .. h_k \text{ will be consist with } m \text{ examps}}$

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

prob $\boxed{< |H| (1-\epsilon)^m}$

In general for $0 \leq \epsilon \leq 1$ then $(1-\epsilon) \leq e^{-\epsilon}$

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

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):

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

Example: H is Conjunction of Boolean Literals

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

Consider classification problem f:X→Y:

- instances: <X_1 X_2 X_3 X_4> where each X_i is boolean
- learned hypotheses are rules 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

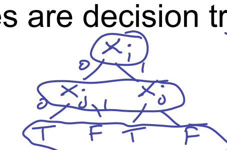
How many training examples *m* suffice to assure that with probability at least 0.9, *any* consistent learner will output a hypothesis with true error at most 0.05?

Example: H is Decision Tree with depth=2

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

Consider classification problem f:X→Y:

- instances: <X_1 ... X_N> where each X_i is boolean
- learned hypotheses are decision trees of depth 2, using only two variables



$\binom{N}{2} \cdot 16 = |H| =$

$(N \cdot N-1)\frac{1}{2} \cdot 16$

$1-\delta, \delta = 0.1$

How many training examples *m* suffice to assure that with probability at least 0.9, *any* consistent learner will output a hypothesis with true error at most 0.05?

ϵ

$$m \geq \frac{1}{0.05}\left(\ln(8N^2 - 8N) + \ln\left(\frac{1}{0.1}\right)\right)$$

$2 \ln N = \ln N^2$

for $N = 2$, $m \geq 101$

for $N = 10$, $m \geq 164$

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

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 $0 < \delta < 1/2$,
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Sufficient condition:

Holds if 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?

note ε here is the difference between the training error and true error

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

derived from Hoeffding bounds:

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

true error training error degree of overfitting

Additive Hoeffding Bounds – Agnostic Learning

- Given *m* independent coin flips of coin with Pr(heads) = θ bound the error in the maximum likelihood estimate $\hat{\theta}$

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

- 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 the mean θ inside [a,b] from *m* examples

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

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

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

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

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

What if H is not finite?

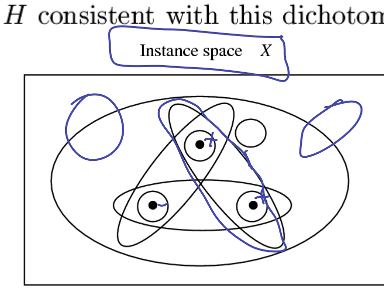
- Can't use our result for finite H
- Need some other measure of complexity for H
  - Vapnik-Chervonenkis (VC) dimension!

Shattering a Set of Instances

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

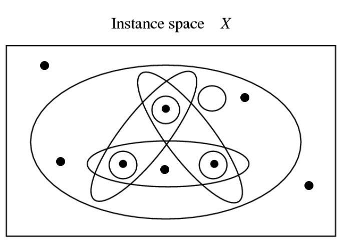
Definition: a set of instances S is **shattered** by hypothesis space H if and only if for every dichotomy of S there exists some hypothesis in H consistent with this dichotomy.

every possible labeling



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

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

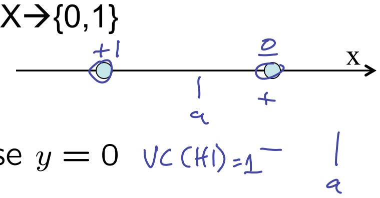
Compare to our earlier results based on |*H*|:

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

VC dimension: examples

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

What is VC dimension of



- Open intervals: parameter defining H

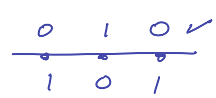
  $\boxed{\text{H1}}$: if $x > a$ then $y = 1$ else $y = 0$ VC(H1)=1

  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:

  $\boxed{\text{H3:}}$ if $a < x < b$ then $y = 1$ else $y = 0$

  VC(H3)=2

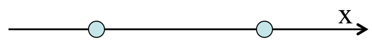


  H4: if $a < x < b$ then $y = 1$ else $y = 0$
  or, if $a < x < b$ then $y = 0$ else $y = 1$

VC 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

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 $y = 1$