Machine Learning 10-701

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February 24, 2011

Today:

- Computational Learning Theory
- PAC learning theorem
- VC dimension

Recommended reading:

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

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

* see Annual Conference on Learning Theory (COLT)

Sample Complexity

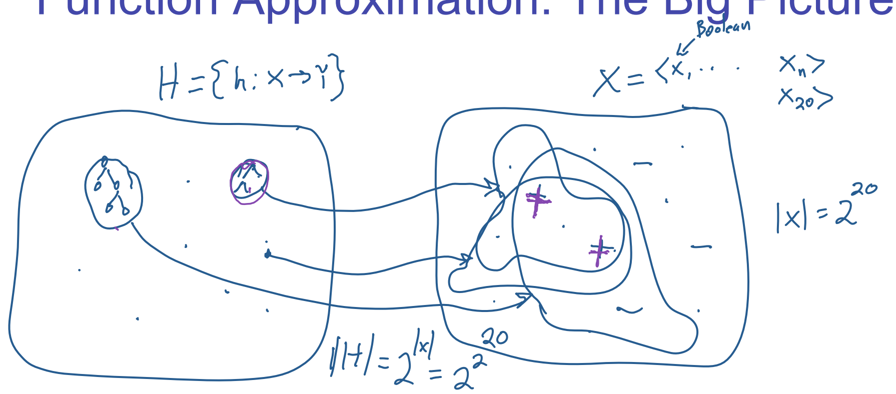
How many training examples are sufficient to learn the target concept?

Target concept is the boolean-valued fn to be learned

c: X → {0,1}

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
   - instance x generated randomly, teacher provides $c(x)$

Function Approximation: The Big Picture



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 <u>unless</u> we add more assumptions (eg. priors over H)

Sample Complexity: 3

Given:

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

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

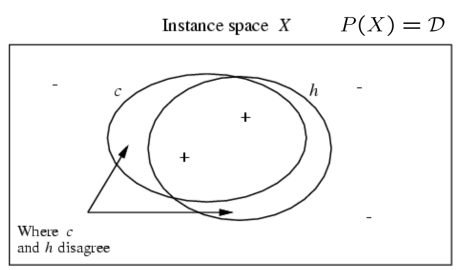
- instances x are drawn from distribution $\mathcal{D}$
- teacher provides target value $c(x)$ for each

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



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

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

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 $\mathcal{D}$

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Probability distribution P(x)

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

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training examples

Can we bound $error_{\mathcal{D}}(h)$ true

in terms of $error_{D}(h)$ train

??

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

Probability distribution P(x)

test error

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:

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

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

Version Spaces

c: X → {0,1}

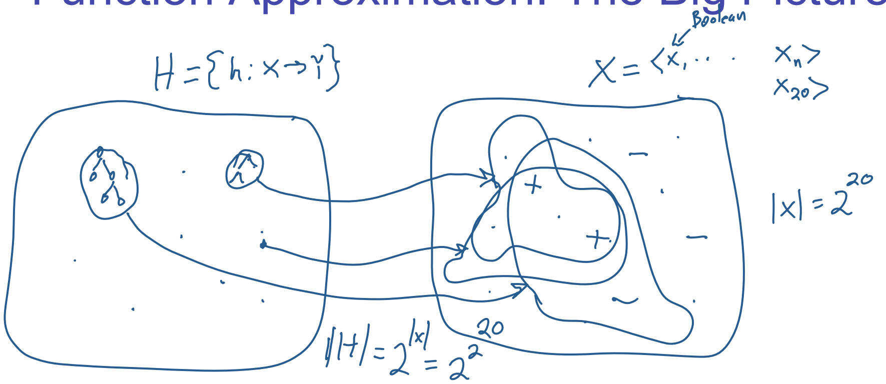
A hypothesis h is **consistent** with a set of training examples D of target concept c if and only if $h(x) = c(x)$ for each training example $\langle x, c(x) \rangle$ in D.

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

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.

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

Function Approximation: The Big Picture



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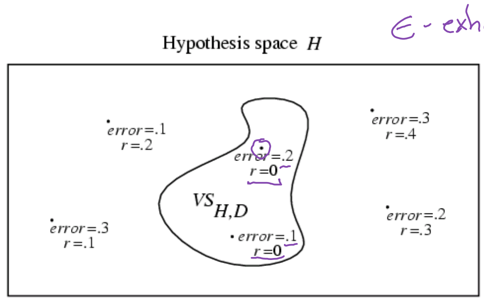
Exhausting the Version Space

ε - exhausted for ε > .2



(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

instances X

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

m labeled examps

error tolerance ϵ

let $h_1, \ldots h_k$ be the hyps $h \in H$ with true error $\geq \epsilon$

Prob that h_1 will be consistent with first training example
$\leq (1-\epsilon)$

" h_1 will be cons. w/ m indep drawn examps?
$\leq (1-\epsilon)^m$

" that at least of $h_1 \cdots h_k$ will be consist w/ m ?

$k \leq |H|$

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

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

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

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

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: $X = \langle X_1\ X_2\ X_3\ X_4 \rangle$ where each X_i is boolean
- learned hypotheses are rules of the form:
  - IF $\langle X_1\ X_2\ X_3\ X_4 \rangle = \langle 0,?,1,? \rangle$, 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 will output a hypothesis with true error at most 0.05?

$m \geq \frac{1}{.05}\left(\ln|H| + \ln\left(\frac{1}{.01}\right)\right)$, $|H| = 3^n$, $\ln|H| = n \ln 3$

n=4 → m ≥ 180 ← 3^4, n=4

n=10 ≥ 312

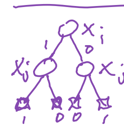
n=100 ≥ 2290

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



$\binom{N}{2} \cdot 16 = \frac{N(N-1)}{2} \cdot 16$ 8

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?

$|H| = 8N^2 - 8N$

$m \geq \frac{1}{0.05}\left(\ln(8N^2 - 8N) + \ln\left(\frac{1}{0.01}\right)\right)$

N=4 m ≥ 184

N=10 m ≥ 224

N=100 m ≥ 318

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 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?

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

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

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 true Pr(heads) = θ bound the error in the maximum likelihood estimate $\widehat{\theta}$

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

- 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

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

- 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

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

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

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

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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)