## Hypothesis Testing and Computational Learning Theory

EECS 349 Machine Learning
With slides from Bryan Pardo, Tom Mitchell

## Overview

- Hypothesis Testing: How do we know our learners are "good"?
- What does performance on test data imply/guarantee about future performance?
- Computational Learning Theory:Are there general laws that govern learning?
- Sample Complexity: How many training examples are needed to learn a successful hypothesis?
- Computational Complexity: How much computational effort is needed to learn a successful hypothesis?


## Some terms

$X \quad$ is the set of all possible instances
$C$ is the set of all possible concepts $c$ where $c: X \rightarrow\{0,1\}$
$H$ is the set of hypotheses considered by a learner, $H \subseteq C$
$L \quad$ is the learner
$D \quad$ is a probability distribution over $X$ that generates observed instances

## Definition

- The true error of hypothesis $h$, with respect to the target concept $c$ and observation distribution $D$ is the probability that $h$ will misclassify an instance drawn according to $D$

$$
\operatorname{error}_{D} \equiv \underset{x \in D}{P}[c(x) \neq h(x)]
$$

- In a perfect world, we'd like the true error to be 0


## Definition

- The sample error of hypothesis $h$, with respect to the target concept $c$ and sample $S$ is the proportion of $S$ that that $h$ misclassifies:

$$
\operatorname{error}_{s}(h)=\mathrm{I} /|S| \sum_{x \in S} \delta(c(x), h(x))
$$

where $\delta(c(x), h(x))=0$ if $c(x)=h(x)$,
I otherwise

## Problems Estimating Error

1. Bias: If $S$ is training set, $\operatorname{error}_{S}(h)$ is optimistically biased

$$
\text { bias } \equiv E\left[\operatorname{error}_{S}(h)\right]-\operatorname{error}_{\mathcal{D}}(h)
$$

For unbiased estimate, $h$ and $S$ must be chosen independently
2. Variance: Even with unbiased $S$, error $_{S}(h)$ may still vary from $\operatorname{error}_{\mathcal{D}}(h)$

## Example on Independent Test Set

Hypothesis $h$ misclassifies 12 of the 40 examples in $S$

$$
\operatorname{error}_{S}(h)=\frac{12}{40}=.30
$$

What is $\operatorname{error}_{\mathcal{D}}(h)$ ?

## Estimators

Experiment:

1. choose sample $S$ of size $n$ according to distribution $\mathcal{D}$
2. measure error $_{S}(h)$
error $_{S}(h)$ is a random variable (i.e., result of an experiment)
$\operatorname{error}_{S}(h)$ is an unbiased estimator for $\operatorname{error}_{\mathcal{D}}(h)$
Given observed error $_{S}(h)$ what can we conclude about $\operatorname{error}_{\mathcal{D}}(h)$ ?

## Confidence Intervals

If

- $S$ contains $n$ examples, drawn independently of $h$ and each other
- $n \geq 30$ and $n^{*}$ error $_{s}(h), n^{*}(1$-error $(h))$ each $>5$

Then

- With approximately $95 \%$ probability, $\operatorname{error}_{\mathcal{D}}(h)$ lies in interval

$$
\operatorname{error}_{S}(h) \pm 1.96 \sqrt{\frac{\operatorname{error}_{S}(h)\left(1-\operatorname{error}_{S}(h)\right)}{n}}
$$

## Confidence Intervals

- Under same conditions...
- With approximately N\% probability, error $_{\mathcal{D}}(h)$ lies in interval

$$
\operatorname{error}_{S}(h) \pm z_{N} \sqrt{\frac{\operatorname{error}_{S}(h)\left(1-\operatorname{eror}_{S}(h)\right)}{n}}
$$

where

$$
\begin{array}{|c|ccccccc|}
\hline N \%: & 50 \% & 68 \% & 80 \% & 90 \% & 95 \% & 98 \% & 99 \% \\
z_{N}: & 0.67 & 1.00 & 1.28 & 1.64 & 1.96 & 2.33 & 2.58 \\
\hline
\end{array}
$$

## Life Skills

" "Convincing demonstration" that certain enhancements improve performance?

- Use online Fisher Exact or Chi Square tests to evaluate hypotheses, e.g:
- http://people.ku.edu/~preacher/chisq/chisq.htm


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## Computational Learning Theory

- Are there general laws that govern learning?
- No Free Lunch Theorem: The expected accuracy of any learning algorithm across all concepts is $50 \%$.
- But can we still say something positive?
- Yes.
- Probably Approximately Correct (PAC) learning


## The world isn't perfect

- If we can't provide every instance for training, a consistent hypothesis may have error on unobserved instances.

- How many training examples do we need to bound the likelihood of error to a reasonable level?
When is our hypothesis Probably Approximately Correct (PAC)?


## Definitions

- A hypothesis is consistent if it has zero error on training examples
- The version space $\left(\mathrm{VS}_{\mathrm{H}, \mathrm{T}}\right)$ is the set of all hypotheses consistent on training set T in our hypothesis space H
- (reminder:hypothesis space is the set of concepts we're considering, e.g. depth-2 decision trees)


## Definition: $\varepsilon$-exhausted

## IN ENGLISH:

The set of hypotheses consistent with the training data $\boldsymbol{T}$ is $\boldsymbol{\varepsilon}$-exhausted if, when you test them on the actual distribution of instances, all consistent hypotheses have error below $\varepsilon$
IN MATH:
$V S_{H, T}$ is $\varepsilon$-exhausted for concept $c$ and sample distributi on $D$, if....
$\forall h \in V S_{H, T}$, error $_{D}(h)<\varepsilon$

## A Theorem

If hypothesis space $H$ is finite, \& training set $T$ contains $m$ independen t randomly drawn examples of concept $c$

THEN, for any $0 \leq \varepsilon \leq 1 \ldots$
$P\left(V S_{H, T}\right.$ is NOT $\varepsilon$-exhausted $) \leq|H| e^{-\varepsilon m}$

## Proof of Theorem

If hypothesis $h$ has true error $\varepsilon$, the probabilit y of it getting a single random exampe right is :
$P(h$ got 1 example right $)=1-\varepsilon$

Ergo the probabilit $y$ of $h$ getting $m$ examples right is :
$P(h$ got $m$ examples right $)=(1-\varepsilon)^{m}$

## Proof of Theorem

If there are $k$ hypotheses in $H$ with error at least $\varepsilon$, call the probabilit y at least of those $k$ hypotheses got $m$ instances right $P$ ( at least one bad $h$ looks good ).

This prob. is BOUNDED by $k(1-\varepsilon)^{m}$

$$
P(\text { at least one bad } h \text { looks good }) \leq k(1-\varepsilon)^{m}
$$

## Proof of Theorem (continued)

Since $k \leq|H|, \quad$ it follows that $k(1-\varepsilon)^{m} \leq|\mathrm{H}|(1-\varepsilon)^{m}$
If $0 \leq \varepsilon \leq 1$, then $(1-\varepsilon) \leq e^{-\varepsilon}$

Therefore.
$P($ at least one bad $h$ looks good $) \leq k(1-\varepsilon)^{m} \leq|\mathrm{H}|(1-\varepsilon)^{m} \leq|\mathrm{H}| e^{-\varepsilon m}$

Proof complete!
We now have a bound on the likelihood that a hypothsesi s consistent with the training data will have error $\geq \varepsilon$

## Using the theorem

Let' s rearrange to see how many train ing examples we need to set a bound $\delta$ on the likelihood our true error is $\varepsilon$.

$$
|\mathrm{H}| e^{-\varepsilon m} \leq \delta
$$

$$
\ln \left(|\mathrm{H}| e^{-\varepsilon m}\right) \leq \ln (\delta)
$$

$$
\ln (|\mathrm{H}|)+\ln \left(e^{-\varepsilon m}\right) \leq \ln (\delta)
$$

$$
\ln (|\mathrm{H}|)-\varepsilon m \leq \ln (\delta)
$$

$$
\ln (|\mathrm{H}|)-\ln (\delta) \leq \varepsilon m
$$

$$
\begin{gathered}
\frac{1}{\varepsilon}(\ln (|\mathrm{H}|)-\ln (\delta)) \leq m \\
\frac{1}{\varepsilon}\left(\ln (|\mathrm{H}|)+\ln \left(\frac{1}{\delta}\right)\right) \leq m
\end{gathered}
$$

## Probably Approximately Correct (PAC)

## $\frac{1}{-}(\ln (|\mathrm{H}|)-\ln (\delta)) \leq m$

The worst error we'll tolerate
hypothesis
space size

The likelihood a hypothesis consistent with the training data will have error $\varepsilon$

## Using the bound

$$
\frac{1}{\varepsilon}(\ln (|\mathrm{H}|)-\ln (\delta)) \leq m
$$

Plug in $\boldsymbol{\varepsilon}, \boldsymbol{\delta}$, and $\boldsymbol{H}$ to get a number of training examples $\boldsymbol{m}$ that will "guarantee" your learner will generate a hypothesis that is Probably Approximately Correct.

NOTE:This assumes that the concept is actually IN H, that H is finite, and that your training set is drawn using distribution D

## Think/Pair/Share

Average accuracy of any learner across all concepts is $50 \%$, but also:

$$
\frac{1}{\varepsilon}(\ln (|\mathrm{H}|)-\ln (\delta)) \leq m
$$

How can both be true?

## Think

Start
End

## Think/Pair/Share

Average accuracy of any learner across all concepts is $50 \%$, but also:

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How can both be true?
|Pair
Start
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How can both be true?

## Share

## Problems with PAC

- The PAC Learning framework has 2 disadvantages:
I) It can lead to weak bounds
2)Sample Complexity bound cannot be established for infinite hypothesis spaces
- We introduce the VC dimension for dealing with these problems


## Shattering

Def: A set of instances $\boldsymbol{S}$ is shattered by hypothesis set $\boldsymbol{H}$ iff for every possible concept $\boldsymbol{c}$ on $\boldsymbol{S}$ there exists a hypothesis $\boldsymbol{h}$ in $\boldsymbol{H}$ that is consistent with that concept.


## Can a linear separator shatter this?

## NO!

The ability of H to shatter a set of instances is a measure of its capacity to represent target concepts defined over those instances

## Can a quadratic separator shatter this?

## Can a quadratic separator shatter this?



Start
End

## Can a quadratic separator shatter this?



Pair
Start


End

## Can a quadratic separator shatter this?



Share

## Vapnik-Chervonenkis Dimension

Def: The Vapnik-Chervonenkis dimension, VC(H) of hypothesis space $\boldsymbol{H}$ defined over instance space $\boldsymbol{X}$ is the size of the largest finite subset of $\boldsymbol{X}$ shattered by $\boldsymbol{H}$. If arbitrarily large finite sets can be shattered by $\boldsymbol{H}$, then $\mathbf{V C}(H)$ is infinite.

## How many training examples needed?

- Upper bound on $m$ using VC(H)

$$
m \geq \frac{1}{\varepsilon}\left(4 \log _{2}(2 / \delta)+8 V C(H) \log _{2}(13 / \varepsilon)\right)
$$

## Infinite VC dimension?

## Think/Pair/Share

What kind of classifier (that we've talked about) has infinite VC dimension?

> |Think

Start


## Think/Pair/Share

What kind of classifier (that we've talked about) has infinite VC dimension?

## Pair <br> Start



## Think/Pair/Share

What kind of classifier (that we've talked about) has infinite VC dimension?

## Share

