Basic Sample Complexity

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http://www.cs.cmu.edu/~jcl/research/tutorial/tutorial.ps
http://www.cs.cmu.edu/~jcl/presentation/tutorial/index.htm (Need MathML. Use mozilla.)

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Goals

1. How can we measure learning?
2. How can we design training algorithms?

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Goals

1. Sample Complexity Model
2. Test Set Bound
3. Application: Learning Measurement
4. Train Set Bound
5. Application: viability and learning algorithm design

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Model

- $X \equiv$ Input space to Classifier
- $Y \equiv \{0,\ 1\} \equiv$ Output space of Classifier
- $D \equiv$ Distribution over $X \times Y$
- $S \equiv$ A set of examples drawn i.i.d. from D.
- $m \equiv |S| \equiv$ the number of examples.
- $c : X \rightarrow Y \equiv$ a classifier.

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Model Notes

Independence is a fundamental assumption.

Model like information theory: $D \sim X \times Y$ rather than $D \sim X$.

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Example

Goal: Predict Rain or Not Rain given sensor data

X = Barometric Pressure, Cloudy/Not Cloudy
Y = Rain or Not Rain
D = Distribution over weather
S = 100 examples i.i.d from D
$c : X \rightarrow Y$ function predicting rain/not rain

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Derived Quantities

True error = $e_D(c) \equiv \Pr_D(c(x) \neq y)$
(= Generalization error)

Empirical error = $\widehat{e}_S(c) \equiv \Pr_{U(S)}(c(x) \neq y)$
(= $\frac{1}{m}\sum_{i=1}^{m} I(c(x_i) \neq y_i)$ = observed error)

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Example (continued)

Suppose: $\forall\ x \quad c(x) =$ Not Rain

Empirical error = $\hat{e}_S(c) = \frac{38}{100}$

True error unknown, maybe 0.5.

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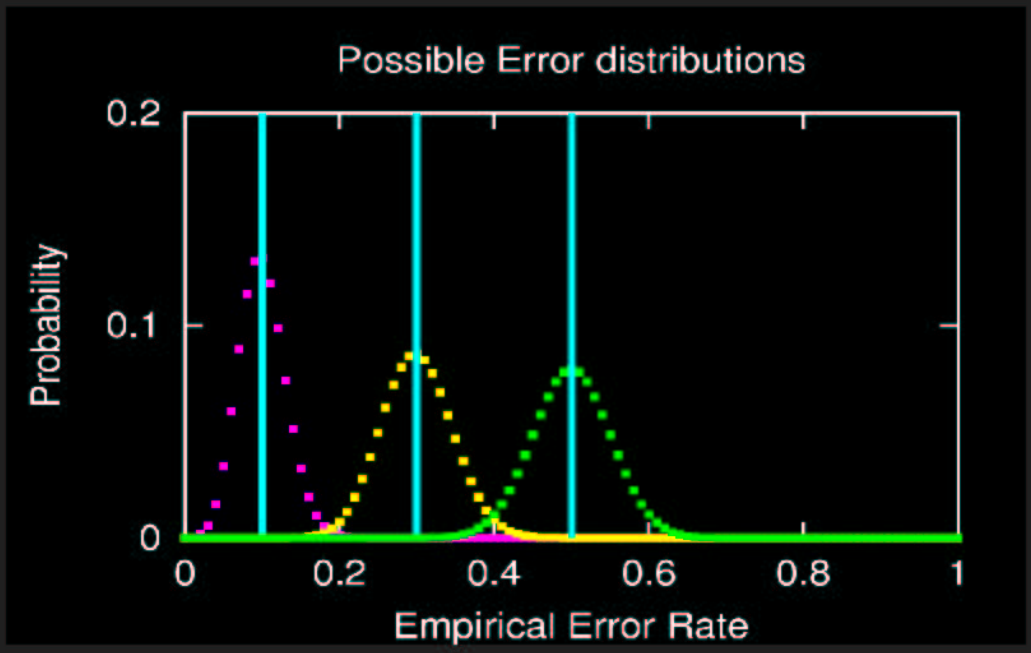
What is the distribution of $\hat{e}_S(c)$?



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Test Set Bound

$\mathrm{Bin}\left(m, \frac{k}{m}, p\right) = \Pr_{X_1, \ldots, X_m}\left(\sum_{i=1}^{m} X_i \leq k \middle| p\right)$
(= Binomial cumulative distribution)

$\overline{\mathrm{Bin}}\left(\frac{k}{m}, \delta\right) = \max_p \{p : \quad \mathrm{Bin}\left(m, \hat{e}_S(c), p\right) = \delta\}$

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Theorem (Test Set Bound):

$$\Pr_{S \sim D^m}\left(e_D(c) \geq \overline{\mathrm{Bin}}\left(\hat{e}_S(c), \delta\right)\right) \leq \delta$$

(note randomization)

Test Set Notes

"Perfectly" tight: there exist true error rates which achieve the bound.

Test Set lower bound of the same form.

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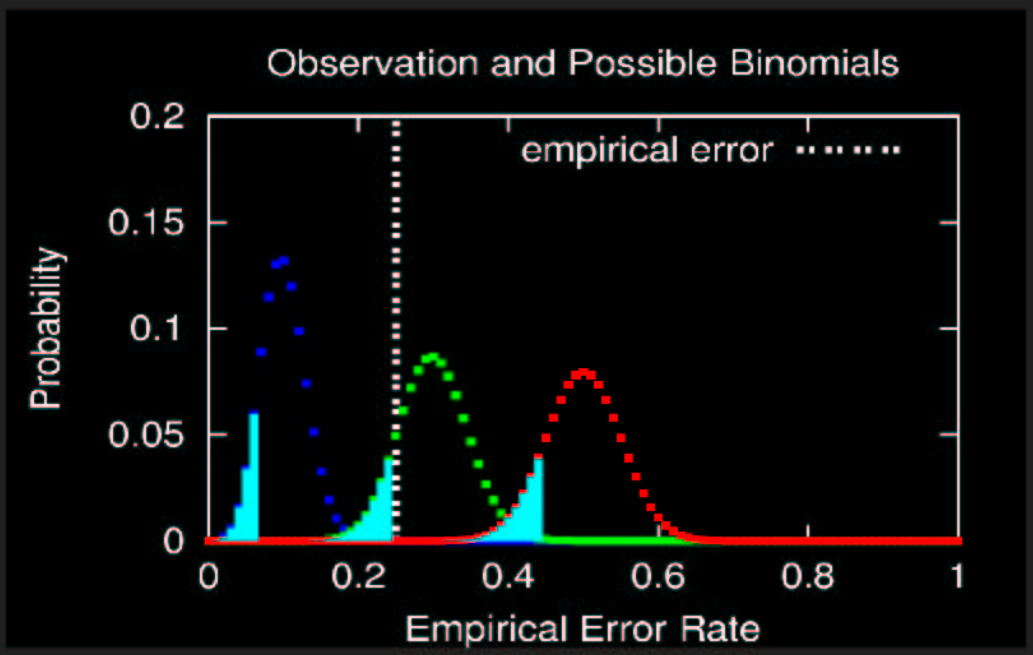
Proof (in pictures)



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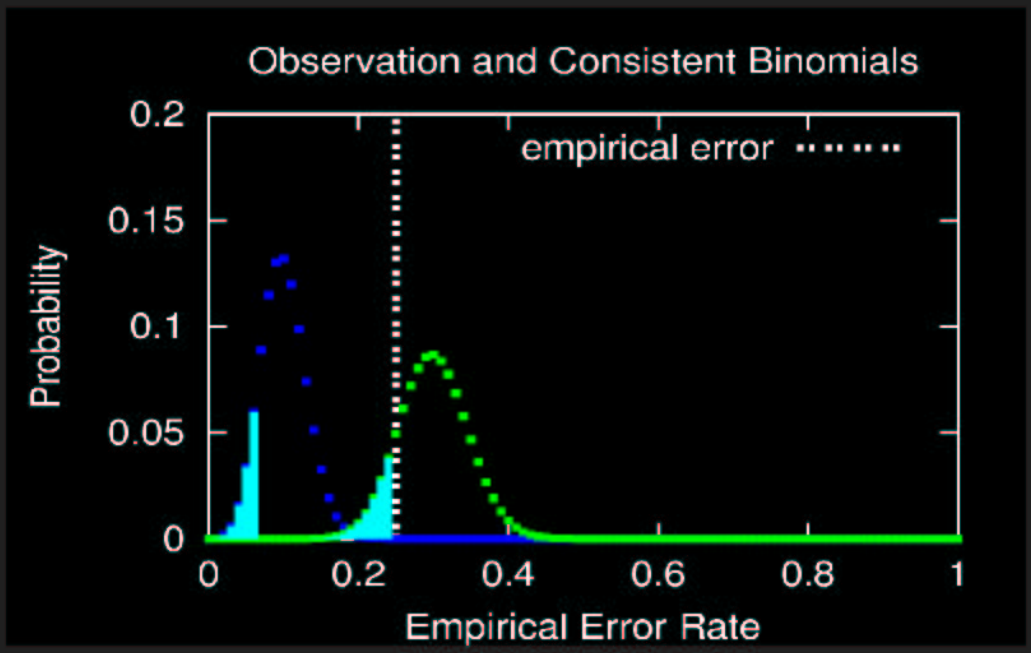
Proof (in pictures)



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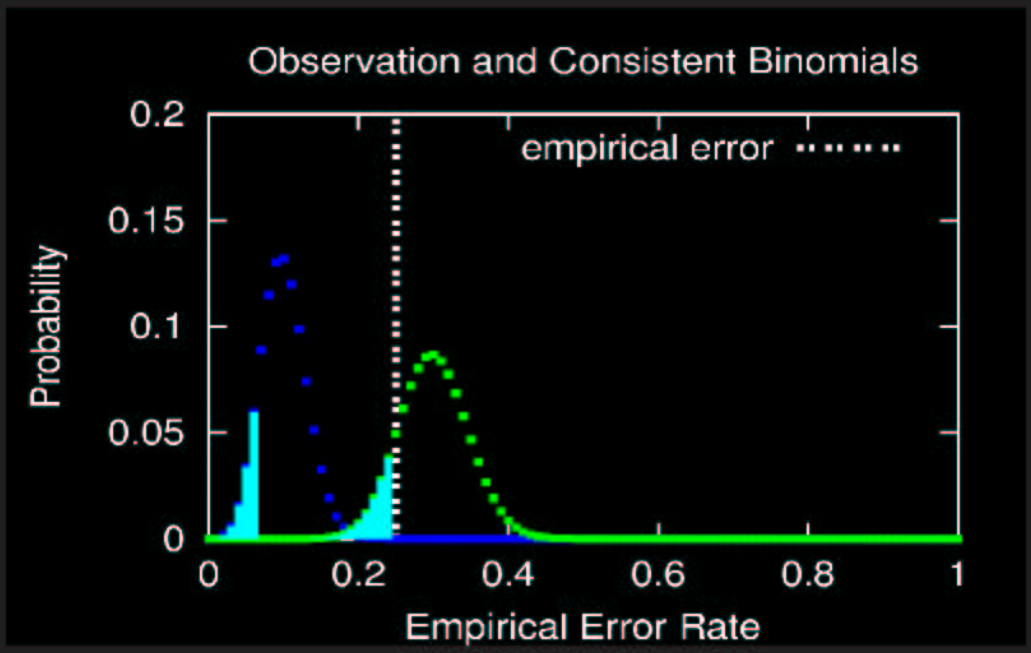
Proof (in pictures)



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Test Set Bound Approximations

Corollary: (Realizable Test Set Bound)

$$\Pr_{S \sim D^m}\left(\hat{e}_S(c) = 0 \,\middle|\, e_D(c) \geq \frac{\ln \frac{1}{\delta}}{m}\right) \leq \delta$$

Proof: specialization

Corollary: (Agnostic Test Set Bound)

$$\Pr_{S \sim D^m}\left(e_D(c) \geq \hat{e}_S(c) + \sqrt{\frac{\ln \frac{1}{\delta}}{2m}}\right) \leq \delta$$

Proof: Hoeffding approximation to Binomial tail bound.

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Test Set Use

Primary use: verification of succesful learning

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The Sigma Approach

1. $\widehat{\mu} \leftarrow \widehat{e}_{S_{\text{textrm test}}}(h) = \frac{1}{m}\sum_{i=1}^{m} I(h(x_i) \neq y_i)$
2. $\widehat{\sigma}^2 = \frac{1}{m-1}\sum_{i=1}^{m} (I(h(x_i) \neq y_i) - \widehat{\mu})^2$
3. Pretend data is drawn from $N(\widehat{\mu}, \widehat{\sigma})$ gaussian, calculate confidence intervals.

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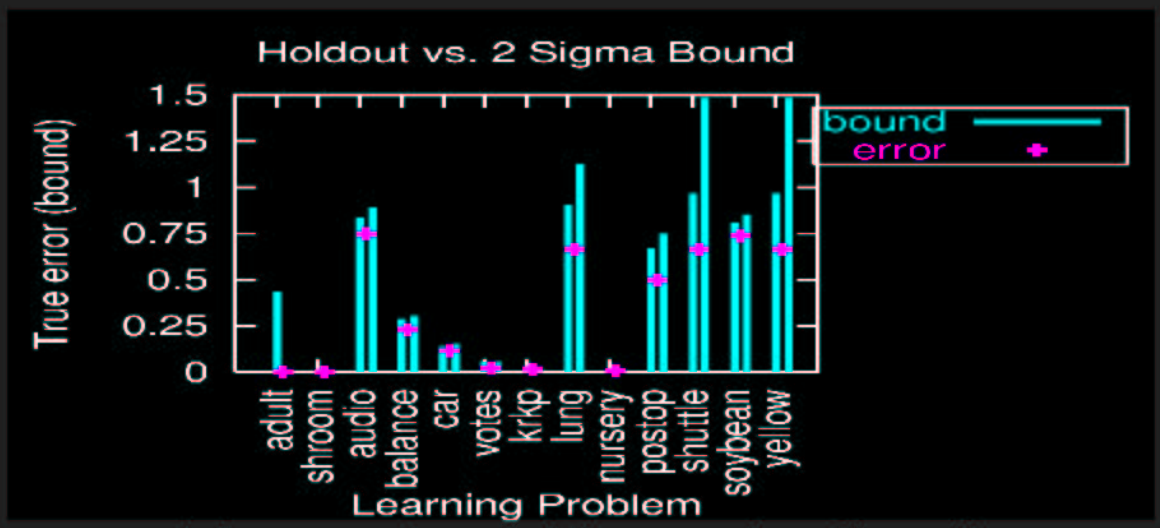
Test Set vs. Sigma



left = test set bound, right = two sigma "bound"

Learning = seeking "bad" bias.

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Test Set vs. Sigma Notes

Sigma approach (and related) = relic of noncomputerized days.

1. Test set approach *never* overoptimistic.
2. Test Set approch works well for all true error rates.

Bound program available at:
http://www.cs.cmu.edu/~jcl/programs/bound/bound.html

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Example (continued)

Suppose we have:
$m = 100$ test examples
$\hat{e}_S(c) = \frac{38}{100}$
$\delta = 0.1$.

Hoeffding approximation:

$$e_D(c) \in [0.26,\ 0.50]$$

Exact calculation:

$$e_D(c) \in [0.30,\ 0.47]$$

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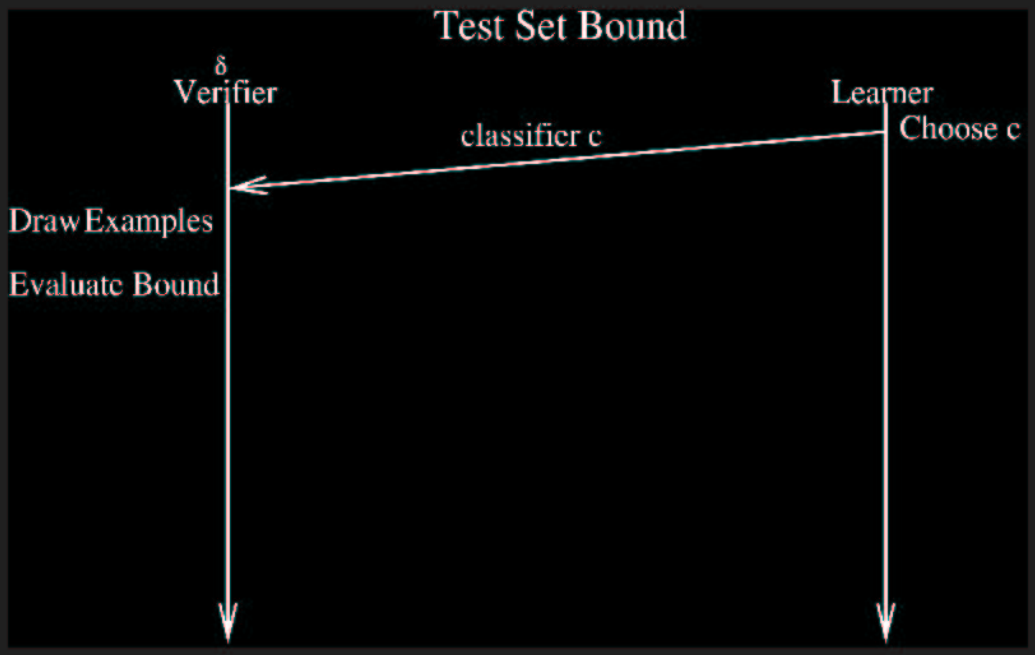
Test Set Protocol



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The state of the art (test sets)

- Test set bound very well understood.
- Cross validation techniques somewhat understood.
  - Understood for Nearest Neighbor.
  - Weak results for arbitrary algorithms.
- Many others not understood.

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Why Train set bounds?

1. Sometimes an extra few examples are *critical.*
2. Train set bounds can be used in the learning algorithm.
3. Train set bounds teach us about ways to learn.

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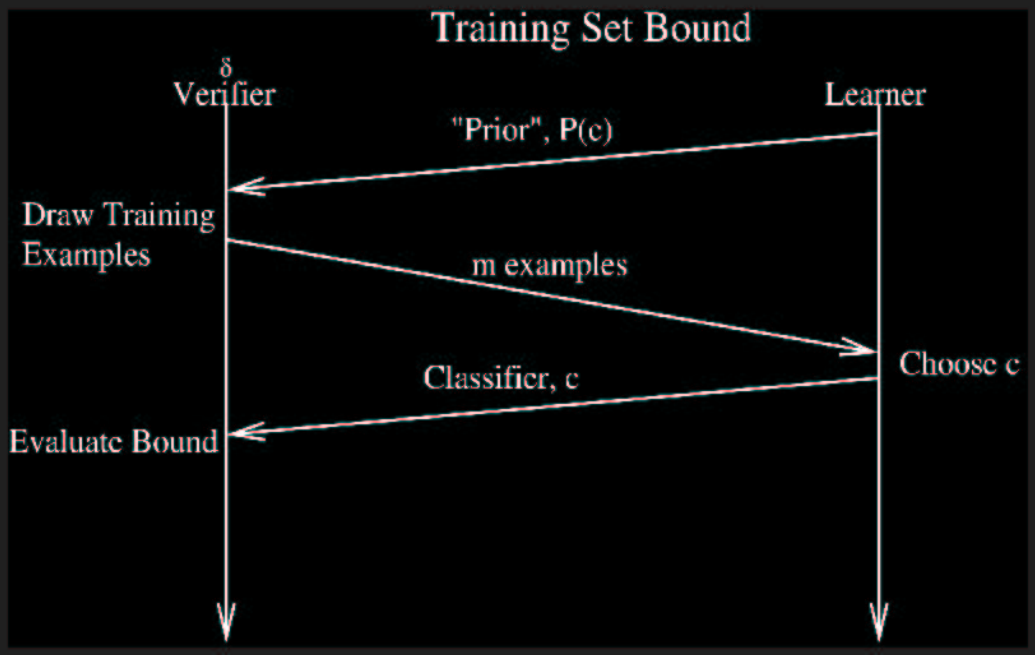
Train Set Protocol



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Train Set Bound

Theorem: (Occam's Razor Bound) $\forall\ p(c)$

$$\Pr_{S \sim D^m}\left(\exists\ c:\ \ e_D(c) \geq \overline{\mathrm{Bin}}\left(\hat{e}_S(c), \delta\, p(c)\right)\right) \leq \delta$$

Corollary: $\forall\ p(c)$

$$\Pr_{S \sim D^m}\left(\exists\ c:\ \ e_D(c) \geq \hat{e}_S(c) + \sqrt{\frac{\ln \frac{1}{p(c)} + \ln \frac{1}{\delta}}{2m}}\right) \leq \delta$$

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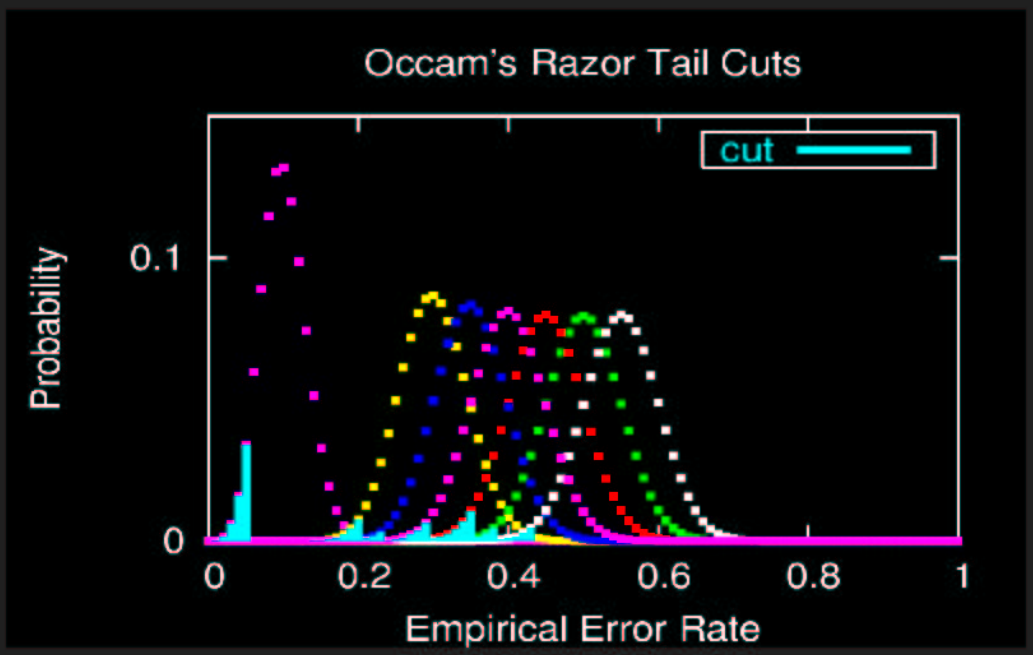
Proof (in pictures)



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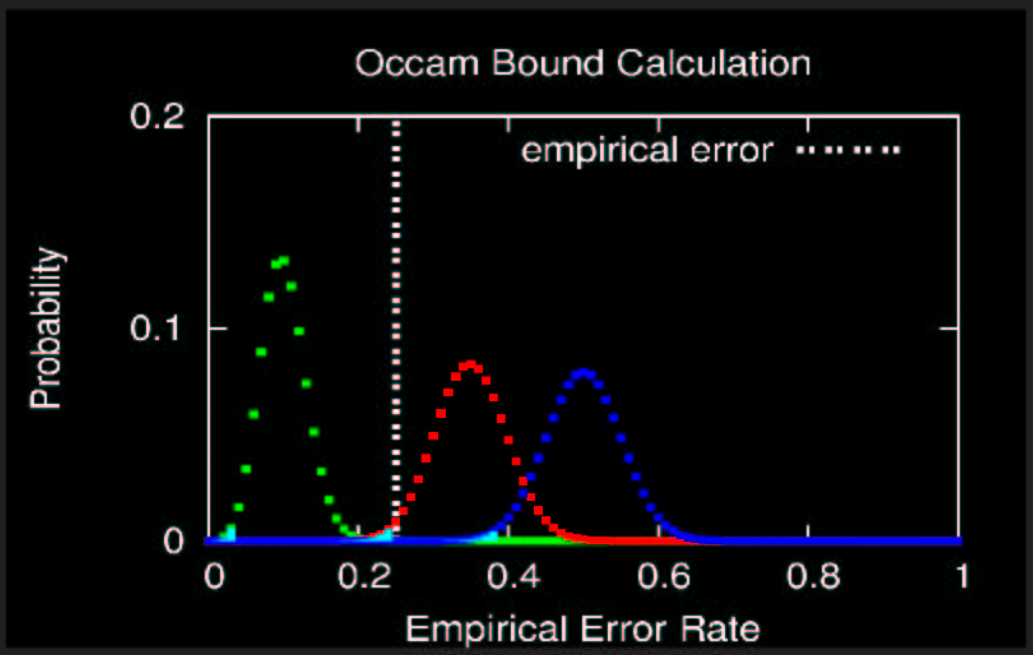
Proof (in pictures)



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Proof (in pictures)

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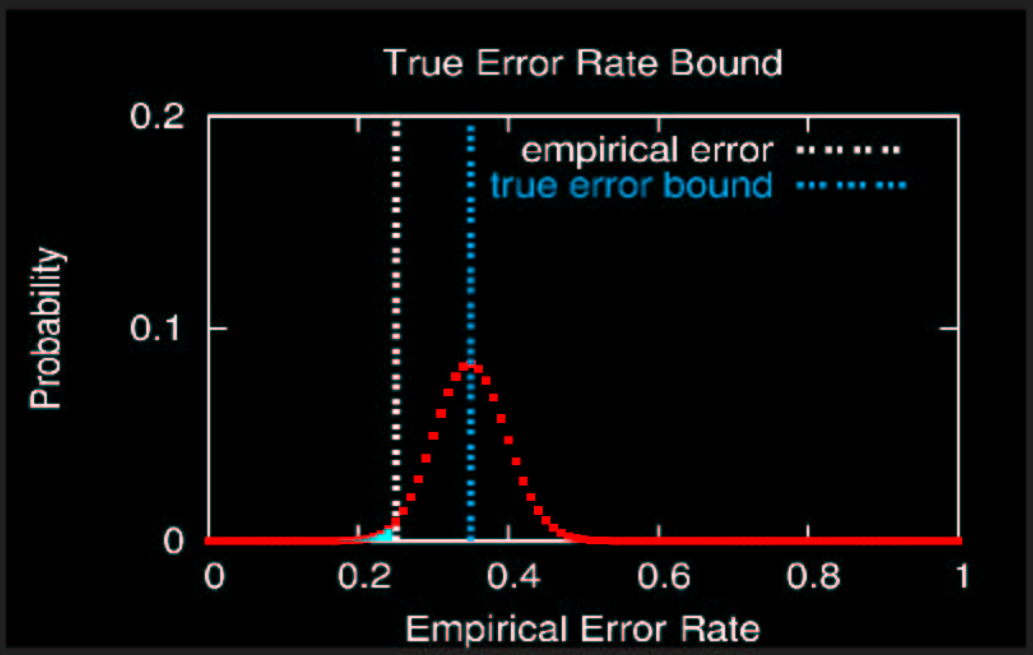
Proof (in pictures)



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Train Set setup

- Discrete classification problems.
- Decision tree algorithm.
- d = description length = description of data-dependent choices made to construct tree.
- "prior" = 2^{-d}

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Train Set Bound Uses

- Verification of learning
- Decision tree pruning criteria
- Method for learning

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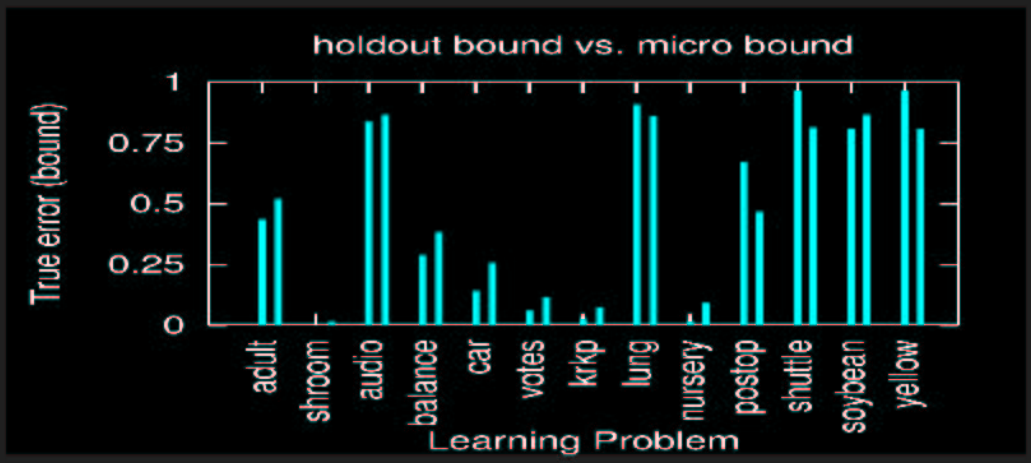
Train Set Verification



- Left = Test set bound in 80/20 train/test split
- Right = Train set bound in 100/0 train/test split

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Example

Suppose $p(c) = 0.1$ with $m = 100$ train examples and error rate $\widehat{e}_S(c) = \frac{38}{100}$.

Hoeffding approximation:

$$e_D(c) \in [0.22,\ 0.54]$$

Exact calculation:

$$e_D(c) \in [0.26,\ 0.51]$$

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Train Set Induction

Bound $\Rightarrow$ learning algorithm (= Optimize bound)

Note learning algorithm is often *bad*.

1. Many bounds too loose to justify use. Let $f(k/m) > 0$

$$\Pr_{S \sim D^m}\left[e_D(c) \leq 1 + f\left(\hat{e}_S(c)\right)\right] = 1$$

2. Learning algorithm = minimize worst case.
   1. Optimize for best case?
   2. Optimized for average case?

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The State of the Art (Train Sets)

Much work

- VC bounds (reinterpreted...)
- PAC bounds (reinterpreted...)
- PAC-Bayes bounds
- Shell bounds
- Combined Train and Test Bounds

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Conclusion

1. Test set bound = "right" way to verify learning.
2. Train set bound:
    1. more developmental
    2. Can be useful now
    3. suggest learning algorithms

http://www.cs.cmu.edu/~jcl/research/tutorial/tutorial.ps

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