# Practical Prediction Theory

John Langford

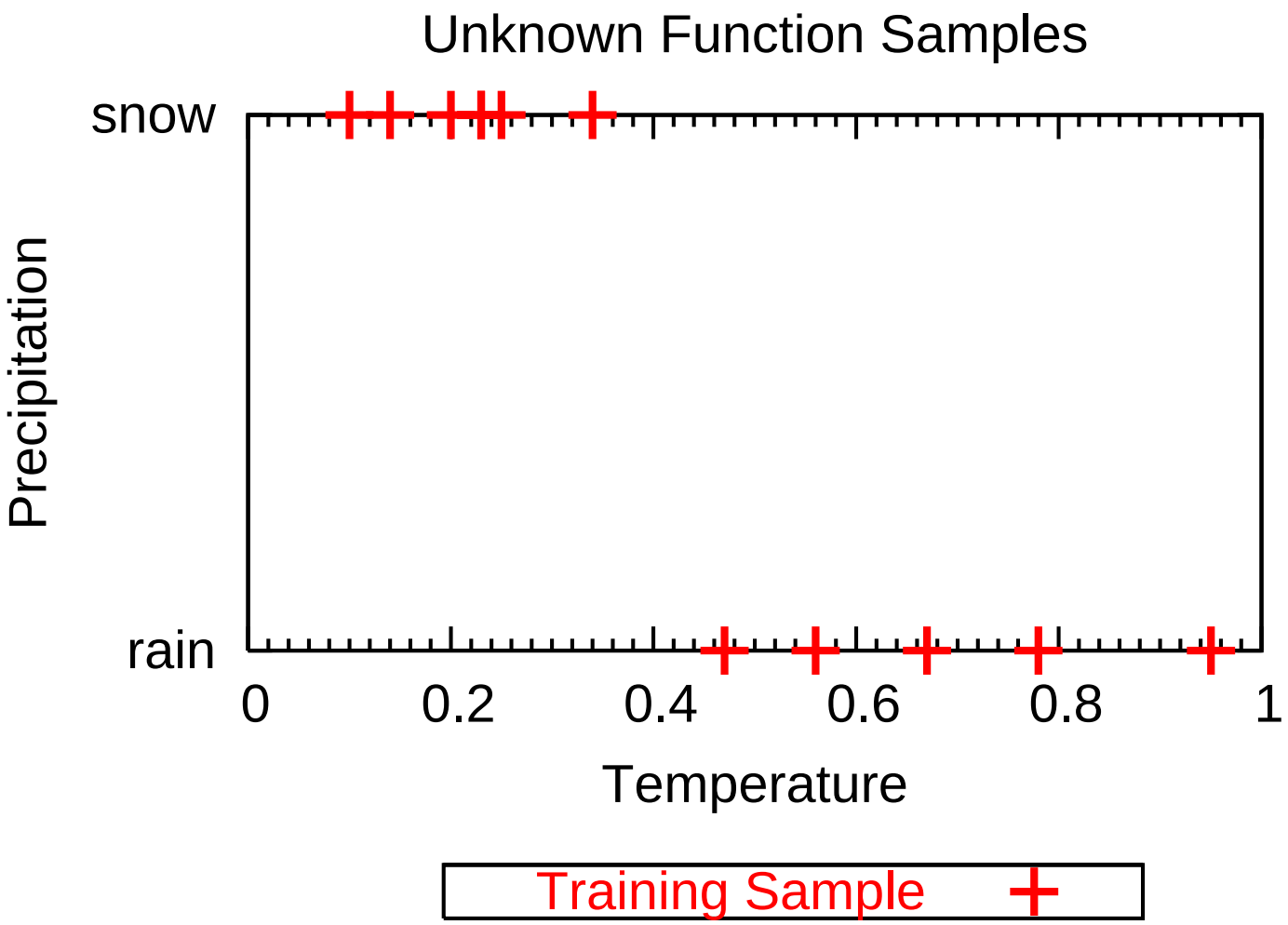
IBM Research

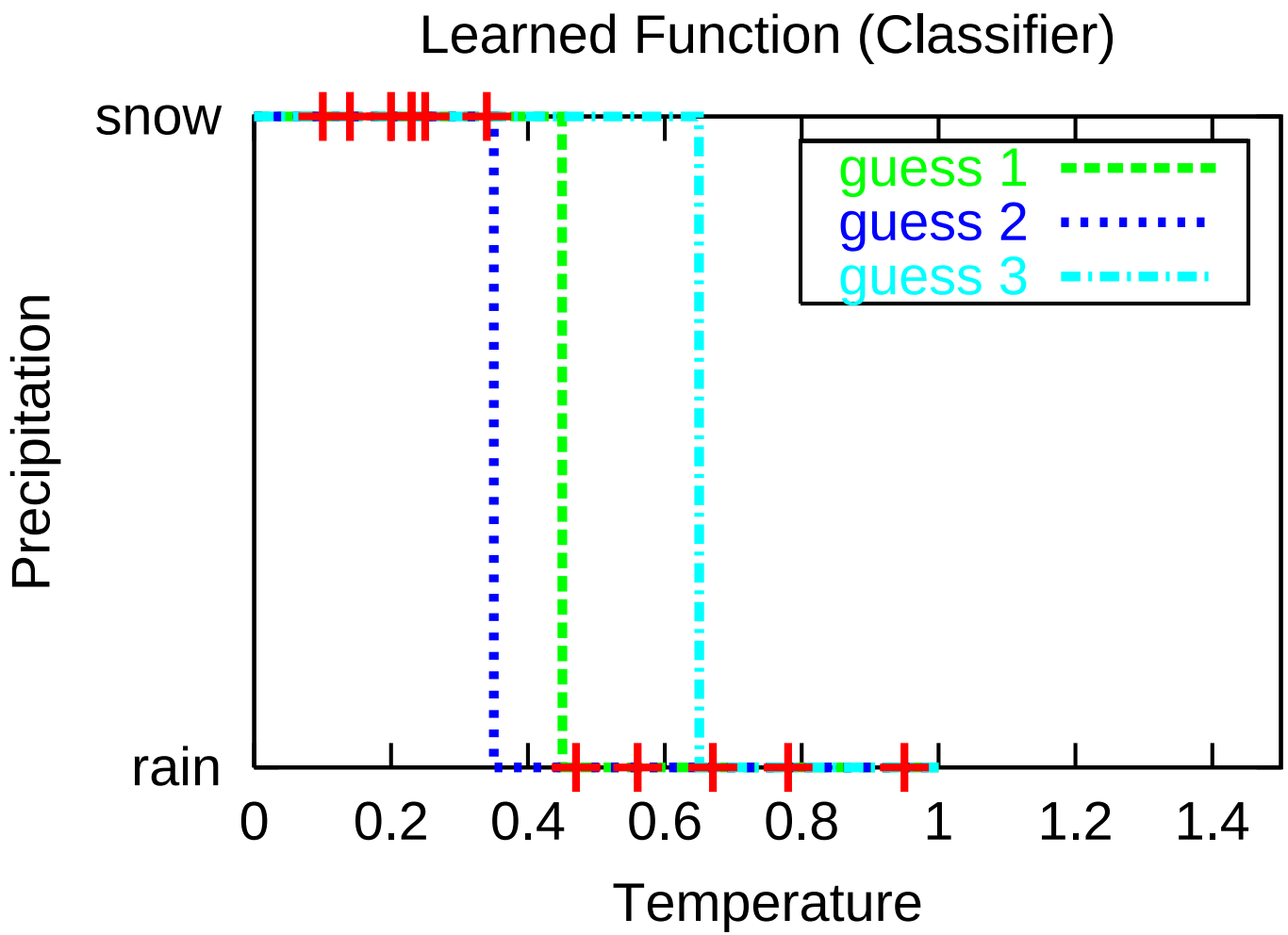
The Classification Problem:

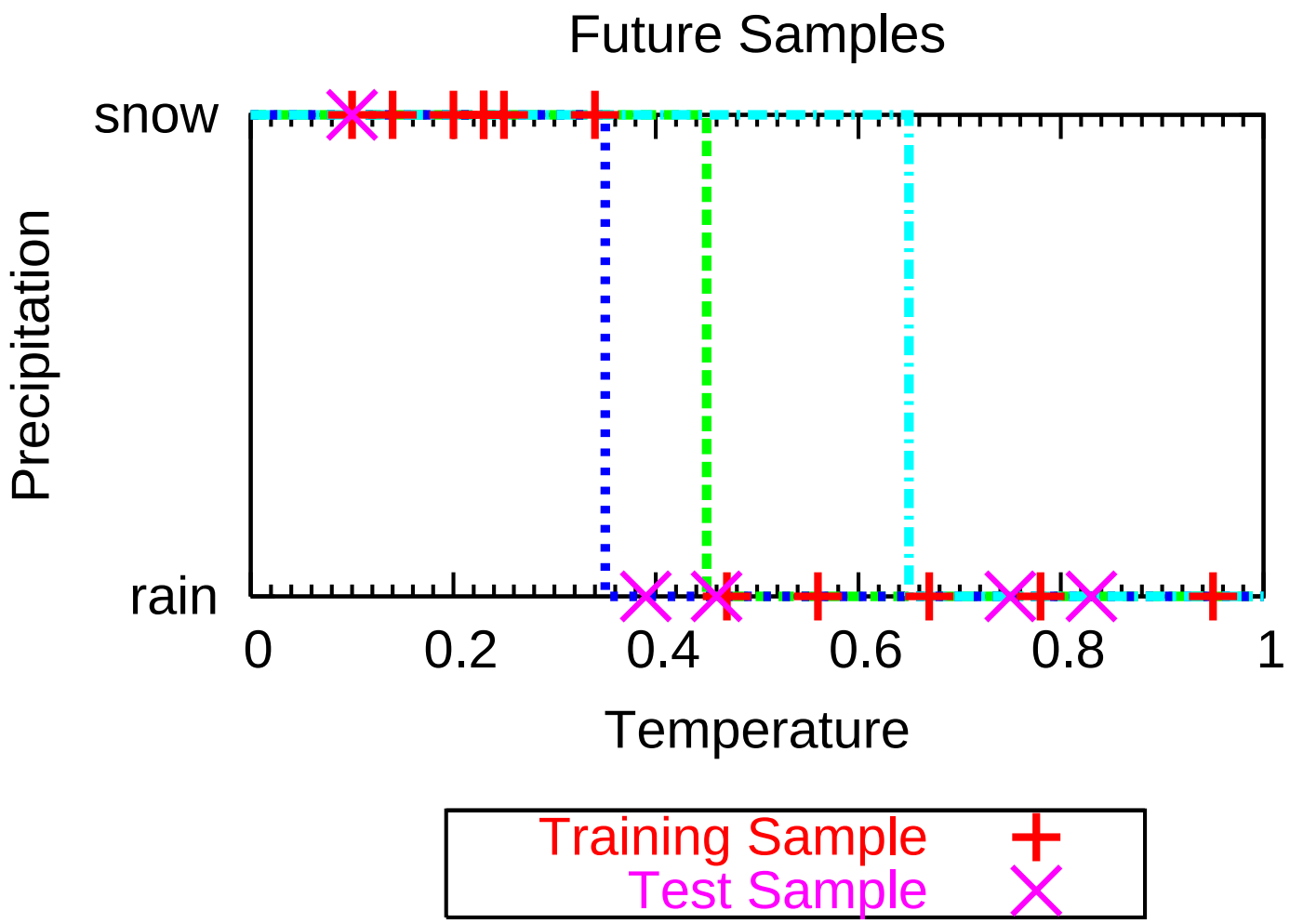
1. Get (input, class label) pairs from unknown function

2. Find the unknown function

3. ... to minimize errors on future inputs


Unknown Function Samples
snow
rain
Precipitation
0
0.2
0.4
0.6
0.8
1
Temperature
Training Sample


Learned Function (Classifier)
snow
rain
Precipitation
guess 1
guess 2
guess 3
0
0.2
0.4
0.6
0.8
1
1.2
1.4
Temperature


Future Samples
snow
rain
Precipitation
0
0.2
0.4
0.6
0.8
1
Temperature
Training Sample
Test Sample

Learning = Prediction ability

- We can't expect any prediction ability, in general.

- We can expect prediction ability, if examples come independently, sometimes.

Here we study prediction ability, assuming indepedence.

Why study prediction theory?

1. Better methods for learning and verifying predictive ability

2. To gain insight into learning.

# Better Methods for Learning & Verification

Standard technique:

1. Divide samples into train and test set
2. Train on train set
3. Test on test set

We can do better.

To gain insight into learning

1. Overfitting: sample complexity quantifies overfitting.

2. Learning algorithm design: What is a good pruning criterion? Why are large margins good? What other algorithms are likely to yield good results?

# Outline

1. The Basic Model
2. The Test Set Bound
3. Occam's Razor Bound
4. PAC-Bayes Bound
5. Sample Compression Bound

## Model: Definitions

$X$ = input space

$Y = \{0, 1\}$ = output space

$c : X \to Y$ = classifier

## Model: Basic Assumption

All samples are drawn independently from some unknown distribution $D(x, y)$.

$S = (x, y)^m \sim D^m$ is a sample set.

## Model: Derived quantities

The thing we want to know:

$$c_D \equiv \Pr_{x,y \sim D}(c(x) \neq y) = \text{true error}$$

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The thing we want to know:

$$c_D \equiv \Pr_{x,y \sim D}(c(x) \neq y) = \text{true error}$$

The thing we have:

$$\widehat{c}_S \equiv \Pr_{x,y \sim S}(c(x) \neq y) = \frac{1}{m} \sum_{i=1}^{m} I\left[c(x) \neq y\right]$$

= "train error", "test error", or "observed error", depending on context.

(note: we identify the set $S$ with the uniform distribution on $S$)

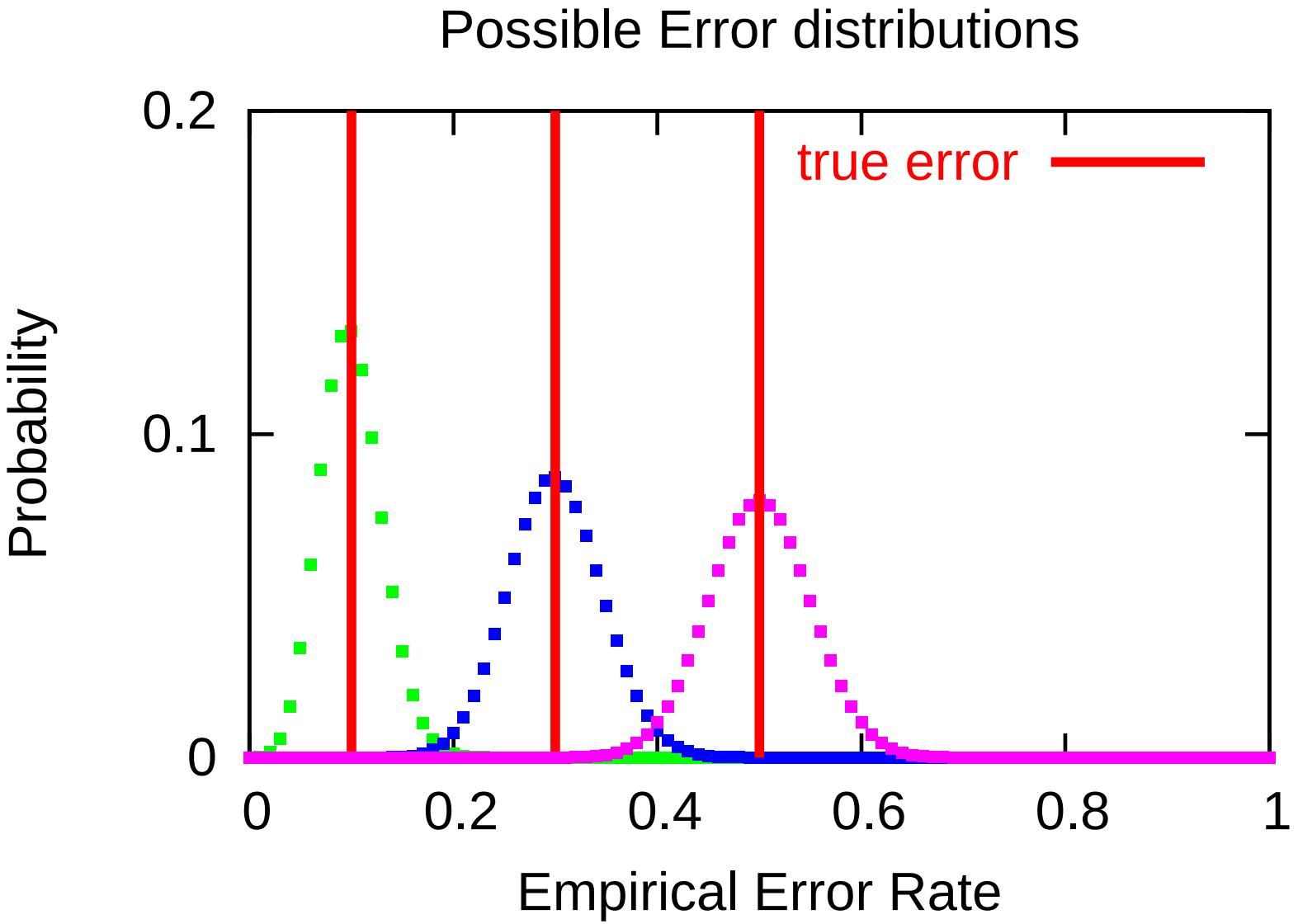
## Model: Basic Observations

Q: What is the distribution of $\widehat{c}_S$?

A: A Binomial.

$$\Pr_{S \sim D^m}\left(\widehat{c}_S = \frac{k}{m} \middle| c_D\right) = \binom{m}{k} c_D^k (1 - c_D)^{m-k}$$

= probability of $k$ heads (errors) in $m$ flips of a coin with bias $c_D$.


Possible Error distributions
0.2
0.1
0
Probability
true error
0
0.2
0.4
0.6
0.8
1
Empirical Error Rate

## Model: basic quantities

We use the cumulative:

$$\begin{aligned} \mathsf{Bin}\left(\tfrac{k}{m}, c_D\right) &= \mathsf{Pr}_{S\sim D^m}\left(\widehat{c}_S \leq \tfrac{k}{m} \middle| \, c_D\right) \\ &= \textstyle\sum_{i=0}^{k} \left( \begin{array}{c} m \\ i \end{array} \right) c_D^i (1-c_D)^{m-i} \end{aligned}$$

$=$ probability of observing $k$ or fewer "heads" (errors) with $m$ coins.

## Model: basic quantities

Need confidence intervals $\Rightarrow$ use the pivot of the cumulative instead

$$\overline{\mathsf{Bin}}\left(\frac{k}{m}, \delta\right) = \max\left\{p : \mathsf{Bin}\left(\frac{k}{m}, p\right) \geq \delta\right\}$$

$=$ the largest true error such that the probability of observing $k$ or fewer "heads" (errors) is at least $\delta$.

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# Test Set Bound: Setting

Standard technique:

1. Cut the data into train set and test set
2. Train on the train set
3. Test on the test set

What does Sample Complexity say about this method?

# Test Set Bound: Theorem

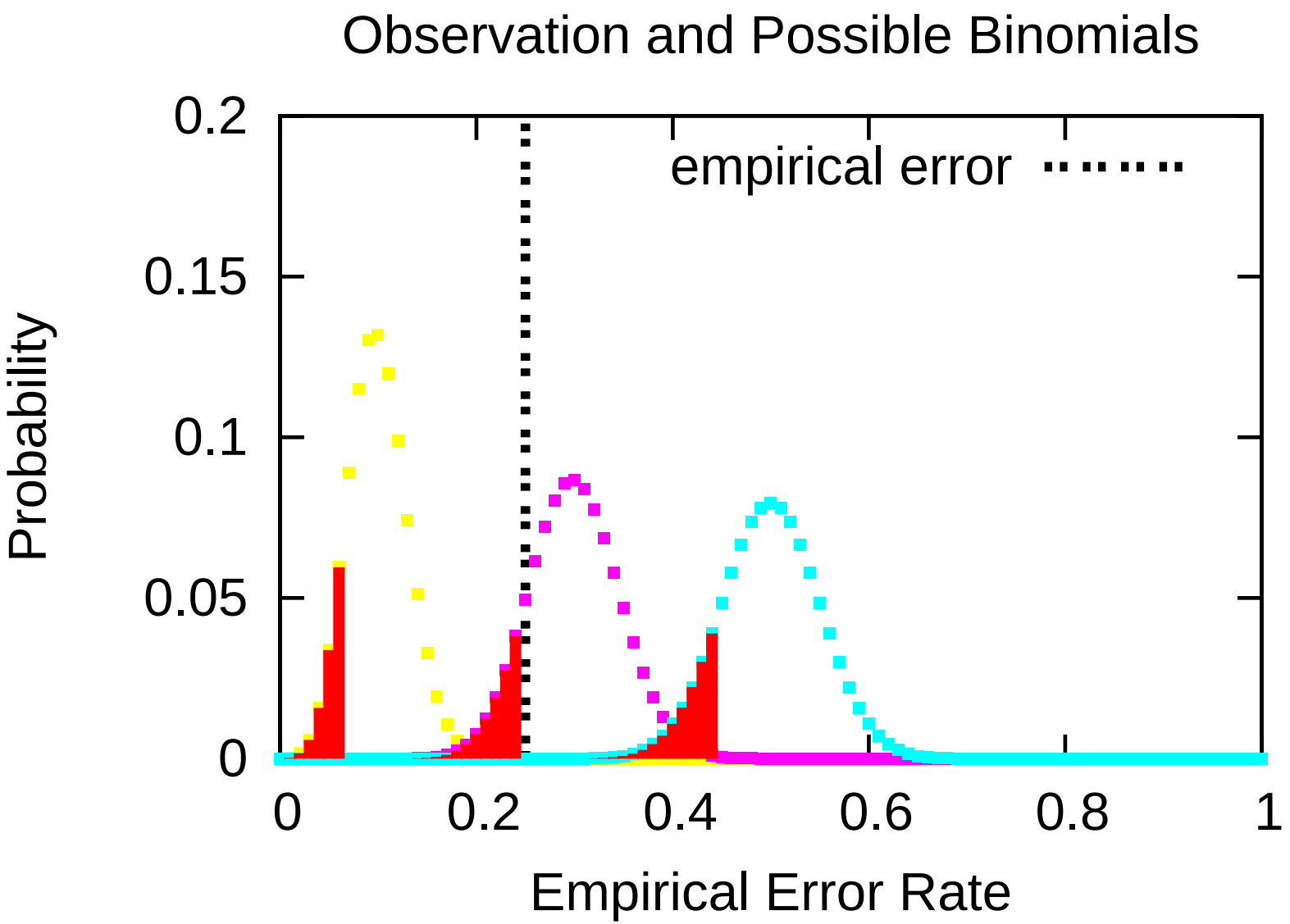
Theorem: (Test Set Bound) For all classifiers $c$, for all $D$, for all $\delta \in (0, 1]$:

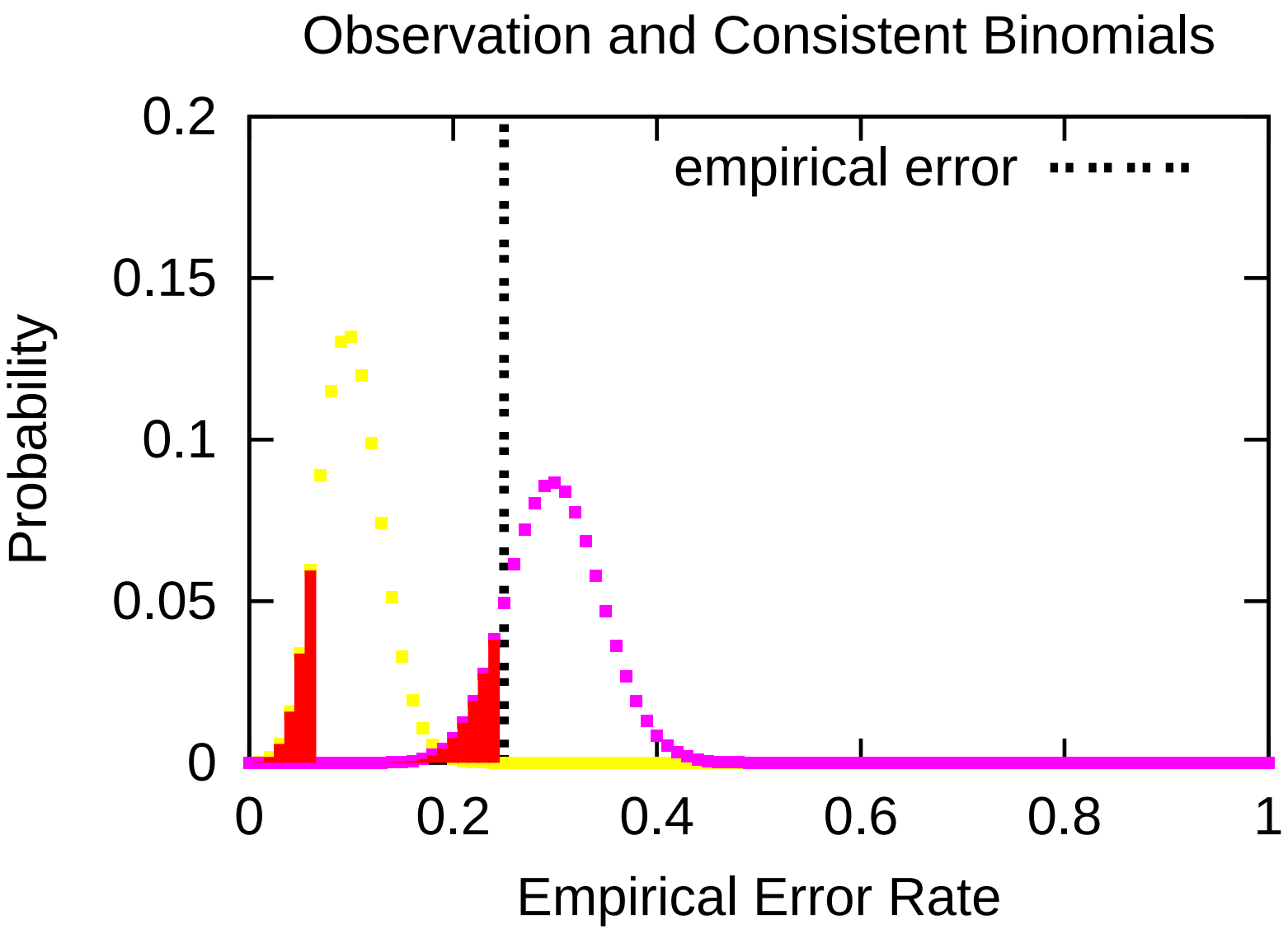
$$\Pr_{S \sim D^m} \left( c_D \leq \overline{\mathsf{Bin}} \left( \hat{c}_S, \delta \right) \right) \geq 1 - \delta$$

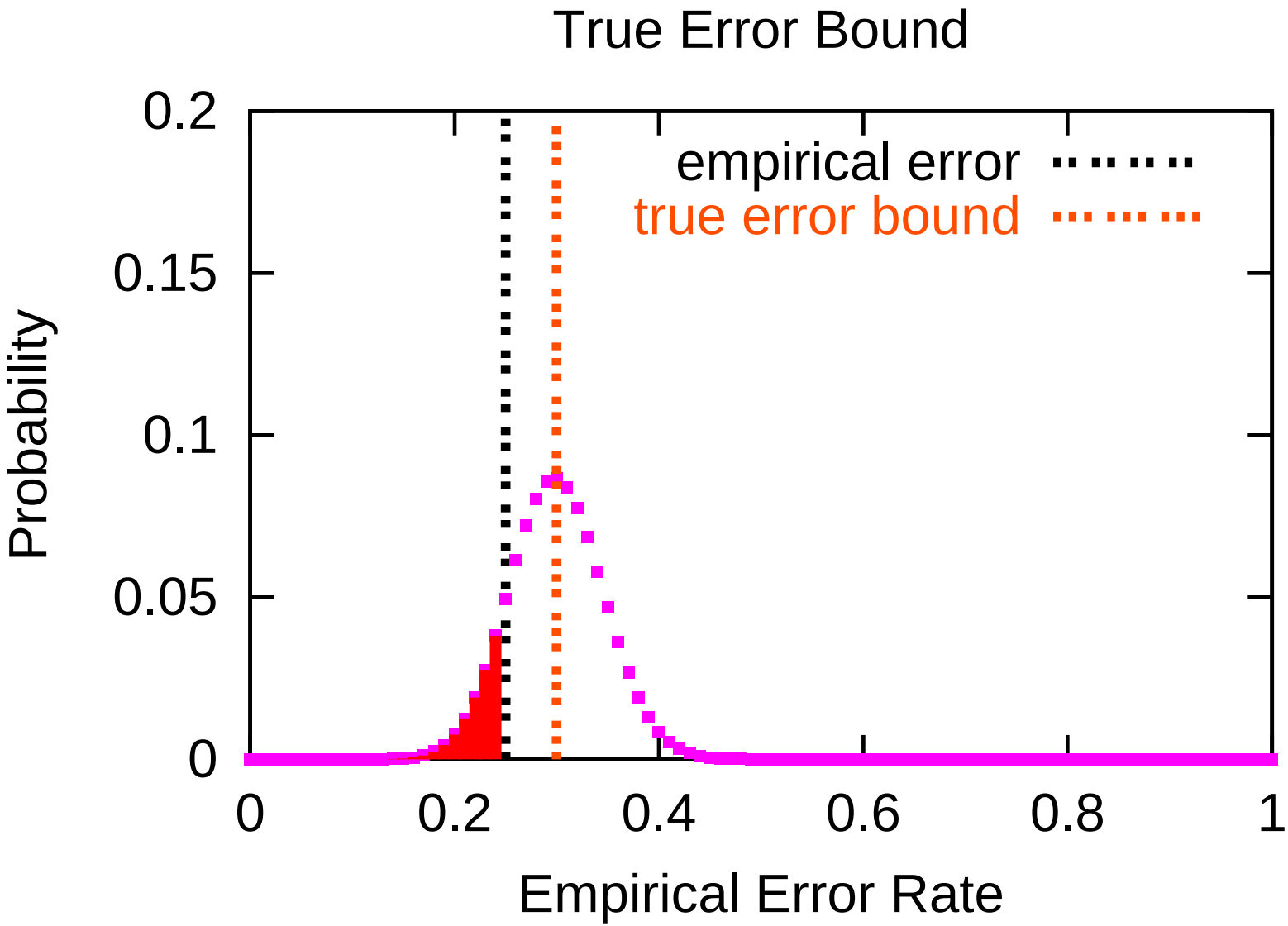
World's easiest proof: (by contradiction).

Assume $\mathsf{Bin} \left( \frac{k}{m}, c_D \right) \geq \delta$ (which is true with probability $1 - \delta$).

Then by definition, $\overline{\mathsf{Bin}} \left( \hat{c}_S, \delta \right) \geq c_D$


Observation and Possible Binomials
empirical error
Probability
0.2
0.15
0.1
0.05
0
0
0.2
0.4
0.6
0.8
1
Empirical Error Rate


Observation and Consistent Binomials
empirical error
Probability
Empirical Error Rate
0
0.05
0.1
0.15
0.2
0
0.2
0.4
0.6
0.8
1


True Error Bound
0.2
0.15
0.1
0.05
0
Probability
empirical error
true error bound
0
0.2
0.4
0.6
0.8
1
Empirical Error Rate

# Test Set Bound Notes

Perfectly tight: There exist true error rates achieving the bound

Lower bound of the same form.

Primary use: verification of succesful learning

## What does Test Set Bound mean?

Corollary: For all classifiers $c$, for all $D$, for all $\delta \in (0, 1]$:

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

Proof: Use the Chernoff approximation,

$$\overline{\mathrm{Bin}}\left(\hat{c}_S, \delta\right) \leq \hat{c}_S + \sqrt{\frac{\ln \frac{1}{\delta}}{2m}}$$

Note: NOT tight when $\hat{c}_S$ near 0 (our goal!)

# Test Set Bound: Example

Suppose $\delta = 0.1$

Suppose $m = 100$

Suppose $\widehat{c}_S = \frac{38}{100}$

Square root Chernoff bound: $\Rightarrow c_D \in [0.26, 0.50]$

Exact calculation $\Rightarrow c_D \in [0.30, 0.47]$

## Test Set Bound Comparison: Empirical "confidence" intervals

$k$ = number of test errors, $m$ = number of examples

$\mu = \frac{k}{m}$

$\sigma^2 = \frac{1}{m-1} \sum_{i=1}^{m} \left(\mu - I\left[c(x_i) \neq y_i\right]\right)^2$

pick bound = $\frac{k}{m} + 2\sigma$

How do they compare?

Test Set Bound vs. 2 Sigma Bound
True error (bound)
1.5
1.25
1
0.75
0.5
0.25
0
Learning Problem
adult
shroom
audio
balance
car
votes
krkp
lung
nursery
postop
shuttle
soybean
yellow
bound
error

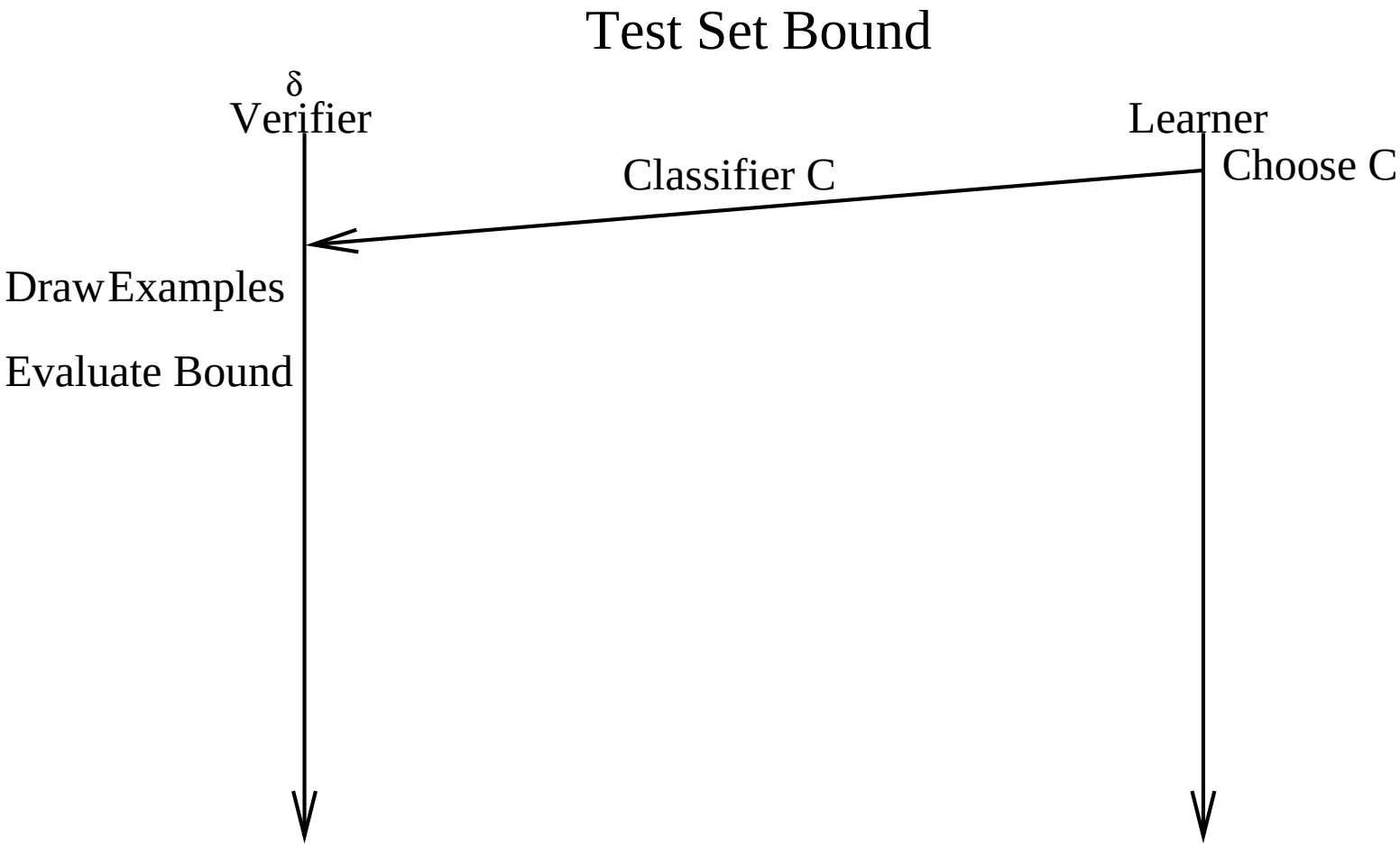
## Test Set Bound vs Empirical Confidence Interval

1. empirical confidence intervals are sometimes pessimistic

2. empirical confidence intervals are sometimes optimistic

3. the test set bound always works

# Interpretation: Interactive Proof of Learning



## $K$-fold Cross Validation

Divide $m$ examples into $K$ subsets.

Repat $K$ times: Train on $K-1$ subsets, test on heldout subset.

Not well understood theoretically.

Best Result: Confidence interval smaller than a test set of size $\frac{m}{K}$.

$\Rightarrow$ leave-one-out cross validation very prone to overfitting.

$\Rightarrow$ Some people fool themselves with overconfidence in Cross Validation.

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## Training Set Bounds in General

- Sometimes the holdout set is *critical* for learning.
- Sometimes we want bounds to guide learning

$\Rightarrow$Train set bounds

Occam's Razor bound is the simplest train set bound.

## A note on Practicality

Many Train set bounds are not practical: They are too loose.

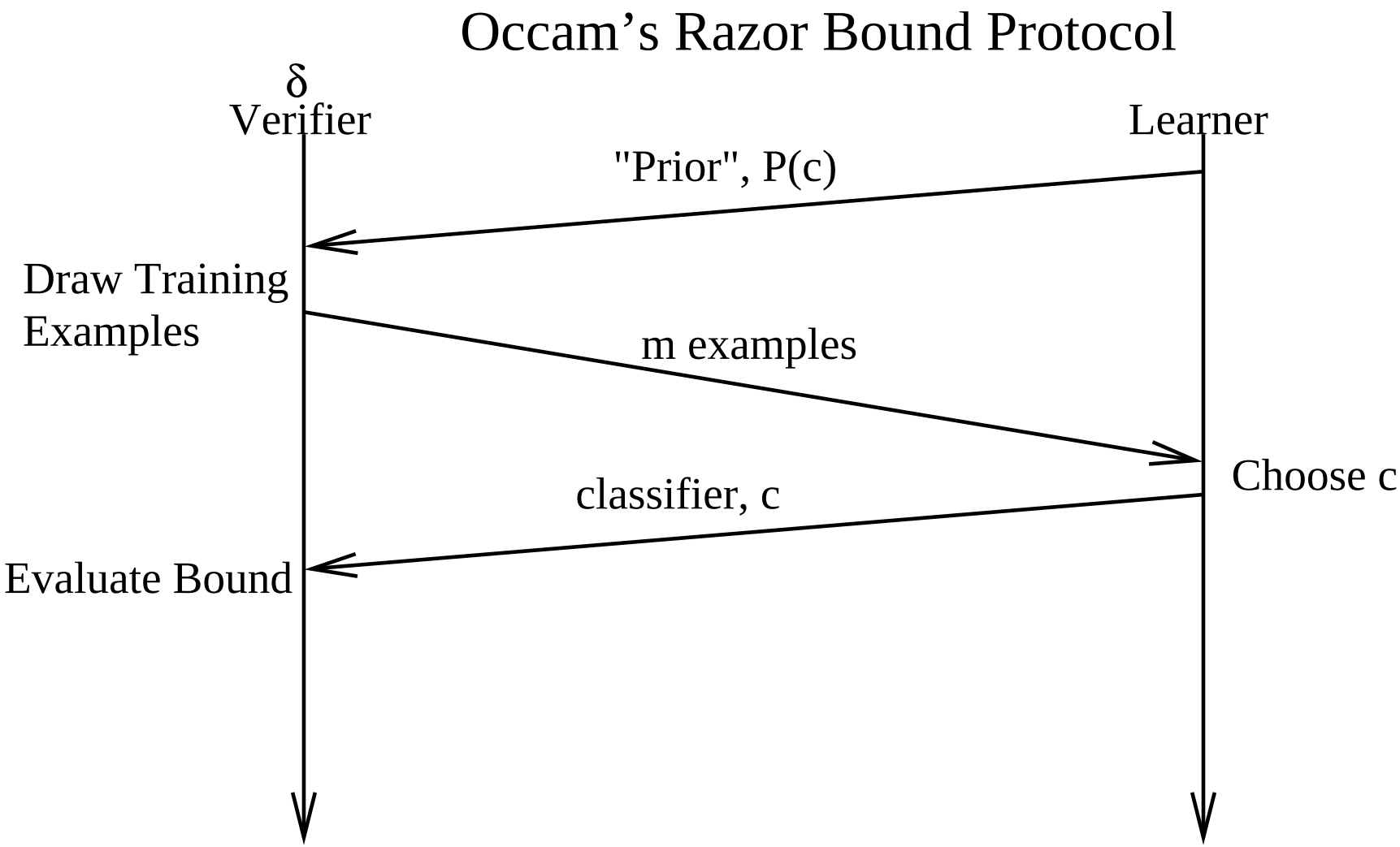
1. VC dimension bounds

2. Fat-shattering dimension bounds

3. Covering number bounds

We do not cover these here: the emphasis is on (in practice) tight bounds.

Despite lack of tightness, these other bounds can motivate learning algorithms.


Occam's Razor Bound Protocol
δ
Verifier
Learner
"Prior", P(c)
Draw Training
Examples
m examples
Choose c
classifier, c
Evaluate Bound

## Occam's Razor Bound

Theorem: (Occam's Razor Bound) For all "priors" $P(c)$ over the classifiers $c$, for all $D$, for all $\delta \in (0, 1]$:

$$\Pr_{S \sim D^m} \left( \forall c : \; c_D \leq \overline{\mathsf{Bin}} \left( \hat{c}_S, \delta P \left( c \right) \right) \right) \geq 1 - \delta$$

Compare with test set bound: $\delta \to \delta P(c)$.

# Occam's Razor Bound: Proof

Test set bound $\Rightarrow$

$$\forall c \quad \Pr_{S \sim D^m} \left( c_D \leq \overline{\mathsf{Bin}} \left( \hat{c}_S, \delta P(c) \right) \right) \geq 1 - \delta P(c)$$

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Negate to get:

$$\forall c \quad \Pr_{S \sim D^m} \left( c_D > \overline{\mathsf{Bin}} \left( \hat{c}_S, \delta P(c) \right) \right) < \delta P(c)$$

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Apply union bound: $\Pr(A \text{ or } B) \leq \Pr(A) + \Pr(B)$ repeatedly.

$$\Pr_{S \sim D^m} \left( \exists c : \ \ c_D > \overline{\mathsf{Bin}} \left( \hat{c}_S, \delta P(c) \right) \right) < \sum_c \delta P(c) = \delta$$

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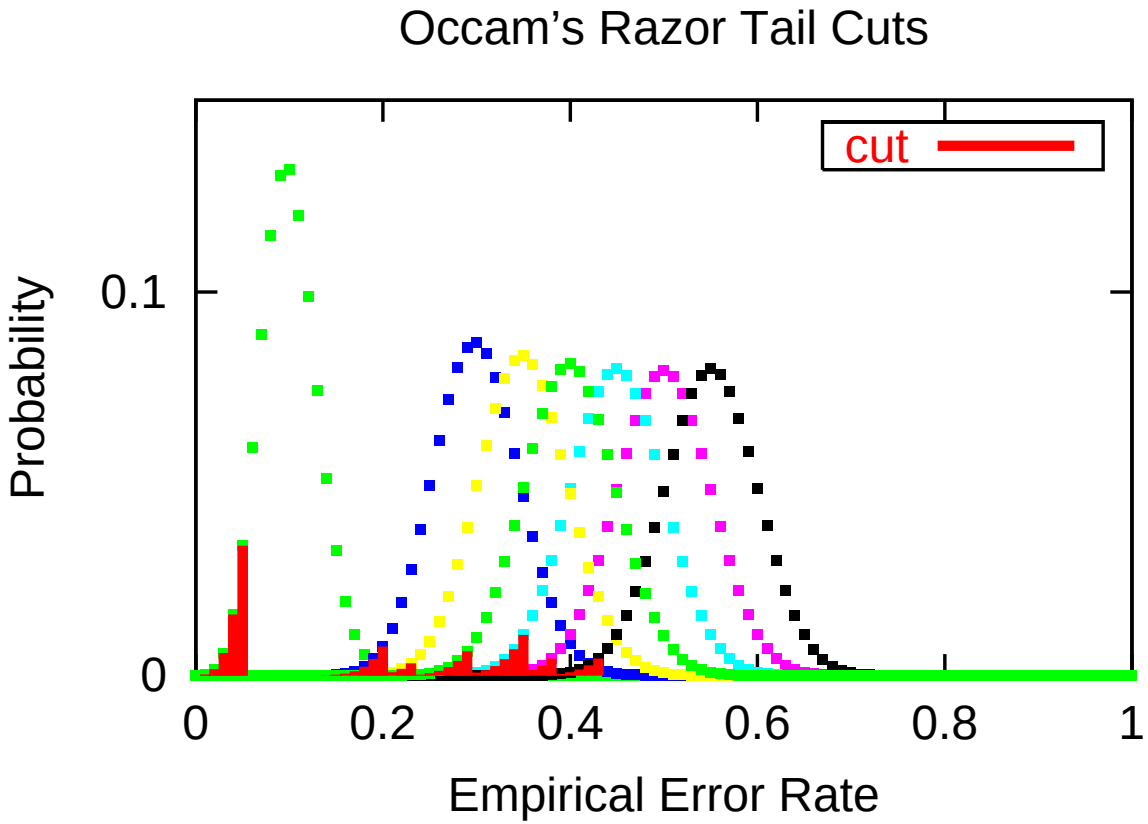
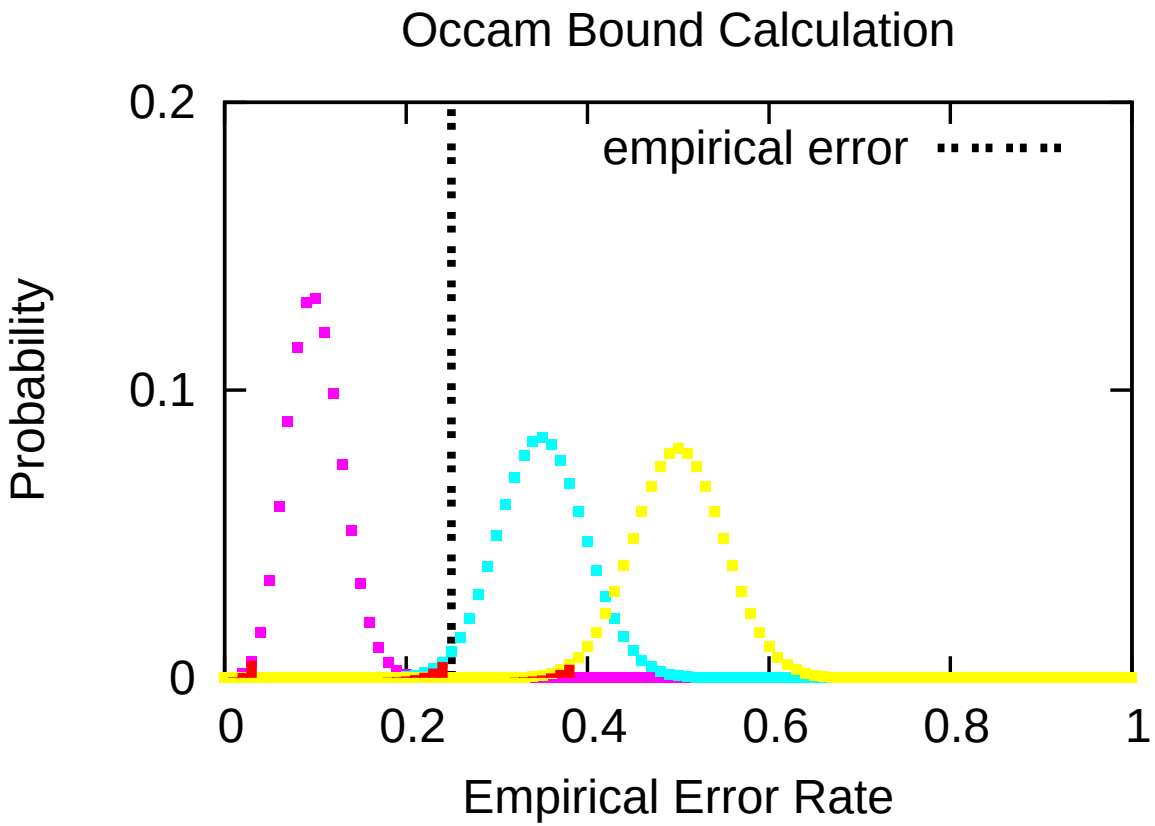
Negate again to get proof.

Next: Graphical proof

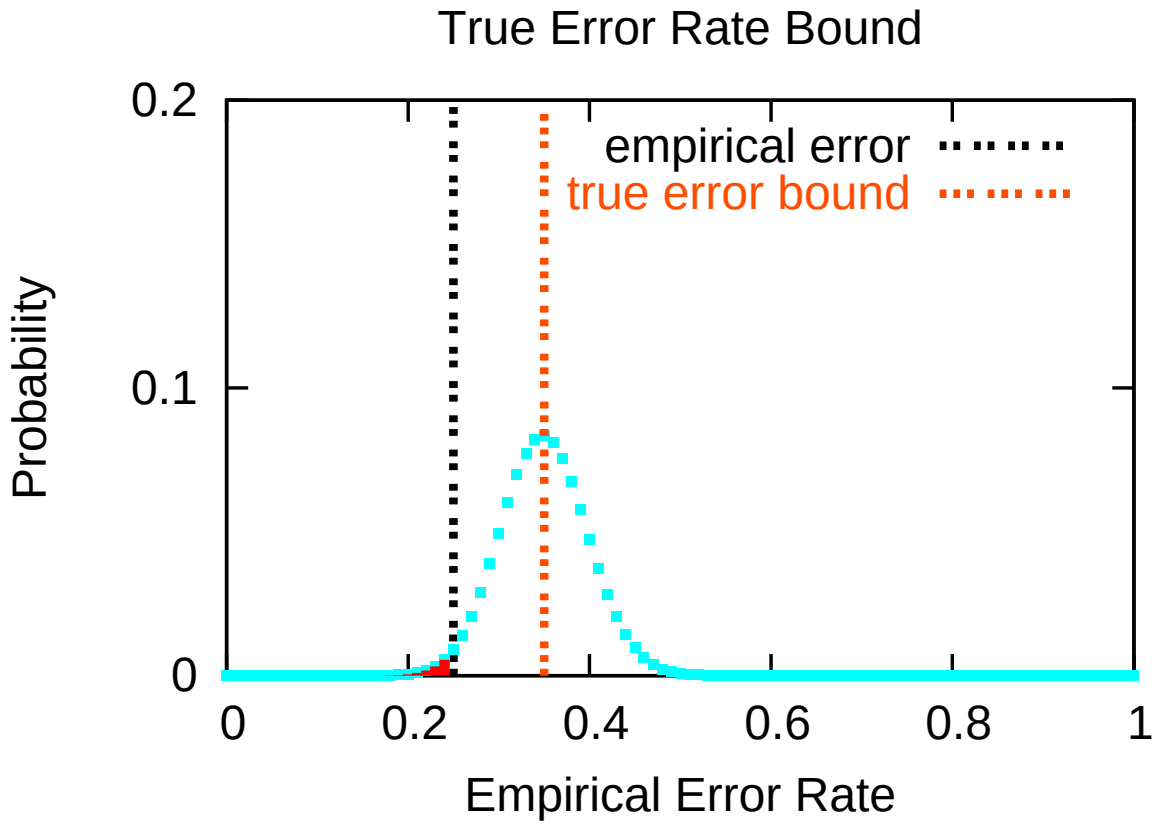



Each classifier is a Binomial with a different size tail cut.

With high probability no error falls in any tail.




The chosen classifier has an unknown true error rate.




Bound = the largest true error rate for which the observation is not in the tail.

# Occam's Razor Bound: Example

Suppose $\delta = 0.1$

Suppose $m = 100$

Suppose $P(c) = 0.1$

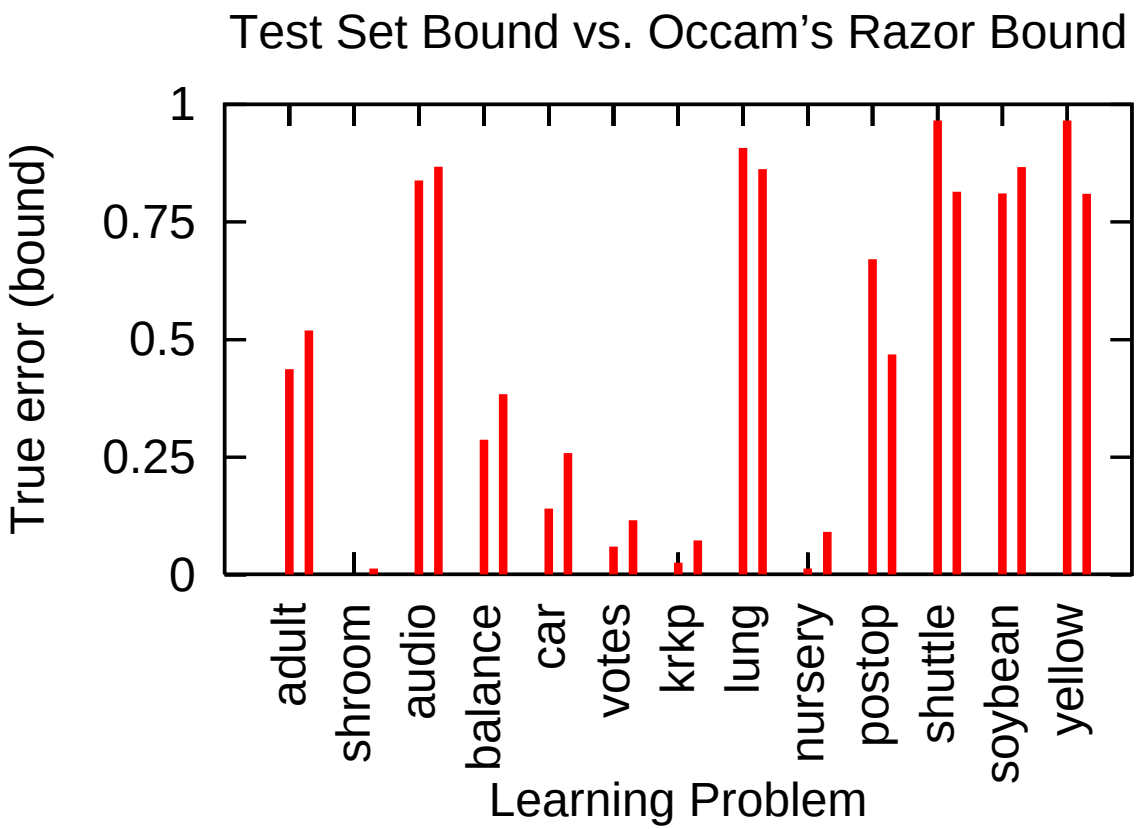
Suppose $\widehat{c}_S = \frac{38}{100}$

Square root Chernoff $\Rightarrow c_D \in [0.22, 0.54]$

Exact calculation $\Rightarrow c_D \in [0, 26, 0.51]$

## Occam's Razor Bound Results Decision Trees

- ID3 decision tree + pruning
- probability of failure $= \delta = 0.1$
- Discrete problems from UCI database of Machine Learning problems.
- 100% of data used for training set bounds
- 80%/20% Train/Test split for test set bounds
- Minimal selection bias




Left bar = test set bound, right bar = Occam's Razor Bound

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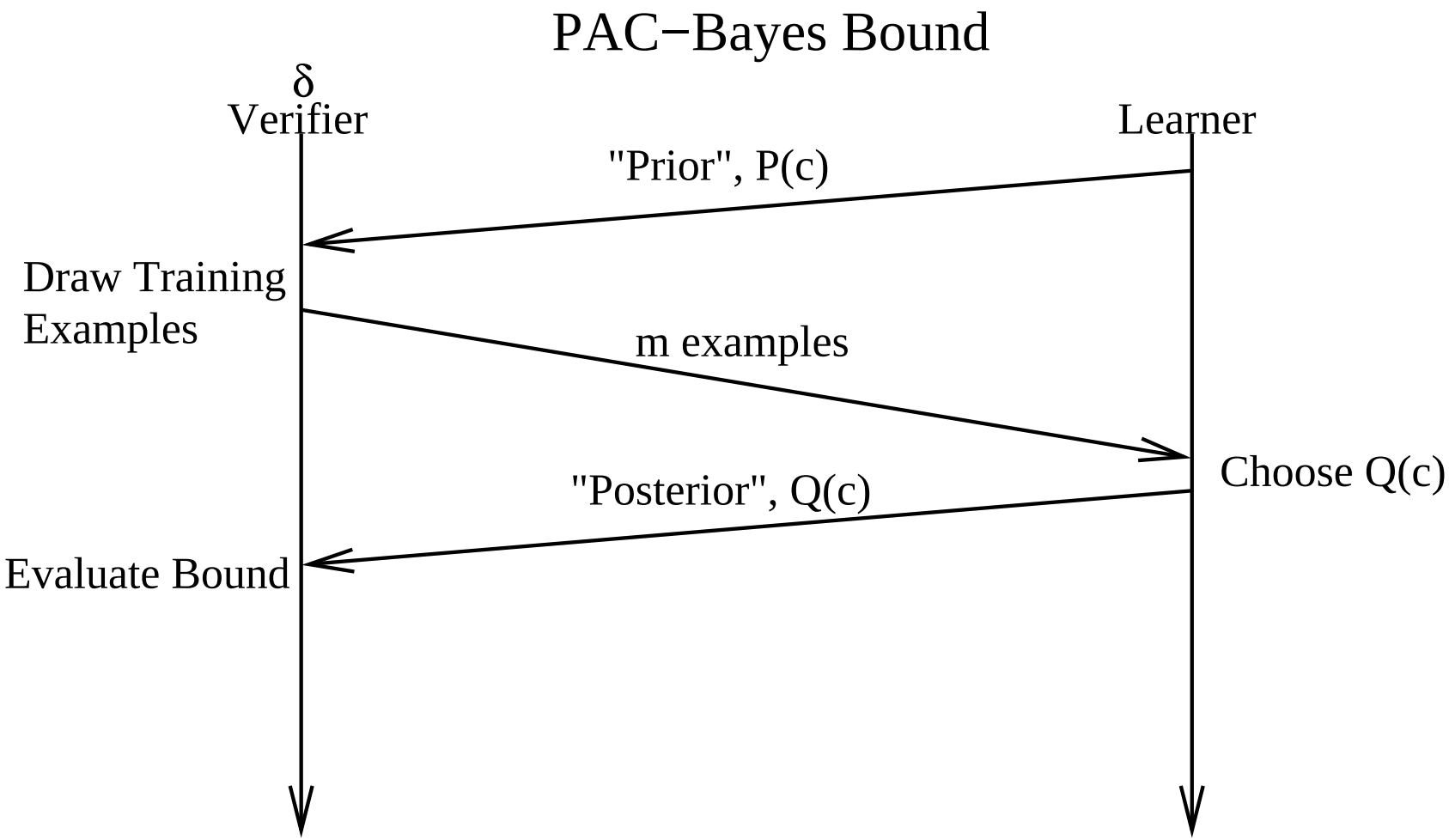
PAC−Bayes Bound
δ
Verifier
Learner
"Prior", P(c)
Draw Training
Examples
m examples
Choose Q(c)
"Posterior", Q(c)
Evaluate Bound

## PAC-Bayes Bound: Basic quantities

$Q_D \equiv E_{c\sim Q}[c_D]$ = average true error

$\widehat{Q}_S \equiv E_{c\sim Q}[\widehat{c}_S]$ = average train error

## PAC-Bayes Bound: Theorem

Theorem: (PAC-Bayes Bound) For all "priors" $P(c)$ over the classifiers $c$, for all $D$, for all $\delta \in (0, 1]$:

$$\Pr_{S \sim D^m} \left( \forall Q(c) : \ \mathsf{KL}\left(\hat{Q}_S || Q_D\right) \leq \frac{\mathsf{KL}(Q||P) + \ln \frac{m+1}{\delta}}{m} \right) \geq 1 - \delta$$

where: $\mathsf{KL}(Q||P) = E_{c \sim Q} \ln \frac{Q(c)}{P(c)}$

$\mathsf{KL}(q||p) = q \ln \frac{q}{p} + (1 - q) \ln \frac{1-q}{1-p}$ for $q < p$

The proof uses two quick lemmas

Lemma 1: For all $P(c)$, for all $D$, for all $\delta \in (0, 1]$:

$$\Pr_{S \sim D^m} \left( E_{c \sim P} \frac{1}{\Pr_{S' \sim D^m} (\widehat{c}_S = \widehat{c}_{S'})} \leq \frac{m+1}{\delta} \right) \geq 1 - \delta$$

Lemma 1: For all $P(c)$, for all $D$, for all $\delta \in (0, 1]$:

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Proof:

$$\forall c \;\; E_{S \sim D^m} \frac{1}{\Pr_{S' \sim D^m}\left(\widehat{c}_S = \widehat{c}_{S'}\right)} = \sum_{\frac{k}{m}} \frac{\Pr_{S \sim D^m}\left(\widehat{c}_S = \frac{k}{m}\right)}{\Pr_{S' \sim D^m}\left(\widehat{c}_{S'} = \frac{k}{m}\right)} = m + 1$$

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Proof:

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$$\Rightarrow E_{S \sim D^m} E_{c \sim P} \frac{1}{\Pr_{S \sim D^m}(\widehat{c}_S)} = m + 1$$

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$$\Rightarrow E_{S \sim D^m} E_{c \sim P} \frac{1}{\Pr_{S' \sim D^m}(\hat{c}_S = \hat{c}_{S'})} = m + 1$$

Use the Markov inequality ($X \geq 0$, $EX = \mu$, $\Rightarrow \Pr(X > \frac{\mu}{\delta}) \leq \delta$):

$$\forall P \;\; \Pr_{S \sim D^m}\left(E_{c \sim P} \frac{1}{\Pr_{S' \sim D^m}(\hat{c}_S = \hat{c}_{S'})} \leq \frac{m+1}{\delta}\right) \leq \delta$$

$\Rightarrow$lemma

Lemma 2: For all $Q(c)$: $\frac{E_{c\sim Q} \ln \frac{1}{\Pr_{S\sim D^m}(\hat{c}_S)}}{m} \geq \mathsf{KL}(\hat{Q}_S || Q_D)$

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Proof: $\frac{1}{m} E_{c\sim Q} \ln \frac{1}{\binom{m}{m\hat{c}_S} c_D^{m\hat{c}_S} (1-c_D)^{m(1-\hat{c}_S)}}$

$$= E_{c\sim Q}\left[\hat{c}_S \ln \frac{1}{c_D} + (1-\hat{c}_S) \ln \frac{1}{1-c_D}\right] - \frac{E_{c\sim Q} \ln \binom{m}{m\hat{c}_S}}{m}$$

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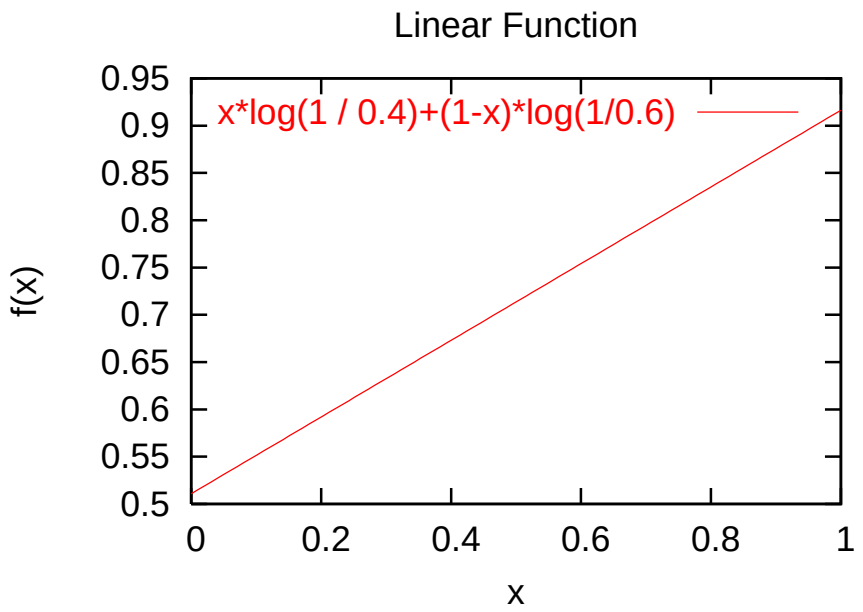
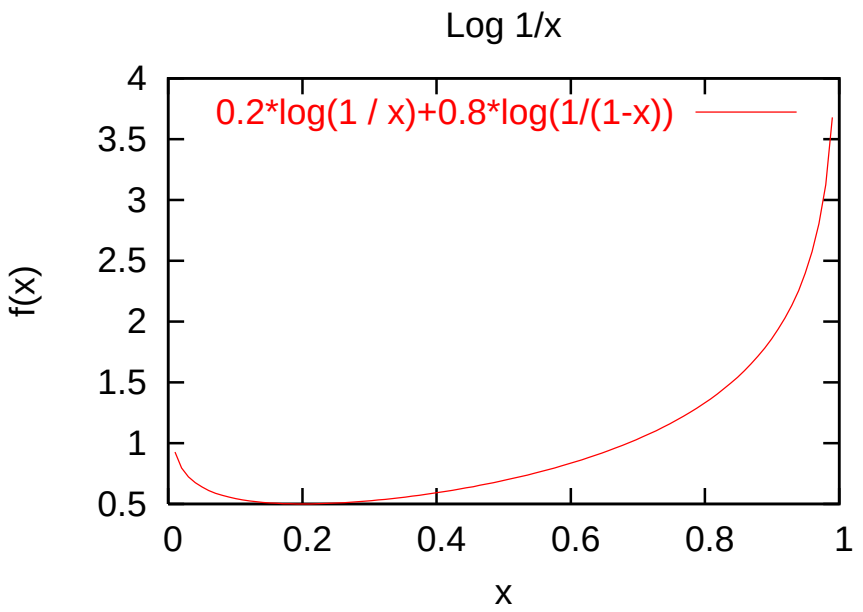
$$= E_{c\sim Q}\left[\hat{c}_S \ln \frac{1}{c_D} + (1-\hat{c}_S)\ln\frac{1}{1-c_D}\right] - \frac{E_{c\sim Q}\ln\binom{m}{m\hat{c}_S}}{m}$$

Jensen's inequality ($f$ concave $\Rightarrow Ef(X) \geq f(EX)$):

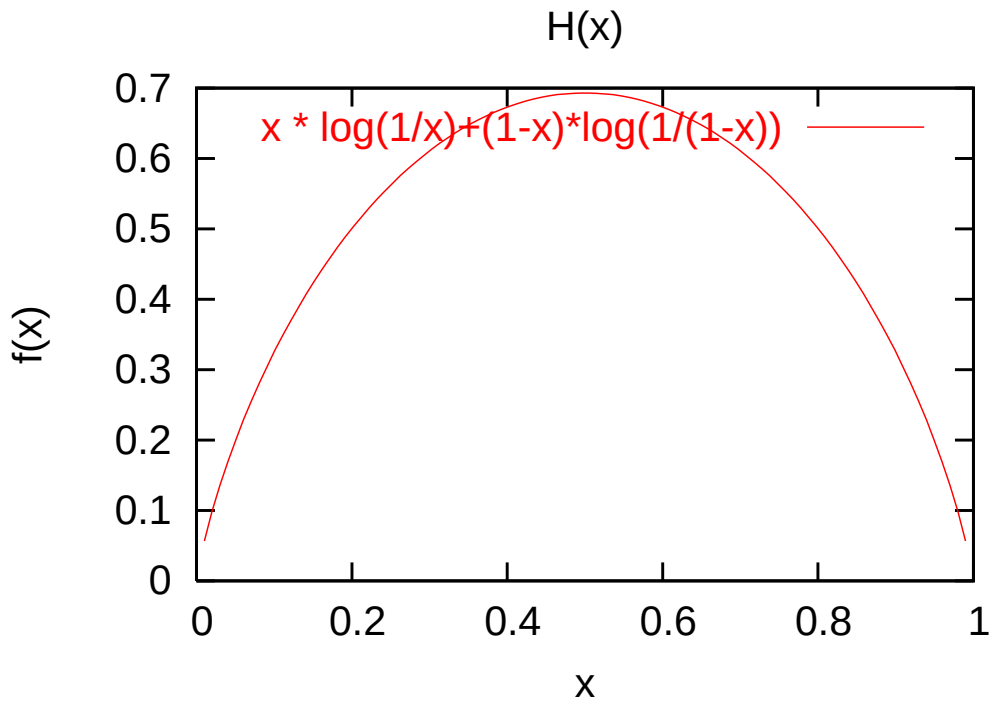
$$E_{c\sim Q}\left[\hat{c}_S \ln \frac{1}{c_D} + (1-\hat{c}_S)\ln\frac{1}{1-c_D}\right] \geq \hat{Q}_S \ln\frac{1}{Q_D} + \left(1-\hat{Q}_S\right)\ln\frac{1}{1-Q_D}$$

$$E_{c\sim Q}\left[\hat{c}_S \ln \frac{1}{c_D} + (1-\hat{c}_S)\ln\frac{1}{1-c_D}\right] \geq \hat{Q}_S \ln\frac{1}{Q_D} + \left(1-\hat{Q}_S\right)\ln\frac{1}{1-Q_D}$$



$$\frac{E_{c\sim Q} \ln \binom{m}{m\hat{c}_S}}{m} \leq \frac{E_{c\sim Q} \ln e^{mH(\hat{c}_S)}}{m} = \frac{E_{c\sim Q} mH(\hat{c}_S)}{m} \leq H\left(\hat{Q}_S\right)$$



Lemma 2: For all $Q(c)$: $\frac{E_{c\sim Q} \ln \frac{1}{\Pr_{S\sim D^m}(\hat{c}_S)}}{m} \geq \mathrm{KL}(\hat{Q}_S || Q_D)$

Proof: $\frac{1}{m} E_{c\sim Q} \ln \frac{1}{\binom{m}{m\hat{c}_S} c_D^{m\hat{c}_S} (1-c_D)^{m(1-\hat{c}_S)}}$

$$= E_{c\sim Q}\left[\hat{c}_S \ln \frac{1}{c_D} + (1-\hat{c}_S) \ln \frac{1}{1-c_D}\right] - \frac{E_{c\sim Q} \ln \binom{m}{m\hat{c}_S}}{m}$$

Jensen's inequality ($f$ concave $\Rightarrow Ef(X) \geq f(EX)$):

$$E_{c\sim Q}\left[\hat{c}_S \ln \frac{1}{c_D} + (1-\hat{c}_S) \ln \frac{1}{1-c_D}\right] \geq \hat{Q}_S \ln \frac{1}{Q_D} + \left(1-\hat{Q}_S\right) \ln \frac{1}{1-Q_D}$$

and $$\frac{E_{c\sim Q} \ln \binom{m}{m\hat{c}_S}}{m} \leq \frac{E_{c\sim Q} \ln e^{mH(\hat{c}_S)}}{m} = \frac{E_{c\sim Q} mH(\hat{c}_S)}{m} \leq H\left(\hat{Q}_S\right)$$

$\Rightarrow$lemma

# PAC-Bayes bound: Proof

Let

$$P_G(c, \hat{c}_S) = \frac{1}{\Pr_{S \sim D^m}(\hat{c}_S)\, E_{c \sim P} \frac{1}{\Pr_{S' \sim D^m}(\hat{c}_S = \hat{c}_{S'})}} P(c)$$

# PAC-Bayes bound: Proof

Let

$$P_G(c, \hat{c}_S) = \frac{1}{\Pr_{S \sim D^m}(\hat{c}_S)\, E_{c \sim P} \frac{1}{\Pr_{S' \sim D^m}(\hat{c}_S = \hat{c}_{S'})}} P(c)$$

$$\Rightarrow 0 \leq \mathrm{KL}(Q||P_G) = E_{c \sim Q} \ln \frac{Q(c)}{P(c)} \Pr_{S \sim D^m}(\hat{c}_S)\, E_{c \sim P} \frac{1}{\Pr_{S' \sim D^m}(\hat{c}_S = \hat{c}_{S'})}$$

$$= \mathrm{KL}(Q||P) - E_{c \sim Q} \ln \frac{1}{\Pr_{S \sim D^m}(\hat{c}_S)} + \ln E_{c \sim P} \frac{1}{\Pr_{S' \sim D^m}(\hat{c}_S = \hat{c}_{S'})}$$

# PAC-Bayes bound: Proof

Let

$$P_G(c, \hat{c}_S) = \frac{1}{\Pr_{S\sim D^m}(\hat{c}_S)\, E_{c\sim P} \frac{1}{\Pr_{S'\sim D^m}(\hat{c}_S = \hat{c}_{S'})}} P(c)$$

$$\Rightarrow 0 \leq \mathrm{KL}(Q||P_G) = E_{c\sim Q} \ln \frac{Q(c)}{P(c)} \Pr_{S\sim D^m}(\hat{c}_S)\, E_{c\sim P} \frac{1}{\Pr_{S'\sim D^m}(\hat{c}_S = \hat{c}_{S'})}$$

$$= \mathrm{KL}(Q||P) - E_{c\sim Q} \ln \frac{1}{\Pr_{S\sim D^m}(\hat{c}_S)} + \ln E_{c\sim P} \frac{1}{\Pr_{S'\sim D^m}(\hat{c}_S = \hat{c}_{S'})}$$

$$\Rightarrow E_{c\sim Q} \ln \frac{1}{\Pr_{S'\sim D^m}(\hat{c}_S = \hat{c}_{S'})} \leq \mathrm{KL}(Q||P) + \ln E_{c\sim P} \frac{1}{\Pr_{S\sim D^m}(\hat{c}_S)}$$

Lemma 1&2 $\Rightarrow$proof

## PAC-Bayes Bound: Application

Is the PAC-Bayes bound tight enough to be useful?

Application: true error bounds for Support Vector Machines.

Classifier form:

$$c(x) = \text{sign}\,(\vec{w} \cdot \vec{x})$$

Also note: Work by Matthias Seeger for Gaussian Processes.

## PAC-Bayes Margin bound

$\bar{F}(x) = \int_x^\infty \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$ = cumulative distribution of a Gaussian

$Q(\vec{w}, \mu) = N(\mu, 1) \times N(0, 1)^{n-1}$ where first direction parallel to $\vec{w}$

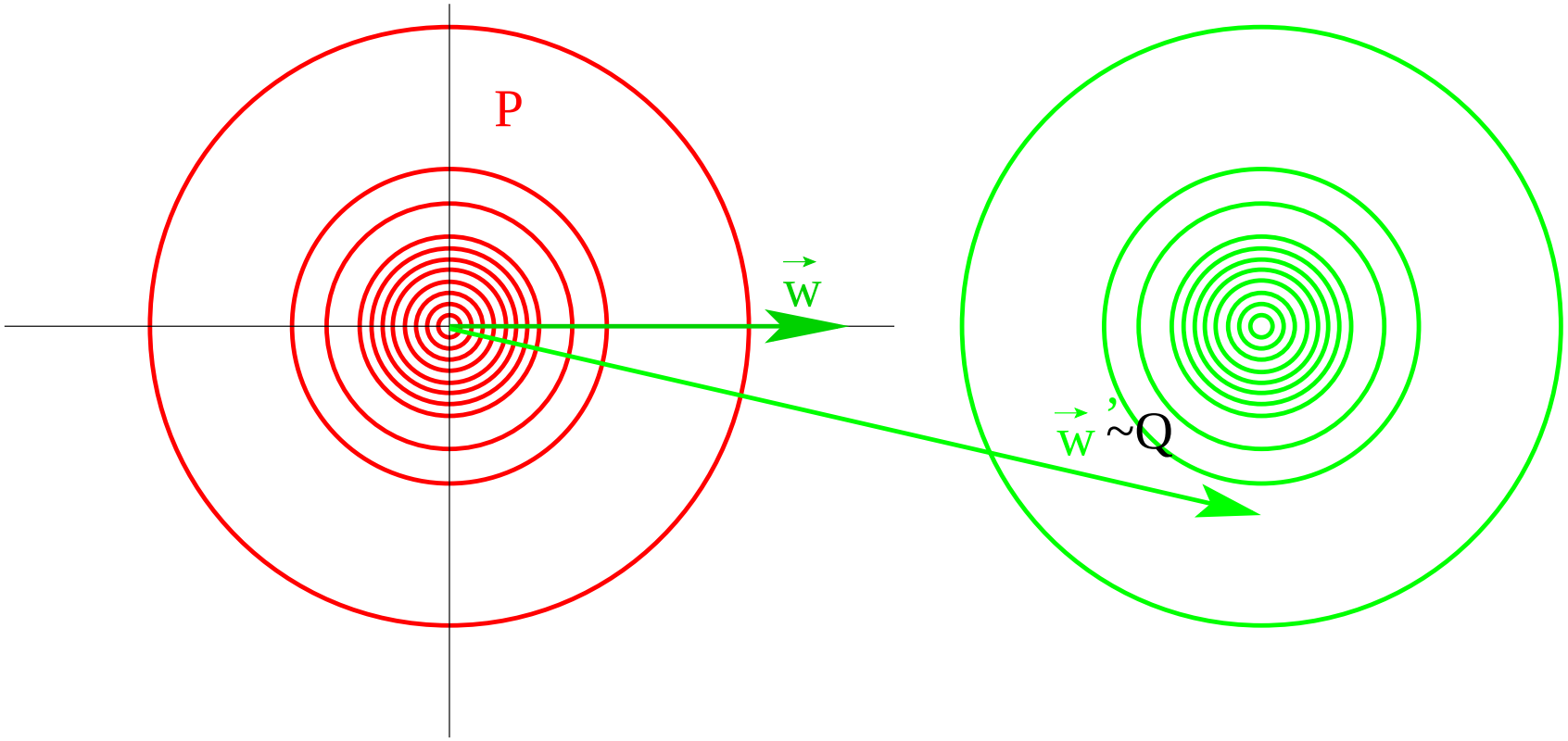
$\gamma(\vec{x}, y) = \frac{y\vec{w} \cdot \vec{x}}{||\vec{w}||||\vec{x}||}$ = normalized margin

$\widehat{Q}(\vec{w}, \mu)_S = E_{\vec{x},y \sim S} \bar{F}\left(\mu \gamma(\vec{x}, y)\right)$ = stochastic error rate

Corollary: (PAC-Bayes Margin Bound) For all distributions $D$, for all $\delta \in (0, 1]$:

$$\Pr_{S \sim D^m}\left(\forall \vec{w}, \mu > 0 : \ \mathrm{KL}\left(\widehat{Q}(\vec{w}, \mu)_S || Q(\vec{w}, \mu)_D\right) \leq \frac{\frac{\mu^2}{2} + \ln \frac{m+1}{\delta}}{m}\right) \geq 1 - \delta$$

# PAC-Bayes Margin Bound: Intuition




Isotropic Gaussian prior and posterior

## PAC-Bayes Margin Bound: Proof

Start with PAC-Bayes bound:

$$\forall P(c) \quad \Pr_{S\sim D^m}\left(\forall Q(c):\ \mathsf{KL}\left(\hat{Q}_S||Q_D\right) \leq \frac{\mathsf{KL}(Q||P)+\ln\frac{m+1}{\delta}}{m}\right) \geq 1-\delta$$

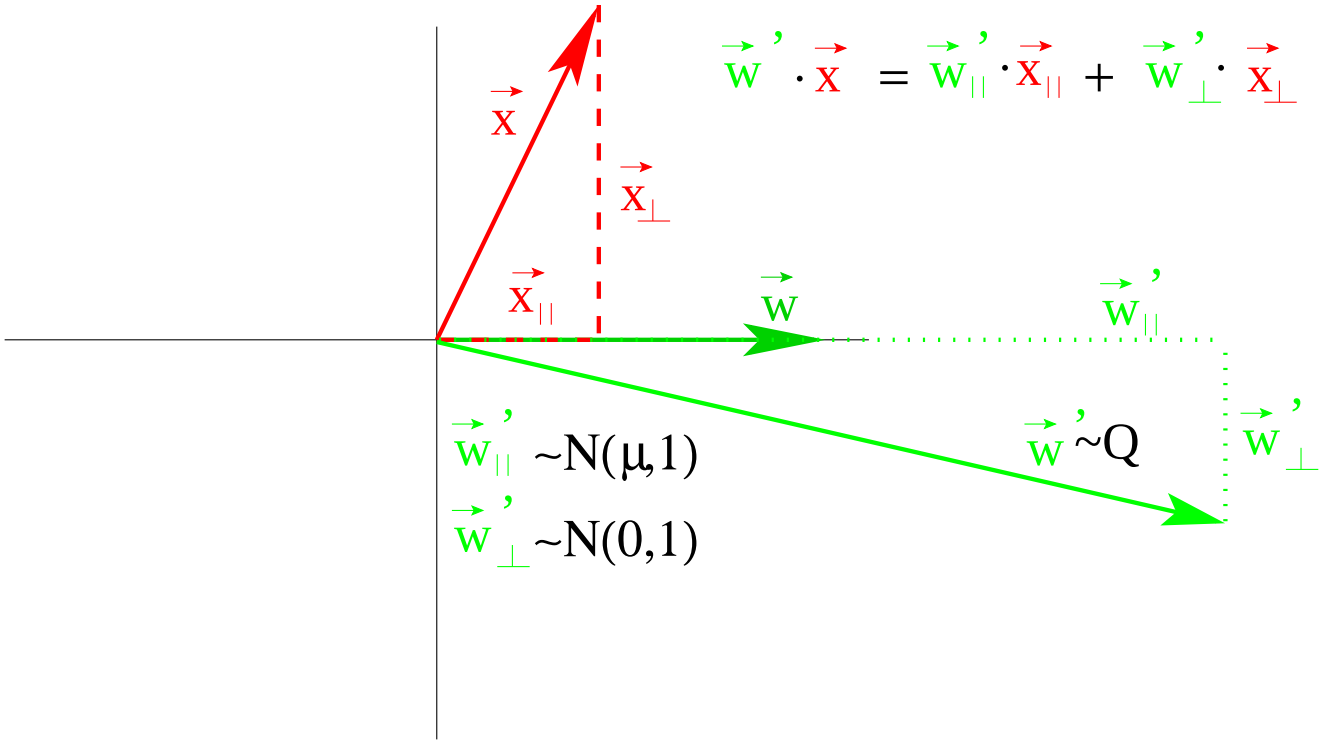
Set $P = N(0,1)^n$

$Q(\vec{w},\mu) = N(\mu,1)\times N(0,1)^{n-1}$ with first direction parallal to $\vec{w}$

Gaussian $\Rightarrow$ coordinate system reorientable

$$\Rightarrow \mathsf{KL}(Q||P) = \mathsf{KL}(N(0,1)^{n-1}||N(0,1)^{n-1}) + \mathsf{KL}(N(\mu,1)||N(0,1))$$

$$= \frac{\mu^2}{2}$$




$$\hat{Q}(\vec{w},\mu)_S = E_{\vec{x},y\sim S,\vec{w}'\sim Q(\vec{w},\mu)} I\left(y \neq \text{sign}\left(\vec{w}' \cdot \vec{x}\right)\right)$$

$$= E_{\vec{x},y\sim S} E_{w'_{||}\sim N(\mu,1)} E_{w'_{\perp}\sim N(0,1)} I\left(y(w'_{||}x_{||} + w'_{\perp}x_{\perp}) \leq 0\right)$$

Use properties of Gaussians to finish proof

## PAC-Bayes Margin proof: the end

$$= E_{\vec{x},y\sim S} E_{z'\sim N(0,1)} E_{w'_\perp \sim N(0,1)} I\left(y\mu \leq -yz' - yw'_\perp \frac{x_\perp}{x_{||}}\right)$$

The sum of two Gaussians is a Gaussian $\Rightarrow$

$$= E_{\vec{x},y\sim S} E_{v\sim N\left(0,1+\frac{x_\perp^2}{x_{||}^2}\right)} I\left(y\mu \leq -yv\right)$$

$$= E_{\vec{x},y\sim S} E_{v\sim N\left(0,\frac{1}{\gamma(\vec{x},y)^2}\right)} I\left(y\mu \leq -yv\right)$$

$$= E_{\vec{x},y\sim S} \bar{F}\left(\mu\gamma(\vec{x},y)\right)$$

$\Rightarrow$ Corollary

## PAC-Bayes: Application to SVM

SVM classifier:

$$c(x) = \text{sign}\left(\sum_{i=1}^{m} \alpha_i k(x_i, x)\right)$$

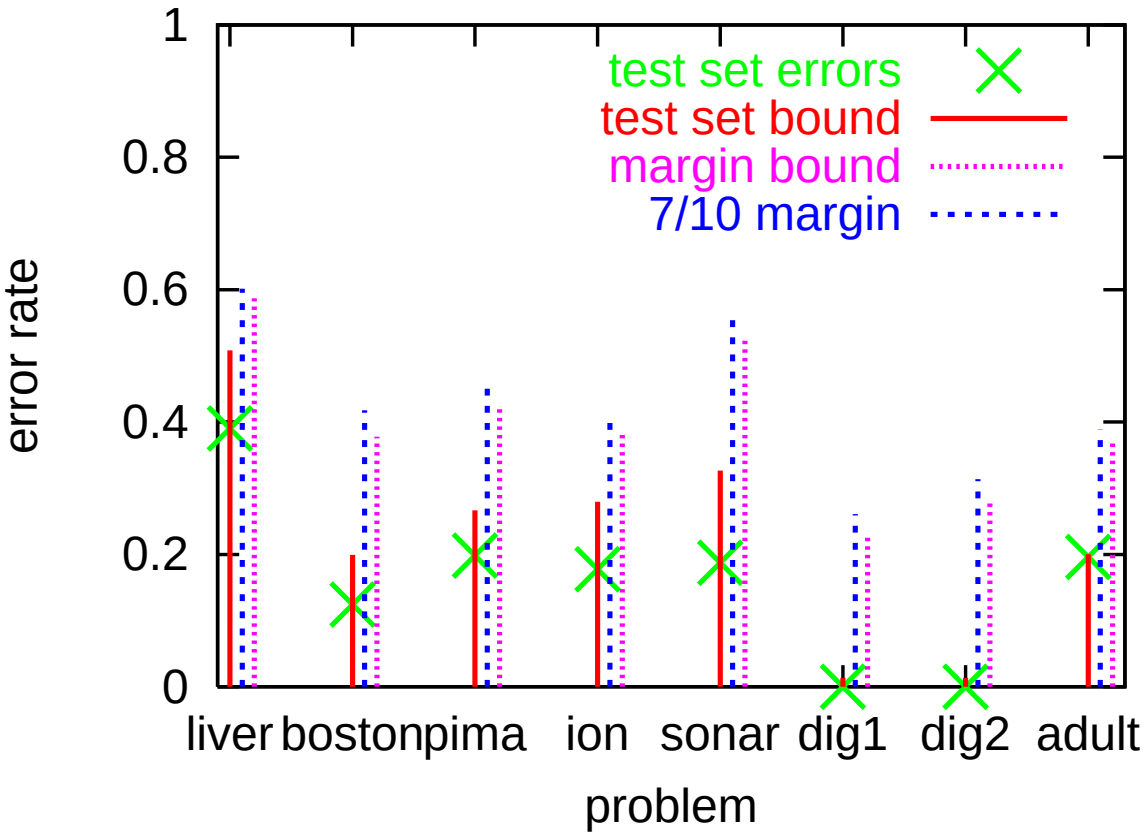
$k$ is a kernel $\Rightarrow \exists \vec{\Phi}: \quad k(x_i, x) = \vec{\Phi}(x_i) \cdot \vec{\Phi}(x)$ so:

$\vec{w} \cdot \vec{x} = \sum_{i=1}^{m} \alpha_i k(x_i, x)$ $\qquad\qquad$ $\vec{w} \cdot \vec{w} = \sum_{i,j} \alpha_i \alpha_j k(x_i, x_j)$

$$\Rightarrow \gamma(x, y) = \frac{\sum_{i=1}^{m} \alpha_i k(x_i, x)}{\sqrt{k(x, x) \sum_{i,j=1,1}^{m,m} \alpha_i \alpha_j k(x_i, x_j)}}$$

$\Rightarrow$ Margin bound applies to support vector machines.

# PAC-Bayes Margin Bound Results



# Outline

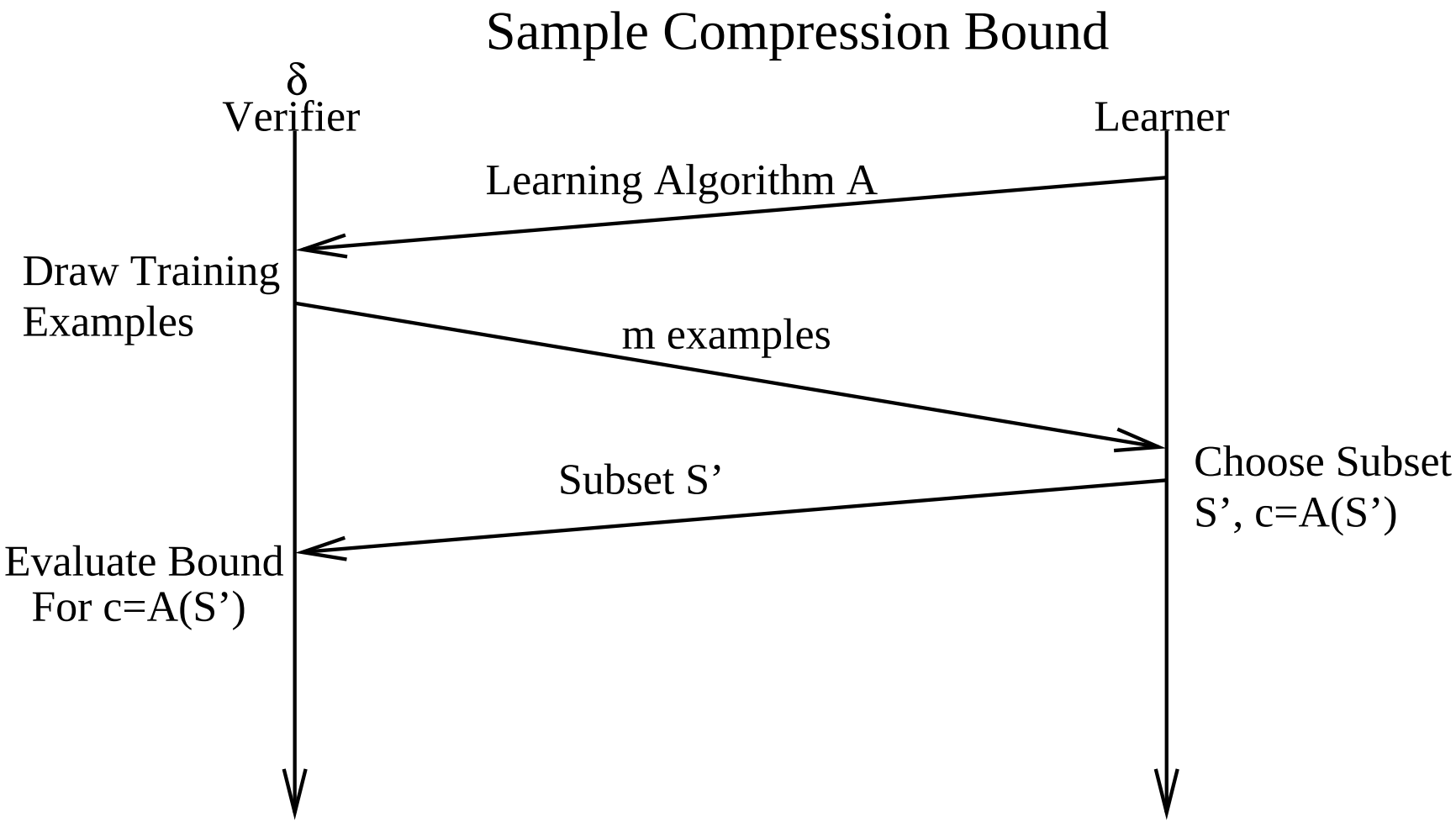
1. The Basic Model
2. The Test Set Bound
3. Occam's Razor Bound
4. PAC-Bayes Bound
5. Sample Compression Bound

## Sample Compression Bound: Basic Quantities

$A$ = learning algorithm

$S' \subseteq S$ = subset of training set.

The idea: if we knew $S'$ in advance that $S - S'$ would act as a test set. We don't know $S'$ in advance so the bound is looser.


Sample Compression Bound
δ
Verifier
Learner
Learning Algorithm A
Draw Training
Examples
m examples
Choose Subset
S', c=A(S')
Subset S'
Evaluate Bound
For c=A(S')

## Sample Compression Bound: Theorem

Theorem: (Sample Compression Bound) For all algorithms $A$, for all distributions $D$, for all $\delta \in (0, 1]$:

$$\Pr_{S \sim D^m} \left( \forall S' \subseteq S \text{ with } c = A(S') : \; c_D \leq \overline{\text{Bin}} \left( \widehat{c}_{S-S'}, \frac{\delta}{m \binom{m}{|S'|}} \right) \right) \geq 1 - \delta$$

## Sample Compression Bound: Proof

(Note that $S'$ is unambiguous before $S$ is drawn)

$$\forall S' \;\; c = A(S') : \Pr_{S \sim D^m} \left( c_D \leq \overline{\mathsf{Bin}} \left( \hat{c}_{S-S'}, \frac{\delta}{m \binom{m}{|S-S'|}} \right) \right) \geq 1 - \frac{\delta}{m \binom{m}{|S-S'|}}$$

## Sample Compression Bound: Proof

(Note that $S'$ is unambiguous before $S$ is drawn)

$$\forall S' \ c = A(S') \ \Pr_{S \sim D^m} \left( c_D \leq \overline{\mathsf{Bin}} \left( \hat{c}_{S-S'}, \frac{\delta}{m \binom{m}{|S-S'|}} \right) \right) \geq 1 - \frac{\delta}{m \binom{m}{|S-S'|}}$$

Negate to get:

$$\forall S' \ c = A(S') : \Pr_{S \sim D^m} \left( c_D > \overline{\mathsf{Bin}} \left( \hat{c}_{S-S'}, \frac{\delta}{m \binom{m}{|S-S'|}} \right) \right) < \frac{\delta}{m \binom{m}{|S-S'|}}$$

## Sample Compression Bound: Proof

(Note that $S'$ is unambiguous before $S$ is drawn)

$$\forall S' \ c = A(S') \ \Pr_{S \sim D^m}\left(c_D \leq \overline{\mathsf{Bin}}\left(\hat{c}_{S-S'}, \frac{\delta}{m\binom{m}{|S-S'|}}\right)\right) \geq 1 - \frac{\delta}{m\binom{m}{|S-S'|}}$$

Negate to get:

$$\forall S' \ c = A(S') : \ \Pr_{S \sim D^m}\left(c_D > \overline{\mathsf{Bin}}\left(\hat{c}_{S-S'}, \frac{\delta}{m\binom{m}{|S-S'|}}\right)\right) < \frac{\delta}{m\binom{m}{|S-S'|}}$$

Use union bound ($\Pr(A \text{ or } B) \leq \Pr(A) + \Pr(B)$) over each $S'$

$$\Rightarrow \Pr_{S \sim D^m}\left(\exists S' \ c = A(S') : \ \ c_D > \overline{\mathsf{Bin}}\left(\hat{c}_{S-S'}, \frac{\delta}{m\binom{m}{|S-S'|}}\right)\right) < \delta$$

## Sample Compression Bound: Proof

(Note that $S'$ is unambiguous before $S$ is drawn)

$$\forall S' \;\; c = A(S') \; \Pr_{S \sim D^m} \left( c_D \leq \overline{\text{Bin}} \left( \hat{c}_{S-S'}, \frac{\delta}{m \binom{m}{|S-S'|}} \right) \right) \geq 1 - \frac{\delta}{m \binom{m}{|S-S'|}}$$

Negate to get:

$$\forall S' \;\; c = A(S') : \; \Pr_{S \sim D^m} \left( c_D > \overline{\text{Bin}} \left( \hat{c}_{S-S'}, \frac{\delta}{m \binom{m}{|S-S'|}} \right) \right) < \frac{\delta}{m \binom{m}{|S-S'|}}$$

Use union bound ($\Pr(A \text{ or } B) \leq \Pr(A) + \Pr(B)$) over each $S'$

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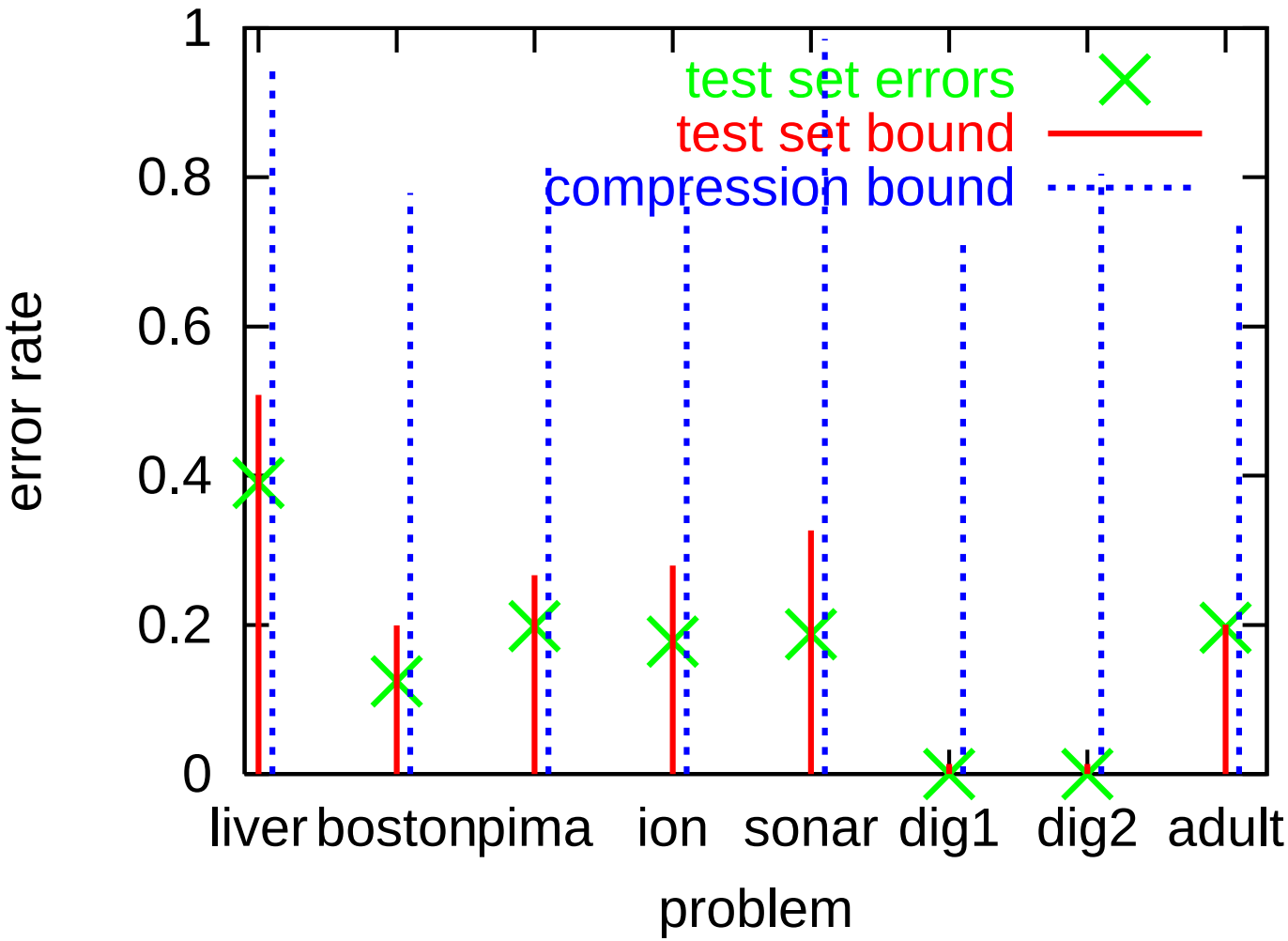
Negate again $\Rightarrow$ theorem

## Sample Compression Bound Application: Support Vector Machines

If $S'$= set of support vectors then $A(S') = A(S)$.

How well does the sample compression bound work with a support vector machine?

Note work by Mario Marchand and John Shawe-Taylor using Sample Compression bound variant for "Set Covering Machine".


1
0.8
0.6
0.4
0.2
0
error rate
test set errors
test set bound
compression bound
liver
boston
pima
ion
sonar
dig1
dig2
adult
problem

## Sample Compression Bound Results

Answer: Sample Compression bound not very tight on SVM.

Why not?

The SVM learning algorithm achieves 'incidental' sparsity rather than optimizing for it explicitly (in contrast to the margin).

## Combining Train Set and Test Set Bounds

Train set and Test set bounds are not exclusive.

The Test Set bound is our most robust known method.

But: we have a training set around anyways.

In general: can combine train set and test set bounds.

Behavior like a test set bound, except occasionally better.

# Conclusion

1. Use real confidence intervals to compare classifiers.

2. Test set bound very simple.

3. Train set bounds on the threshold of quantitatively useful.

Code for bound calculation at:

http://www-2.cs.cmu.edu/~jcl/programs/bound/bound.html