Machine Learning

Boosting

(based on Rob Schapire's IJCAI'99 talk and slides by B. Pardo)

Horse Race Prediction

How to Make $$$ In Horse Races?

- Ask a professional.
- Suppose:
  - Professional <u>cannot</u> give single highly accurate rule
  - …but presented with a set of races, can always generate better-than-random rules
- Can you get rich?

Idea

1) Ask expert for rule-of-thumb
2) Assemble set of cases where rule-of-thumb fails (hard cases)
3) Ask expert for a rule-of-thumb to deal with the hard cases
4) Goto Step 2

- Combine all rules-of-thumb
- Expert could be “weak” learning algorithm

Questions

- How to choose races on each round?
  - concentrate on "hardest" races

    (those most often misclassified by previous rules of thumb)
- How to combine rules of thumb into single prediction rule?
  - take (weighted) majority vote of rules of thumb

Boosting

- boosting = general method of converting rough rules of thumb into highly accurate prediction rule

- more technically:
  - given “weak” learning algorithm that can consistently find hypothesis (classifier) with error $\leq 1/2-\gamma$
  - a boosting algorithm can provably construct single hypothesis with error $\leq \varepsilon$

This Lecture

- Introduction to boosting (AdaBoost)
- Analysis of training error
- Analysis of generalization error based on theory of margins
- Extensions
- Experiments

A Formal View of Boosting

- Given training set $X = \{(x_1, y_1), \ldots, (x_m, y_m)\}$
- $y_i \in \{-1, +1\}$ correct label of instance $x_i \in X$

- for timesteps $t = 1, \ldots, T$:
  - construct a distribution D_t on $\{1, \ldots, m\}$
  - Find a weak hypothesis $h_t : X \to \{-1, +1\}$ with error ε_t on D_t: $\varepsilon_t = \Pr_{D_t}[h_t(x_i) \neq y_i]$

HOW?

- Output a final hypothesis H_{final} that combines the weak hypotheses in a good way

Weighting the Votes

- **H_{final}** is a weighted combination of the choices from all our hypotheses.

How seriously we take hypothesis *t*

What hypothesis *t* guessed

$$H_{\text{final}}(x) = \operatorname{sgn}\left(\sum_t \alpha_t h_t(x) \right)$$

The Hypothesis Weight

- $\boldsymbol{\alpha_t}$ determines how "seriously" we take this particular classifier's answer

The error on training distribution D_t

$$\alpha_t = \frac{1}{2}\ln\left(\frac{1-\varepsilon_t}{\varepsilon_t}\right)$$

The Training Distribution

- **D_t** determines which elements in the training set we focus on.

Size of the training set

$$D_1(i) = \frac{1}{m}$$

The right answer

What we guessed

$$D_{t+1}(i) = \frac{D_t(i)}{Z_t} \cdot \begin{cases} e^{-\alpha_t} & \text{if } y_i = h_t(x_i) \\ e^{\alpha_t} & \text{if } y_i \neq h_t(x_i) \end{cases}$$

Normalization factor

The Hypothesis Weight

$$\alpha_t = \frac{1}{2}\ln\left(\frac{1-\varepsilon_t}{\varepsilon_t}\right) > 0$$

$$D_{t+1} = \frac{D_t}{Z_t} \cdot \begin{cases} e^{-\alpha_t} & \text{if } y_i = h_t(x_i) \\ e^{\alpha_t} & \text{if } y_i \neq h_t(x_i) \end{cases}$$

AdaBoost [Freund&Schapire '97]

- constructing D_t:
  - $D_1(i) = \frac{1}{m}$
  - given D_t and h_t:

$$D_{t+1} = \frac{D_t}{Z_t} \cdot \begin{cases} e^{-\alpha_t} & \text{if } y_i = h_t(x_i) \\ e^{\alpha_t} & \text{if } y_i \neq h_t(x_i) \end{cases}$$

$$= \frac{D_t}{Z_t} \cdot \exp(-\alpha_t \cdot y_i \cdot h_t(x_i))$$

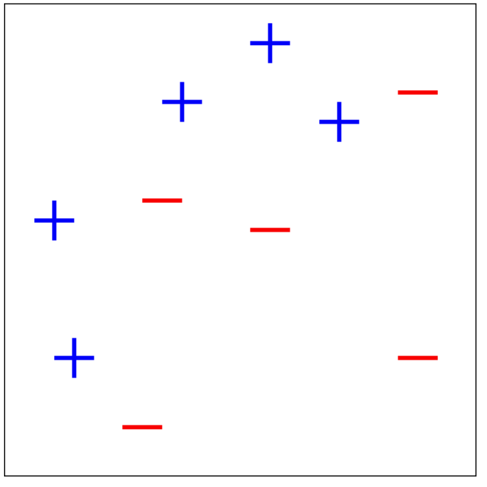
where: Z_t = normalization constant

$$\alpha_t = \frac{1}{2} \ln\left(\frac{1-\varepsilon_t}{\varepsilon_t} \right) > 0$$

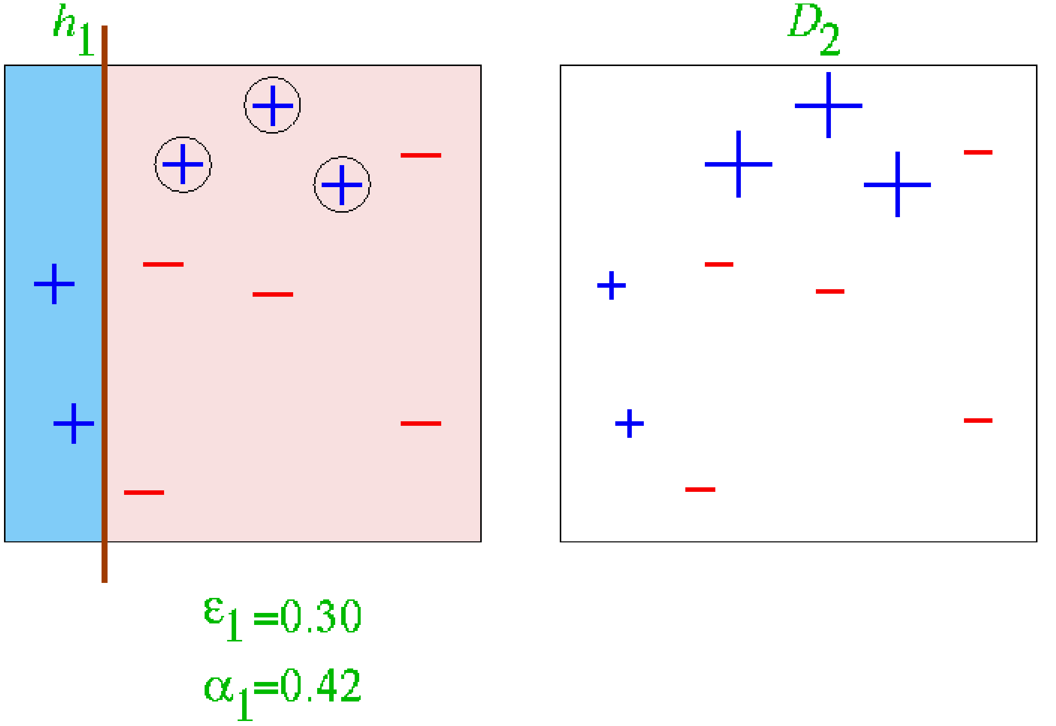
- final hypothesis: $H_{\text{final}}(x) = \text{sgn}\left(\sum_t \alpha_t h_t(x) \right)$

Toy Example

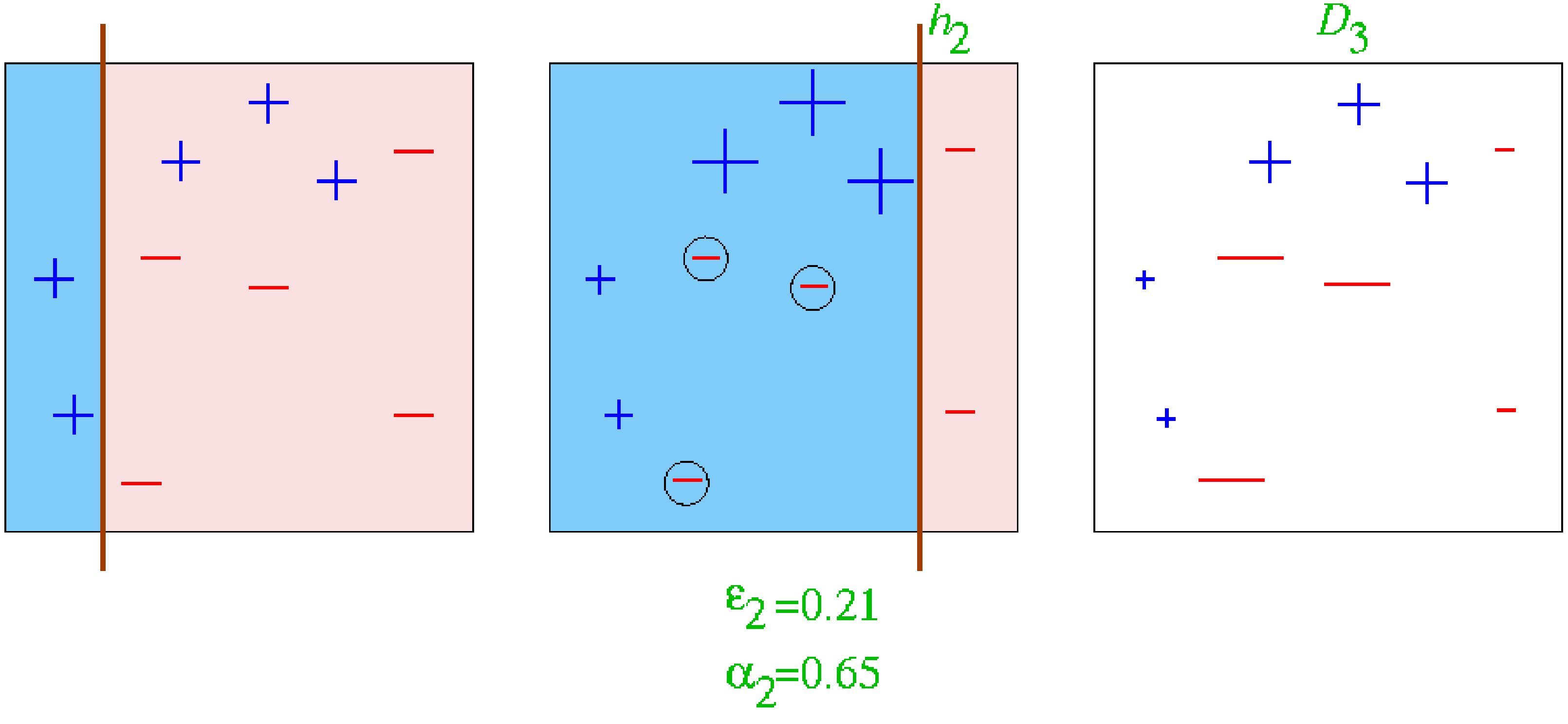
D_1



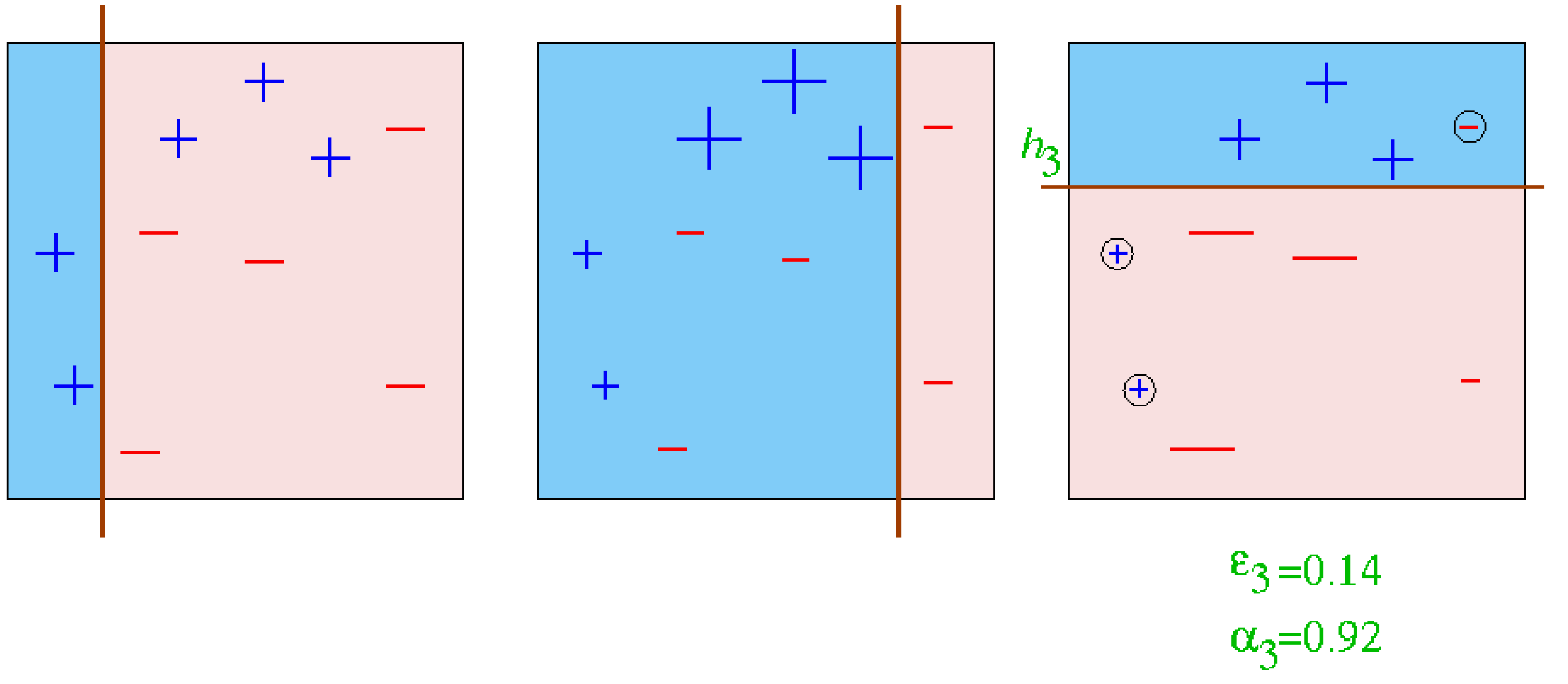
Round 1



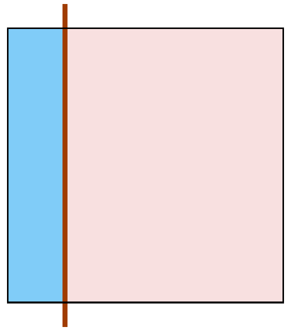
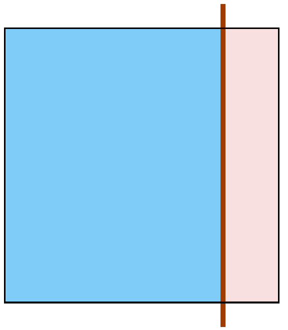
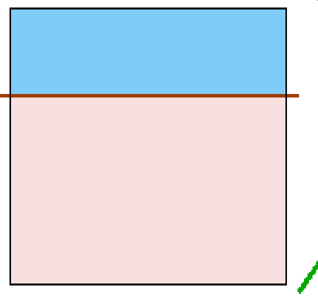
Round 2

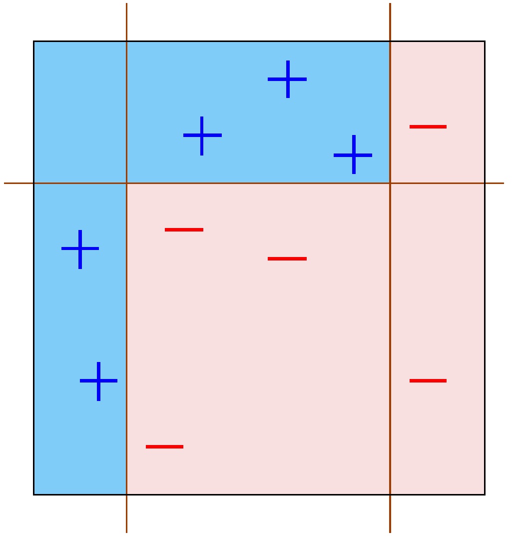


Round 3



Final Hypothesis

$H_{\text{final}} = \text{sign}\Big(0.42$  $+\ 0.65$  $+\ 0.92$  $\Big)$

$=$ 

Analyzing the Training Error

- Theorem [Freund&Schapire '97]:

write ε_t as ½-γ_t

$$\text{then, training error}(H_{\text{final}}) \le \exp\left(-2\sum_t \gamma_t^2\right)$$

so if $\forall t$: $\gamma_t \ge \gamma > 0$ then

$$\text{then, training error}(H_{\text{final}}) \le e^{-2\gamma^2 T}$$

Analyzing the Training Error

So what? This means AdaBoost is adaptive:

- does not need to know γ or T a priori
- Works as long as $\gamma_t > 0$

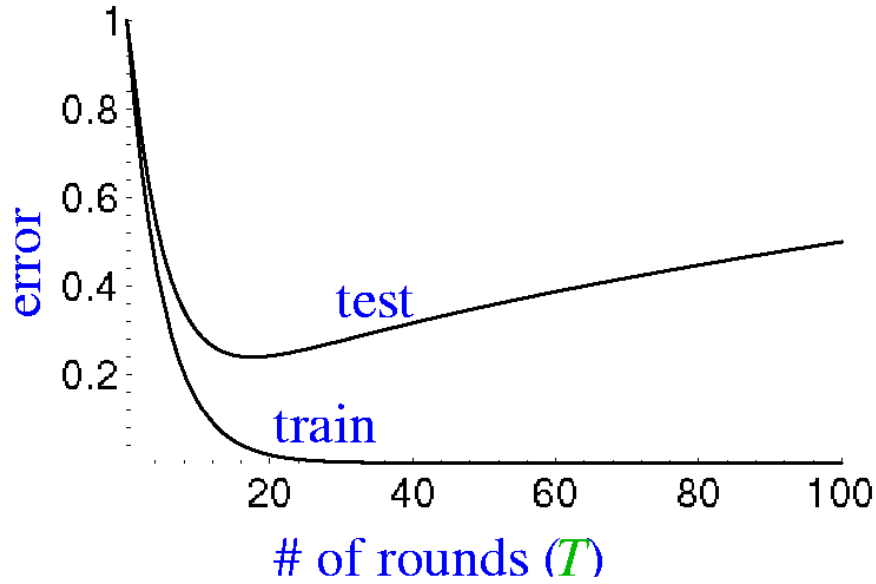
Proof Intuition

- on round t:
  increase weight of examples incorrectly classified by h_t

- if x_i incorrectly classified by H_{final}
  then x_i incorrectly classified by weighted majority of h_t's
  then x_i must have "large" weight under final dist. D_{T+1}

- since total weight ≤ 1:
  number of incorrectly classified examples "small"

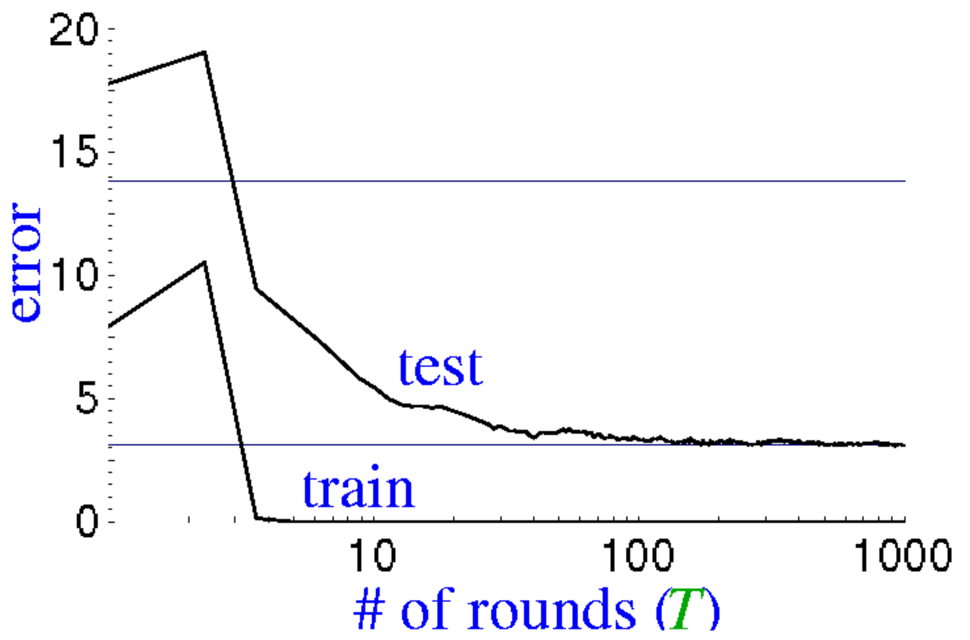
Analyzing Generalization Error



we expect:

- training error to continue to drop (or reach zero)
- test error to <u>increase</u> when H_{final} becomes "too complex" (Occam's razor)

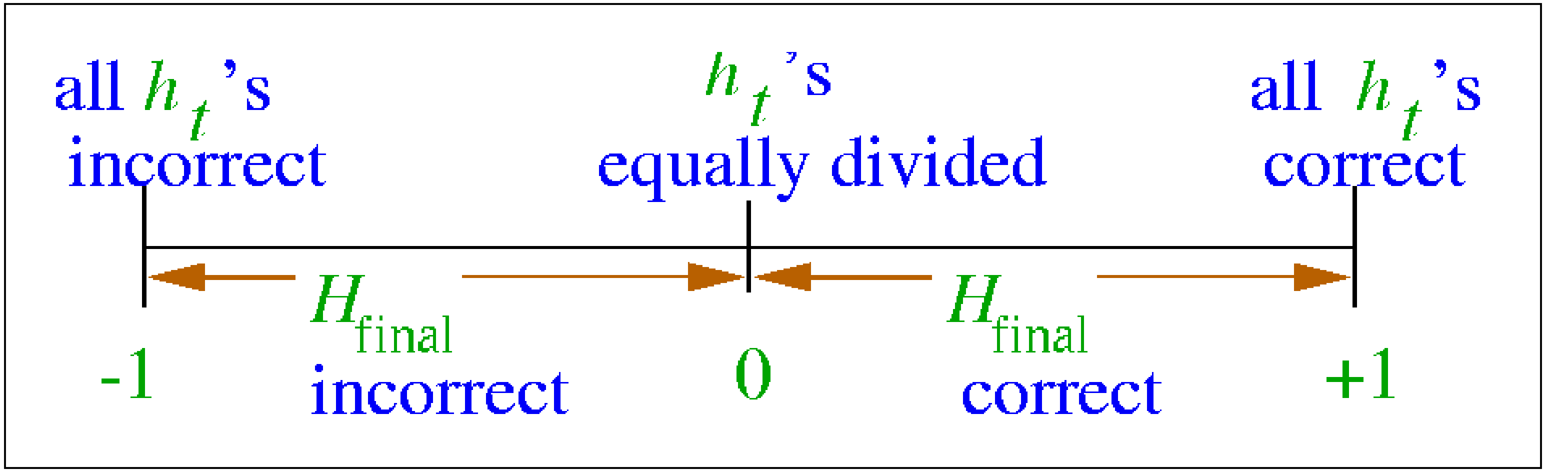
A Typical Run



(boosting on C4.5 on "letter" dataset)

- Test error does <u>not</u> increase even after 1,000 rounds (~2,000,000 nodes)
- Test error continues to drop after training error is zero!
- Occam's razor <u>wrongly</u> predicts "simpler" rule is better.

A Better Story: Margins



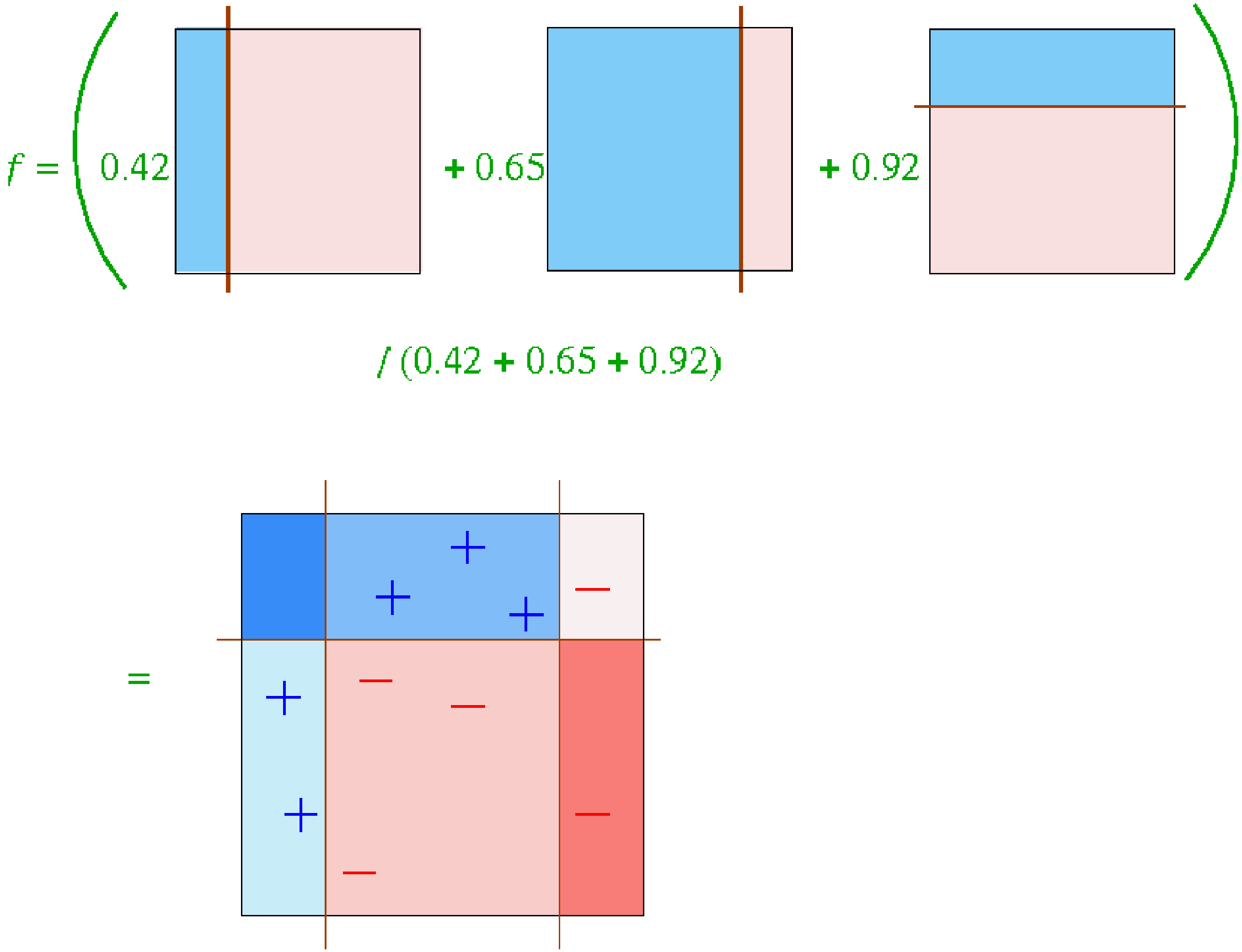
Key idea: Consider confidence (margin):

- with

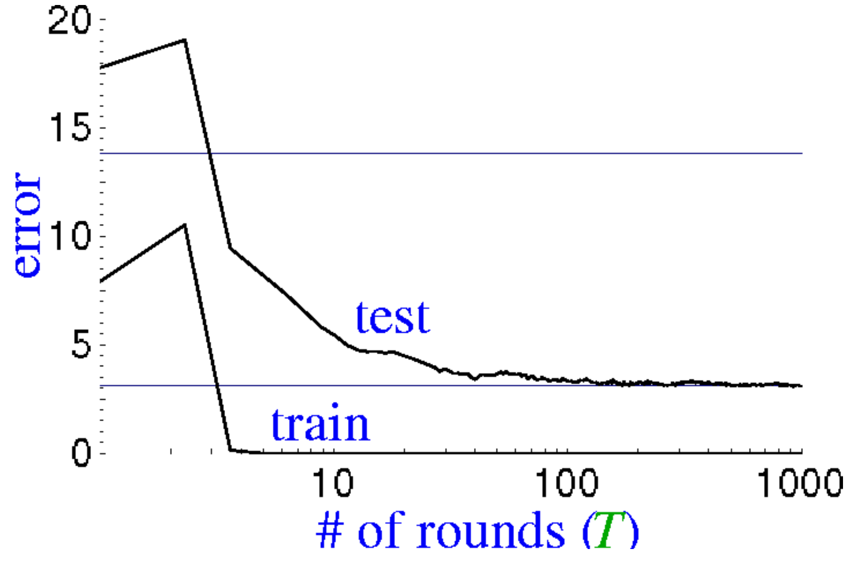
$$H_{\text{final}}(x) = \text{sgn}(f(x)) \qquad f(x) = \frac{\sum_t \alpha_t h_t(x)}{\sum_t \alpha_t} \in [-1,1]$$

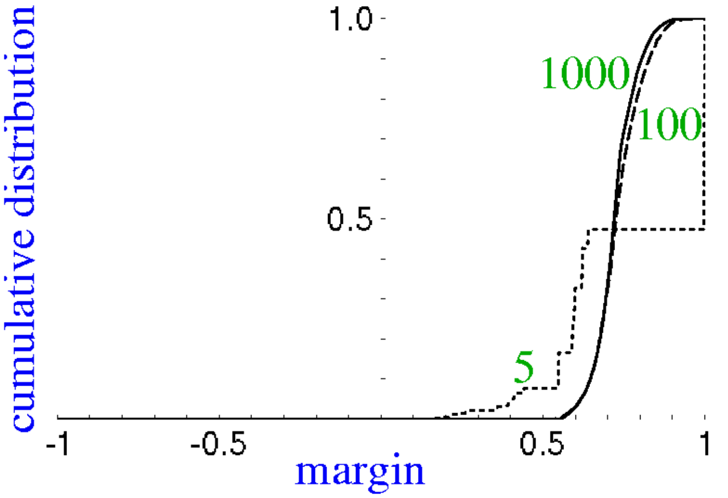
- define: margin of $(x,y) = y \cdot f(x)$

Margins for Toy Example



The Margin Distribution





epoch	5	100	1000
training error	0.0	0.0	0.0
test error	8.4	3.3	3.1
%margins≤0.5	7.7	0.0	0.0
Minimum margin	0.14	0.52	0.55

Boosting Maximizes Margins

- Can be shown to minimize

$$\sum_i e^{-y_i f(x_i)} = \sum_i e^{-y_i \sum_t \alpha_t h_t(x_i)}$$

$\propto$ to margin of (x_i, y_i)

Analyzing Boosting Using Margins

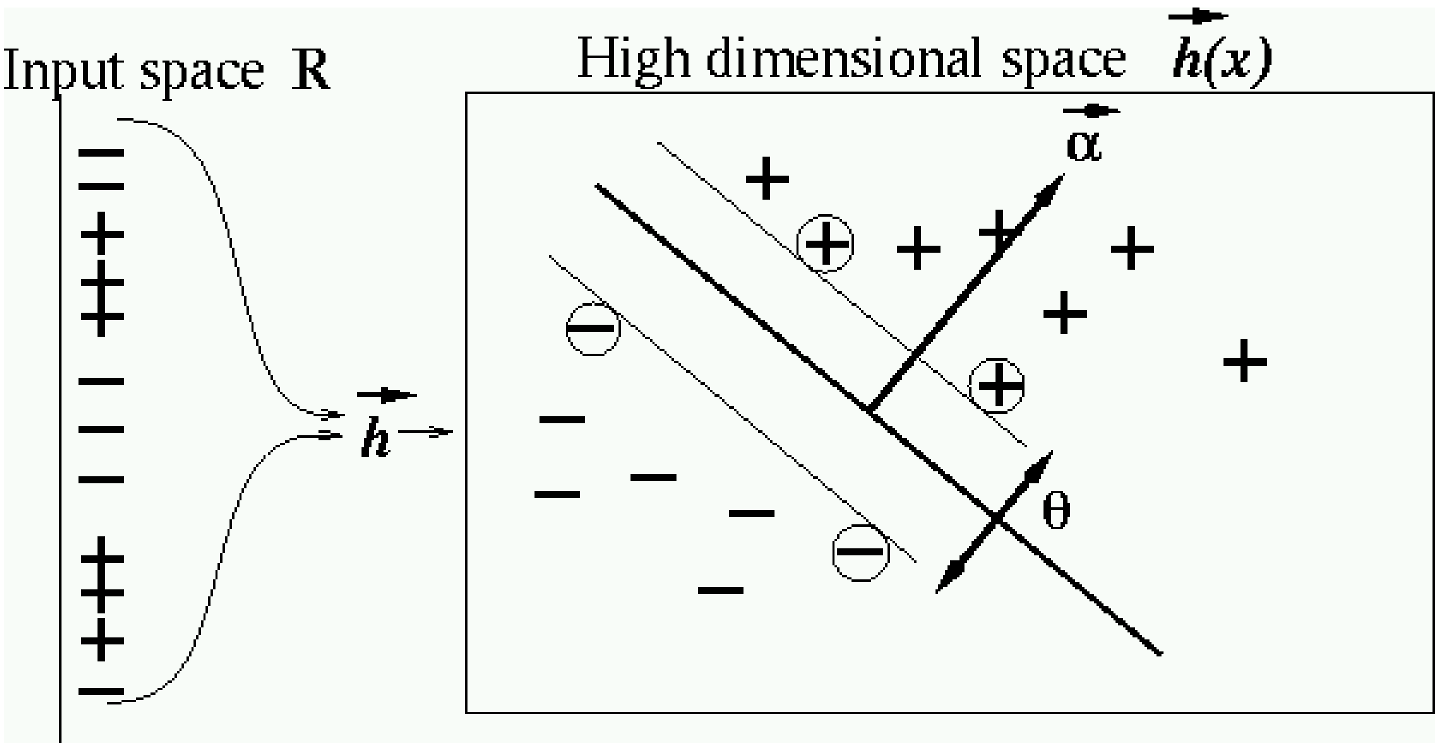
generalization error bounded by function of training sample margins:

$$\text{error} \;\leq\; \hat{\Pr}[\text{margin}_f(x,y) \leq \theta] + \tilde{O}\left(\sqrt{\frac{\text{VC}(H)}{m\theta^2}}\right)$$

- larger margin $\Rightarrow$ better bound
- bound independent on # of epochs
- boosting tends to increase margins of training examples by concentrating on those with smallest margin

Relation to SVMs

SVM: map x into high-dim space, separate data linearly



Relation to SVMs (cont.)

$$H(x) = \begin{cases} +1 & \text{if } 2x^5 - 5x^2 + x > 10 \\ -1 & \text{otherwise} \end{cases}$$

$$\vec{h}(x) = (1, x, x^2, x^3, x^4, x^5)$$

$$\vec{\alpha} = (-10, 1, -5, 0, 0, 2)$$

$$H(x) = \begin{cases} +1 & \text{if } \vec{\alpha} \cdot \vec{h}(x) > 0 \\ -1 & \text{otherwise} \end{cases}$$

Relation to SVMs

- Both maximize margins:

$$\theta \doteq \max_{w} \min_{i} \frac{(\vec{\alpha} \cdot \vec{h}(x_i))\, y_i}{\| \vec{\alpha} \|}$$

- SVM: $\| \vec{\alpha} \|_2$ Euclidean norm (L_2)
- AdaBoost: $\| \vec{\alpha} \|_1$ Manhattan norm (L_1)

- Has implications for optimization, PAC bounds

See [Freund et al '98] for details

Extensions: Multiclass Problems

- Reduce to binary problem by creating several binary questions for each example:

  - “does or does not example x belong to class 1?”
  - “does or does not example x belong to class 2?”
  - “does or does not example x belong to class 3?”

$$\vdots$$

Extensions: Confidences and Probabilities

- Prediction of hypothesis h_t: $\operatorname{sgn}(h_t(x))$

- Confidence of hypothesis h_t: $|h_t(x)|$

- Probability of H_{final}: $\Pr_f[y = +1 | x] = \dfrac{e^{f(x)}}{e^{f(x)} + e^{-f(x)}}$

[Schapire&Singer '98], [Friedman, Hastie & Tibshirani '98]

Practical Advantages of AdaBoost

- (quite) fast
- simple + easy to program
- only a single parameter to tune (T)
- no prior knowledge
- flexible: can be combined with any classifier (neural net, C4.5, …)
- provably effective (assuming weak learner)
  - shift in mind set: goal now is merely to find hypotheses that are better than random guessing
- finds outliers

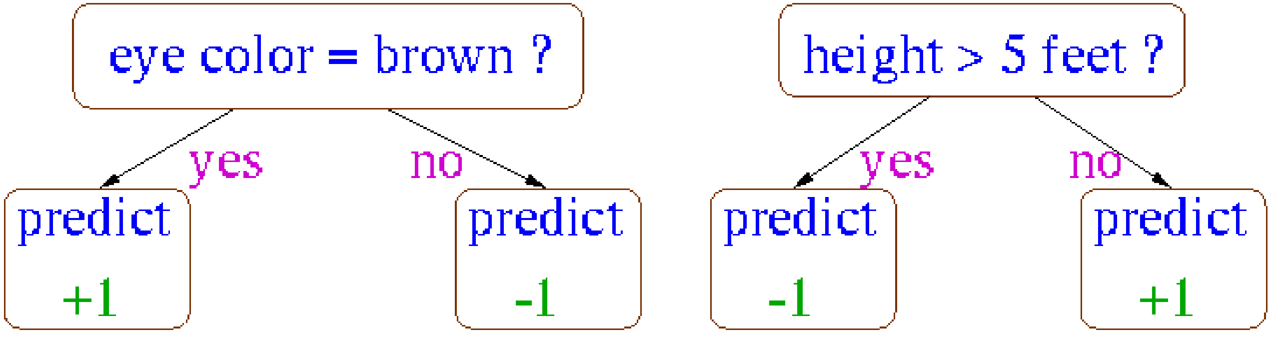
Caveats

- performance depends on data & weak learner
- AdaBoost can fail if
  - weak hypothesis too complex (overfitting)
  - weak hypothesis too weak ($\gamma_t \to 0$ too quickly),
    - underfitting
    - Low margins $\rightarrow$ overfitting
- empirically, AdaBoost seems susceptible to noise

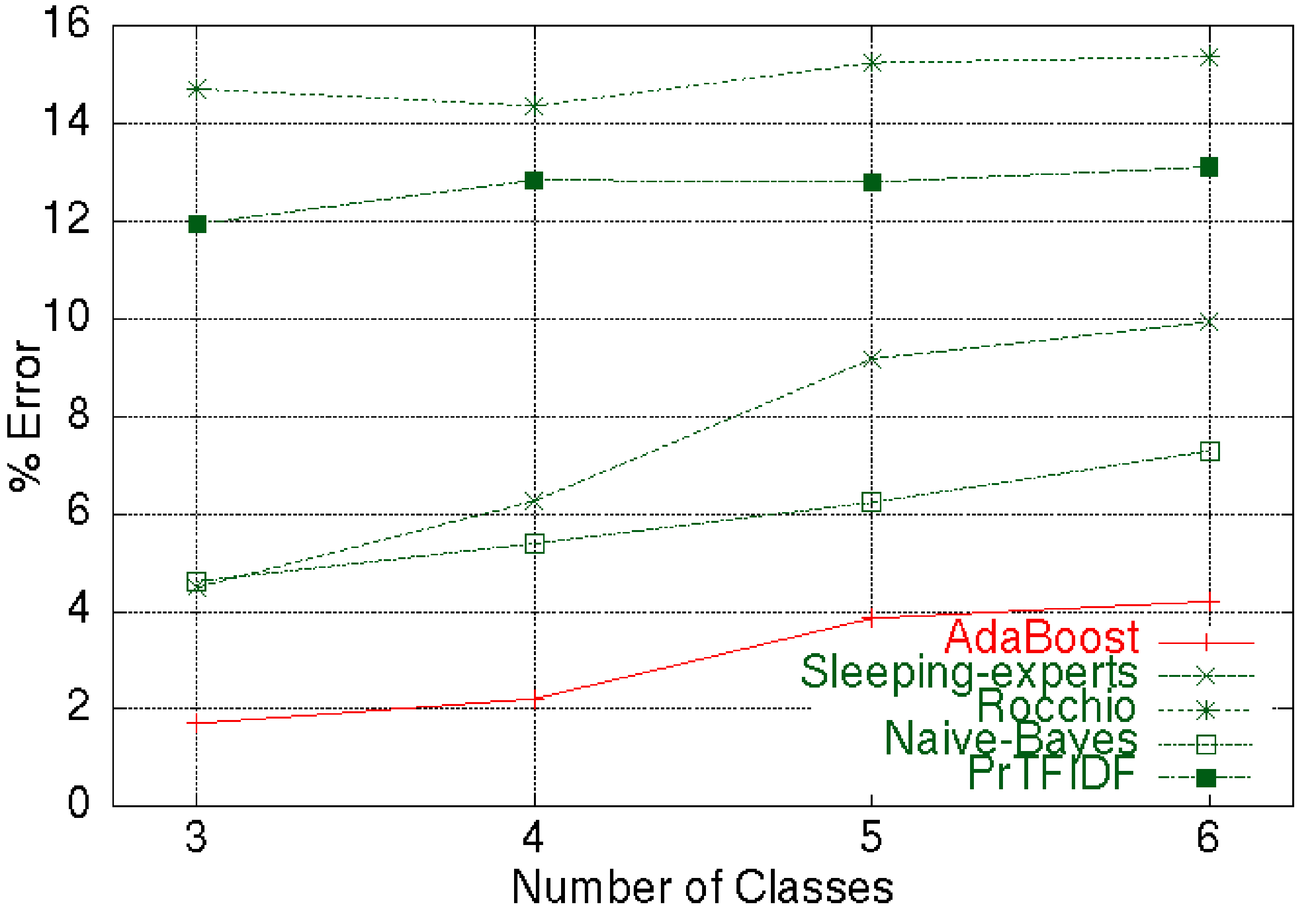
UCI Benchmarks

Comparison with

- C4.5 (Quinlan's Decision Tree Algorithm)
- Decision Stumps (only single attribute)



Text Categorization



database: Reuters

Conclusion

- boosting useful tool for classification problems
  - grounded in rich theory
  - performs well experimentally
  - often (but not always) resistant to overfitting
  - many applications
- but
  - slower classifiers
  - result less comprehensible
  - sometime susceptible to noise

Other Ensembles

- Bagging
- Stacking

Background

- [Valiant'84]

  introduced theoretical PAC model for studying machine learning

- [Kearns&Valiant'88]

  open problem of finding a boosting algorithm

- [Schapire'89], [Freund'90]

  first polynomial-time boosting algorithms

- [Drucker, Schapire&Simard '92]

  first experiments using boosting

Background (cont.)

- [Freund&Schapire '95]
  - introduced AdaBoost algorithm
  - strong practical advantages over previous boosting algorithms
- experiments using AdaBoost:

  [Drucker&Cortes '95] [Schapire&Singer '98]
  [Jackson&Cravon '96] [Maclin&Opitz '97]
  [Freund&Schapire '96] [Bauer&Kohavi '97]
  [Quinlan '96] [Schwenk&Bengio '98]
  [Breiman '96] [Dietterich'98]
- continuing development of theory & algorithms:

  [Schapire,Freund,Bartlett&Lee '97] [Schapire&Singer '98]
  [Breiman '97] [Mason, Bartlett&Baxter '98]
  [Grive and Schuurmans'98] [Friedman, Hastie&Tibshirani '98]