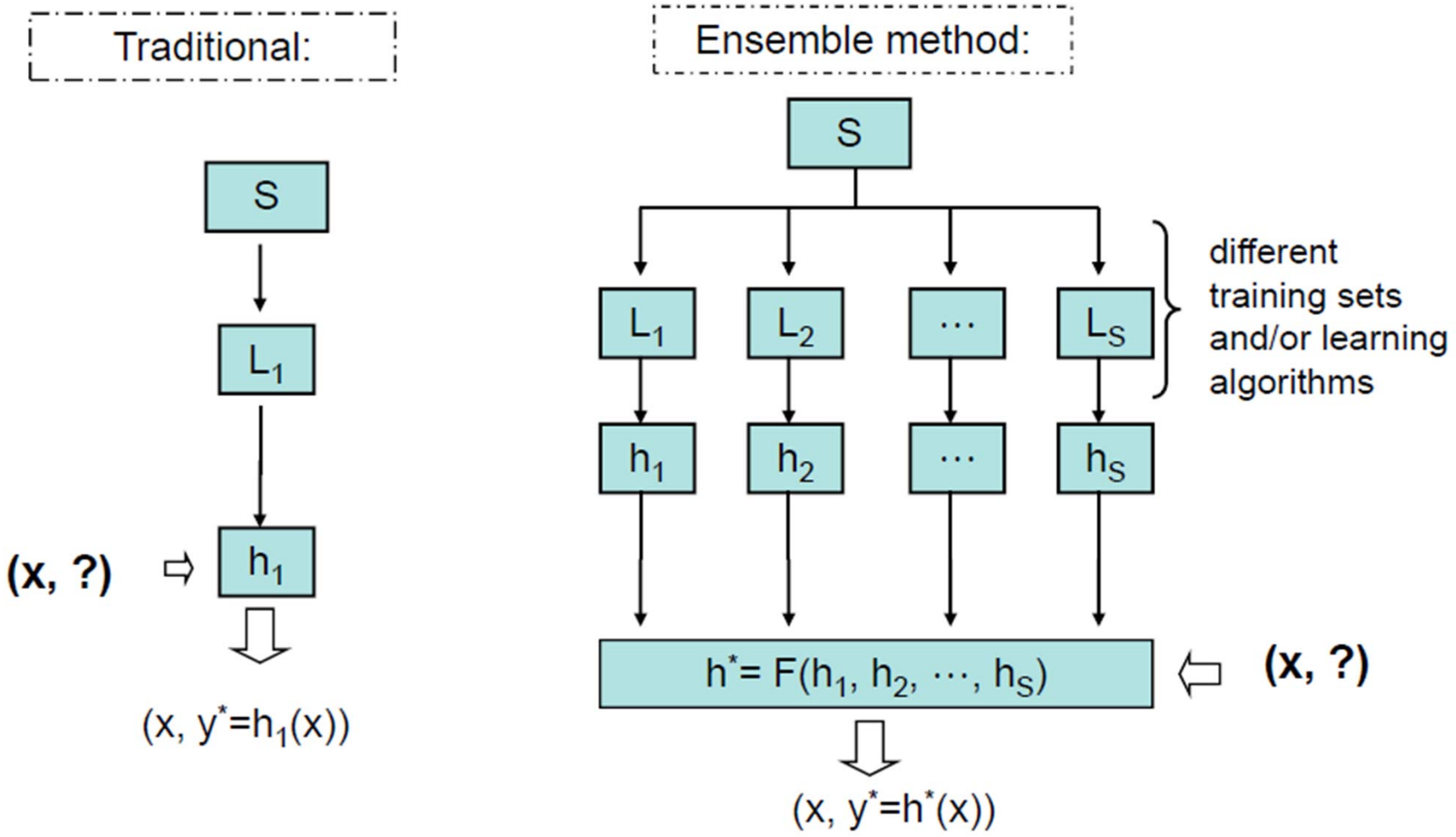
Ensemble Learning

CS534

Ensemble Learning



How to generate ensembles?

- There have been a wide range of methods developed
- We will study to popular approaches
  - Bagging
  - Boosting
- Both methods take a single (base) learning algorithm and generate ensembles

Base Learning Algorithm

- We are given a '*black box*' learning algorithm *Learn* referred to as the base learner.

Protocol to *Learn*:

Input:

S - set of labeled training instances.

Output:

h - a hypothesis from hypothesis space H.

Bootstrap **Agg**regat**ing** (Bagging)

- Leo Breiman, “Bagging Predictors”, *Machine Learning*, 24, 123-140 (1996)
- Consider creating many training data sets by drawing instances from some distribution and then using *Learn* to output a hypothesis for each dataset.
- The resulting hypotheses will likely vary in performance due to variation in the training sets
- What happens if we combine these hypothesesusing a majority vote?

Bagging Algorithm

Given training set S, bagging works as follows:

1. Create *T* ***bootstrap samples*** $\{S_1, \dots, S_T\}$of *S* as follows:
   – For each S_i: Randomly drawing |S| examples from *S* with replacement
2. For each $i = 1, \dots, T, h_i = Learn(S_i)$
3. Output $H =< \{h_1, \dots, h_T\}, majorityVote >$

With large |S|, each S_i will contain $1 - \frac{1}{e} \approx 63.2\%$ unique examples

Stability of Learn

- A learning algorithm is **unstable** if small changes in the training data can produce large changes in the output hypothesis (otherwise **stable**).
- Clearly bagging will have little benefit when used with stable base learning algorithms (i.e., most ensemble members will be very similar).
- Bagging generally works best when used with unstable yet relatively accurate base learners

The Bias-Variance Decomposition

$$\text{expected loss} = (\text{bias})^2 + \text{variance} + \text{noise}$$

Where

y(x; D) is the learned hypothesis given training set D

h(x) is the target underlying function

$$(\text{bias})^2 = \int \{\mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})] - h(\mathbf{x})\}^2 p(\mathbf{x})\,\mathrm{d}\mathbf{x}$$

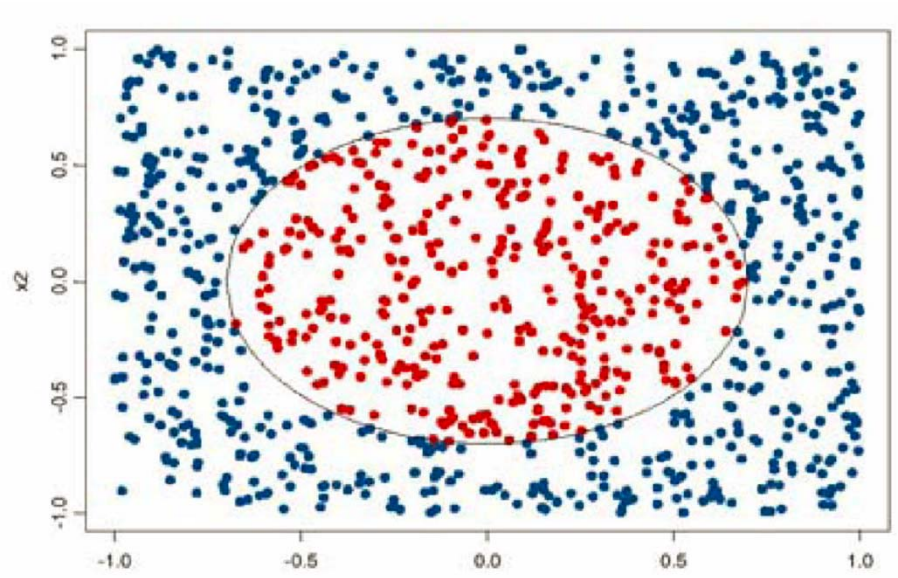
$$\text{variance} = \int \mathbb{E}_{\mathcal{D}}\left[\{y(\mathbf{x};\mathcal{D}) - \mathbb{E}_{\mathcal{D}}[y(\mathbf{x};\mathcal{D})]\}^2\right] p(\mathbf{x})\,\mathrm{d}\mathbf{x}$$

$$\text{noise} = \int\int \{h(\mathbf{x}) - t\}^2 p(\mathbf{x}, t)\,\mathrm{d}\mathbf{x}\,\mathrm{d}t$$

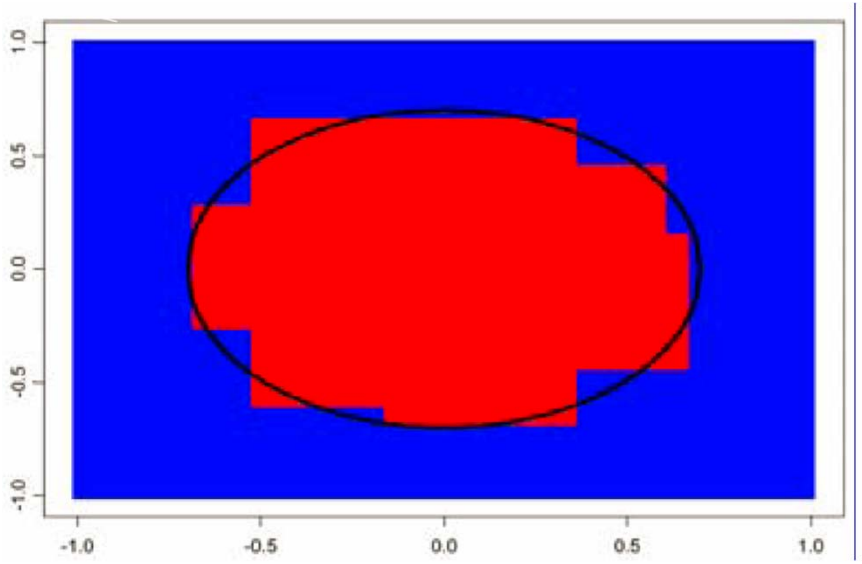
t(x) = h(x) + noise is the observed noisy target value

Bagging reduces variance of a classifier. Most appropriate for classifiers of low bias and high variance (e.g., decision tree).

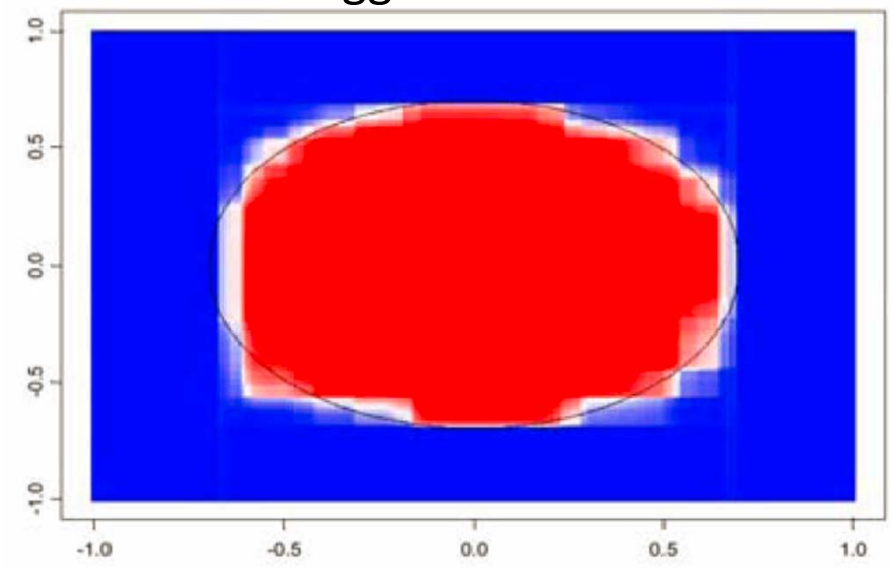
Target concept



Single decision tree

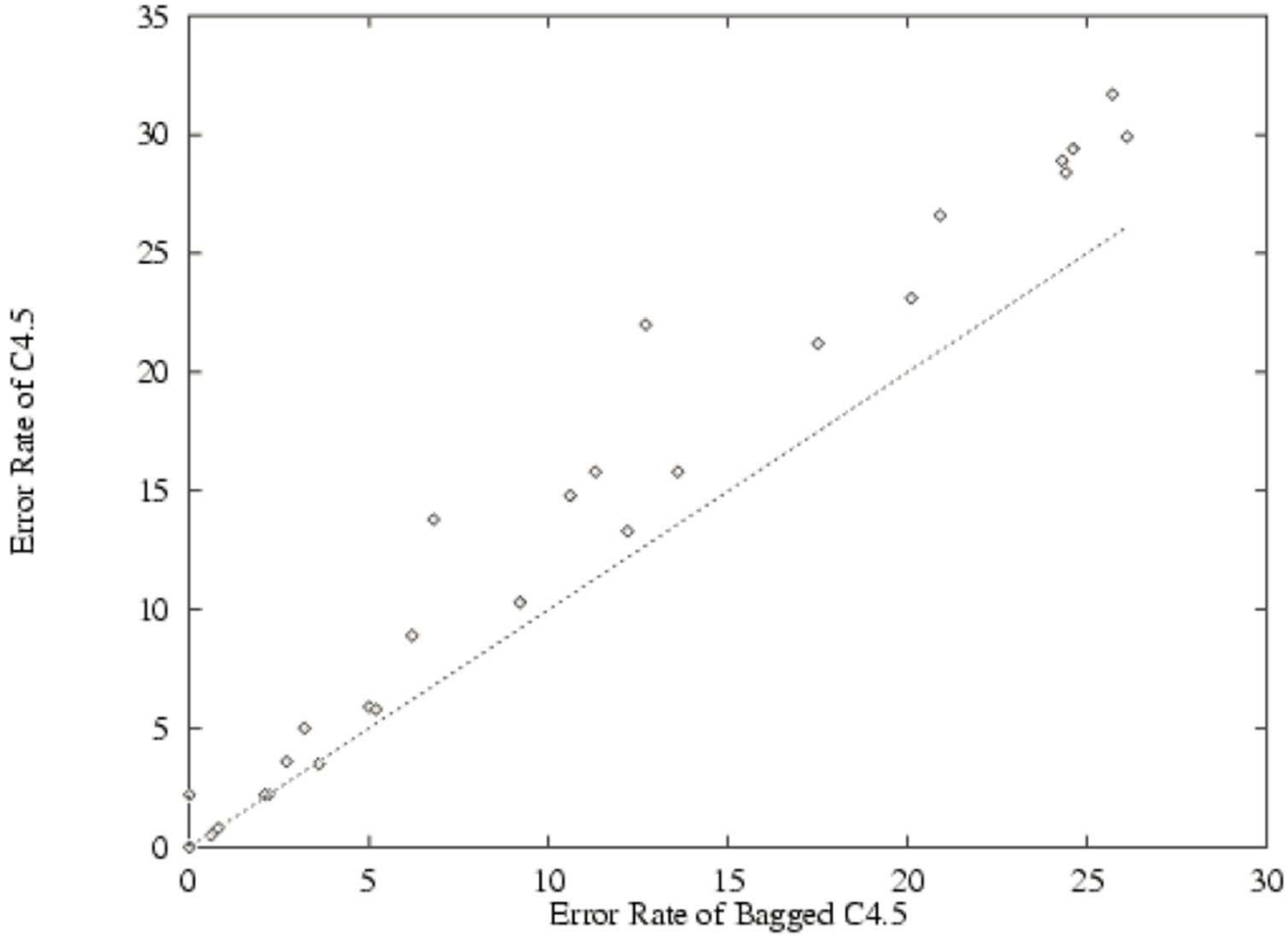


100 bagged decision tree



Bagging Decision Trees

(Freund & Schapire)



Boosting

Key difference compared to bagging?

- Its iterative.
  - **Bagging :** Individual classifiers were independent.
  - **Boosting:**
    - Look at **errors from previous classifiers** to decide what to **focus** on for the next iteration over data
    - Successive classifiers depends upon its predecessors.
    - Result: more weights on ‘hard’ examples. (the ones on which we committed mistakes in the previous iterations)

Some Boosting History

- The idea of boosting began with a learning theory question first asked in the late 80's.
- The question was answered in 1989 by Robert Shapire resulting in the first theoretical boosting algorithm
- Shapire and Freund later developed a practical boosting algorithm called Adaboost
- Many empirical studies show that Adaboost is highly effective (very often they outperform ensembles produced by bagging)

History: Strong vs weak learning

Strong Learning	**Weak Learning**
$\exists$ algorithm A	$\exists$ algorithm A
$\forall c \in \mathcal{C}$	$\exists \gamma > 0$
$\forall D$	$\forall c \in \mathcal{C}$
$\forall \epsilon > 0$	$\forall D$
$\forall \delta > 0$	$\forall \epsilon \geq \frac{1}{2} - \gamma$ say, ε=0.49
	$\forall \delta > 0$
A produces $h \in \mathcal{H}$:	A produces $h \in \mathcal{H}$:
$Pr[err(h) > \epsilon] \leq \delta$	$Pr[err(h) > \epsilon] \leq \delta$

Strong = weak?

Strong = Weak PAC learning

The key idea is that we can learn a little on every distribution

Produce 3 hypothesis as follows

h_1 is the result of applying *Learn* to all training data.

h_2 is the result of applying *Learn* to filtered data distribution such that h_1 has only 50% accuracy on the data.

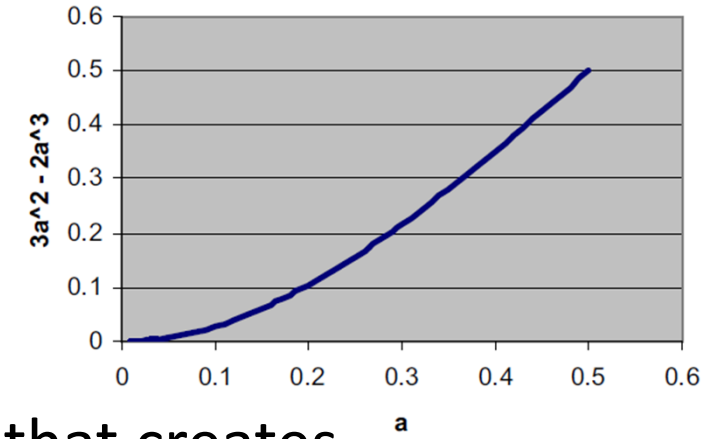
(e.g., to generate an example flip a coin, if head then draw examples until h_1 makes an error, and give it to *Learn*; if tail then wait until h_1 is correct, and give it to *Learn*)

h_3 is the result of applying *Learn* to training data on which h_1 and h_2 disagree.

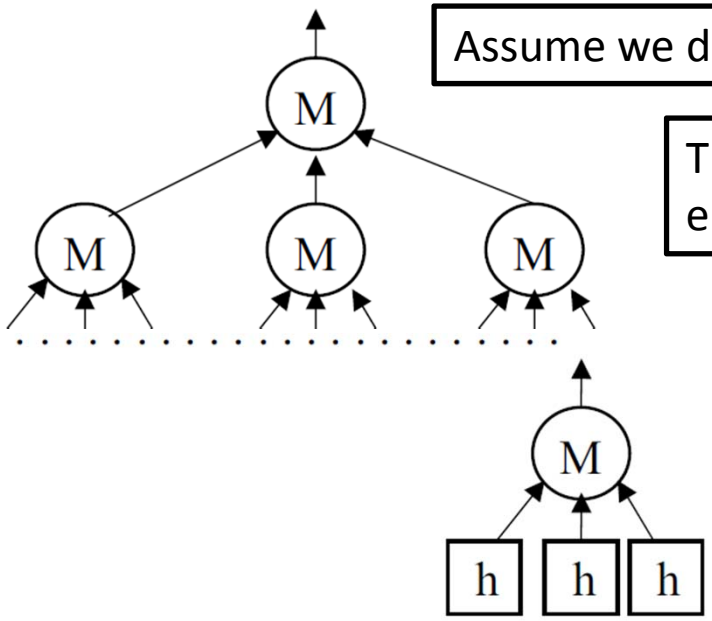
- We can then let them vote, the resulting error rate will be improved. We can repeat this until reaching the target error rate

Consider *E* = <$\{h_1, h_2, h_3\}$, *majorityVote*>.

- If h_1, h_2, h_3 have error rates less than a, it can be shown that the error rate of E is upper-bounded by $g(a)$: $3a^2 - 2a^3 < a$



This fact leads to a recursive algorithm that creates a hypothesis of arbitrary accuracy from weak hypotheses.



Assume we desire an error rate less than *e*.

These need only achieve an error rate less than $g^{-1}(e)$

As we move down the tree, the error we needs to achieve increases according to g^{-1}

Eventually the error rate needed will be attainable by the weak learner

AdaBoost

- The boosting algorithm derived from the original proof is impractical
  - requires to many calls to *Learn*, though only polynomially many
- Practically efficient boosting algorithm
  - Adaboost
  - Makes more effective use of each call of *Learn*

Specifying Input Distributions

- AdaBoost works by invoking *Learn* many times on different distributions over the training data set.
- Need to modify base learner protocol to accept a training set distribution as an input.

Protocol to *Learn*:

Input:

S - Set of N labelled training instances.

D - Distribution over S where $D(i)$ is the weight of the i'th training instance (interpreted as the probability of observing i'th instance). Where $\sum_{i=1}^{N} D(i) = 1$.

Output:

h - a hypothesis from hypothesis space H

D(i) can be viewed as indicating to base learner *Learn* the importance of correctly classifying the *i'th* training instance

AdaBoost (High level steps)

- AdaBoost performs *L* boosting rounds, the operations in each boosting round l are:

1. Call *Learn* on data set *S* with distribution D_l to produce *l'th* ensemble member h_l, where D_l is the distribution of round l.
2. Compute the $l + 1\ th$ round distribution D_{l+1} by putting more weight on instances that h_l makes mistakes on
3. Compute a voting weight α_l for h_l

The ensemble hypothesis returned is:

$$H=<\{h_1, \dots, h_L\}, weightedVote(\alpha_1, \dots, \alpha_L)>$$

AdaBoost algorithm:

Input: *Learn* - Base learning algorithm.

S - Set of *N* labeled training instances.

Output: $H = \langle \{h_1, \ldots, h_L\}, WeightedVote(\alpha_1, \ldots, \alpha_L) \rangle$

Initialize $D_1(i) = 1/N$, for all i from 1 to N. (uniform distribution)

FOR $l = 1, 2, \ldots, L$ **DO**

$h_l = Learn(S, D_l)$

$\varepsilon_l = error(h_l, S, D_l)$

$$\alpha_l = \frac{1}{2}\ln\left(\frac{1-\varepsilon_l}{\varepsilon_l}\right)$$;; if $\varepsilon_l < 0.5$ implies $\alpha_l > 0$

$$D_{l+1}(i) = D_l(i) \times \begin{cases} e^{\alpha_l}, & h_l(x_i) \neq y_i \\ e^{-\alpha_l}, & h_l(x_i) = y_i \end{cases}$$ for i from 1 to N

Normalize D_{l+1} ;; can show that h_l has 0.5 error on D_{l+1}

Note that $\varepsilon_l < 0.5$ implies $\alpha_l > 0$ so weight is decreased for instances h_t predicts correctly and increases for incorrect instances

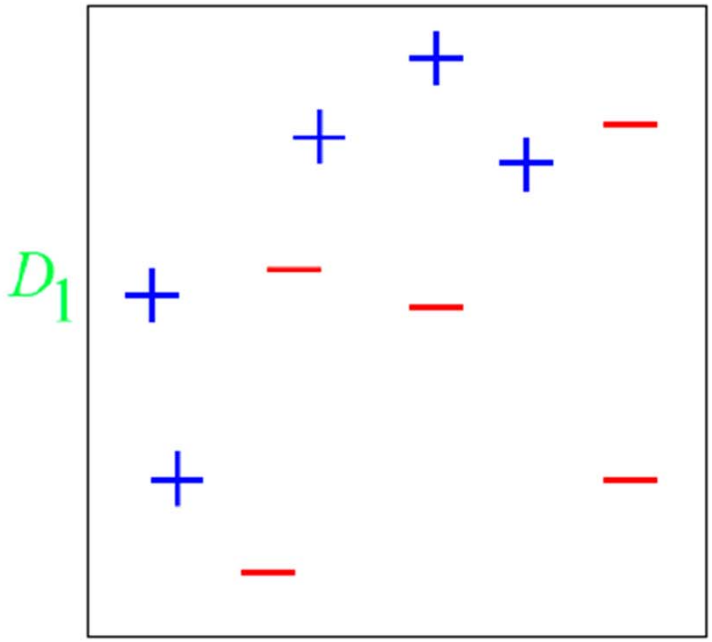
Learning with Weights

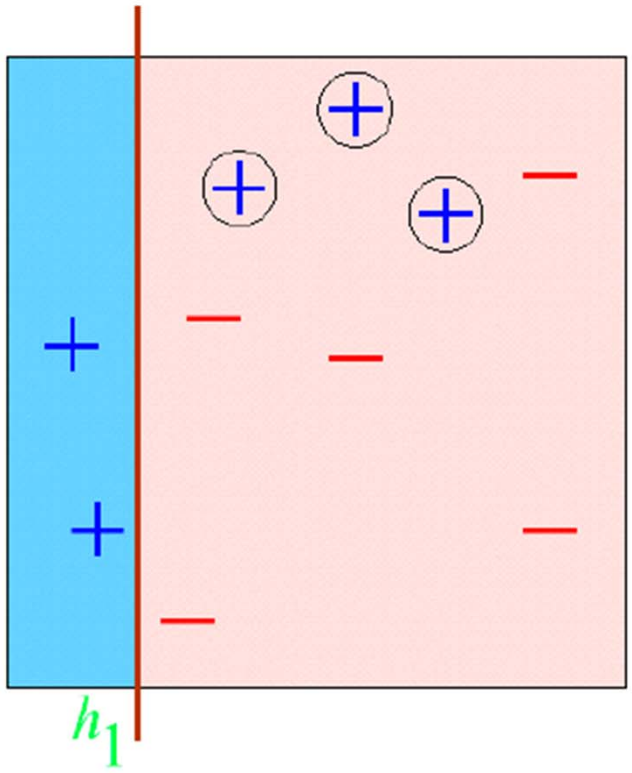
- It is often straightforward to convert a base learner to take into account an input distribution *D*.
  - Decision trees?
  - Neural nets?
  - Logistic regression?
- When it's not straightforward, we can resample the training data according to D

AdaBoost(Example)

Base Learner: Decision Stump Learner (i.e. single test decision trees)

Original Training set : Equal
Weights to all training samples



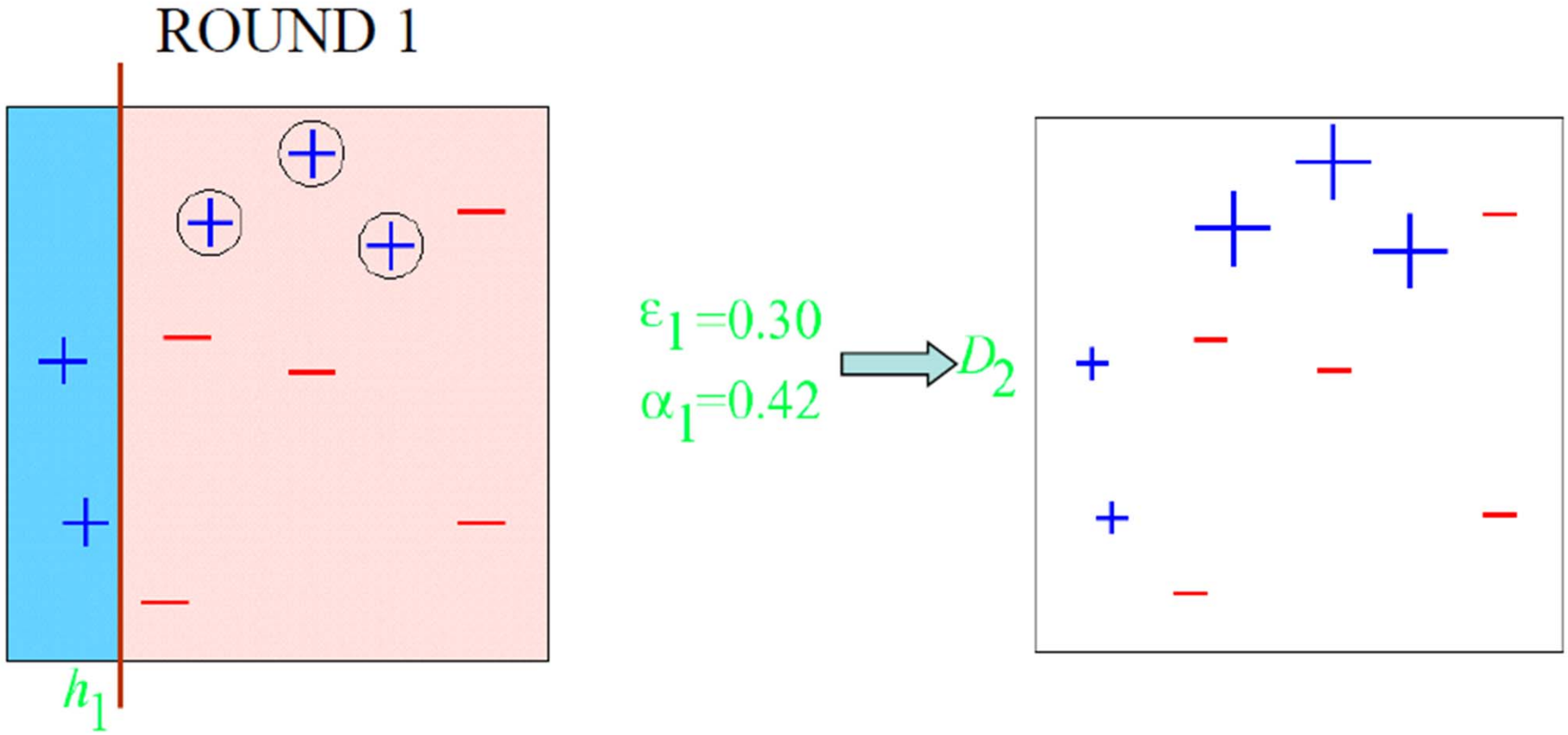


$\varepsilon_1 = 0.30$

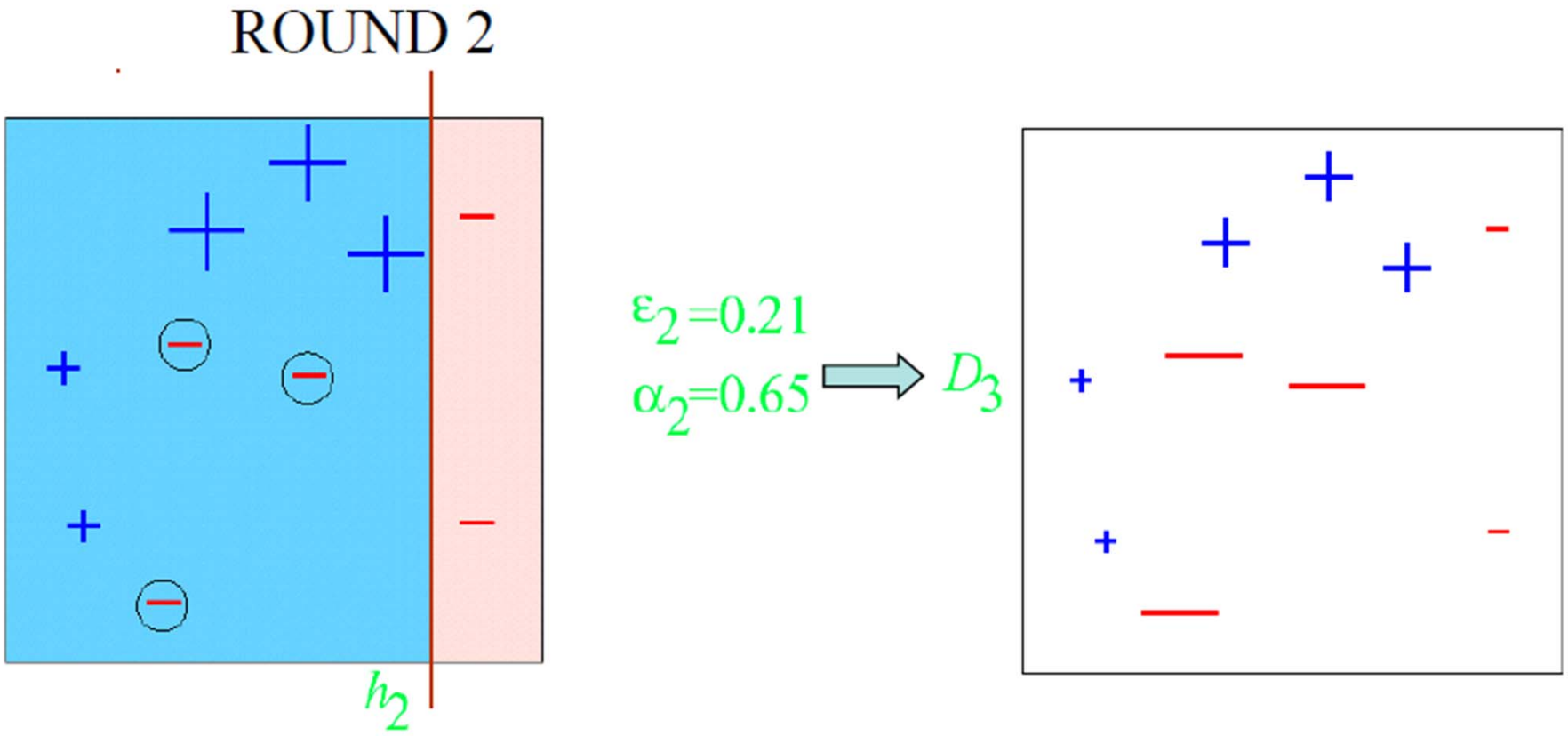
$\alpha_1 = 0.42$

Taken from "**A Tutorial on Boosting" by** Yoav Freund and Rob Schapire

AdaBoost(Example)

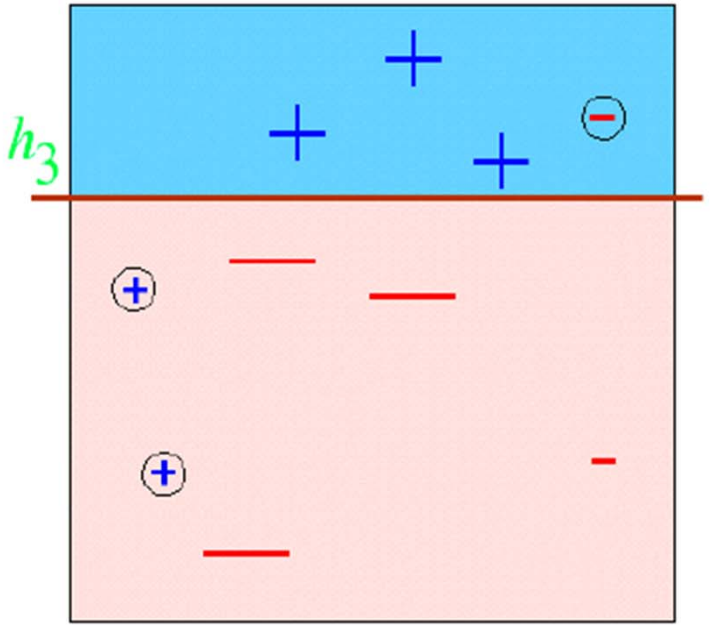


AdaBoost(Example)



AdaBoost(Example)

ROUND 3

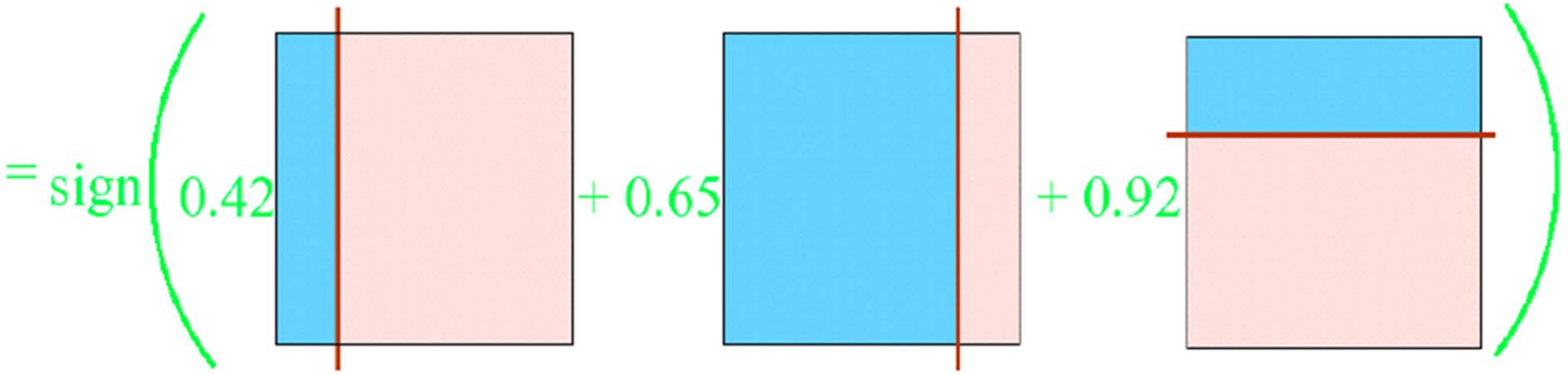


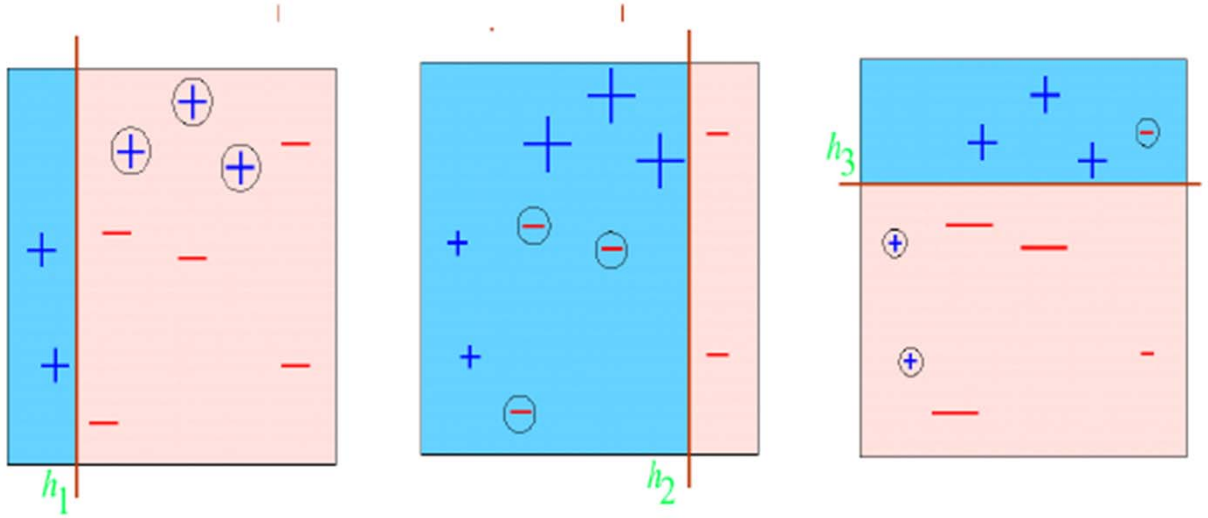
$\varepsilon_3 = 0.14$

$\alpha_3 = 0.92$

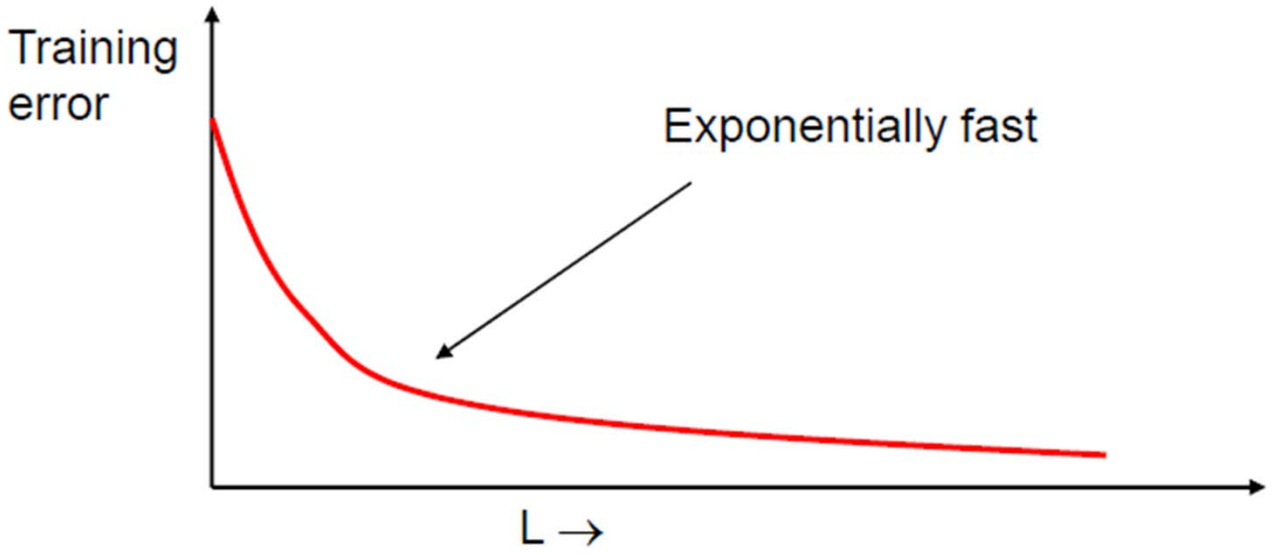
AdaBoost(Example)

H_{final}





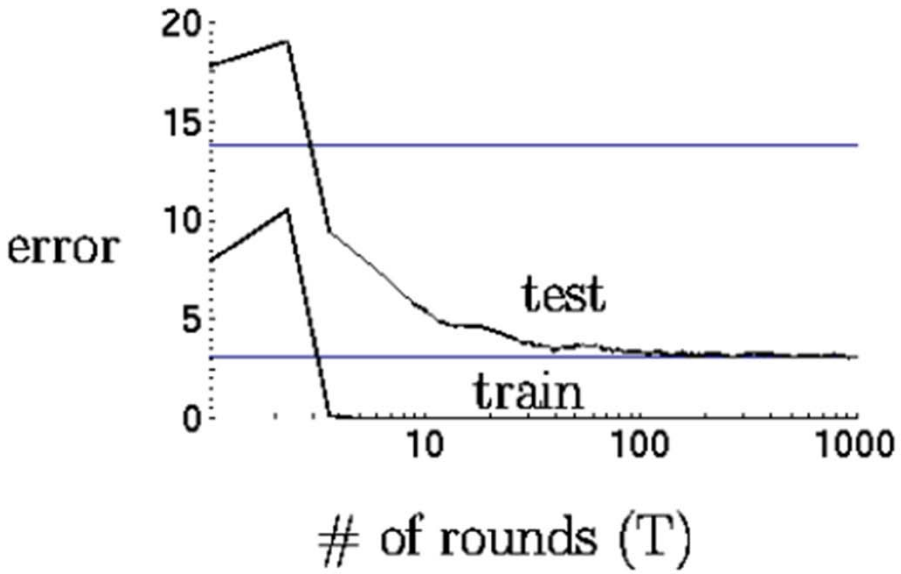
Property of Adaboost



- Suppose L is a weak learner
  - $\varepsilon_l < 0.5$ (slightly better than random guesses)
  - Training error goes to zero exponentially fast

Overfitting?

- Boosting drives training error to zero, will it overfit?
- Curious phenomenon



Schapire 1989.
Letter recognition

- Boosting is often robust to overfitting (not always)
- Test error continues to decrease even after training error goes to zero

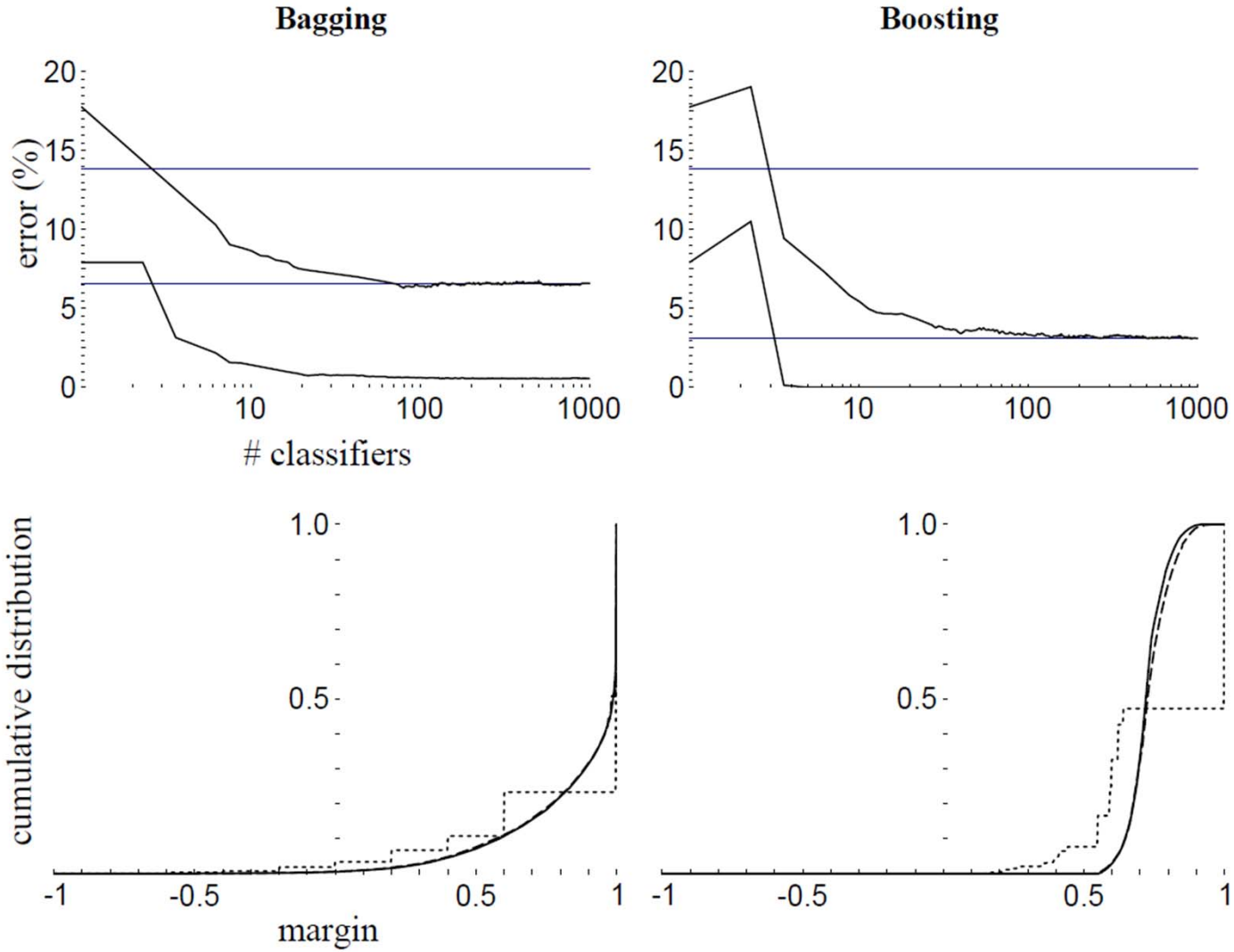


Figure 1: Error curves and margin distribution graphs for bagging and boosting C4.5 on the letter dataset. Learning curves are shown directly above corresponding margin distribution graphs. Each learning-curve figure shows the training and test error curves (lower and upper curves, respectively) of the combined classifier as a function of the number of classifiers combined. Horizontal lines indicate the test error rate of the base classifier as well as the test error of the final combined classifier. The margin distribution graphs show the cumulative distribution of margins of the training instances after 5, 100 and 1000 iterations, indicated by short-dashed, long-dashed (mostly hidden) and solid curves, respectively.

Margin Based Error bound

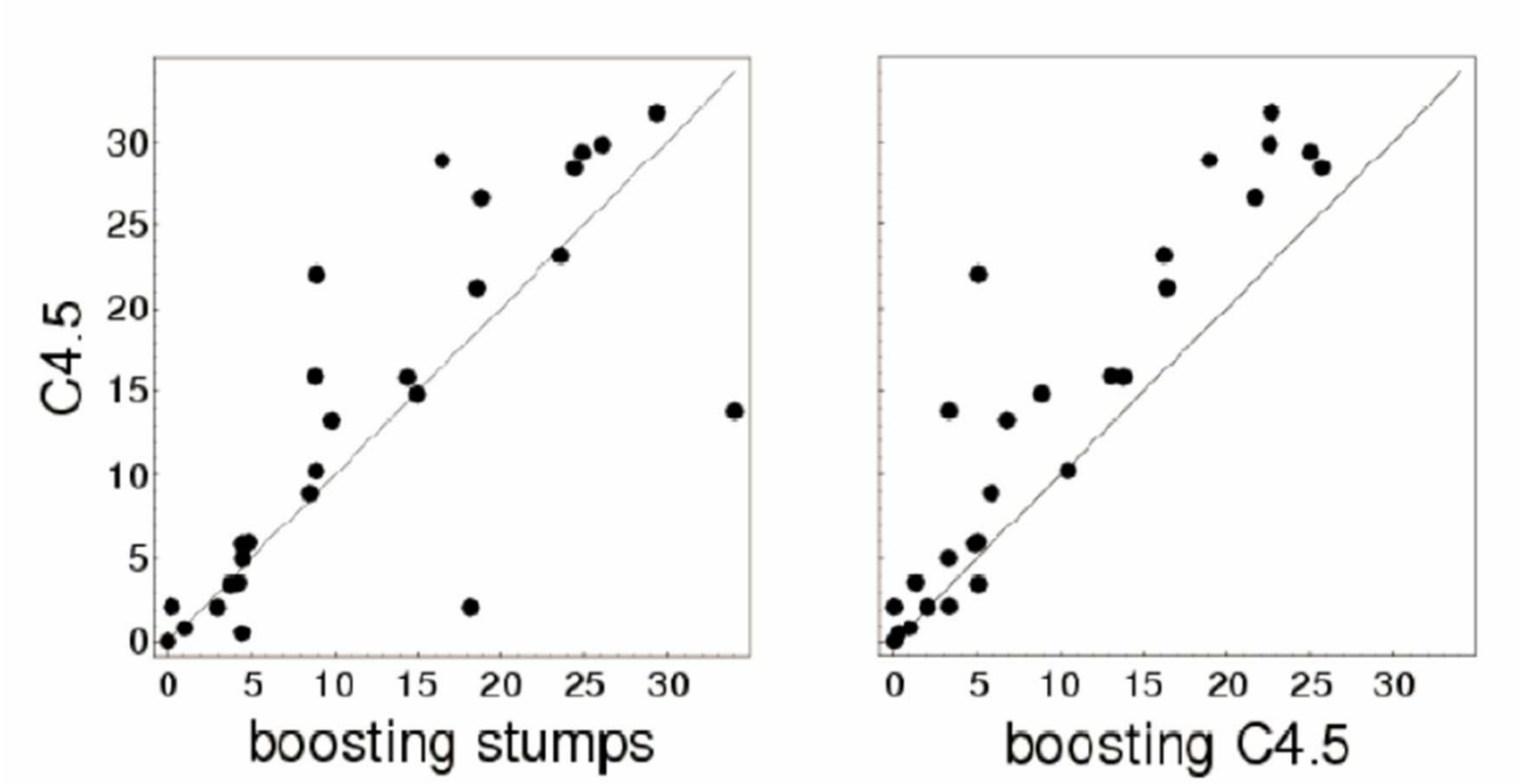
(schapire, Freund, Bartlett and Lee 1989)

$$\mathbf{P}_{\mathcal{D}}\left[yf(x) \leq 0\right] \leq \mathbf{P}_{S}\left[yf(x) \leq \theta\right] + O\left(\frac{1}{\sqrt{m}}\left(\frac{d\log^2(m/d)}{\theta^2} + \log(1/\delta)\right)^{1/2}\right).$$

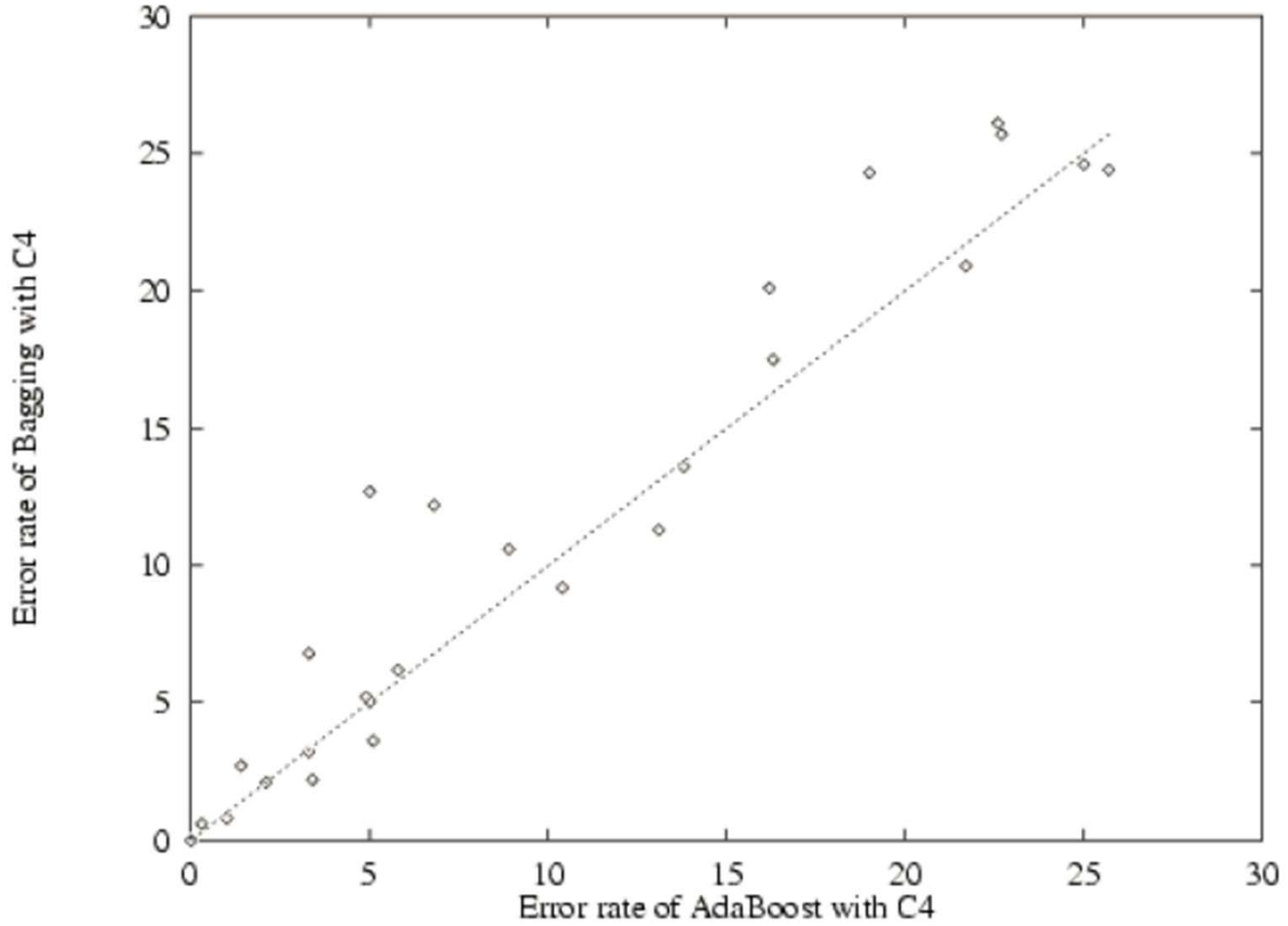
- Boosting increases the margin very aggressively since it concentrates on the hardest examples.
- If margin is large, more weak learners agree and hence more rounds does not necessarily imply that final classifier is getting more complex.
- Bound is independent of number of rounds T!
- Boosting can still overfit if margin is too small , weak learners are too complex or perform arbitrarily close to random guessing

Boosting Performance

- Comparing C4.5, boosting decision stumps, boosting C4.5 using 27 UCI data set
  - C4.5 is a popular decision tree learner



Boosting vs Bagging of Decision Trees



AdaBoost as a Additive Model

- We will now derive AdaBoost in a way that can be adapted in various ways
- This recipe will let you derive “boosting-style” algorithms for particular learning settings of interest
  - E.g., general misprediction cost, semi-supervised learning
- these boosting-style algorithms will not generally be boosting algorithms in the theoretical sense but they often work quite well

AdaBoost: Iterative Learning of Additive Models

- Consider the final hypothesis: it takes the sign of an ***additive expansion of a set of base classifiers***

$$H(\mathbf{x}) = sign\ [f(\mathbf{x})] = sign\ [\sum_{l=1}^{L} \alpha_l h_l(\mathbf{x})]$$

- AdaBoost iteratively finds at each iteration an $h(\cdot)$ to add to $f(\cdot)$

$$f_l(\mathbf{x}) = f_{l-1}(\mathbf{x}) + \alpha_l h_l(\mathbf{x})$$

- The goal is to minimize a loss function on the training example:

$$\sum_{i=1}^{N} L\left(y^i, \sum_{l=1}^{L} \alpha_l h_l(\mathbf{x}^i)\right)$$

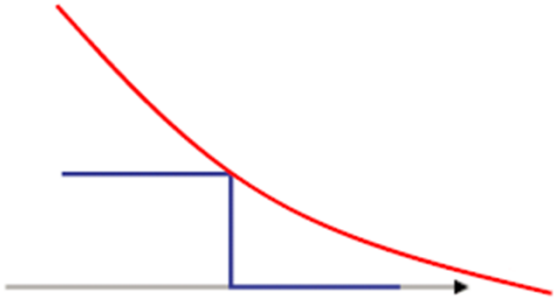
- We would like to minimize the error:

$$L(y^i, f(\mathbf{x}^i)) = [y^i \neq sgn(f(\mathbf{x}^i))]$$

Note y ∈ {-1, 1}

- Instead, Adaboost can be viewed as minimizing an exponential loss function, which is a smooth upper bound on 0/1 error:

$$L(y^i, f(\mathbf{x}^i)) = e^{-y^i f(\mathbf{x}^i)}$$



$$\arg\min_f \sum_{i=1}^{N} L(y^i, f(\mathbf{x}^i))$$

$$= \arg\min_{\alpha, h_l} \sum_{i=1}^{N} e^{-y^i \cdot [f_{l-1}(\mathbf{x}^i) + \alpha \cdot h_l(\mathbf{x}^i)]}$$

at Iteration l, look for h_l and α

$$= \arg\min_{\alpha, h_l} \sum_{i=1}^{N} e^{-y^i \cdot f_{l-1}(\mathbf{x}^i)} \cdot e^{-y^i \cdot \alpha \cdot h_l(\mathbf{x}^i)}$$

Fix α and optimize h_l

$$\arg\min_{h_l} \sum_{i=1}^{N} e^{-y^i \cdot f_{l-1}(\mathbf{x}^i)} \cdot e^{-y^i \cdot \alpha \cdot h_l(\mathbf{x}^i)}$$

$$= \arg\min_{h_l} \sum_{i=1}^{N} w_l^i \cdot e^{-y^i \cdot \alpha \cdot h_l(\mathbf{x}^i)}$$

$$= \arg\min_{h_l} \sum_{y^i = h_l(\mathbf{x}^i)}^{N} w_l^i \cdot e^{-\alpha} + \sum_{y^i \neq h_l(\mathbf{x}^i)}^{N} w_l^i \cdot e^{\alpha}$$

$$= \arg\min_{h_l} \sum_{i=1}^{N} w_l^i \cdot e^{-\alpha} - \sum_{y^i \neq h_l(\mathbf{x}^i)}^{N} w_l^i \cdot e^{-\alpha} + \sum_{y^i \neq h_l(\mathbf{x}^i)}^{N} w_l^i \cdot e^{\alpha}$$

$$= \arg\min_{h_l} \; e^{-\alpha} \sum_{i=1}^{N} w_l^i + (e^{\alpha} - e^{-\alpha}) \cdot \sum_{y^i \neq h_l(\mathbf{x}^i)}^{N} w_l^i$$

$$= \arg\min_{h_l} \; e^{-\alpha} + (e^{\alpha} - e^{-\alpha}) \cdot \frac{\sum_{y^i \neq h_l(\mathbf{x}^i)}^{N} w_l^i}{\sum_{i=1}^{N} w_l^i}$$

$$= \arg\min_{h_l} \; e^{-\alpha} + (e^{\alpha} - e^{-\alpha}) \cdot \sum_{i=1}^{N} \frac{w_l^i}{\sum_{i=1}^{N} w_l^i} \cdot [y^i \neq h_l(\mathbf{x}^i)]$$

Fix $h_l(\cdot)$ and find α

$$\arg\min_{\alpha} \; e^{-\alpha} + (e^{\alpha} - e^{-\alpha}) \cdot \sum_{i=1}^{N} \frac{w_l^i}{\sum_{i=1}^{N} w_l^i} \cdot I[y^i \neq h_l(\mathbf{x}^i)]$$

$$= \arg\min_{\alpha} \; e^{-\alpha} + (e^{\alpha} - e^{-\alpha}) \cdot \epsilon_l$$

$J(\alpha)$

$$\frac{\partial J(\alpha)}{\partial \alpha} = -e^{-\alpha} + \epsilon_l \cdot e^{\alpha} + \epsilon_l \cdot e^{-\alpha}$$

$$= e^{-\alpha} \cdot (\epsilon_l - 1) + e^{\alpha} \cdot \epsilon_l = 0$$

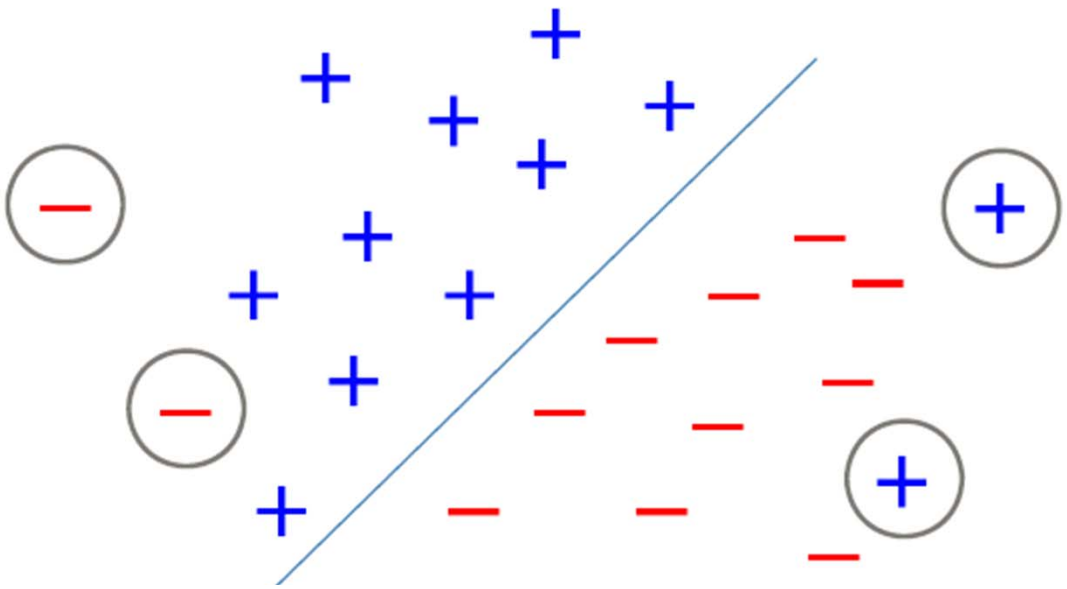
$$\Rightarrow \; e^{\alpha} \cdot \epsilon_l = e^{-\alpha} \cdot (1 - \epsilon_l)$$

$$\Rightarrow \; e^{2\alpha} = \frac{1 - \epsilon_l}{\epsilon_l} \Rightarrow \boxed{\alpha = \frac{1}{2} \ln \frac{1 - \epsilon_l}{\epsilon_l}}$$

Pitfall of Boosting: sensitive to noise and outliers

Good ☺ : Can identify outliers since focuses on examples that are hard to categorize

Bad ☹ : Too many outliers can degrade classification performance dramatically increase time to convergence



Summary: Bagging and Boosting

- Bagging
  - Resample data points
  - Weight of each classifier is the same
  - Only variance reduction
  - Robust to noise and outliers
- Boosting
  - Reweight data points (modify data distribution)
  - Weight of classifier vary depending on accuracy
  - Reduces both bias and variance
  - Can hurt performance with noise and outliers