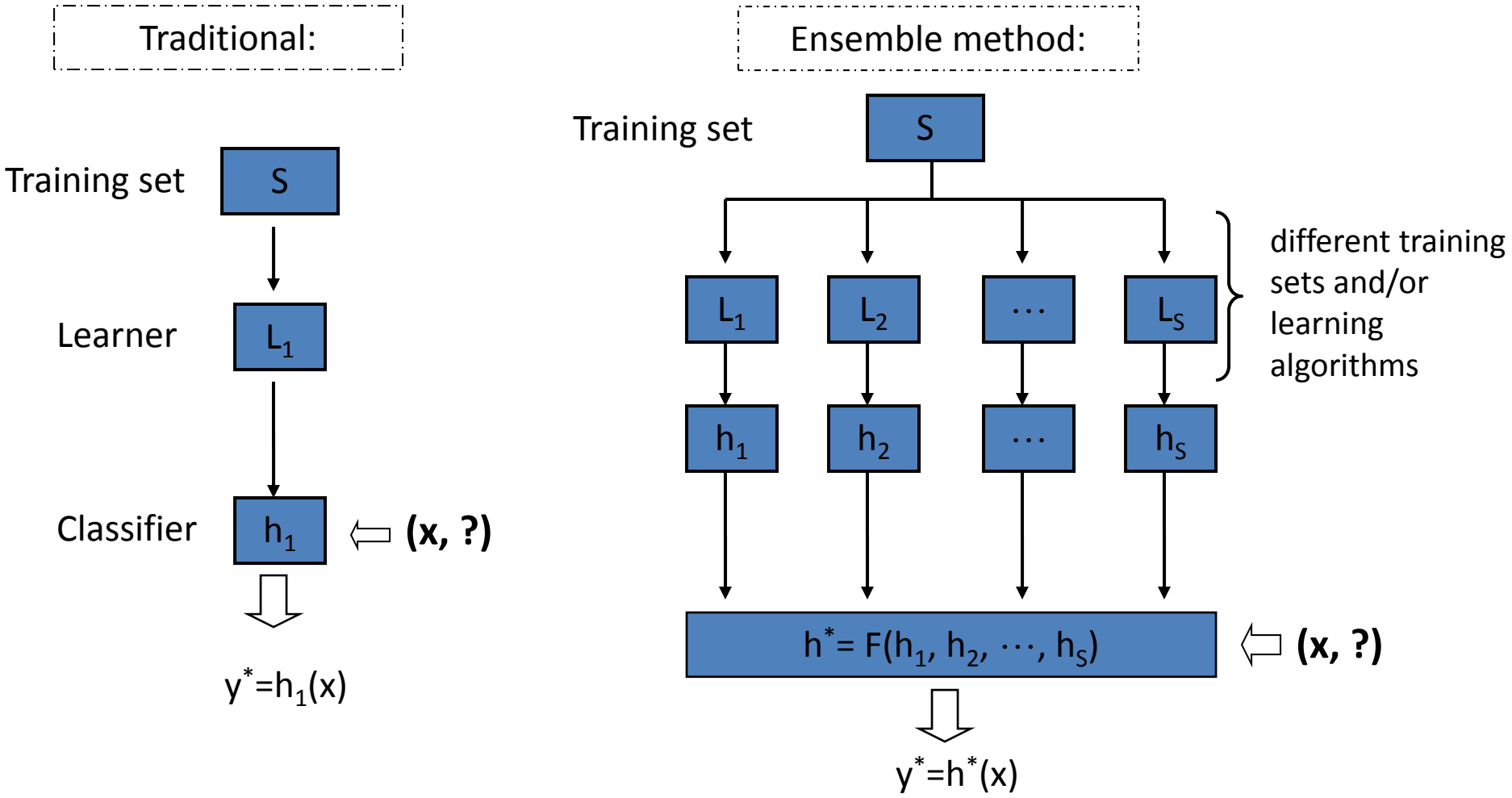
Ensemble Learning

Ensemble Learning

- So far we have seen learning algorithms that take a training set and output a classifier
- What if we want more accuracy than current algorithms afford?
  - Develop new learning algorithm
  - Improve existing algorithms
- Another approach is to leverage the algorithms we have via ensemble methods
  - Instead of calling an algorithm just once and using its classifier
  - Call algorithm multiple times and combine the multiple classifiers

What is Ensemble Learning



Ensemble Learning

- **INTUITION:** Combining predictions of multiple classifiers (an ensemble) is more accurate than a single classifier.
- Justification:
  - easy to find quite good "rules of thumb" however hard to find single highly accurate prediction rule.
  - If the training set is small and the hypothesis space is large then there may be many equally accurate classifiers.
  - Hypothesis space does not contain the true function, but it has several good approximations.
  - Exhaustive global search in the hypothesis space is expensive so we can combine the predictions of several locally accurate classifiers.

How to generate ensemble?

- There are a variety of methods developed
- We will look at two of them:
  - Bagging
  - Boosting (Adaboost: adaptive boosting)
- Both of these methods takes a single learning algorithm (we will call it ***the base learner***) and use it multiple times to generate multiple classifiers

Bagging: Bootstrap Aggregation

(Breiman, 1996)

Bagging carries out the following steps:

S - Training data set.

1. Create T bootstrap training sets $S_1, \ldots, S_T$ from S
   (see next slide for bootstrap procedure)

2. For each i from 1 to T $h_i = Learn(S_i)$.

3. Hypothesis: H(x) = majorityVote(h_1(x), h_2(x), …, h_T(x))

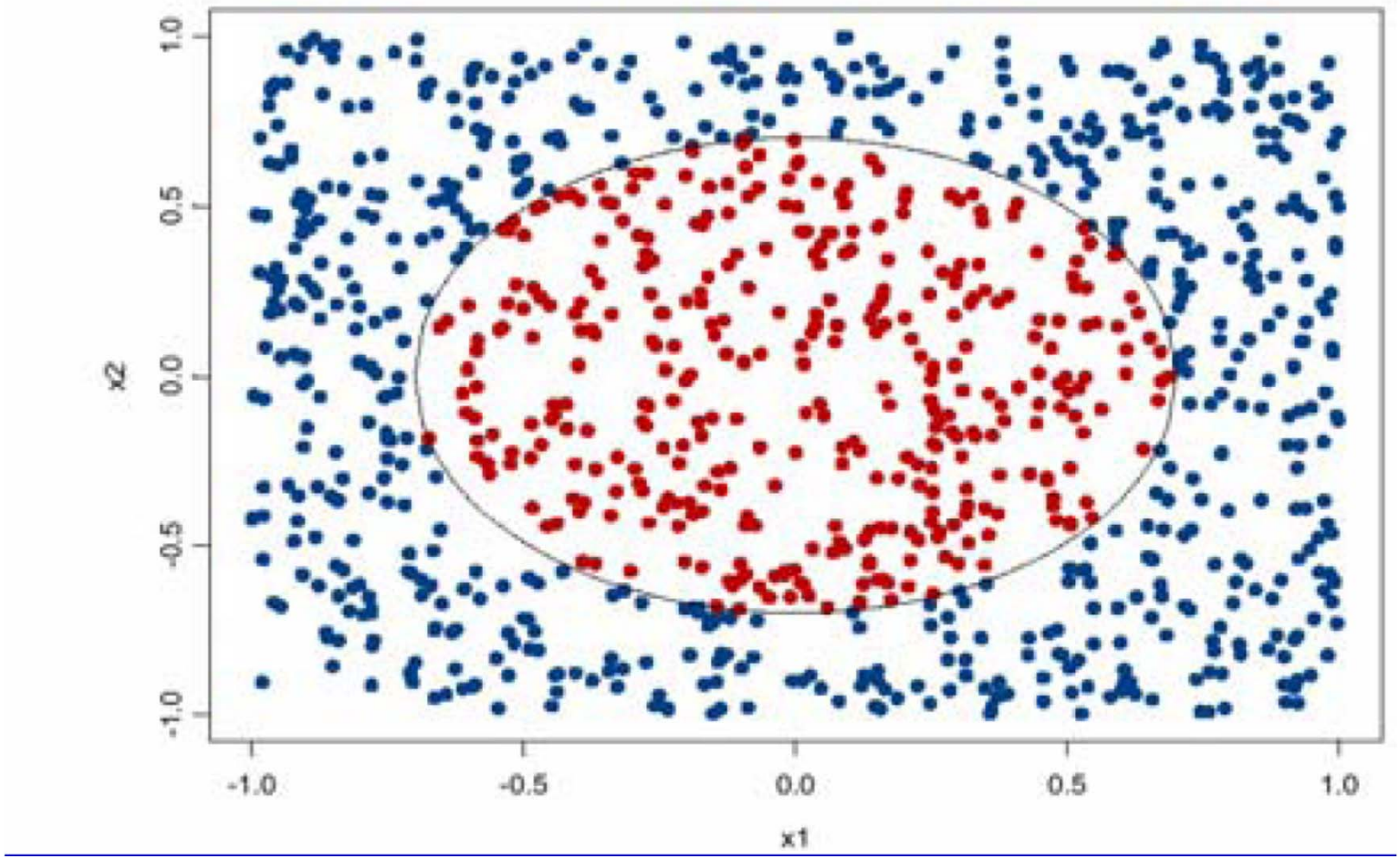
Final hypothesis is just the majority vote of the ensemble members. That is, return the class that gets the most votes.

Generate a Bootstrap sample of S

```
Given S, let S' = {}
For i=1, …, N (the total number of points in S)
        draw a random point from S and add it to S'
End
Return S'
```

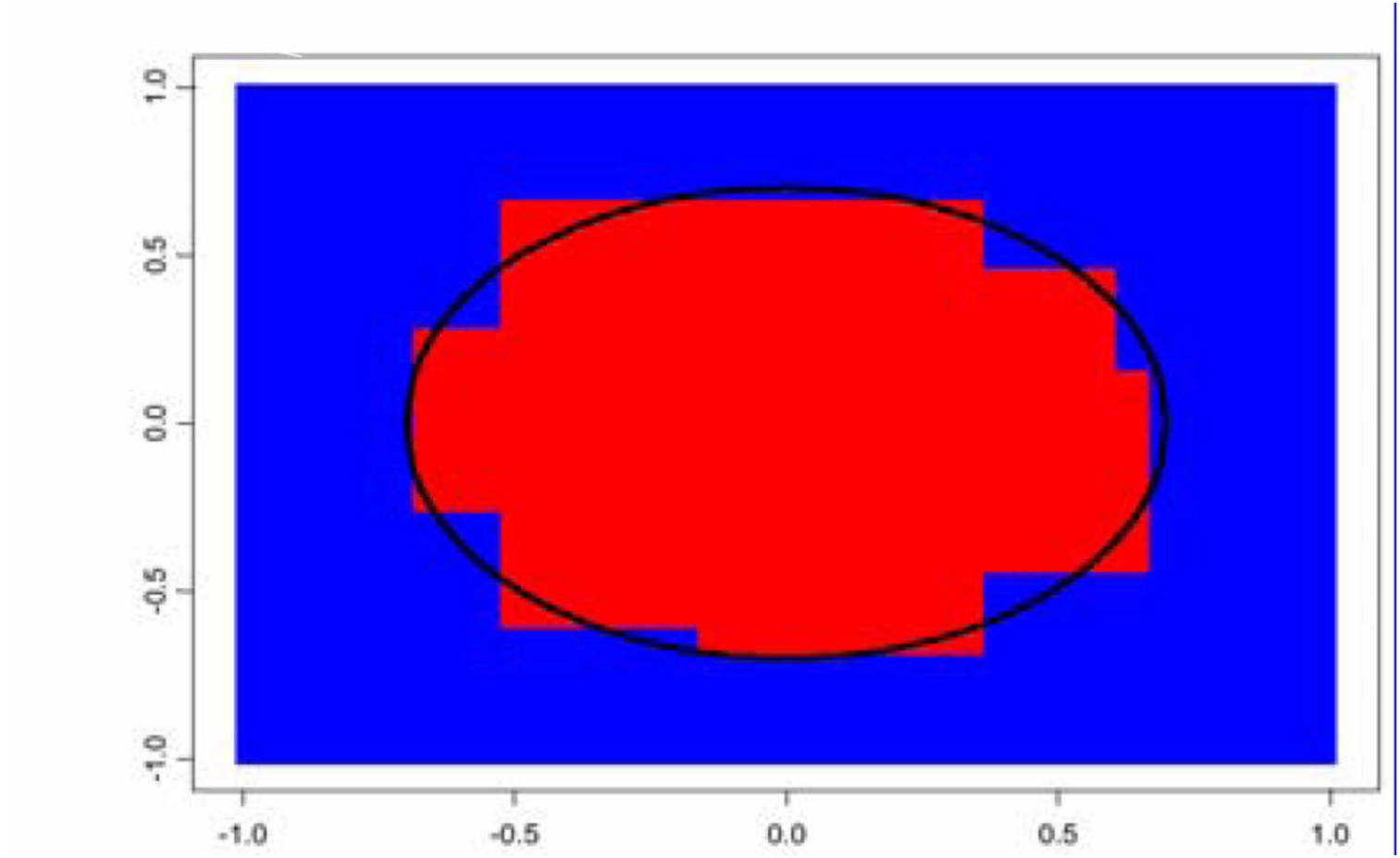
- This procedure is called **sampling with replacement**
  - Each time a point is drawn, it will not be removed
  - This means that we can have multiple copies of the same data point in my sample
  - size of S'= size of S
  - On average, 66.7% of the original points will appear in S'

Bagging Example



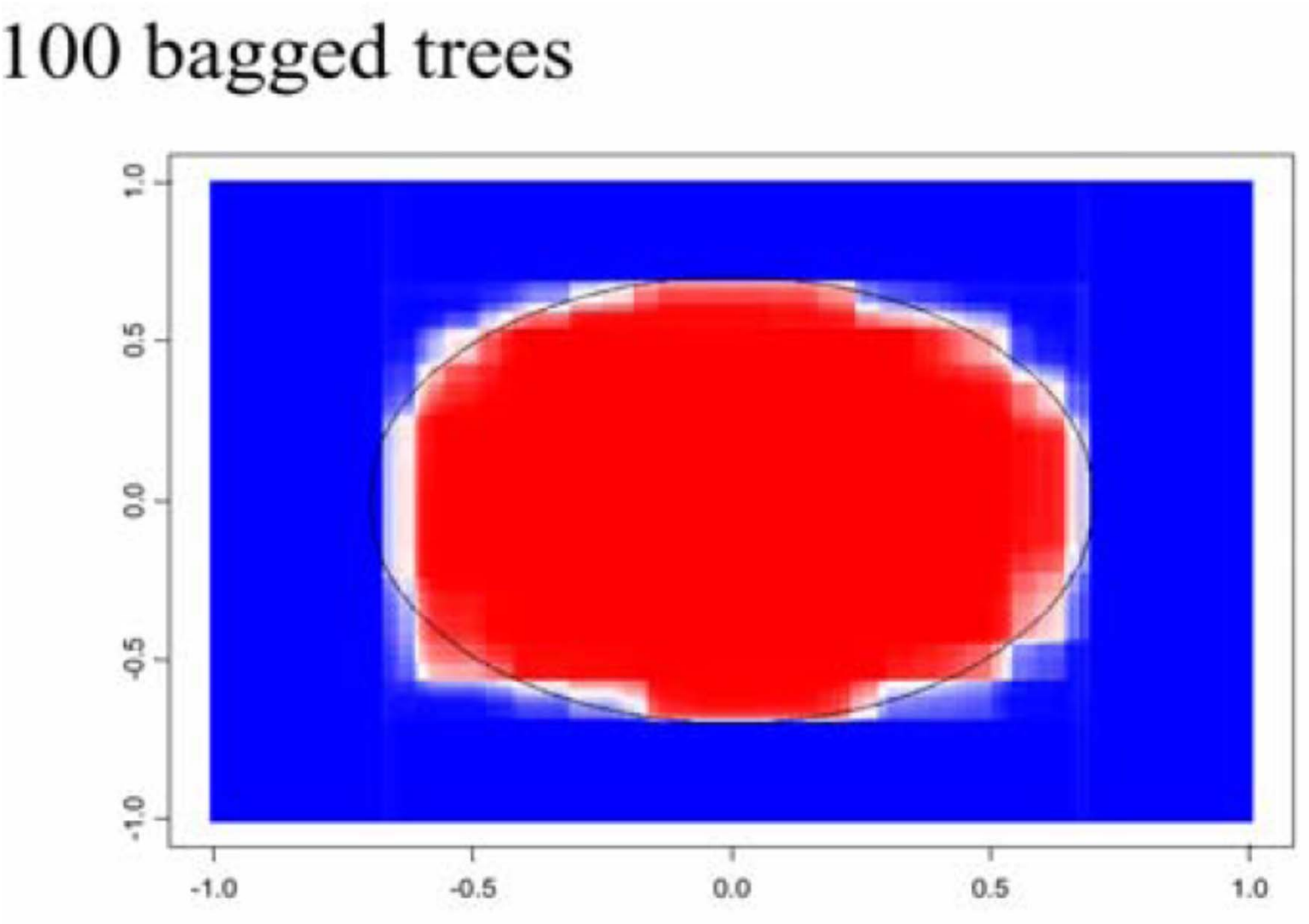
The true decision boundary

Decision Boundary by the CART Decision Tree Algorithm



Note that the decision tree has trouble representing this decision boundary

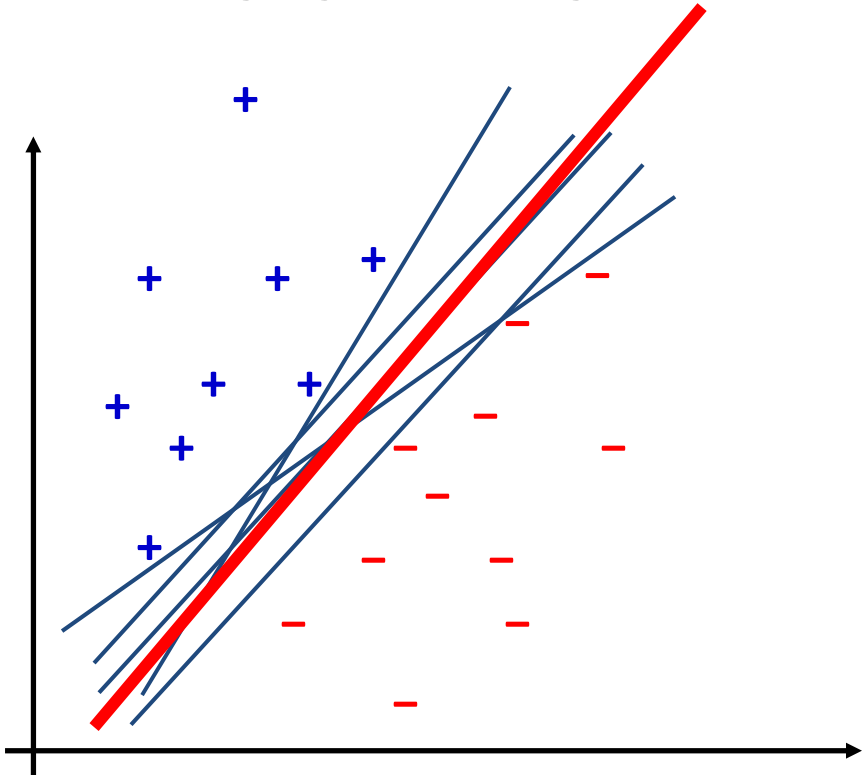
100 bagged trees



By averaging 100 trees, we achieve better approximation of the boundary, together with information regarding how confidence we are about our prediction.

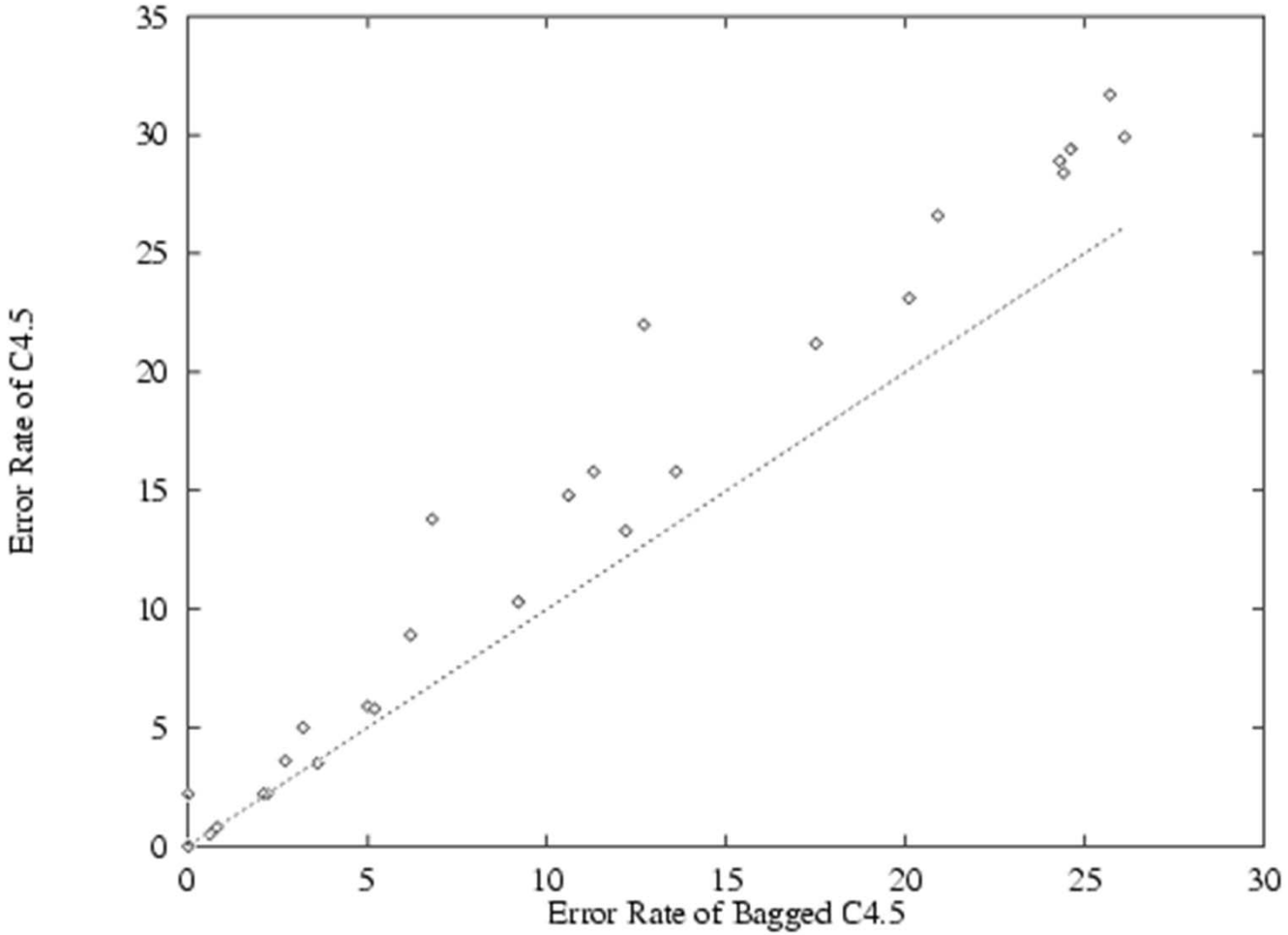
Another Example

- Consider bagging with the linear perceptron base learning algorithm
- Each bootstrap training set will give a different linear separator
- Voting is **similar** to averaging them together (not equivalent)



Empirical Results for Bagging Decision Trees

(Freund & Schapire)

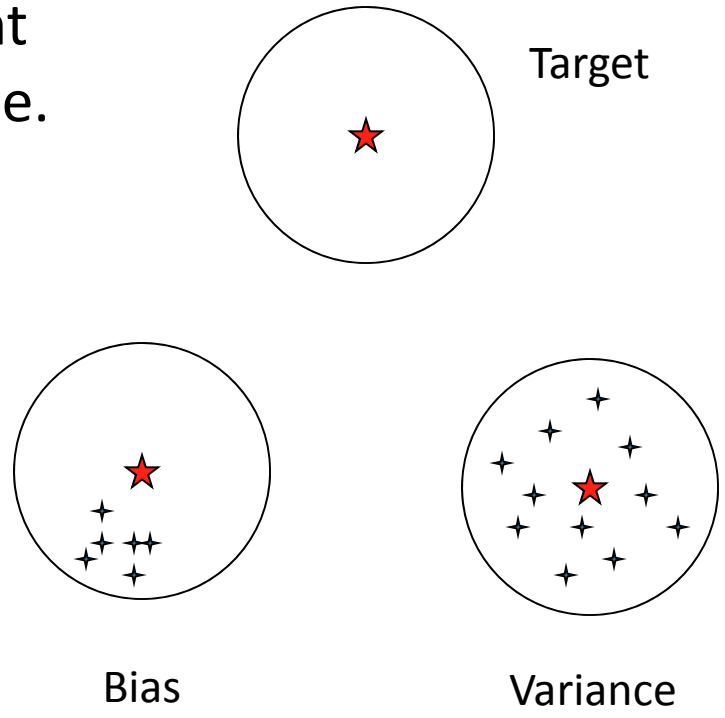


Each point represents the results of one data set

Why can bagging improve the classification accuracy?

The Concept of Bias and Variance

The circles represent the hypothesis space.



Bias/Variance for classifiers

- Bias arises when the classifier cannot represent the true function – that is, the classifier underfits the data
  - If the hypothesis space does not contain the target function, then we have bias

- Variance arises when classifiers learned on minor variations of data result in significantly different classifiers – variations cause the classifier to overfit differently
  - If the hypothesis space has only one function then the variance is zero (but the bias is huge)

- Clearly you would like to have a low bias and low variance classifier!
  - Typically, low bias classifiers (overfitting) have high variance
  - high bias classifiers (underfitting) have low variance
  - We have a trade-off

Effect of Algorithm Parameters on Bias and Variance

- k-nearest neighbor k:

  increasing k typically increases bias and reduces variance

- Decision trees of depth D:

  increasing D typically increases variance and reduces bias

Why does bagging work?

- Bagging takes the average of multiple models --- reduces the variance
- This suggests that bagging works the best with low bias and high variance classifiers such as …
- Un-pruned decision trees
- Bagging typically will not hurt the performace

Boosting

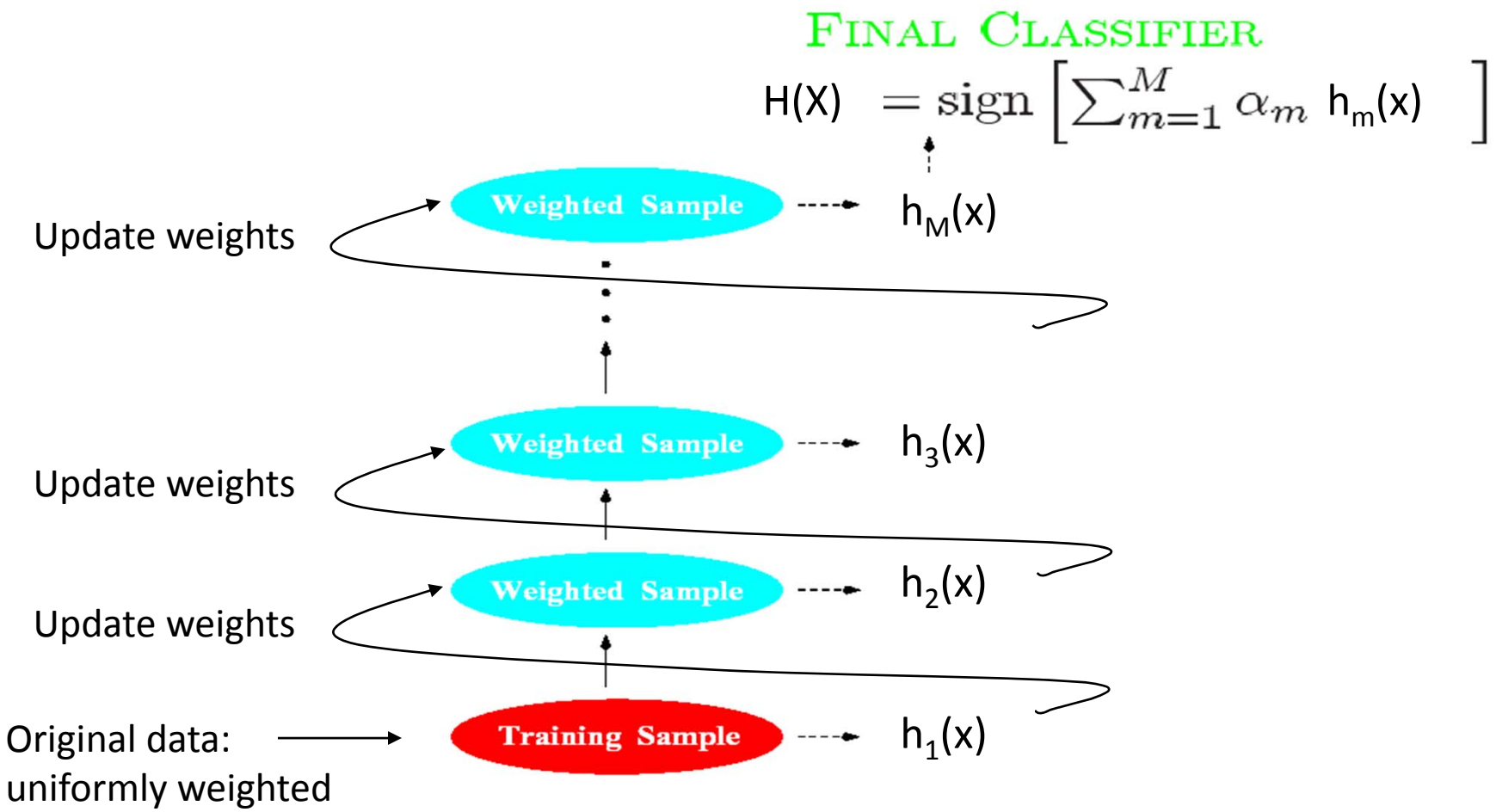
Boosting

- Also an ensemble method: the final prediction is a combination of the prediction of multiple classifiers.
- What is different?
  - It's iterative.

    Boosting: Successive classifiers depends upon its predecessors - look at **errors from previous classifiers** to decide what to **focus** on for the next iteration over data

    Bagging : Individual training sets and classifiers were independent.
  - All training examples are used in each iteration, but with different weights – more weights on difficult examples. (the ones we made mistakes before)

Adaboost: Illustration



AdaBoost (High level steps)

- AdaBoost performs *M* boosting rounds, creating one ensemble member in each round.

Operations in *l'th* boosting round:

1. Call *Learn* on data set *S* and weights D_l to produce *l'th* classifier h_l. Where D_l is the weights of round *l*.

2. Compute the (*l*+1)*'th* round weights D_{l+1} by putting more weight on instances that h_l makes errors on.

3. Compute a voting weight α_l for h_l.

The ensemble hypothesis returned is:

$$H(x) = sign\left[\sum_{m=1}^{M} \alpha_m \cdot h_m(x)\right]$$

Weighted Training Sets

- AdaBoost works by invoking the base learner many times on different weighted versions of the same training data set.
- Thus we assume our base learner takes as input a weighted training set, rather than just a set of training examples

Learn:

Input:

S - Set of *N* labeled training instances.

D - A set of weights over *S*, where *D(i)* is the weight of the *i'th* training instance (interpreted as the probability of observing *i'th* instance), and $\sum_{i=1}^{N} D(i) = 1$. D is also called ***distribution*** of S

Output:

h - hypothesis from hypothesis space *H* with low weighted error

Definition: Weighted Error

- Denote the *i'th* training instance by $<x_i, y_i>$.
- For a training set *S* and distribution *D* the weighed training error is the sum of the weights of incorrect examples

$$error(h, S, D) = \sum_{i=1}^{N} D(i) \cdot [h(x_i) \neq y_i]$$

- The goal of the base learner is to find a hypothesis with a 'small' weighted error.
- Thus *D(i)* can be viewed as indicating to *Learn* the importance of learning the *i'th* training instance.

Weighted Error

• Adaboost calls ***Learn*** with a set of prespecified weights
• It is often straightforward to convert a base learner ***Learn*** to take into account the weights in *D*.

Decision trees?

K Nearest Neighbor?

Naïve Bayes?

• When it is not straightforward we can resample the training data S according to D and then feed the new data set into the learner.

AdaBoost algorithm:

Input: S - Set of N labeled training instances.

Output: $H(x) = sign\left[\sum_{t=1}^{M} \alpha_m \cdot h_m(x)\right]$

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

FOR $t = 1, 2, \ldots, M$ **DO**

$h_t = Learn(S, D_t)$

$\varepsilon_t = error(h_t, S, D_t)$

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

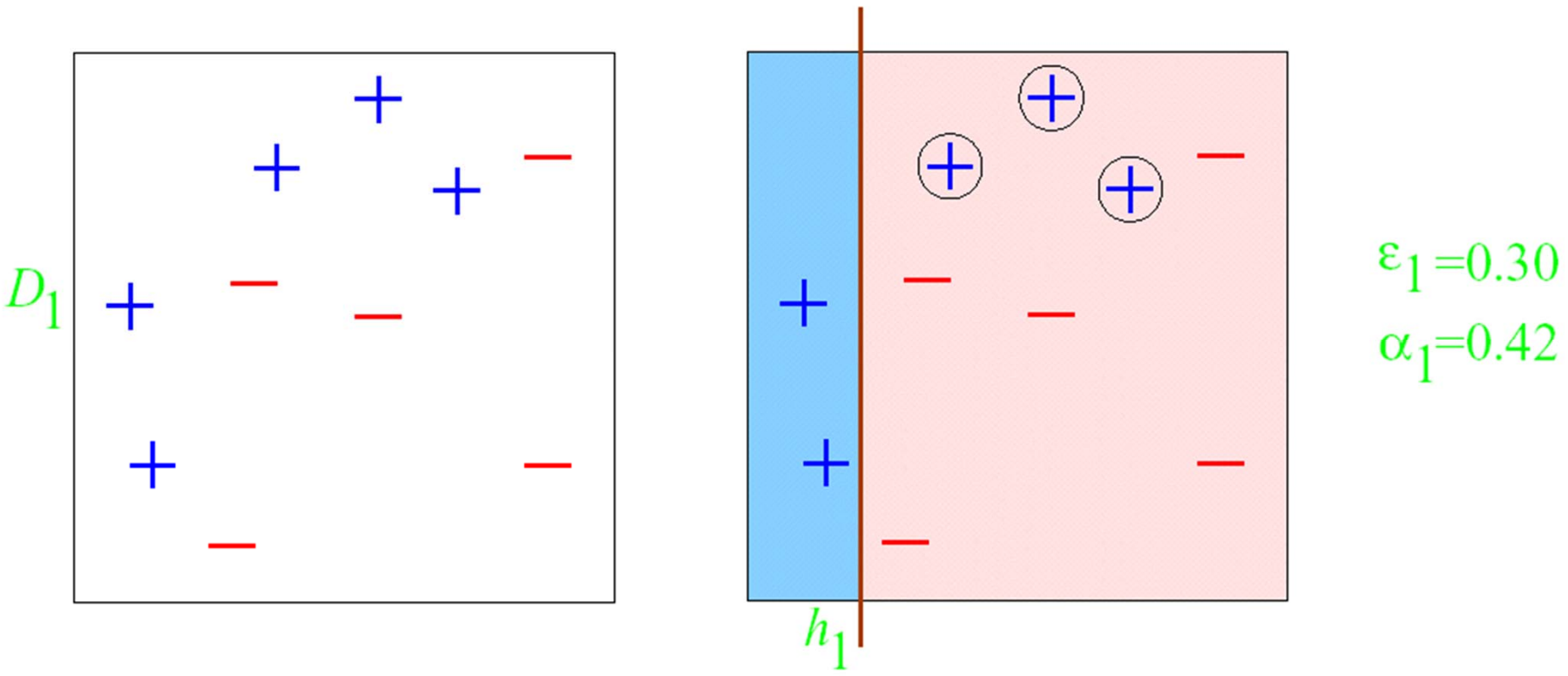
$$D_{t+1}(i) = D_t(i) \times \begin{cases} e^{\alpha_t}, & h_t(x_t) \neq y_t \\ e^{-\alpha_t}, & h_t(x_t) = y_t \end{cases}$$ for i from 1 to N

Normalize D_{t+1} ;; can show that h_t has 0.5 error on D_{t+1}

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

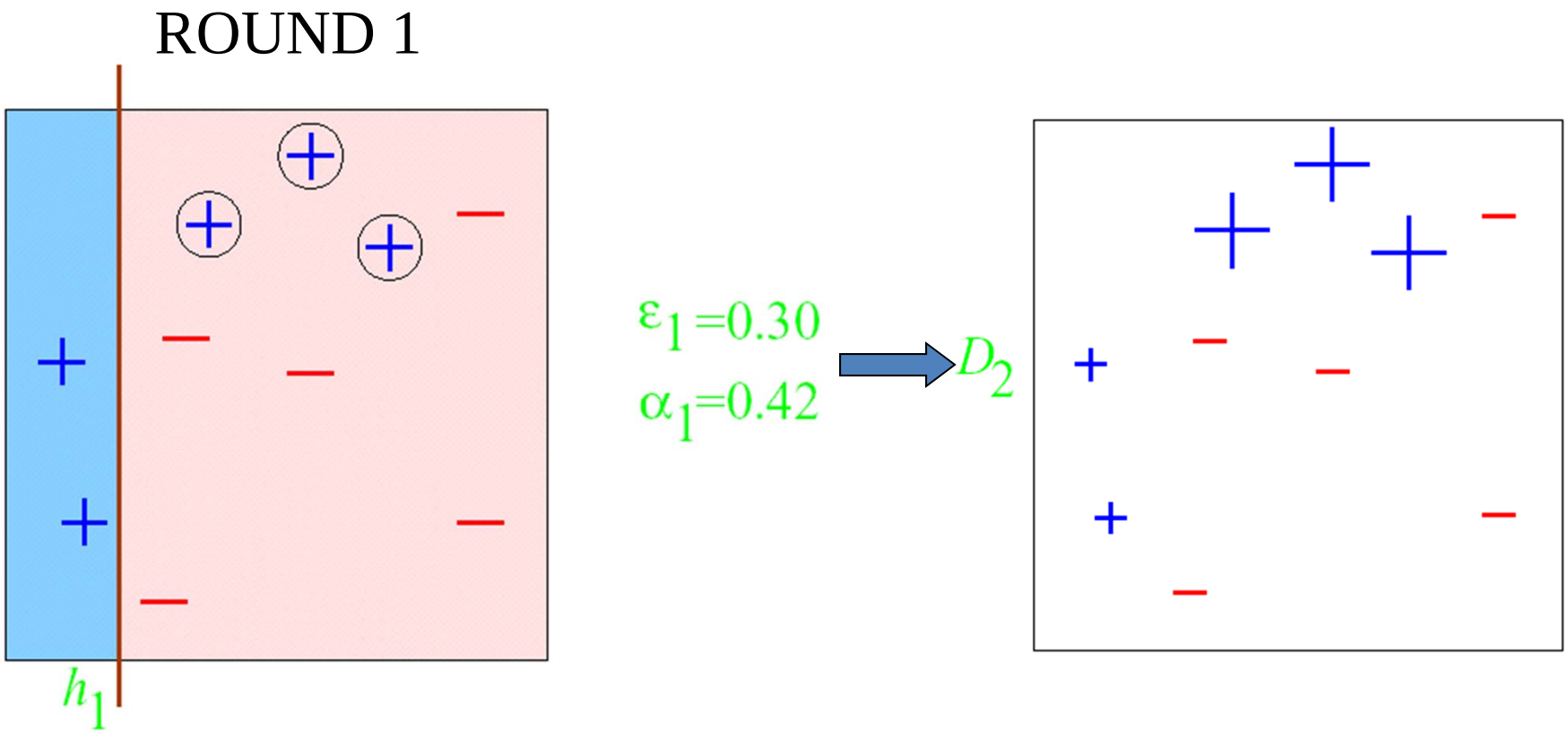
AdaBoost using Decision Stump (Depth-1 decision tree)

Original Training set : Equal
Weights to all training samples

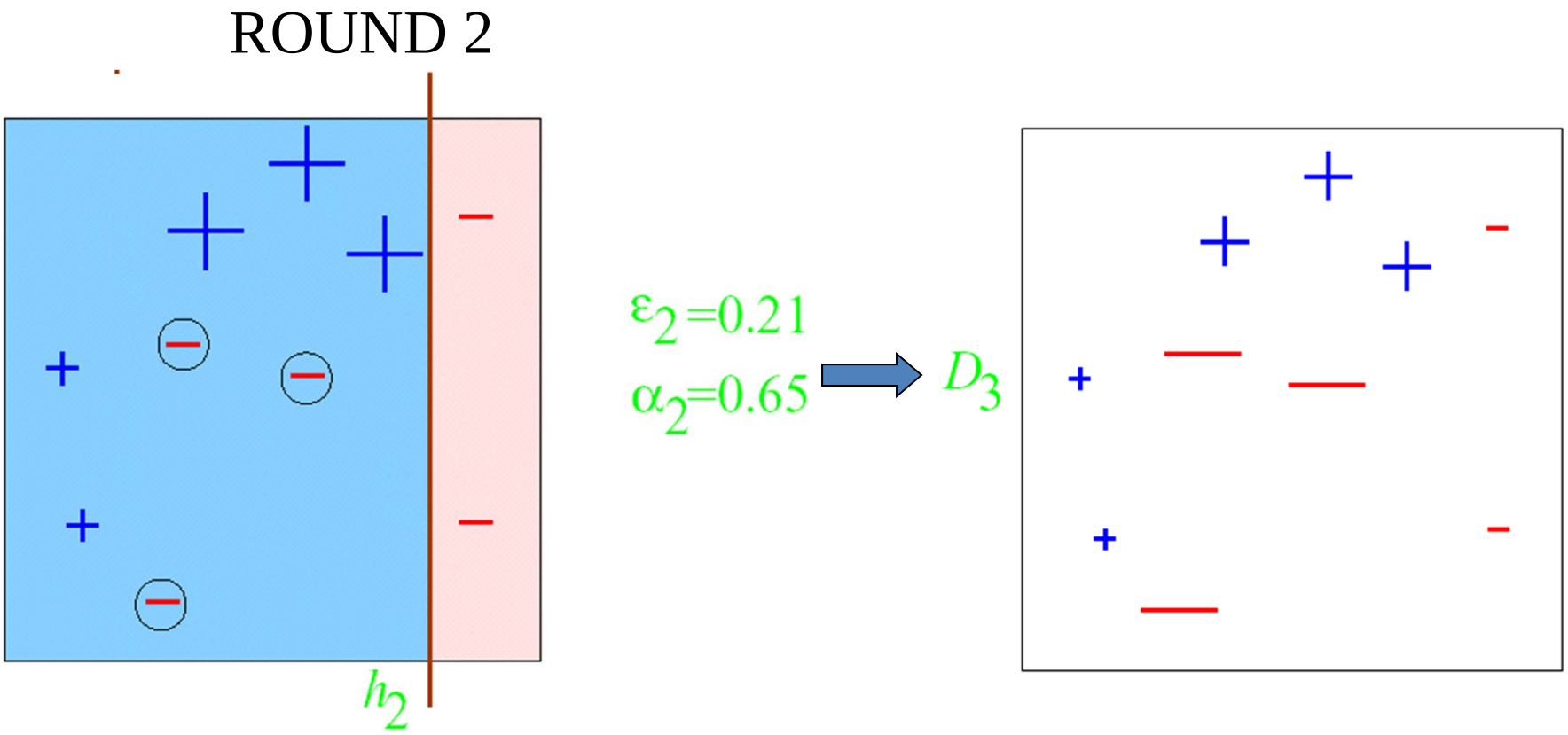


Taken from "**A Tutorial on Boosting" by** Yoav Freund and Rob Schapire

AdaBoost(Example)

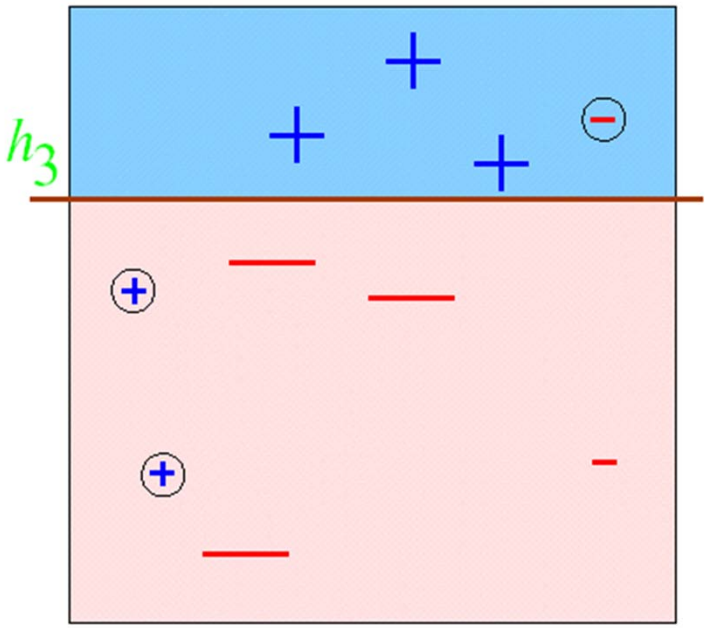


AdaBoost(Example)



AdaBoost(Example)

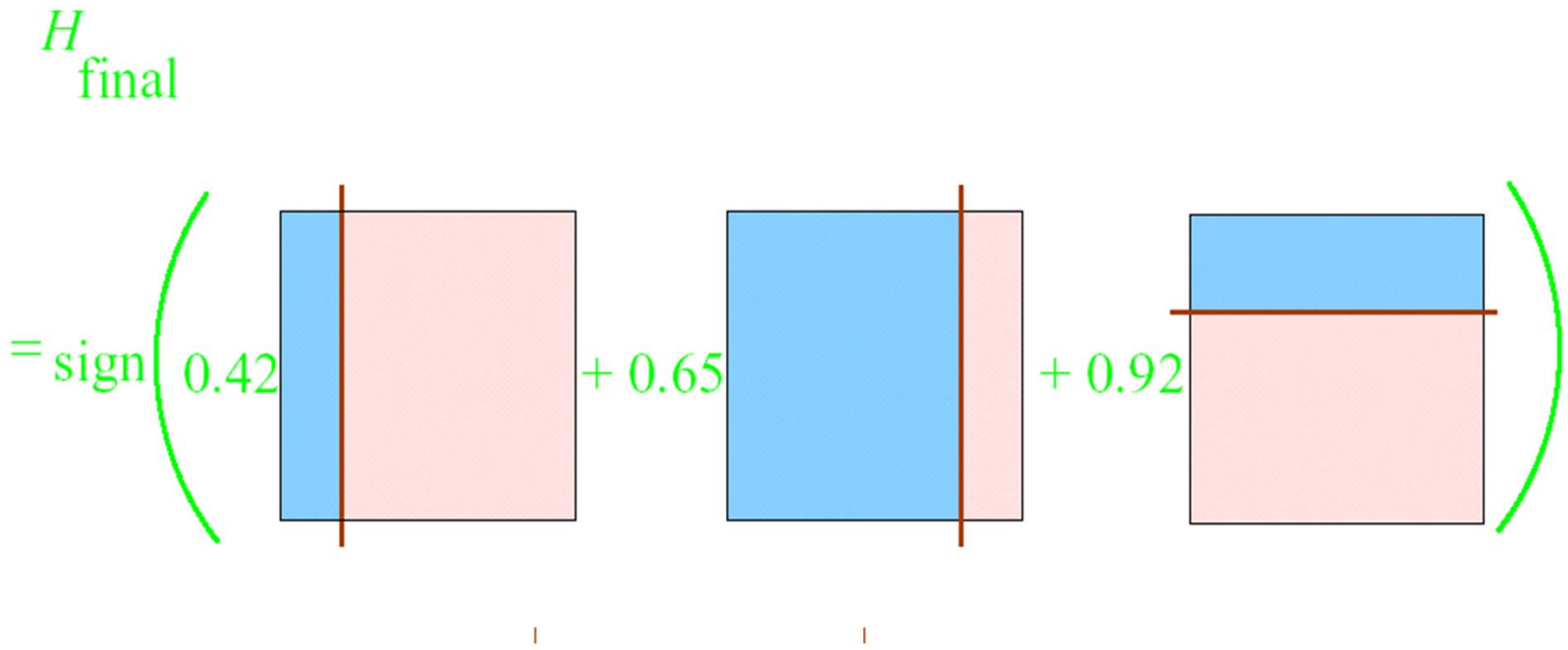
ROUND 3



$\varepsilon_3 = 0.14$

$\alpha_3 = 0.92$

AdaBoost(Example)

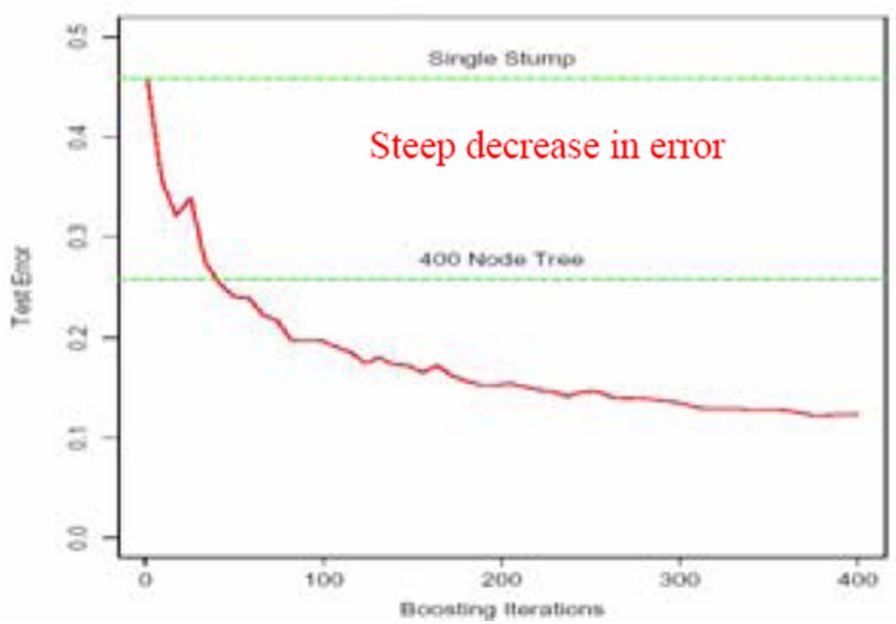


Boosting Decision Stumps

Decision stumps: very simple rules of thumb that test condition on a single attribute.

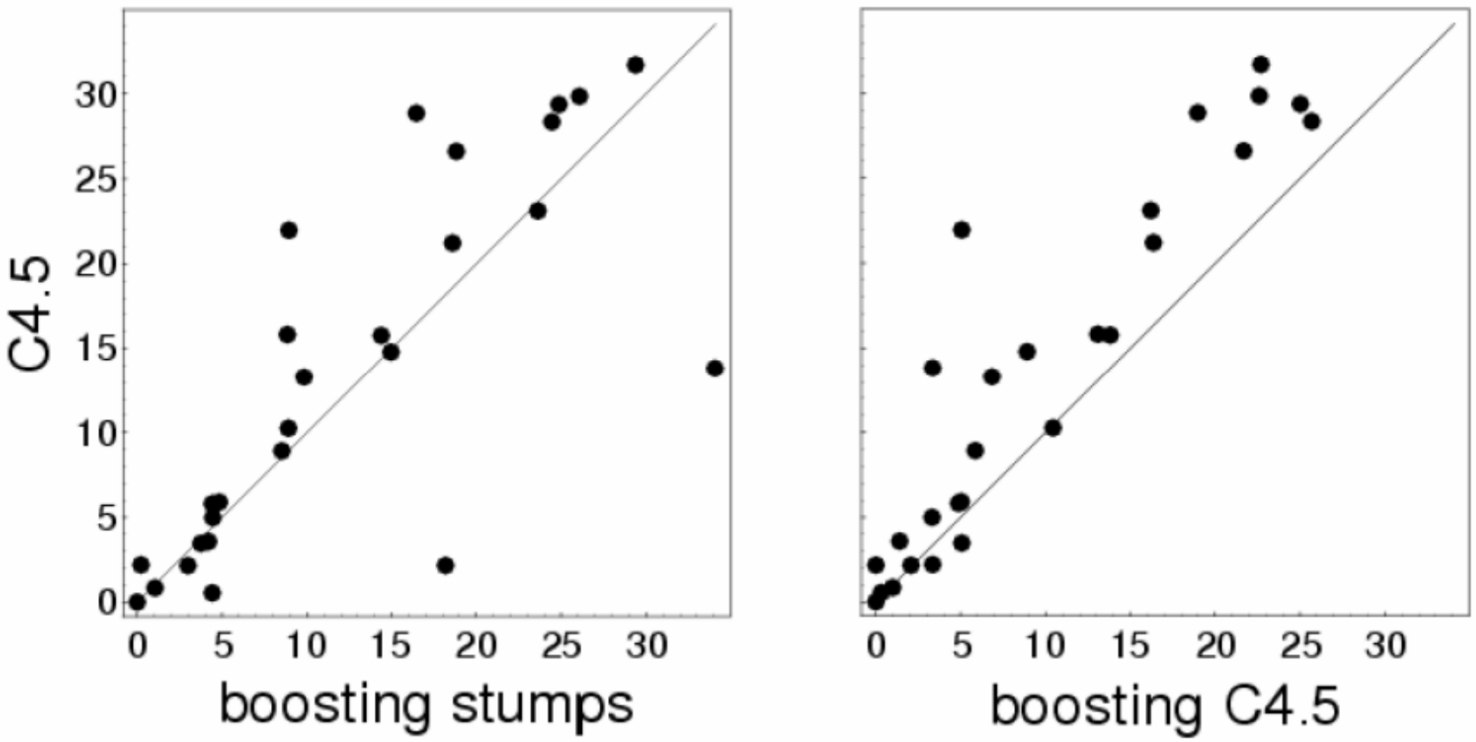
Among the most commonly used base classifiers – truly weak!

Boosting with decision stumps has been shown to achieve better performance compared to unbounded decision trees.

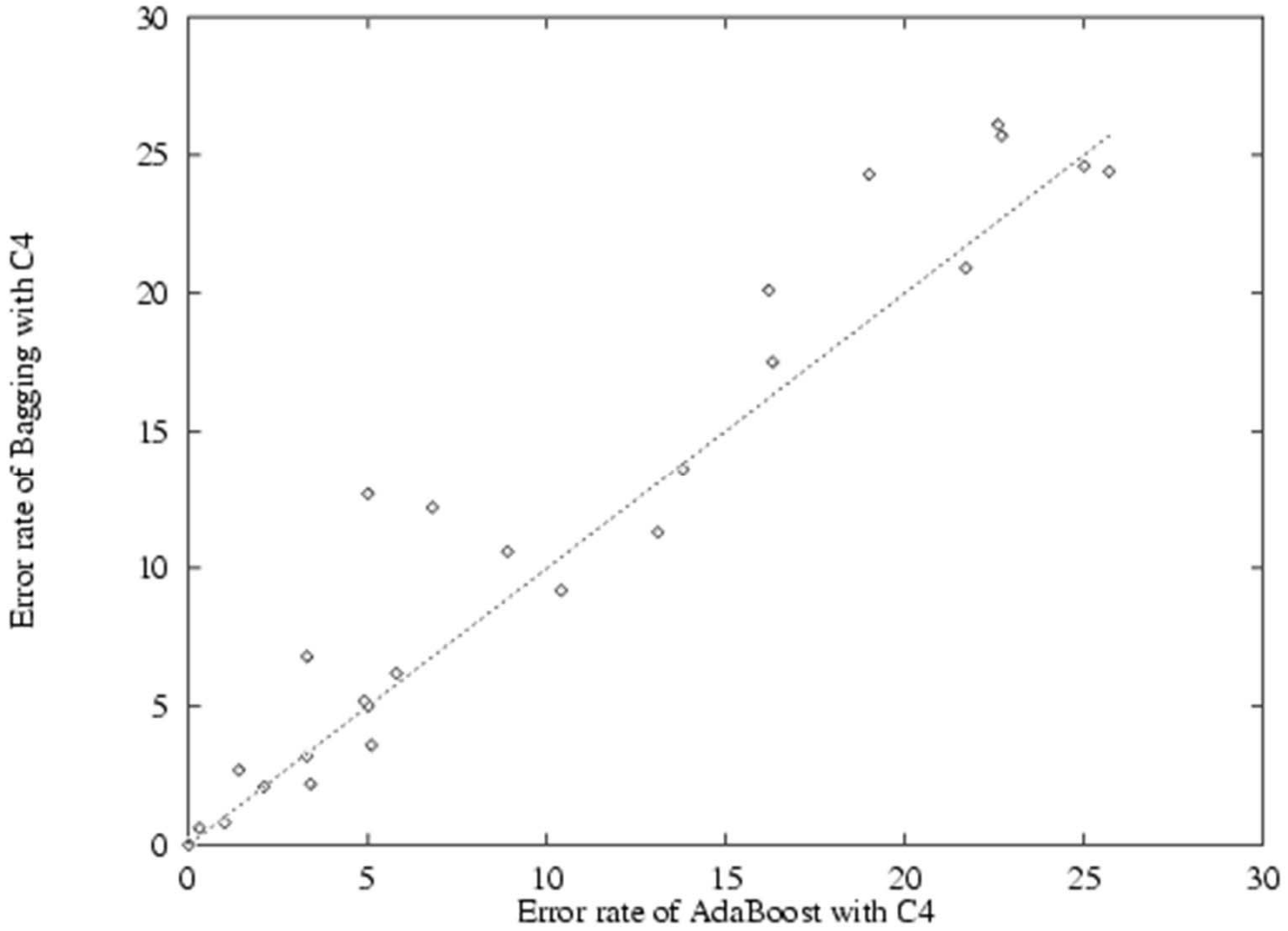


Boosting Performance

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

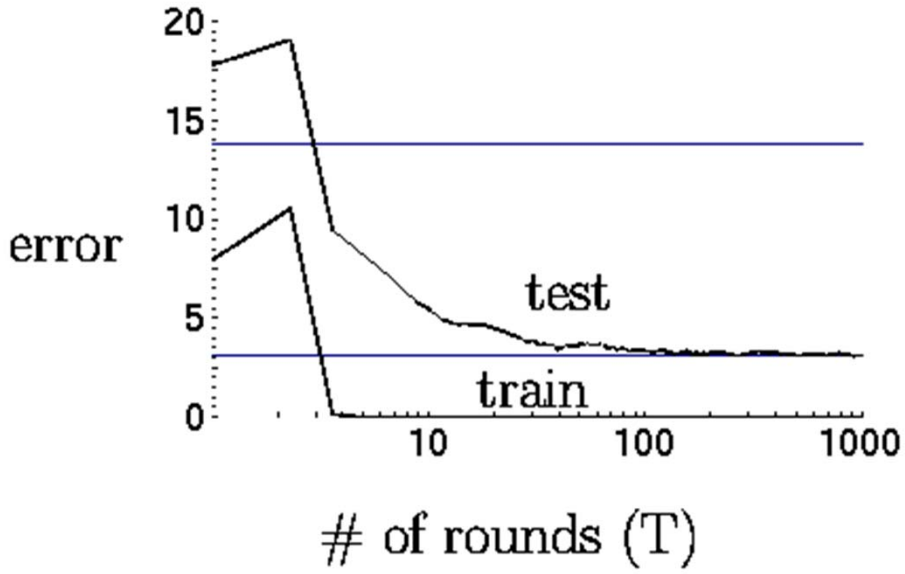


Boosting vs Bagging of Decision Trees



Overfitting?

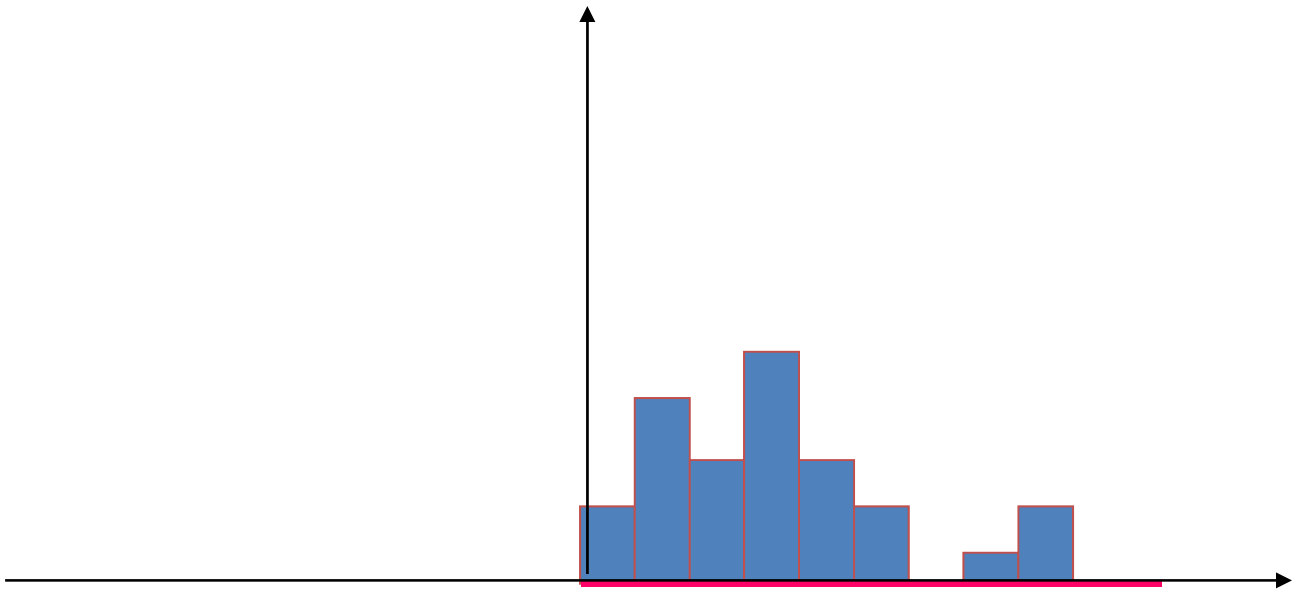
- Boosting drives training error to zero, will it overfit?
- Curious phenomenon



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

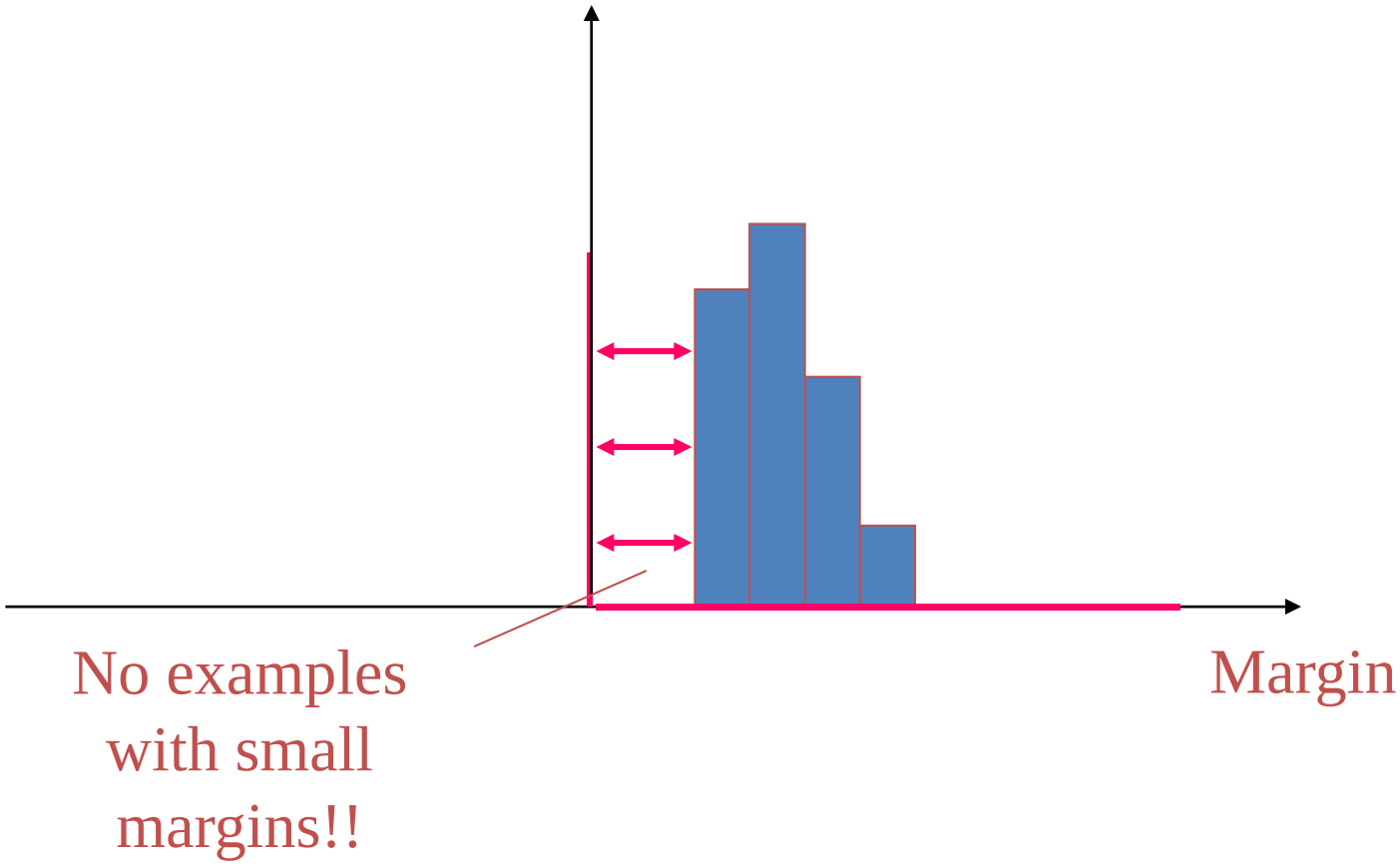
Explanation with Margins

$$f(x) = \sum_{l=1}^{L} w_l \cdot h_l(x)$$



Histogram of functional margin for ensemble just after achieving zero training error

Effect of Boosting: Maximizing Margin



Even after zero training error the margin of examples increases.
This is one reason that the generalization error may continue decreasing.

Bias/variance analysis of Boosting

- In the early iterations, boosting is primary a bias-reducing method
- In later iterations, it appears to be primarily a variance-reducing method

What you need to know about ensemble methods?

- Bagging: a randomized algorithm based on bootstrapping
  - What is bootstrapping
  - Variance reduction
  - What learning algorithms will be good for bagging? - high variance, low bias ones such as unpruned decision trees
- Boosting:
  - Combine weak classifiers (i.e., slightly better than random)
  - Training using the same data set but different weights
  - How to update weights?
  - How to incorporate weights in learning (DT, KNN, Naïve Bayes)
  - One explanation for not overfitting: maximizing the margin