Machine Learning

CSCI 4622

Fall 2019

Prof. Claire Monteleoni

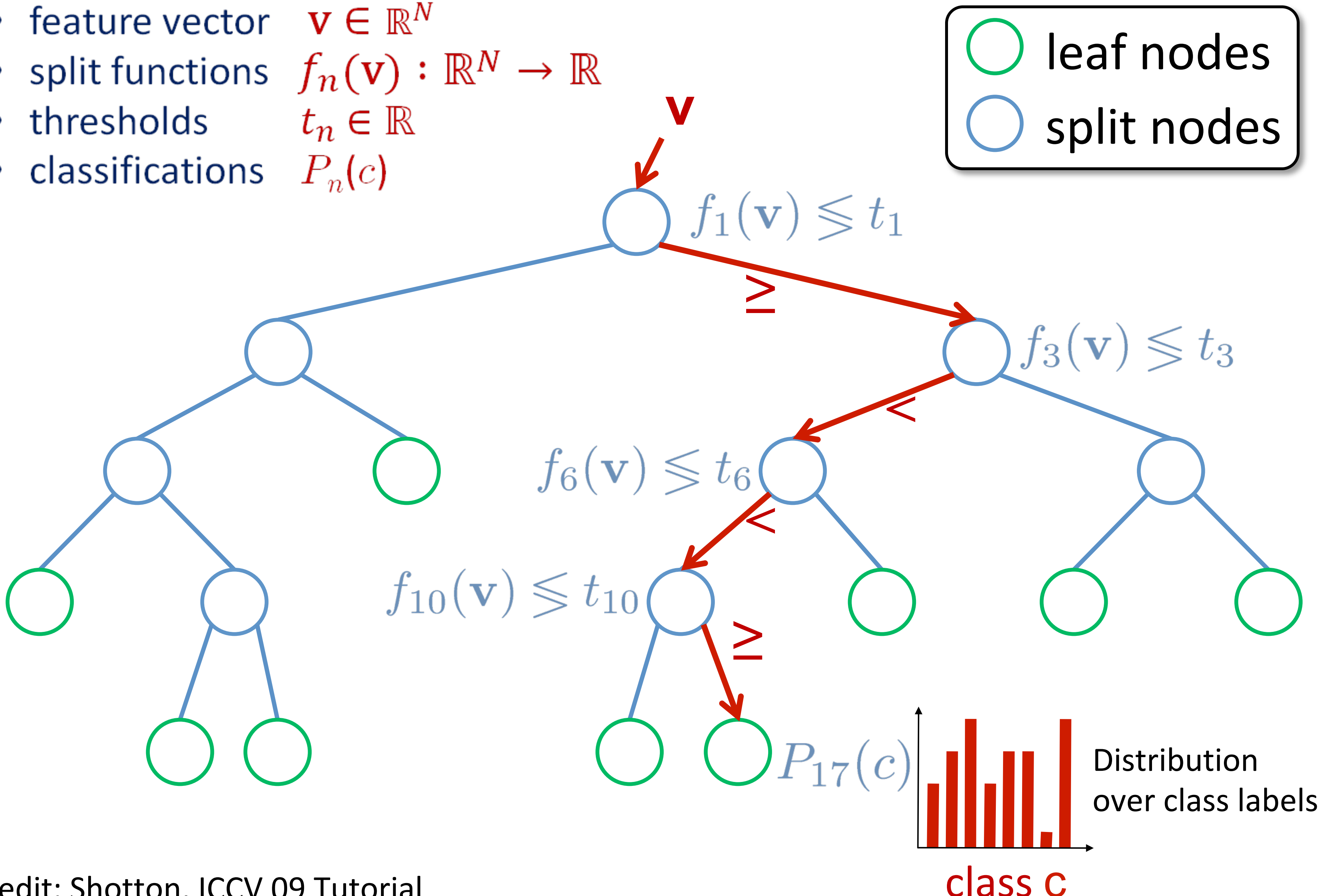
Today: Lecture 10

- Introduction to Ensemble Methods
  - Random Forests
  - Voted Perceptron
  - Boosting (if time)

With slide credits: S. Dasgupta, T. Jaakkola, J. Shotton, C. Tan, and A. Torralba

Review: (Binary) Decision Trees

- feature vector $\mathbf{v} \in \mathbb{R}^N$
- split functions $f_n(\mathbf{v}) : \mathbb{R}^N \rightarrow \mathbb{R}$
- thresholds $t_n \in \mathbb{R}$
- classifications $P_n(c)$



Credit: Shotton, ICCV 09 Tutorial

Speeding up Decision Tree Learning

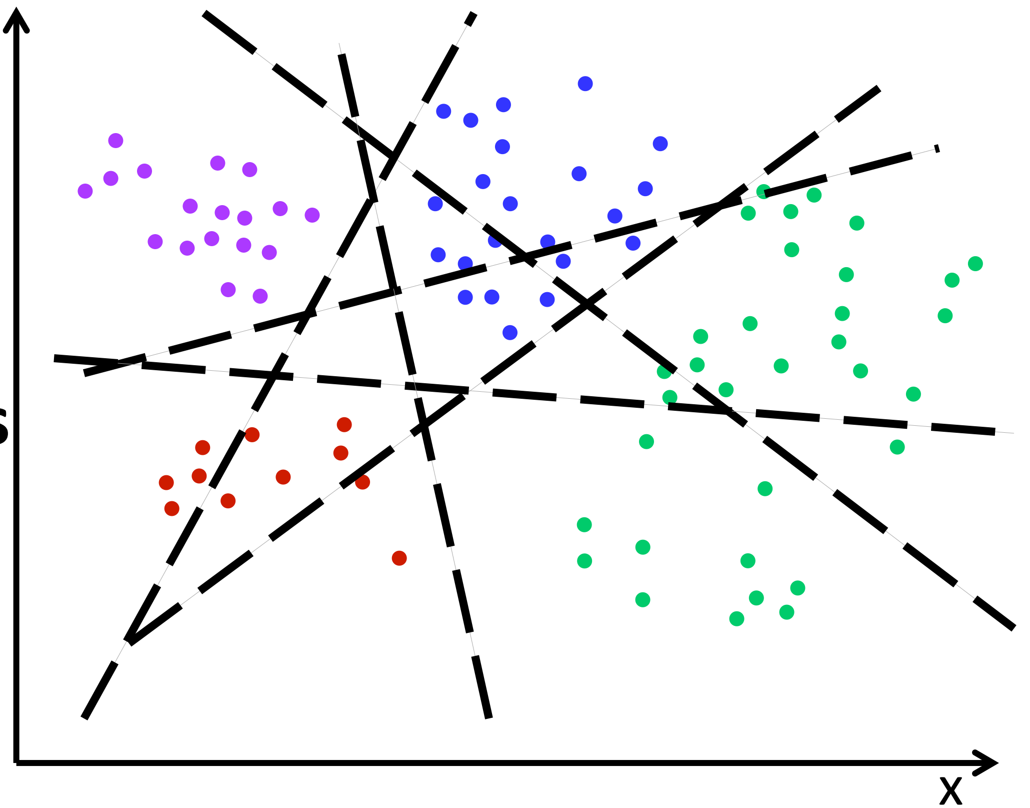
It is cumbersome to test all possible splits

Try several random splits

Keep the split that best separates data

- Reduces uncertainty

Recurse



Animation: Shotton, ICCV 09 Tutorial

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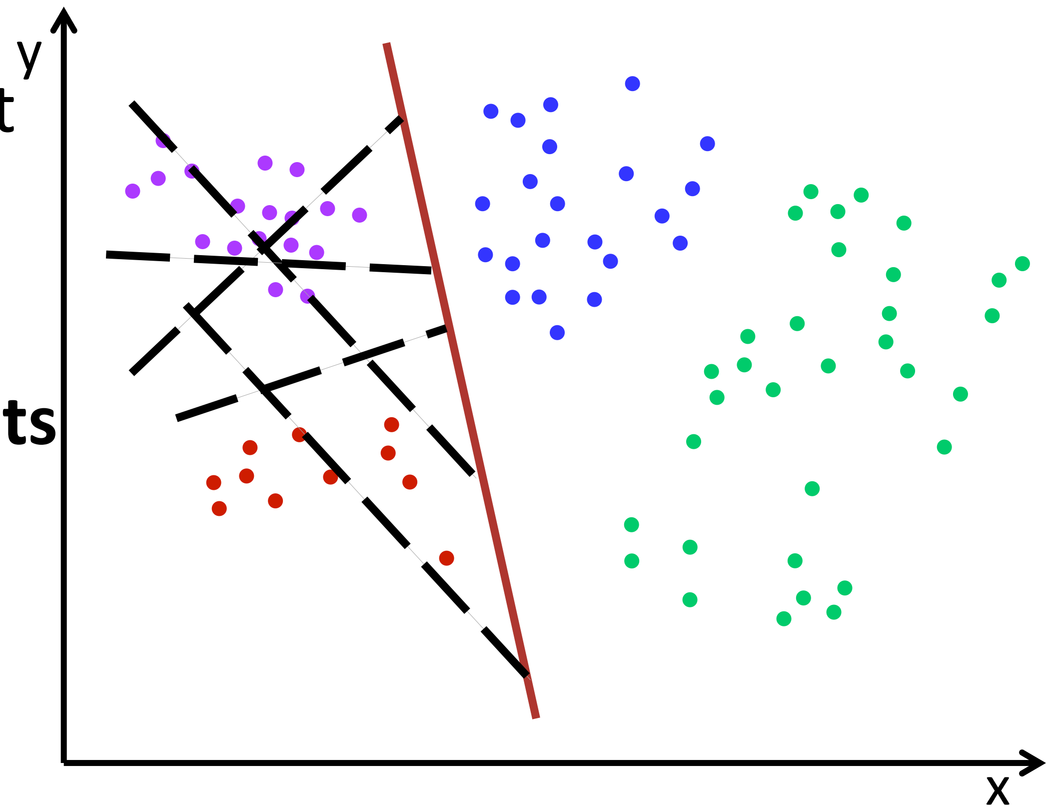

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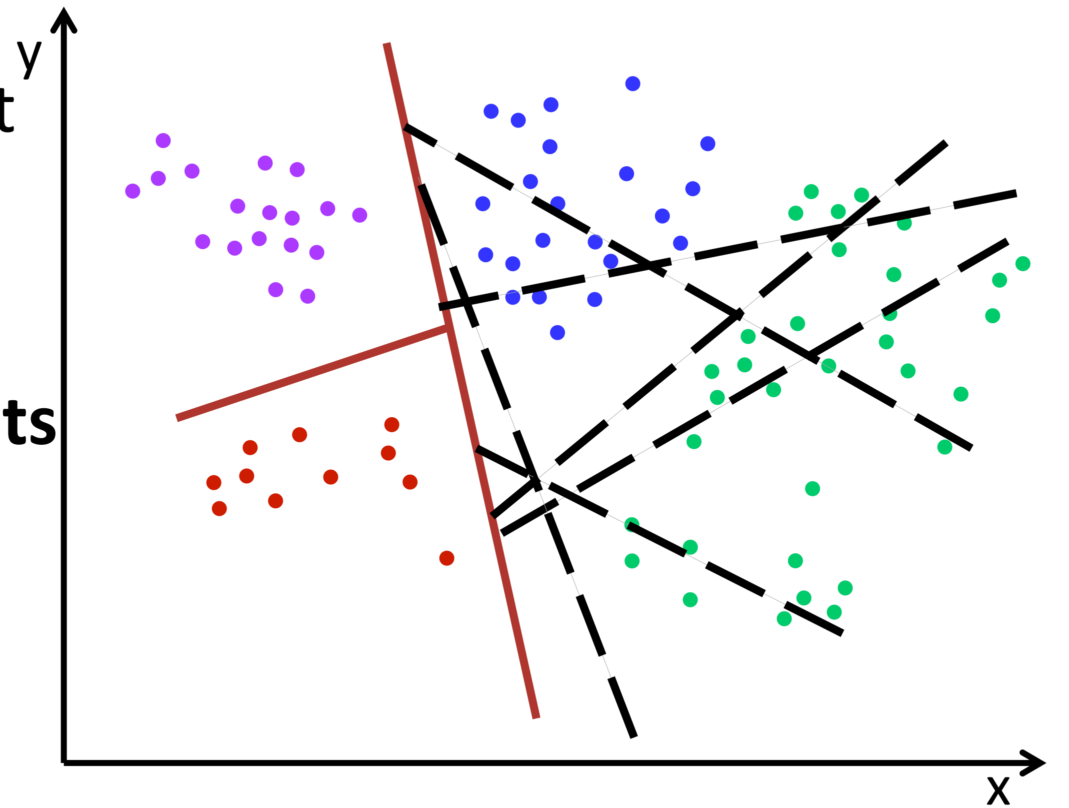

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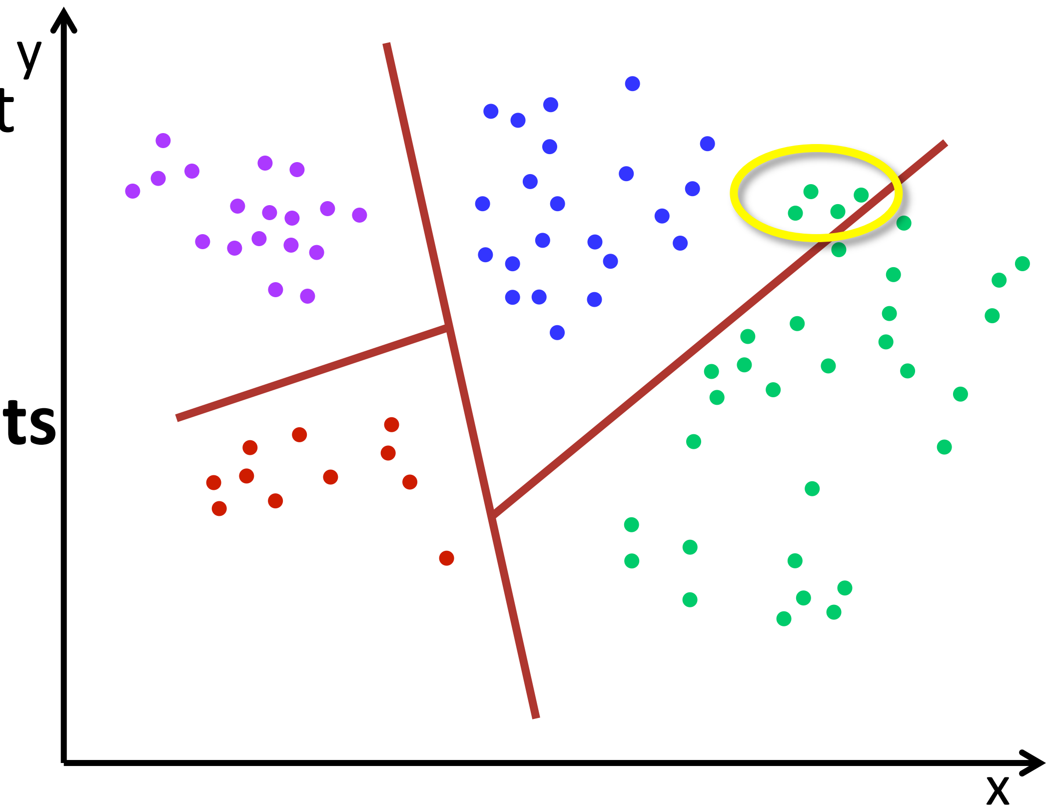

Random Decision Tree

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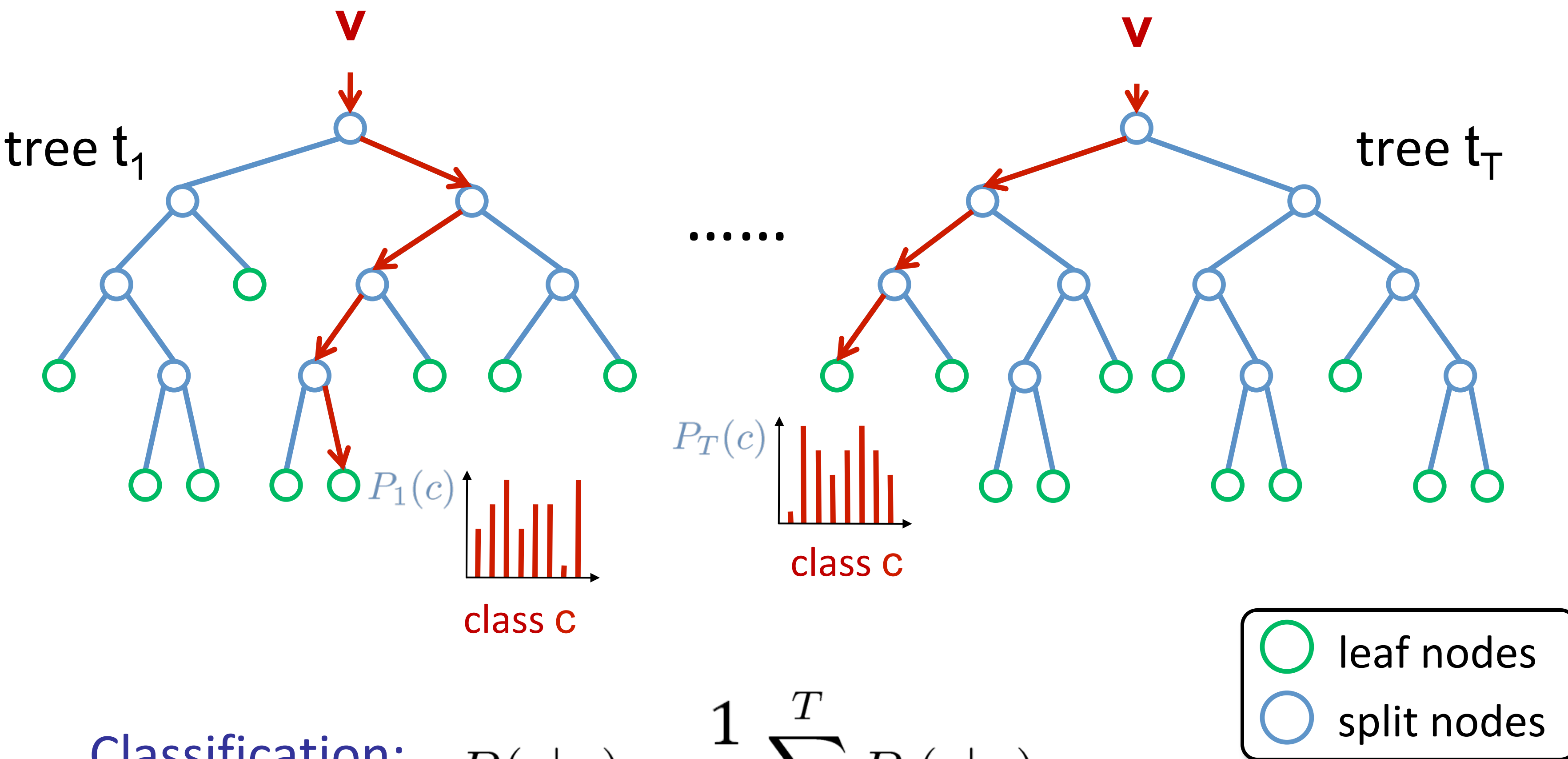
Random Decision Trees

- How many features and thresholds to try?
  - just one: "extremely randomized" [Geurts *et al.* 06]
  - few: fast training, may under-fit
  - many: slower training, may over-fit

- When to stop growing the tree?
  - maximum depth
  - minimum entropy gain
  - threshold changes in class distribution
  - pruning

Decision Forests

- A forest is an ensemble of several decision trees



Classification: $$P(c|\mathbf{v}) = \frac{1}{T}\sum_{t=1}^{T} P_t(c|\mathbf{v})$$

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Learning a Forest

- Divide training examples into T subsets S_t
  - improves generalization
  - reduces memory requirements & training time
- Train each decision tree, *t*, on subset S_t
  - same decision tree learning as before
- Easy to parallelize

Ensemble methods

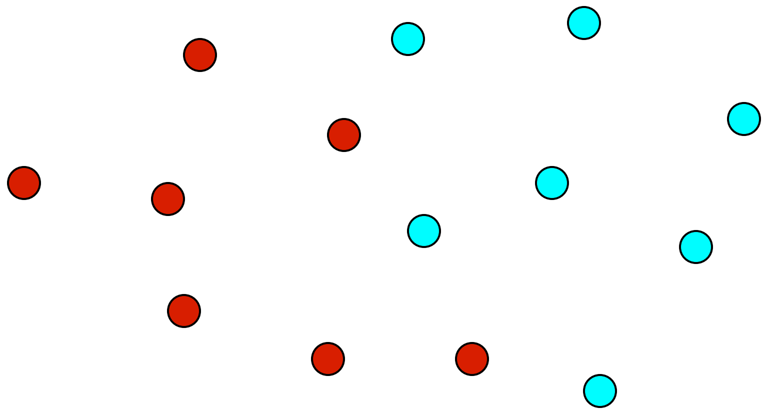
An ensemble classifier combines a set of weak “base” classifiers into a “strong” ensemble classifier.

- “boosted” performance
- more robust against overfitting

- Decision Forests, Random Forests [Breiman ‘01], Bagging
- Voted-Perceptron
- Boosting
- Learning with expert advice
- ….

Perceptron: nonseparable data

What if data is not linearly separable?



In this case: almost linearly separable… how will the perceptron perform?

Batch perceptron

Batch algorithm:

```
w = 0
while some (x_i,y_i) is misclassified:
    w = w + y_i x_i
```

Nonseparable data: this algorithm will never converge. How can this be fixed?

Dream: somehow find the separator that misclassifies the fewest points… **but this is NP-hard** (in fact, even NP-hard to approximately solve).

Fixing the batch perceptron

Idea 1: only go through the data once, or a fixed number of times, K

```
w = 0
for k = 1 to K
    for i = 1 to m
        if (x_i,y_i) is misclassified:
            w = w + y_i x_i
```

At least this stops!

Problem: the final *w* might not be good.

Eg. right before terminating, the algorithm might perform an update on an outlier!

Voted-perceptron

Idea 2: keep around intermediate hypotheses, and have them "vote" [Freund and Schapire, 1998]

```
n = 1
w_1 = 0
c_1 = 0
for k = 1 to K
    for i = 1 to m
        if (x_i, y_i) is misclassified:
            w_{n+1} = w_n + y_i x_i
            c_{n+1} = 1
            n = n + 1
        else
            c_n = c_n + 1
```

At the end, a collection of linear separators w_0, w_1, w_2, …, along with survival times: c_n = amount of time that w_n survived.

Voted-perceptron

Idea 2: keep around intermediate hypotheses, and have them "vote" [Freund and Schapire, 1998]

At the end, a collection of linear separators w_0, w_1, w_2, …, along with survival times: c_n = amount of time that w_n survived.

This c_n is a good measure of the reliability (or confidence) of w_n.

To classify a test point x, use a weighted majority vote:

$$\mathsf{sgn}\left\{\sum_{n=0}^{N} c_n \; \mathsf{sgn}(w_n \cdot x)\right\}$$

Voted-perceptron

Problem: may need to keep around a lot of w_n vectors.

Solutions:

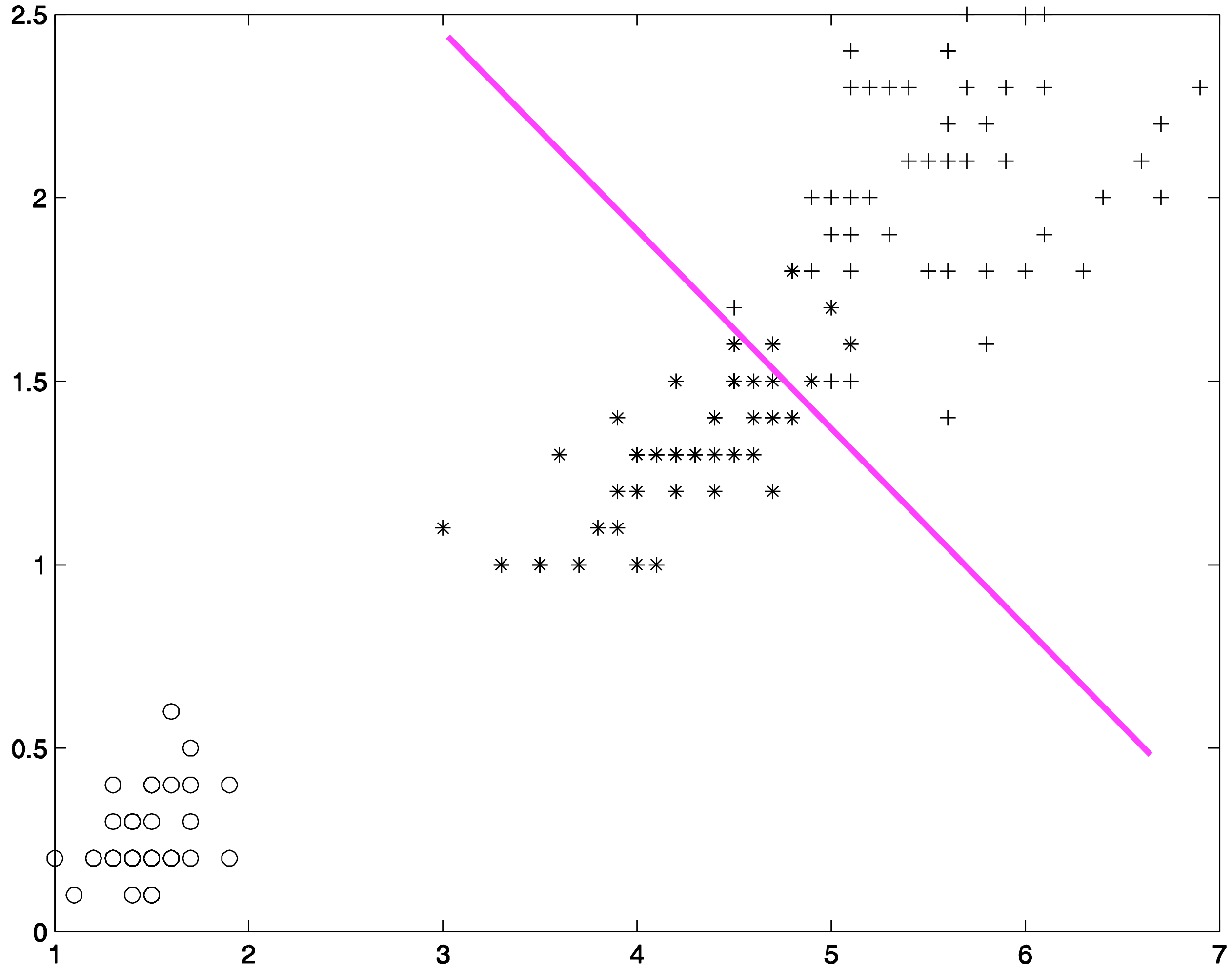
(i) Find "representatives" among the w vectors.

(ii) Alternative prediction rule:

$$\operatorname{sgn}\left\{\sum_{n=0}^{N} c_n \ (w_n \cdot x)\right\} \ = \ \operatorname{sgn}\left\{\left(\sum_{n=0}^{N} c_n \, w_n\right) \cdot x \right\}$$

Just keep track of a running average, w_{avg}

IRIS: features 3 and 4; goal: separate + from o/x



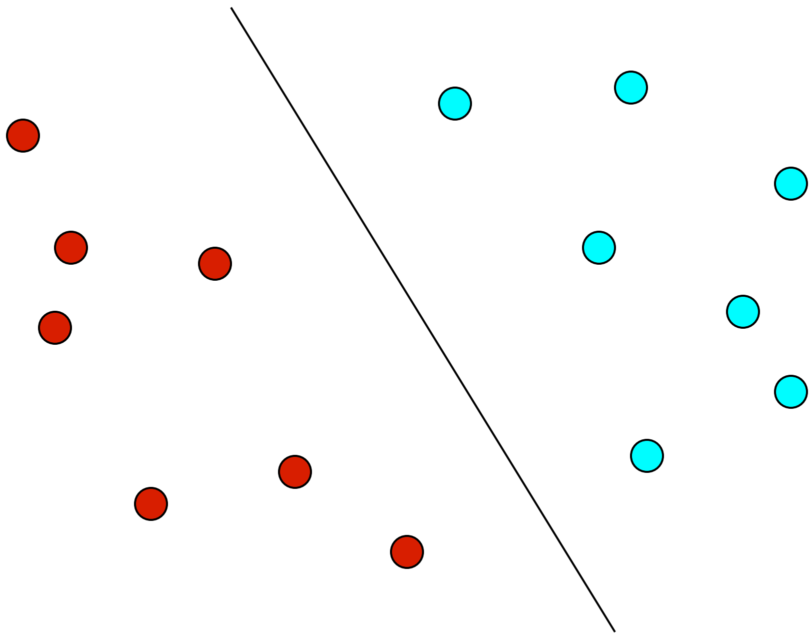
100 rounds, 1595 updates (5 errors)

Final hypothesis: makes 5 errors for voting

Interesting questions

Modify the (voted) perceptron algorithm to:

[1] Find a linear separator with large <u>margin</u>



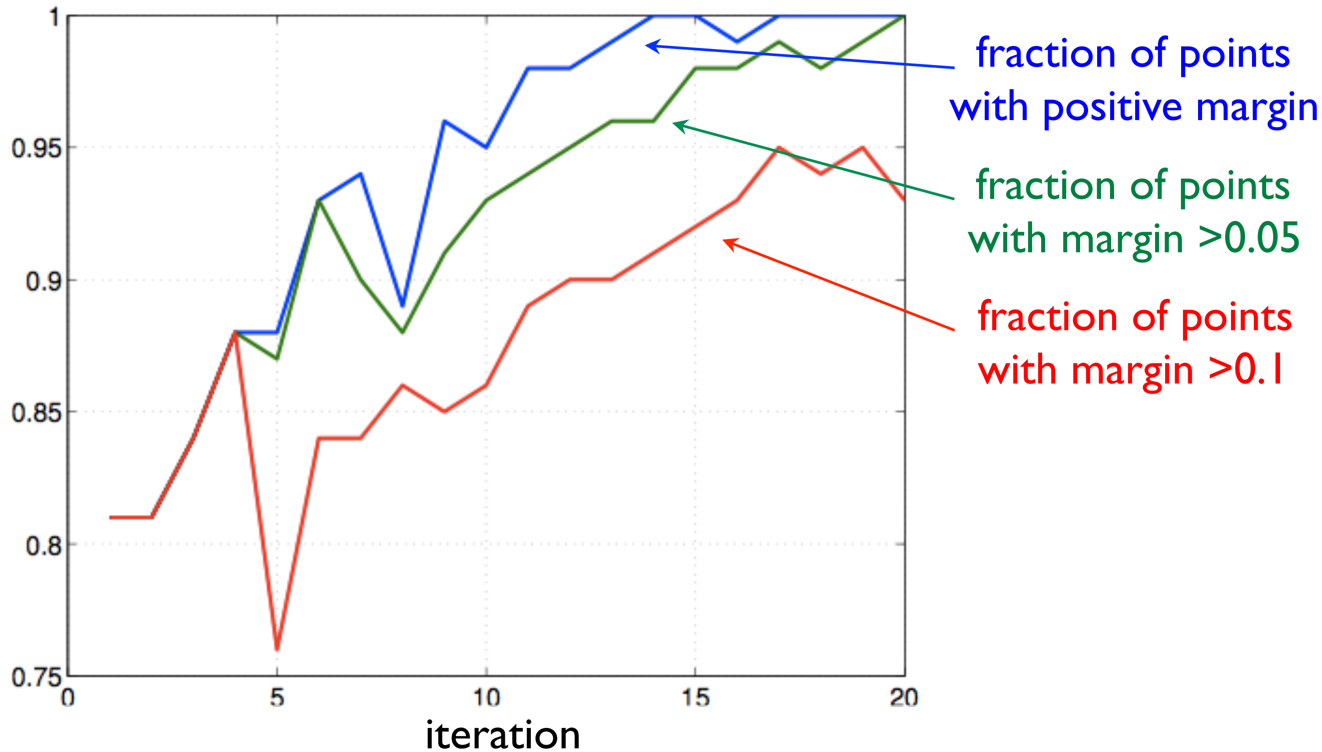
[2] "Give up" on troublesome points after a while

Voting margin and generalization

- If we can obtain a large (positive) voting margin

$$\gamma_t = \frac{y_t h_m(\underline{x}_t)}{\sum_{j=1}^{m} \alpha_j} = \frac{\alpha_1 y_t h(\underline{x}_t; \underline{\theta}_1) + \ldots + \alpha_m y_m h(\underline{x}_t; \underline{\theta}_m)}{\alpha_1 + \ldots + \alpha_m} \in [-1, 1]$$

across the training examples, we will have better generalization guarantees (discussed later)



Boosting

- A simple algorithm for learning robust ensemble classifiers
  - Freund & Shapire, 1995
  - Friedman, Hastie, Tibshhirani, 1998
- Easy to implement, no external optimization tools needed.

Boosting

- Defines a classifier using an additive model:

$$F(x) = \alpha_1 f_1(x) + \alpha_2 f_2(x) + \alpha_3 f_3(x) + \ldots$$

Strong classifier

Weak classifier

Weight

Data point

Boosting

- Defines a classifier using an additive model:

$$F(x) = \alpha_1 f_1(x) + \alpha_2 f_2(x) + \alpha_3 f_3(x) + \ldots$$

Strong classifier

Weak classifier

Weight

Data point

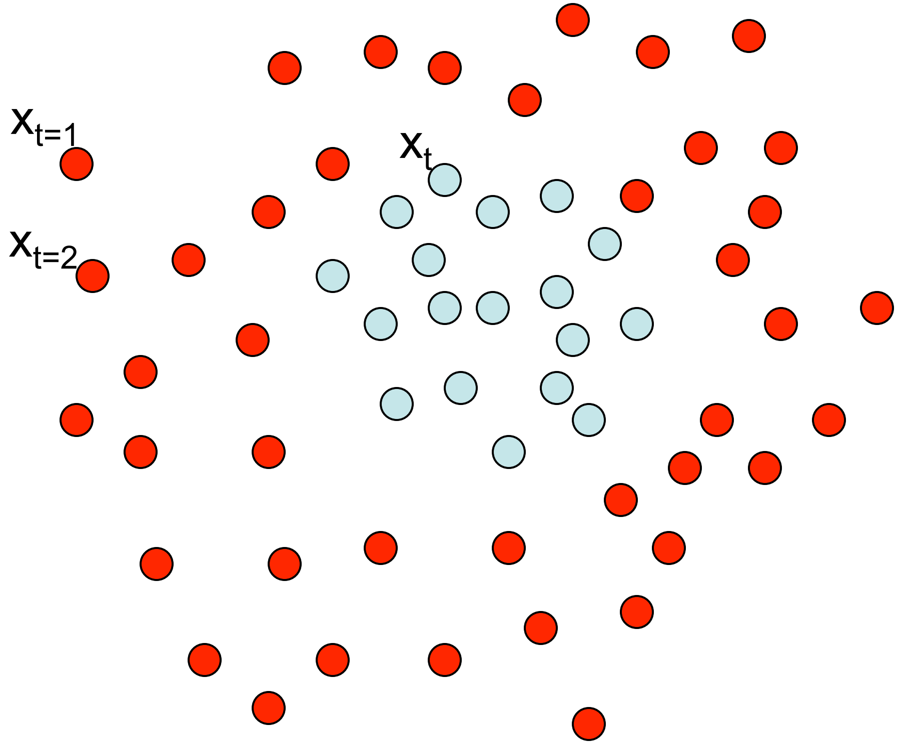
- We need to define a family of weak classifiers

$$f_k(x)$$

  – E.g. linear classifiers, decision trees, or even decision stumps (threshold on one axis-parallel dimension)

Boosting

- Run sequentially on a batch of n data points



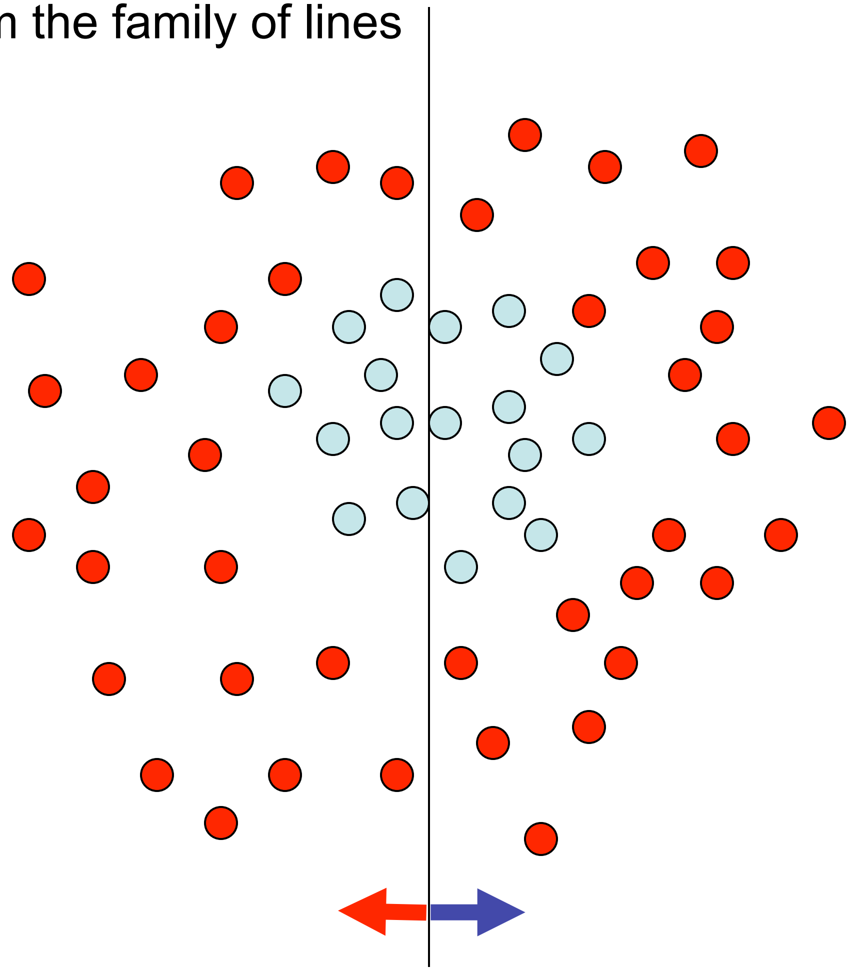
Each data point has a class label:

$$y_t = \begin{cases} +1 \ (\ ) \\ -1 \ (\ ) \end{cases}$$

and a weight, w_t.
- we initialize all $w_t = 1$

Example using linear separators

Weak learners from the family of lines



Each data point has

a class label:

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and a weight:

$w_t = 1$

This linear separator has error rate 50%

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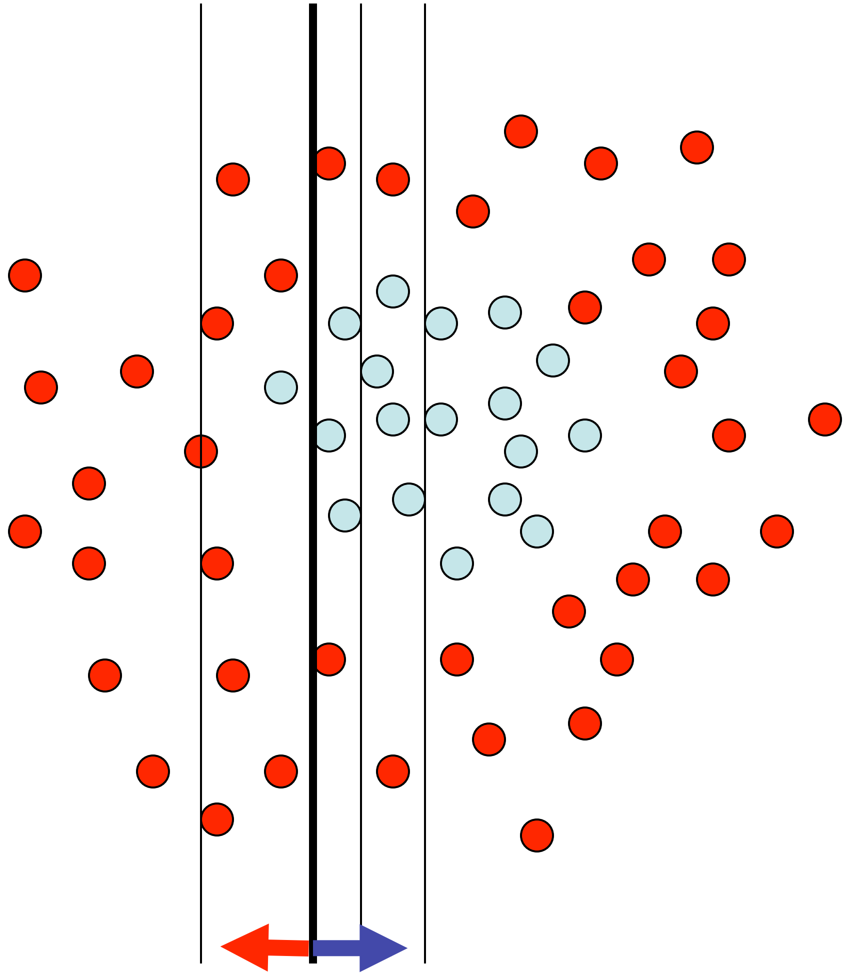
Example using linear separators



Each data point has a class label:

$$y_t = \begin{cases} +1 \\ -1 \end{cases}$$

and a weight:

$w_t = 1$

This one seems to be the best, call it f_1

This is a '**weak classifier**': Its error rate is slightly less than 50%.

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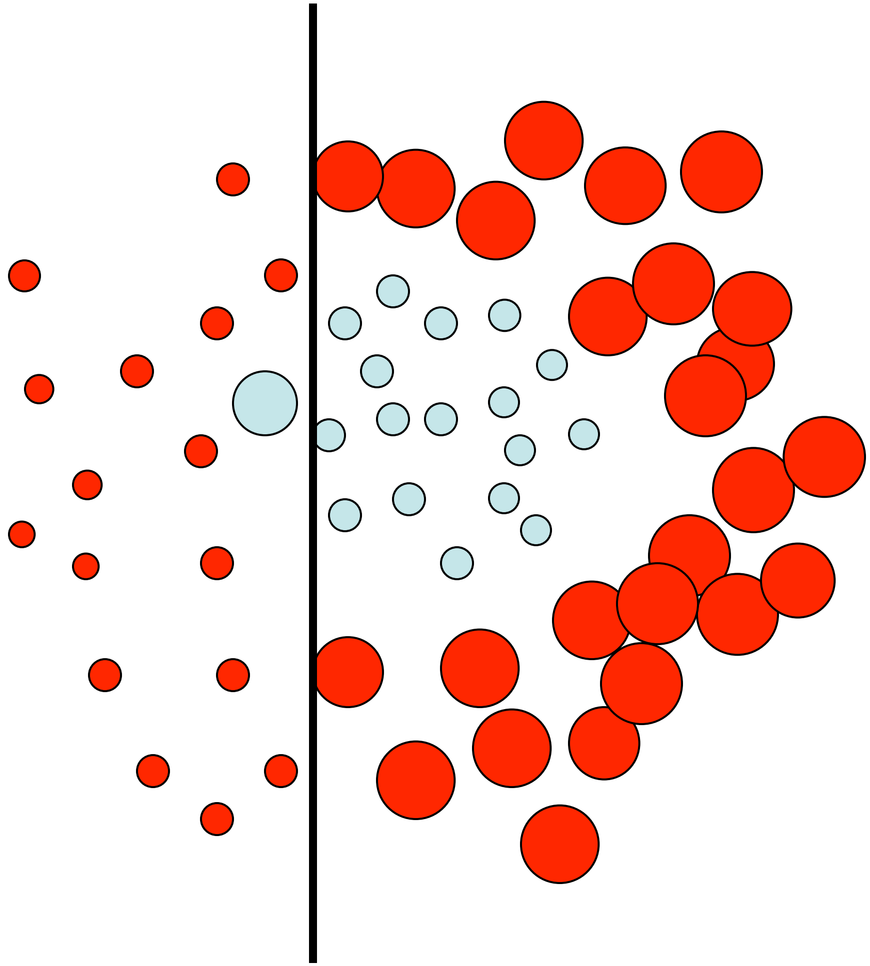
Example using linear separators



Each data point x_i has a class label:

$$y_i = \begin{cases} +1 & (\ ) \\ -1 & (\ ) \end{cases}$$

We update the weights:

$$w_t \leftarrow w_t \exp\{-y_t\, f_m(x_t)\}$$

- Re-weight the points such that the previous weak classifier now has 50% error
- Iterate: find a weak classifier for this new problem

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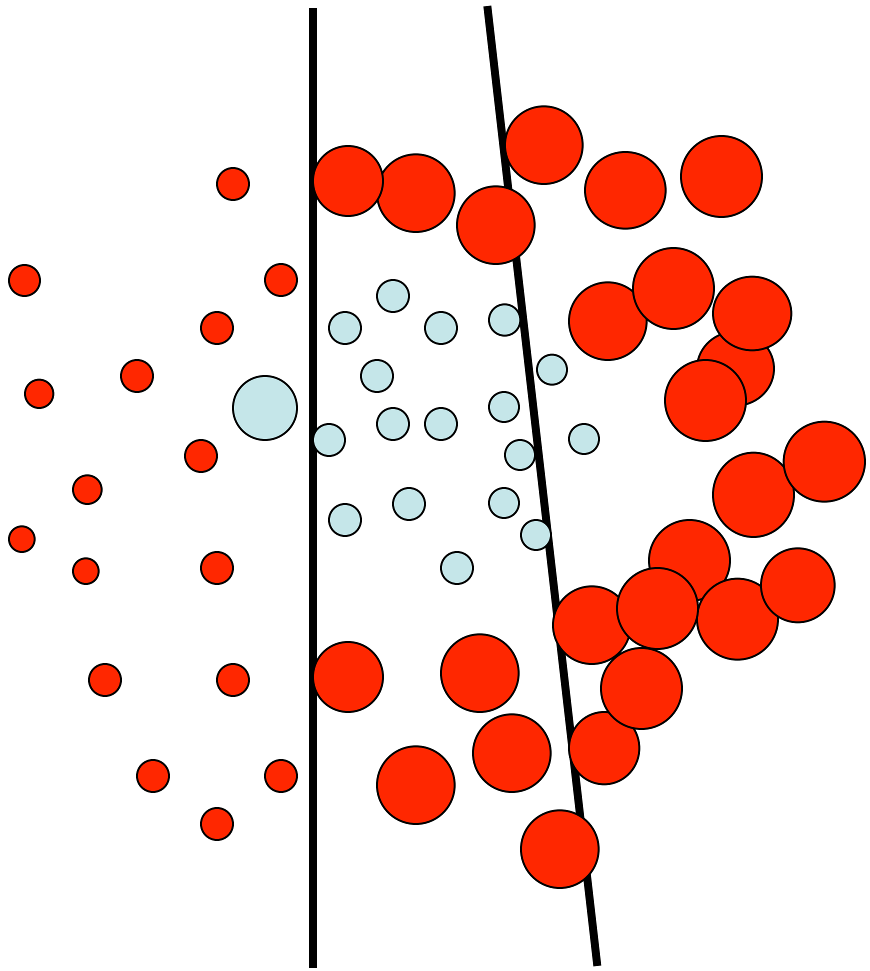
Example using linear separators



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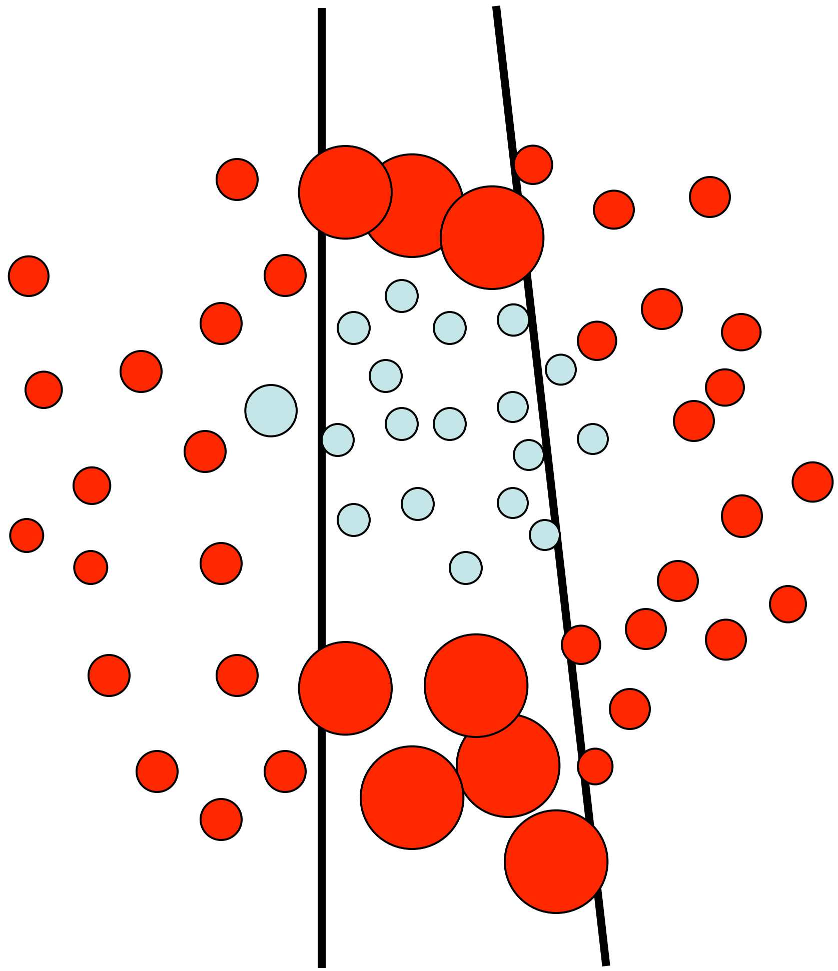

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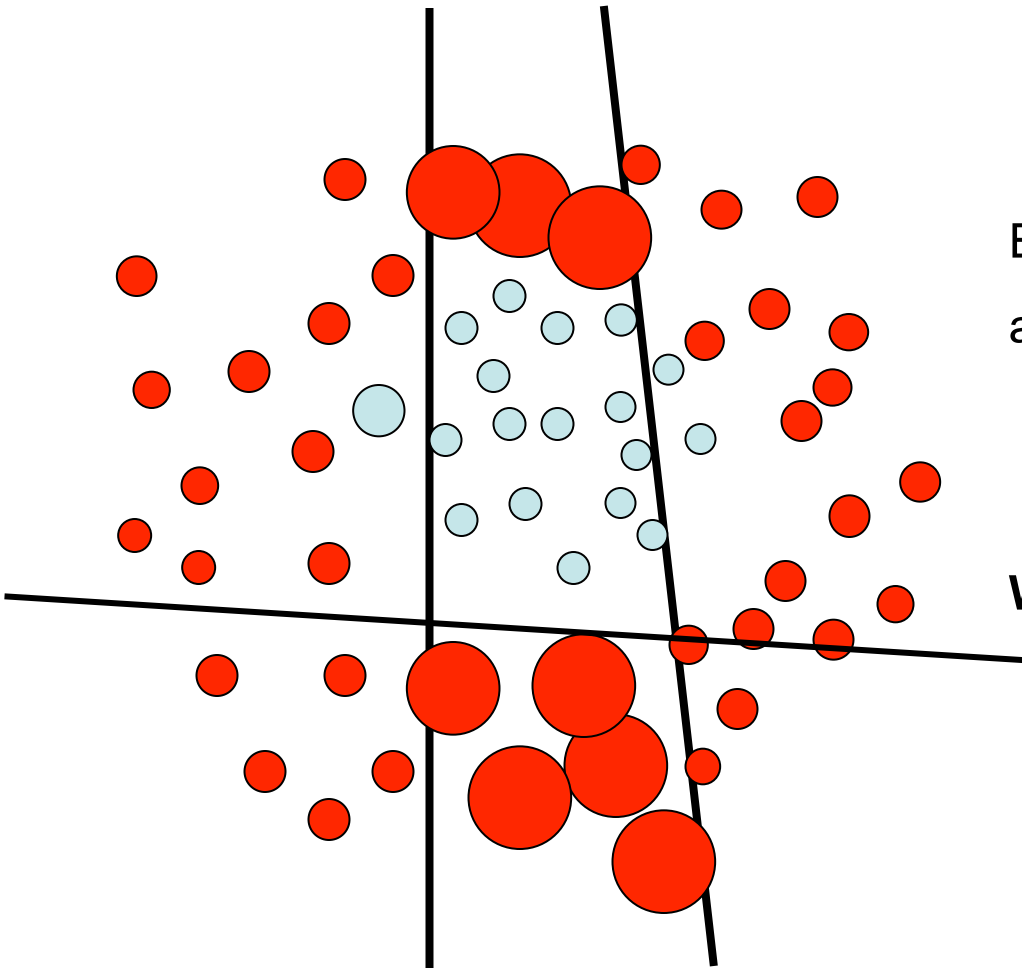

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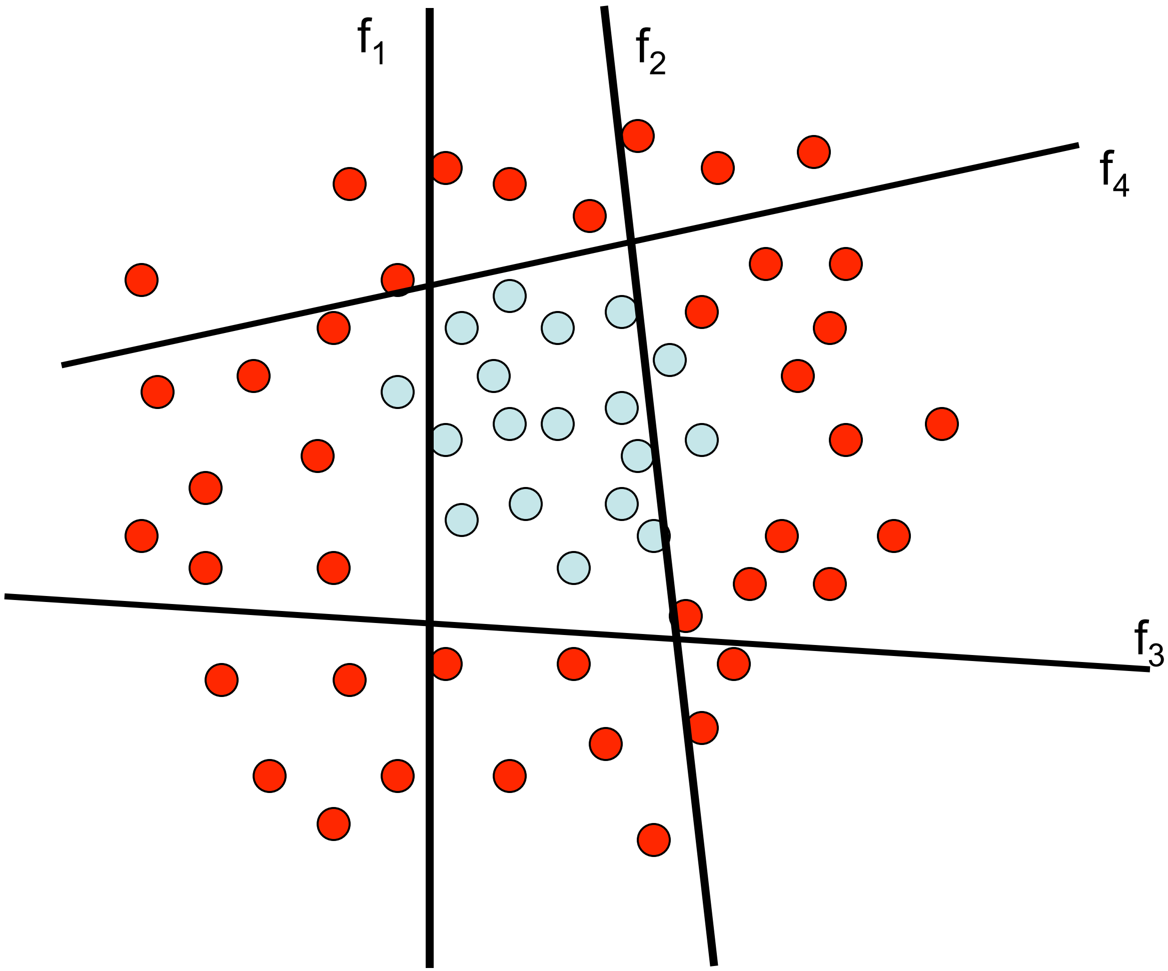

The strong (non-linear) ensemble classifier is built as a weighted combination of all the weak (linear) classifiers.

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Boosting

- AdaBoost (Freund and Shapire, 1995)
- Real AdaBoost (Friedman et al, 1998)
- LogitBoost (Friedman et al, 1998)
- Gentle AdaBoost (Friedman et al, 1998)
- BrownBoosting (Freund, 2000)
- FloatBoost (Li et al, 2002)
- …

Mostly differ in choice of loss function and how it is minimized.

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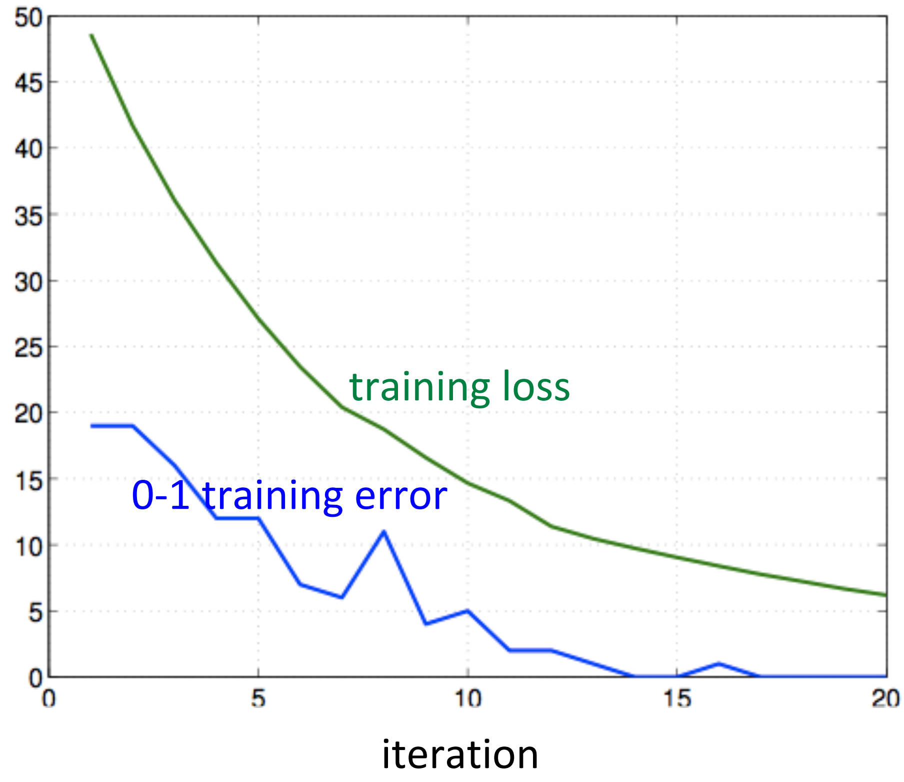
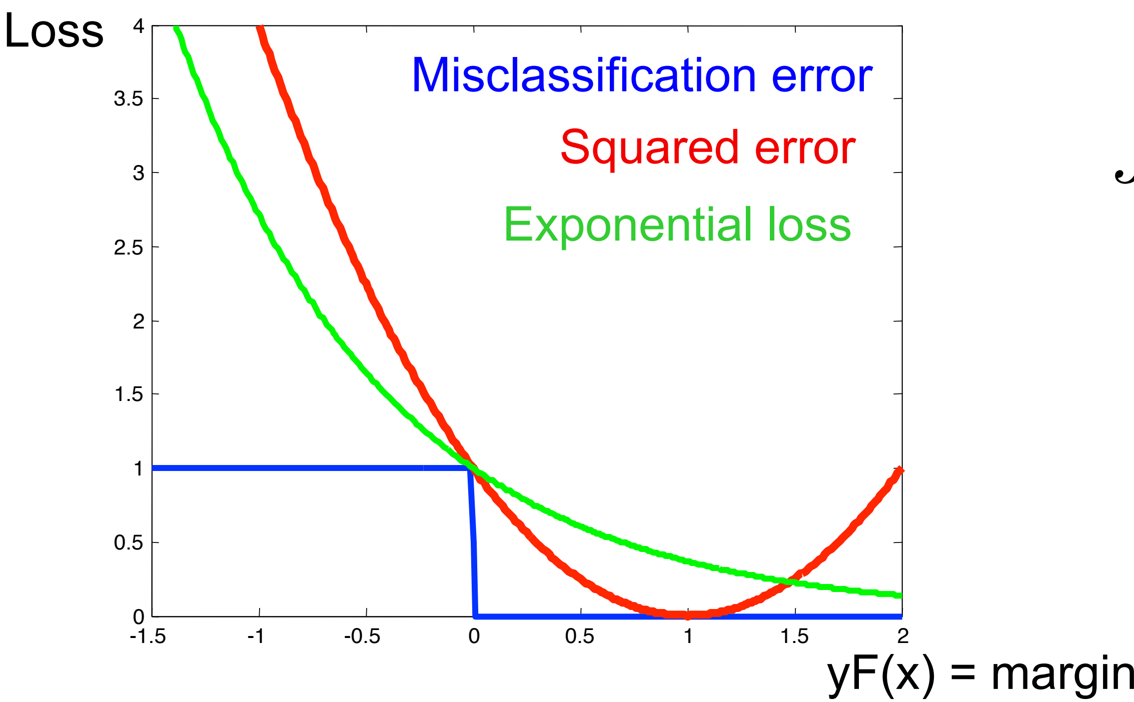
Loss functions: motivation

- Want a smooth upper bound on 0-1 training error.



Loss functions



Squared error

$$J = \sum_{t=1}^{N} [y_t - F(x_t)]^2$$

Exponential loss

$$J = \sum_{t=1}^{N} e^{-y_t F(x_t)}$$

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Boosting

Sequential procedure. At each step we add

$$F(x) \leftarrow F(x) + f_m(x)$$

to minimize the residual loss

$$(\phi_m) = \arg\min_{\phi} \sum_{t=1}^{N} J\left(y_i, F(x_t) + f(x_t; \phi)\right)$$

Parameters weak classifier

Desired output

input

For more details: Friedman, Hastie, Tibshirani. “Additive Logistic Regression: a Statistical View of Boosting” (1998)

How to set the ensemble weights?

- Prediction on a new data point x is typically of the form:

$$F(x) = \sum_{m=1}^{k} \alpha_m f_m(x)$$

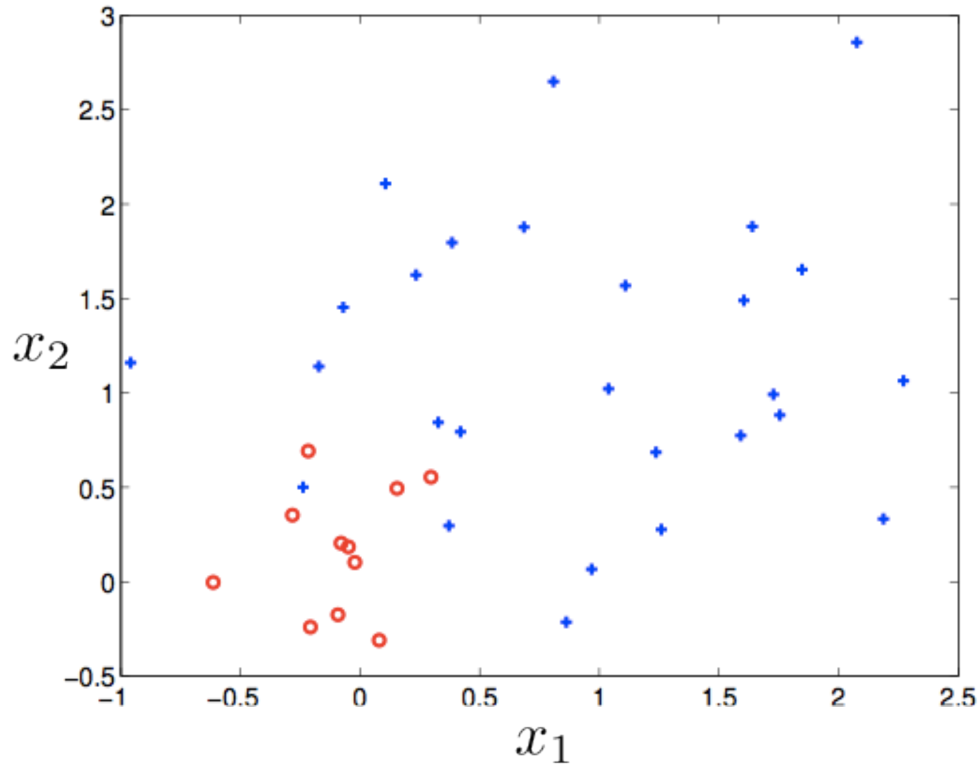
- How to set the α_m values?
- Depends on the algorithm. E.g. in AdaBoost:

$$\alpha_m = \frac{1}{2} \ln \frac{1 - \epsilon_m}{\epsilon_m}$$

- Where ϵ_m is the training error of f_m on the (currently) weighted data set.

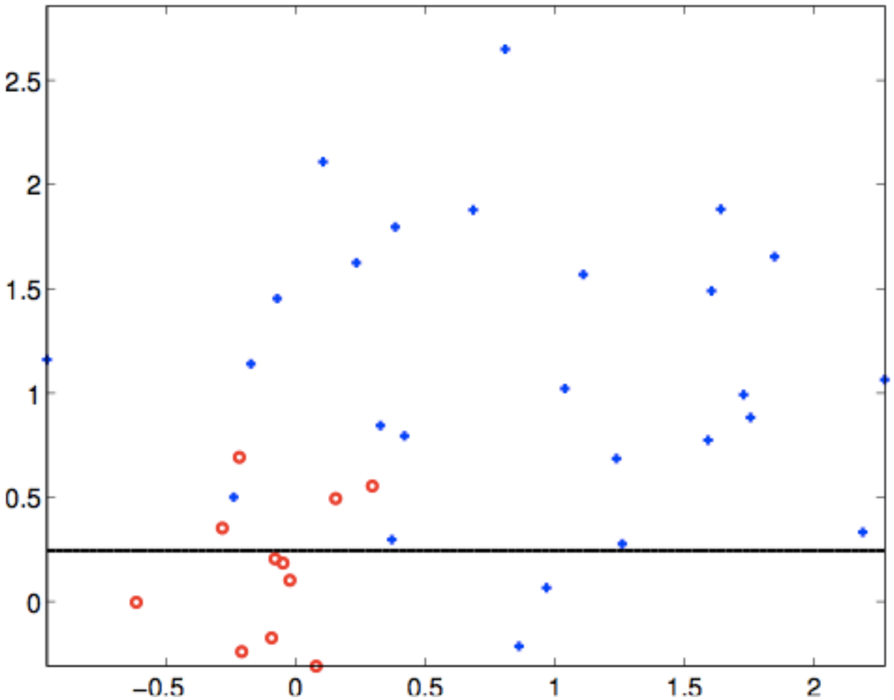
Boosting example

Logistic loss $\text{Loss}(z) = \log(1 + \exp(-z))$

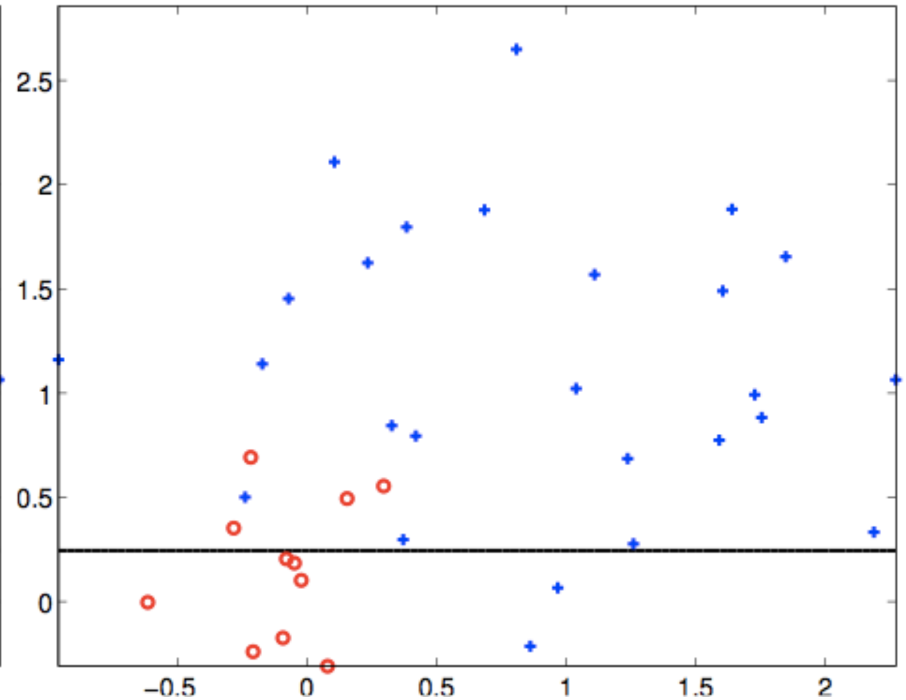


Boosting example

$h(\underline{x};\hat{\underline{\theta}}_1)$

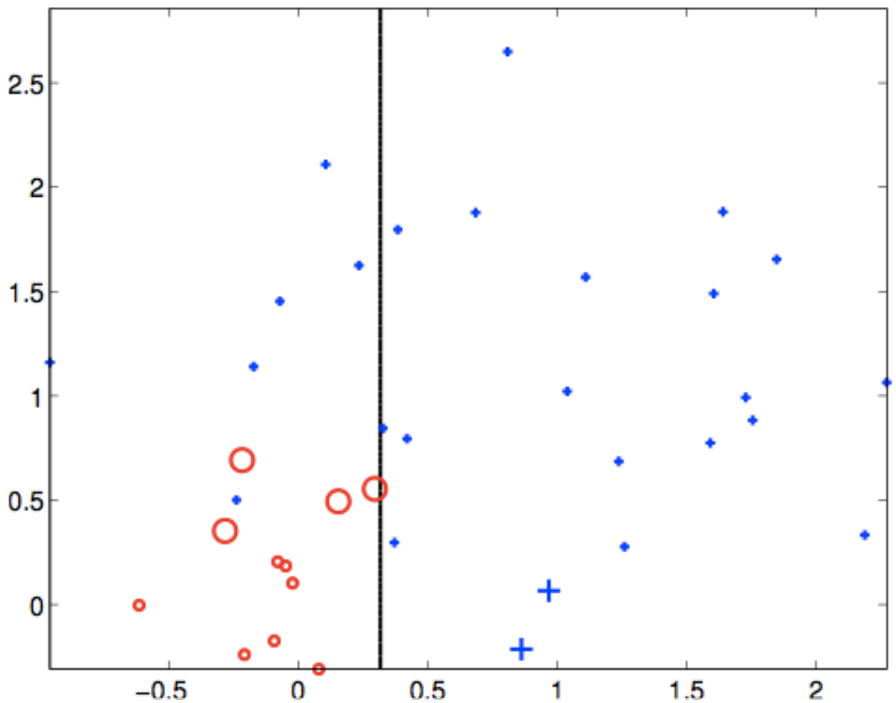


$h_1(\underline{x}) = \hat{\alpha}_1 h(\underline{x};\hat{\underline{\theta}}_1)$

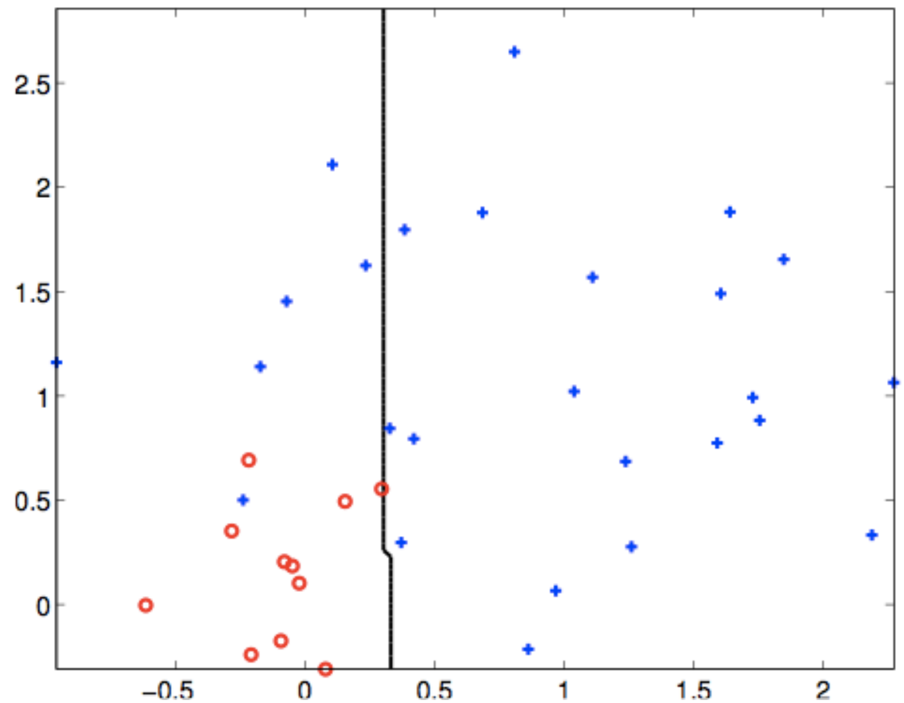


Boosting example

$$h(\underline{x};\hat{\theta}_2)$$

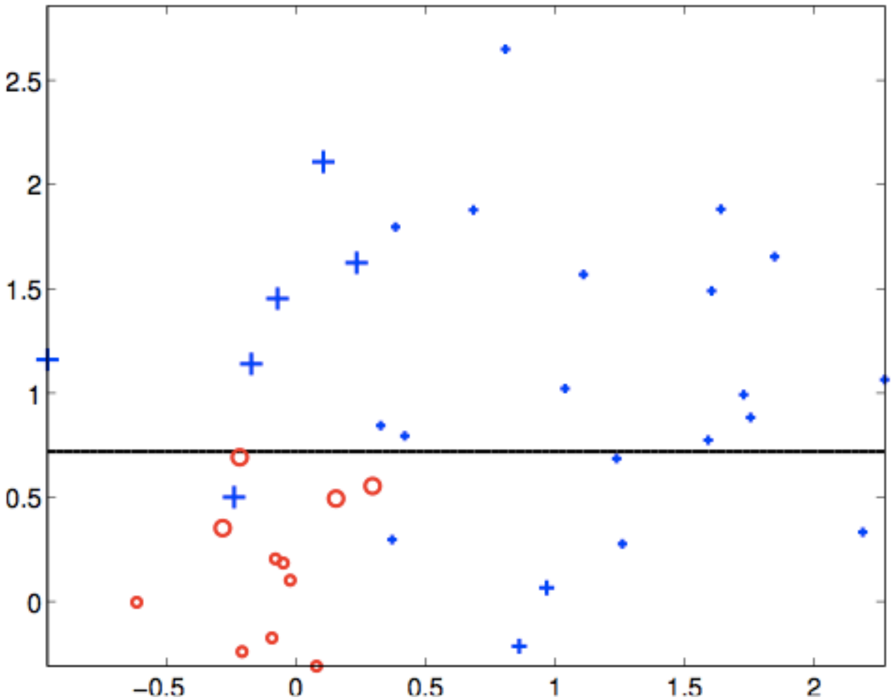


$$h_2(\underline{x}) = \hat{\alpha}_1 h(\underline{x};\hat{\underline{\theta}}_1) + \hat{\alpha}_2 h(\underline{x};\hat{\underline{\theta}}_2)$$

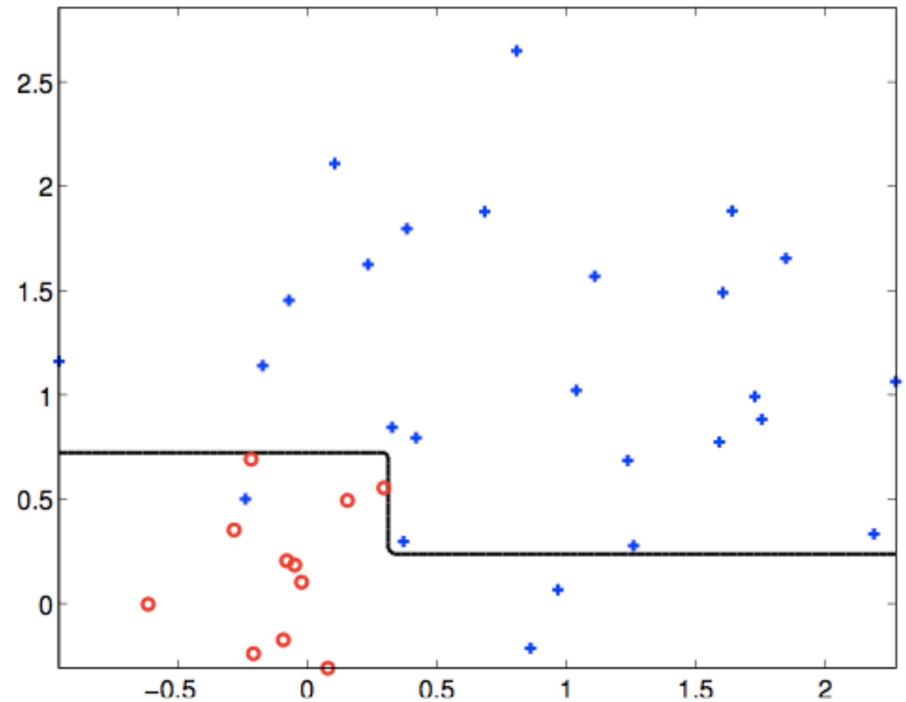


Boosting example

$h(\underline{x}; \underline{\hat{\theta}}_3)$

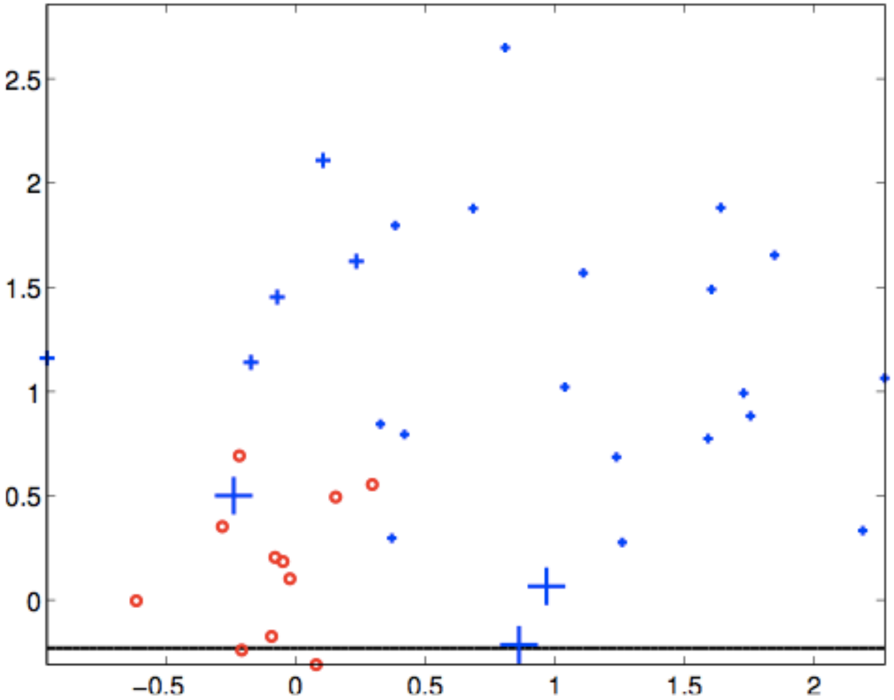


$h_3(\underline{x}) = \hat{\alpha}_1 h(\underline{x}; \underline{\hat{\theta}}_1) + \cdots + \hat{\alpha}_3 h(\underline{x}; \underline{\hat{\theta}}_3)$

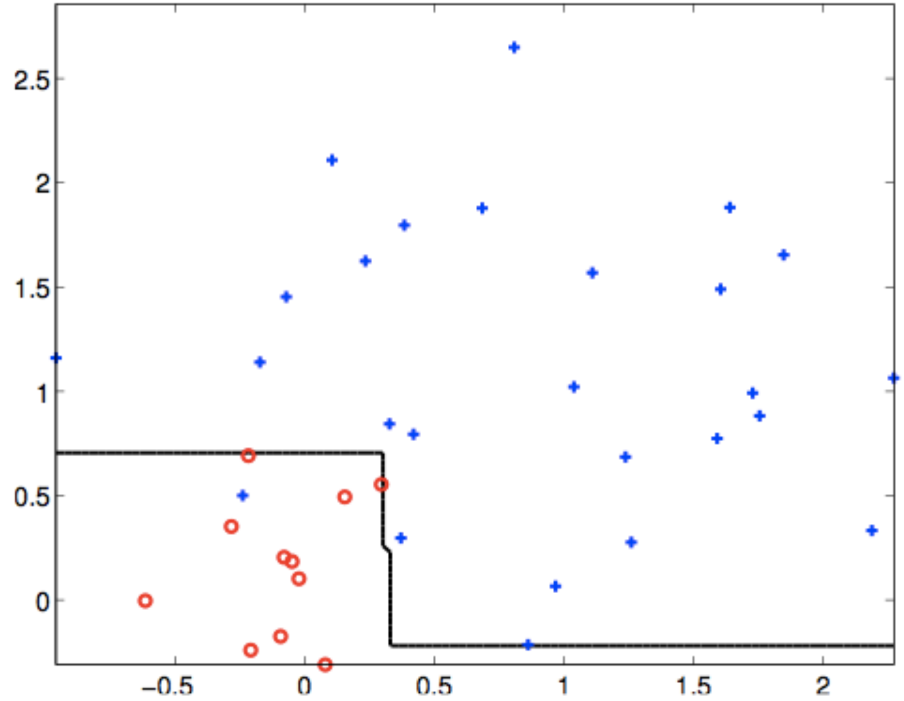


Boosting example

$h(\underline{x}; \hat{\theta}_4)$



$h_4(\underline{x}) = \hat{\alpha}_1 h(\underline{x}; \hat{\theta}_1) + \cdots + \hat{\alpha}_4 h(\underline{x}; \hat{\theta}_4)$



Bias-Variance Error Decomposition

Assume the data *(x,y)* is drawn i.i.d. from *D*, s.t.: $y = f(x) + \epsilon$

where: $\mathrm{E}[\epsilon] = 0$

$\mathrm{Var}(\epsilon) = \sigma^2$

Then, for any data point (x_0, y_0),

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$$= \boxed{\sigma^2} + \mathrm{Var}[h(x_0)] + (\mathrm{Bias}[h(x_0)])^2$$

Irreducible error (can't be changed by choice of h)

where: $\mathrm{Var}[h(x_0)] = \mathrm{E}[h(x_0)^2] - \mathrm{E}[h(x_0)]^2$

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NOTE: All expectations are w.r.t. the random training set *h* is learned from, NOT x_0.

Understanding boosting

- There are four different kinds of errors in the boosting procedure that we can try to understand
  - weighted error that the base learner achieves at each iteration
  - weighted error of the base learner relative to just updated weights (i.e., trying the same base learner again)
  - training error of the ensemble as a function of the number of boosting iterations
  - generalization error of the ensemble