7. Boosting and Bagging

Repetition: Regression

We start with a set of **basis functions**

$$\phi(\mathbf{x}) = (\phi_0(\mathbf{x}), \phi_1(\mathbf{x}), \dots, \phi_{M-1}(\mathbf{x})) \qquad \mathbf{x} \in \mathbb{R}^d$$

The goal is to fit a model into the data

$$y(\mathbf{x}, \mathbf{w}) = \mathbf{w}^T \phi(\mathbf{x})$$

To do this, we need to find an error function, e.g.:

$$E(\mathbf{w}) = \frac{1}{2} \sum_{i=1}^{N} (\mathbf{w}^T \phi(\mathbf{x}_i) - t_i)^2$$

To find the optimal parameters, we derived E with respect to $\mathbf{w}$ and set the derivative to zero.

Some Questions

1. Can we do the same for **classification**?
   As a special case we consider two classes:
   $$t_i \in \{-1, 1\} \quad \forall i = 1, \dots, N$$
2. Can we use a **different** (better?) error function?
3. Can we learn the basis functions **together** with the model parameters?
4. Can we do the learning **sequentially**, i.e. one basis function after another?

Answer to all questions: Yes, using Boosting!

The Loss Function

Definition: a real-valued function $L(t, y(\mathbf{x}))$, where t is a target value and y is a model, is called a **loss function.**

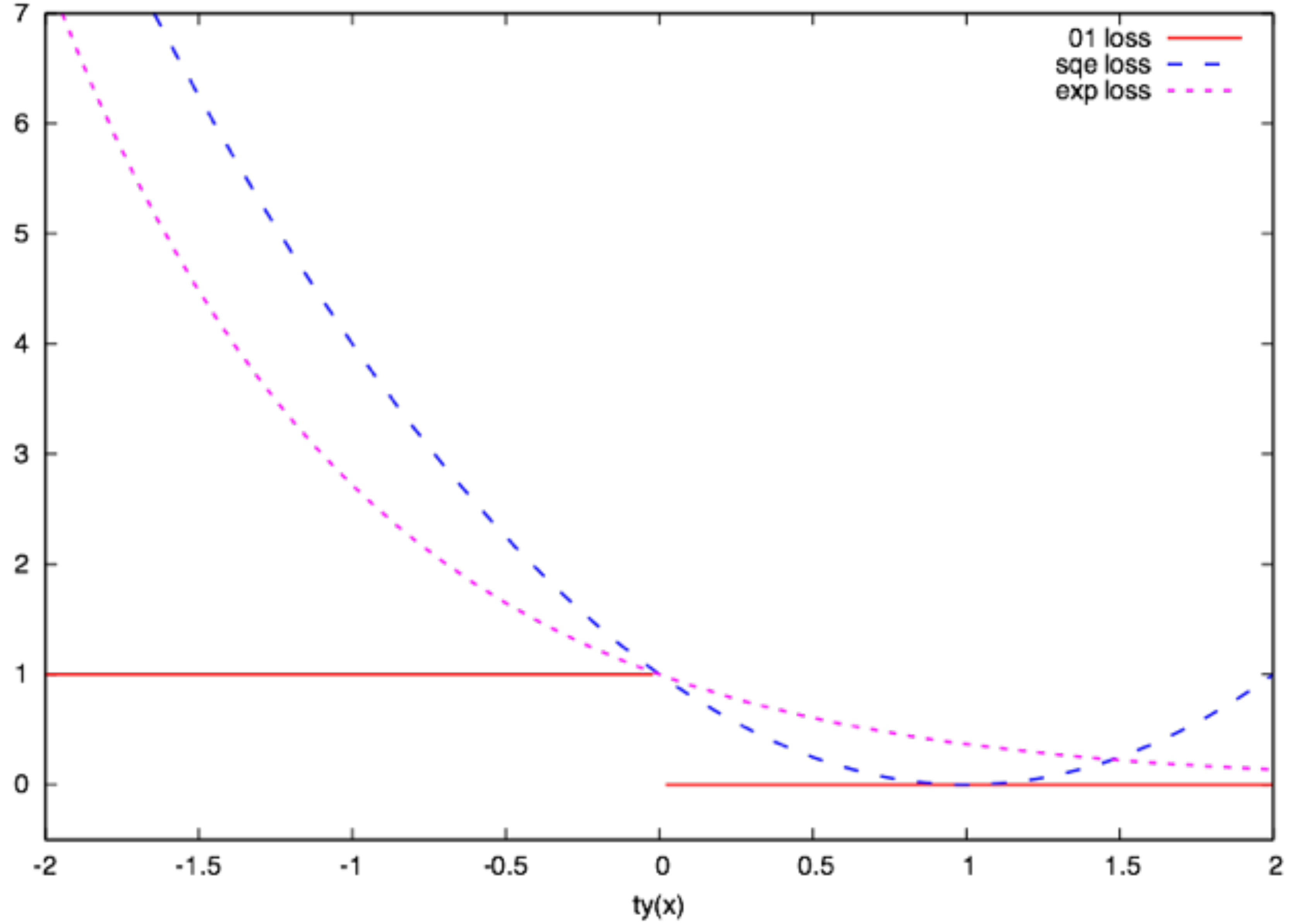
Examples:

01-loss: $$L_{01}(t, y(\mathbf{x})) = \begin{cases} 0 & \text{if } t = y(\mathbf{x}) \\ 1 & \text{else} \end{cases}$$

squared error loss: $$L_{sqe}(t, y(\mathbf{x})) = (t - y(\mathbf{x}))^2$$

exponential loss: $$L_{exp}(t, y(\mathbf{x})) = \exp(-ty(\mathbf{x}))$$

Loss Functions



- 01-loss is not differentiable
- squared error loss has only one optimum

Sequential Fitting of Basis Functions

Idea: We start with a basis function $\phi_0(\mathbf{x})$:

$$y_0(\mathbf{x}, w_0) = w_0 \phi_0(\mathbf{x}) \qquad\qquad w_0 = 1$$

Then, at iteration m, we add a new basis function $\phi_m(\mathbf{x})$ to the model:

$$y_m(\mathbf{x}, w_0, \dots, w_m) = y_{m-1}(\mathbf{x}, w_0, \dots, w_{m-1}) + w_m \phi_m(\mathbf{x})$$

Two questions need to be answered:

1. How do we find a good new basis function?
2. How can we determine a good value for w_m?

Idea: Minimize the **exponential** loss function

Minimizing the Exponential Loss

Aim: find w_m and ϕ_m so that

$$(w_m, \phi_m) = \arg\min_{w,\phi} \sum_{i=1}^{N} L(t_i, y_{m-1}(\mathbf{x}_i) + w\phi(\mathbf{x}_i))$$

where $\qquad L(t, y) = \exp(-ty)$

Minimizing the Exponential Loss

Aim: find w_m and ϕ_m so that

$$(w_m, \phi_m) = \arg\min_{w,\phi} \sum_{i=1}^{N} L(t_i, y_{m-1}(\mathbf{x}_i) + w\phi(\mathbf{x}_i))$$

where $L(t, y) = \exp(-ty)$

Solution: $\phi_m = \arg\min_{\phi} \sum_{i=1}^{N} v_{i,m} \mathbb{I}(t_i \neq \phi(\mathbf{x}_i))$

Minimizing the Exponential Loss

Aim: find w_m and ϕ_m so that

$$(w_m, \phi_m) = \arg\min_{w,\phi} \sum_{i=1}^{N} L(t_i, y_{m-1}(\mathbf{x}_i) + w\phi(\mathbf{x}_i))$$

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Solution: $\phi_m = \arg\min_{\phi} \sum_{i=1}^{N} v_{i,m} \mathbb{I}(t_i \neq \phi(\mathbf{x}_i))$

$$w_m = \frac{1}{2} \log \frac{1 - \mathrm{err}_m}{\mathrm{err}_m}$$

Minimizing the Exponential Loss

Aim: find w_m and ϕ_m so that

$$(w_m, \phi_m) = \arg\min_{w,\phi} \sum_{i=1}^{N} L(t_i, y_{m-1}(\mathbf{x}_i) + w\phi(\mathbf{x}_i))$$

where $$L(t, y) = \exp(-ty)$$

Solution: $$\phi_m = \arg\min_{\phi} \sum_{i=1}^{N} v_{i,m} \mathbb{I}(t_i \neq \phi(\mathbf{x}_i))$$

$$w_m = \frac{1}{2} \log \frac{1 - \mathrm{err}_m}{\mathrm{err}_m} \qquad v_{i,m+1} = v_{i,m} \exp(2 w_m \mathbb{I}(t_i \neq \phi_m(\mathbf{x}_i)))$$

Minimizing the Exponential Loss

Aim: find w_m and ϕ_m so that

$$(w_m, \phi_m) = \arg\min_{w,\phi} \sum_{i=1}^{N} L(t_i, y_{m-1}(\mathbf{x}_i) + w\phi(\mathbf{x}_i))$$

Condition: Must have training error less than 0.5!

where $L(t, y) = \exp(-ty)$

Solution: $\phi_m = \arg\min_{\phi} \sum_{i=1}^{N} v_{i,m} \mathbb{I}(t_i \neq \phi(\mathbf{x}_i))$

$$w_m = \frac{1}{2} \log \frac{1 - \mathrm{err}_m}{\mathrm{err}_m} \qquad v_{i,m+1} = v_{i,m} \exp(2 w_m \mathbb{I}(t_i \neq \phi_m(\mathbf{x}_i)))$$

Factor $\exp(-w_m)$ would be cancelled out later!

The AdaBoost Algorithm

1. For $i = 1, \ldots, N$: $\quad v_i \leftarrow 1/N$
2. For $m = 1, \ldots, M$

   Fit a classifier ("basis function") ϕ_m that minimizes

$$\sum_{i=1}^{N} v_i \mathbb{I}(t_i \neq \phi_m(\mathbf{x}_i))$$

$$\alpha_m := 2w_m$$

   Compute $\mathrm{err}_m = \dfrac{\sum_{i=1}^{N} v_i \mathbb{I}(t_i \neq \phi_m(\mathbf{x}_i))}{\sum_{i=1}^{N} v_i}$ and $\alpha_m = \log \dfrac{1 - \mathrm{err}_m}{\mathrm{err}_m}$

   Update the weights: $\quad v_i \leftarrow v_i \exp(\alpha_m \mathbb{I}(t_i \neq \phi_m(\mathbf{x}_i)))$
3. Use the resulting classifier:

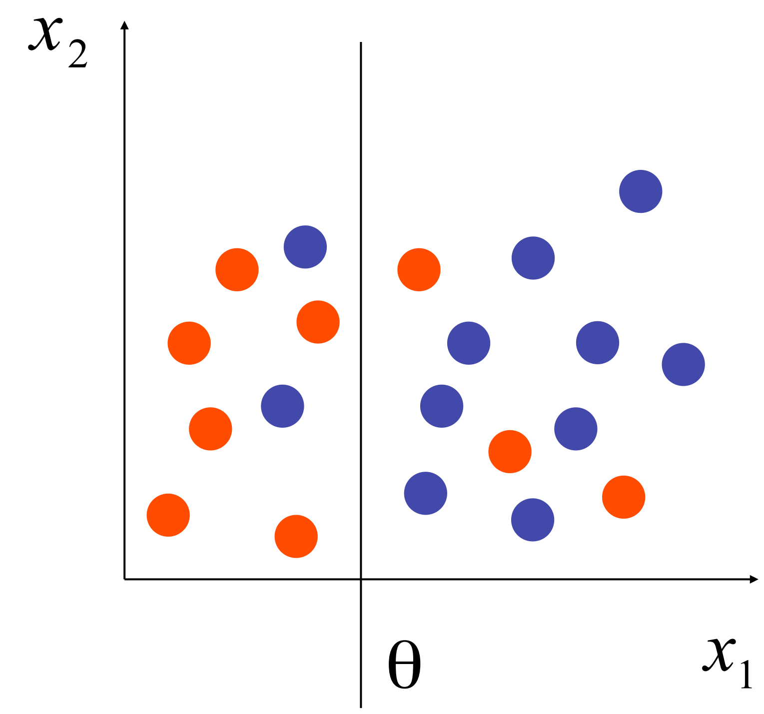
$$y(\mathbf{x}) = \mathrm{sgn} \sum_{m=1}^{M} \alpha_m \phi_m(\mathbf{x})$$

The “Basis Functions”

- Can be any classifier that can deal with weighted data
- Most importantly: if these “base classifiers” provide a training error that is at most as bad as a random classifier would give (i.e. it is a **weak** classifier), then AdaBoost can return an arbitrarily small training error (i.e. AdaBoost is a strong classifier)
- Many possibilities for weak classifiers exist, e.g.:
    - Decision stumps
    - Decision trees

Decision Stumps

Decision Stumps are a kind of very simple weak classifiers.



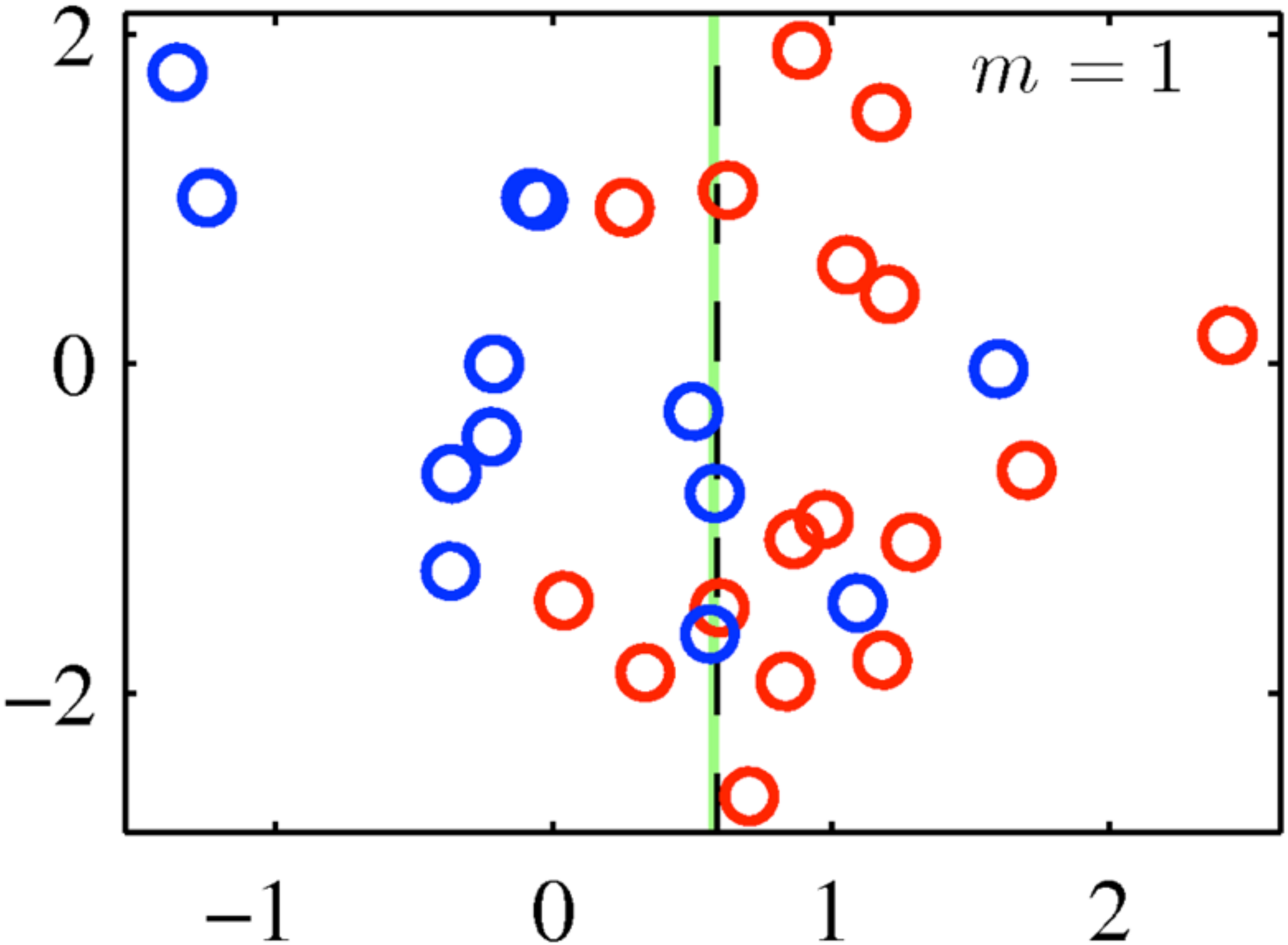
Goal: Find an axis-aligned hyperplane that minimizes the class. error

This can be done for each feature (i.e. for each dimension in feature space)

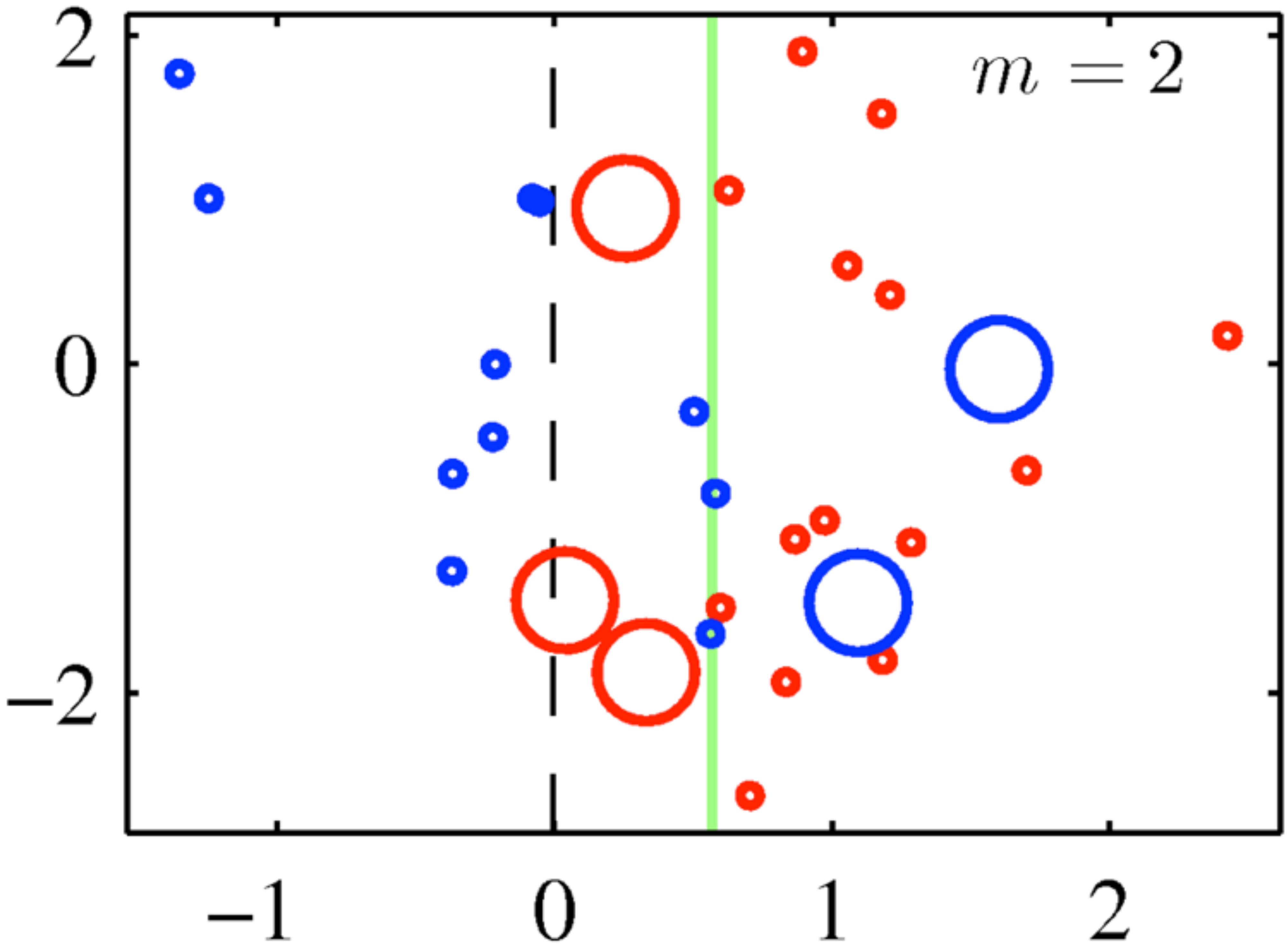
It can be shown that the classif. error is always better than 0.5 (random guessing)

Idea: apply many weak classifiers, where each is trained on the misclassified examples of the previous.

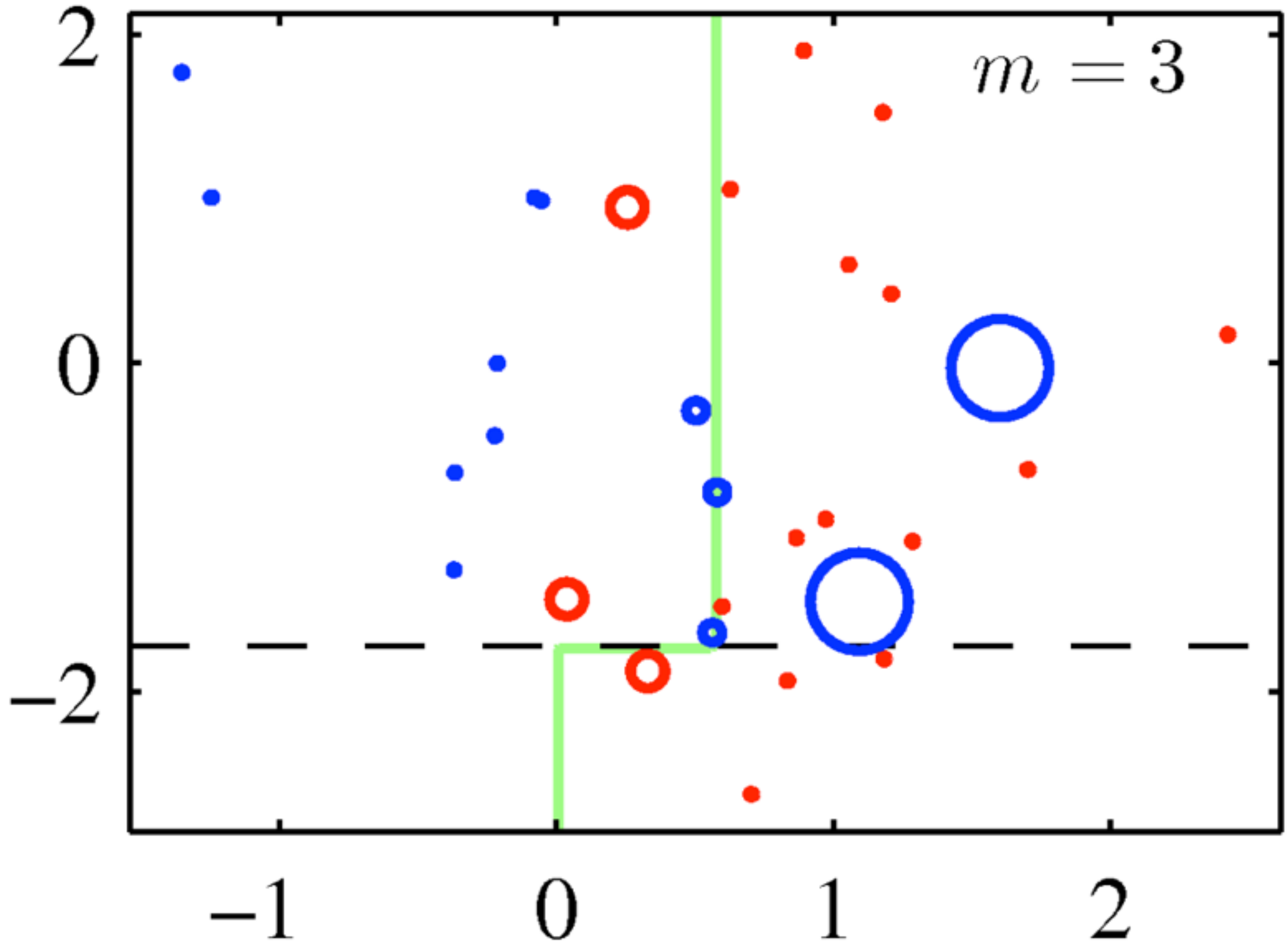
Classification Example



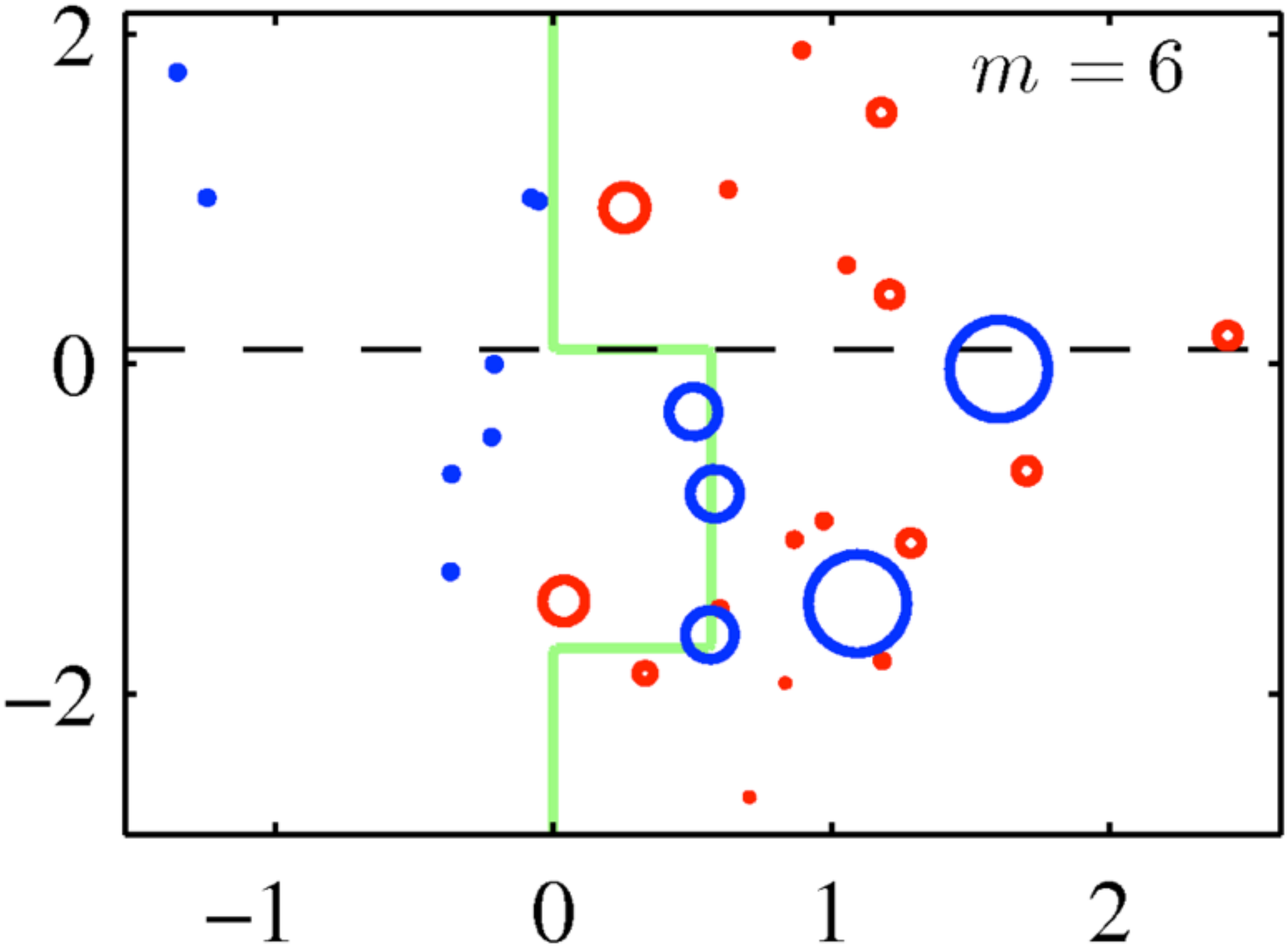
Classification Example



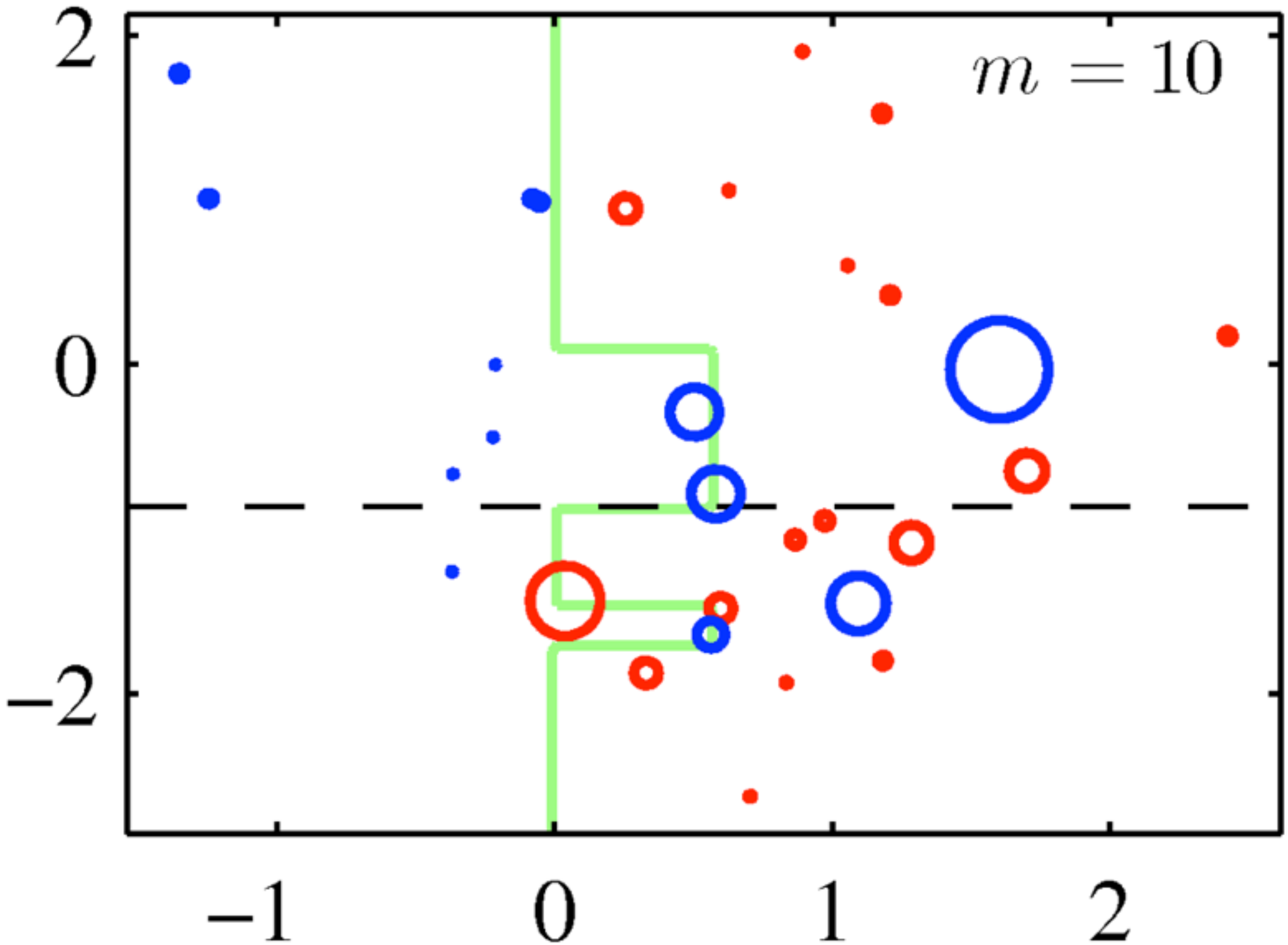
Classification Example



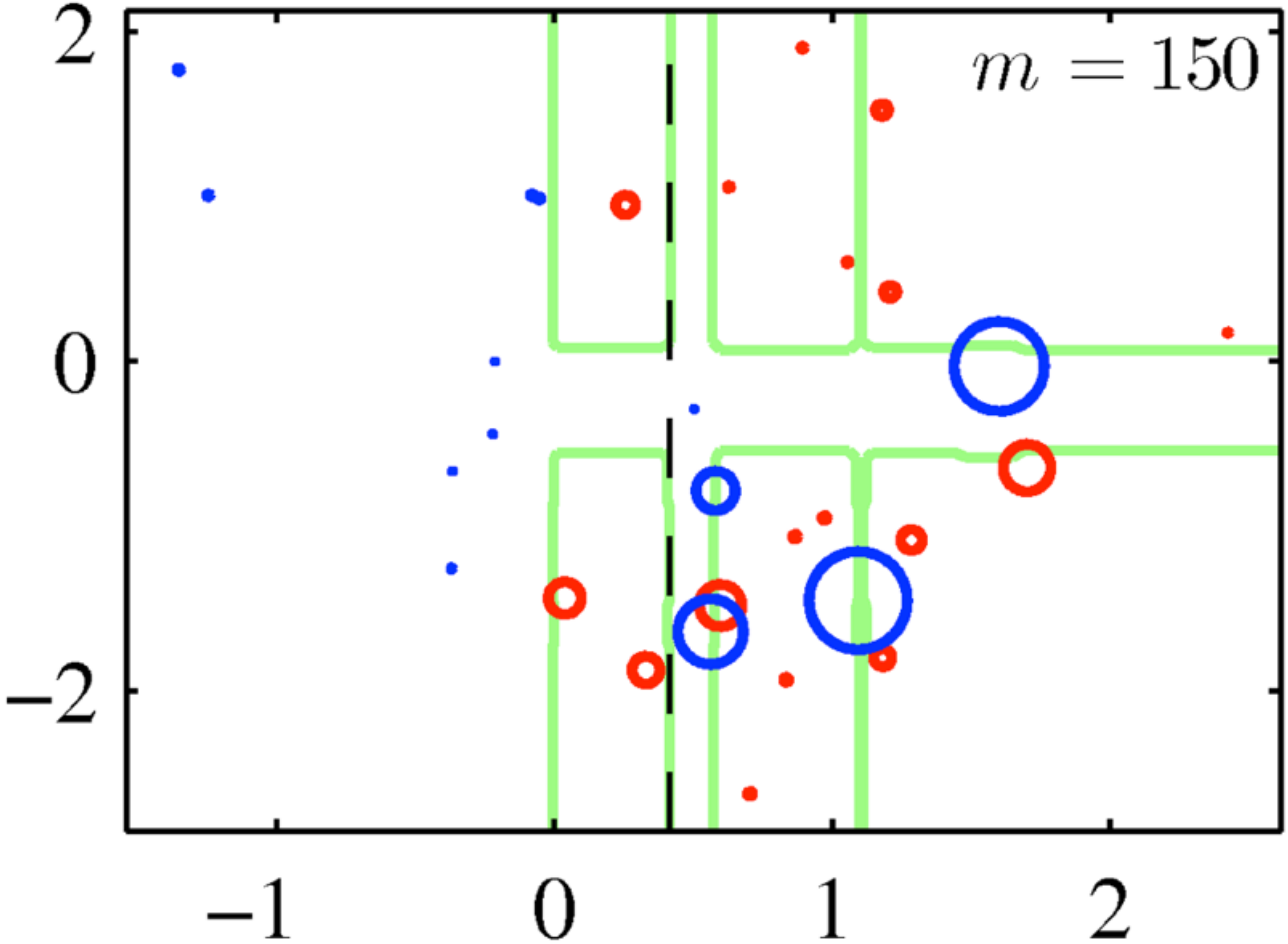
Classification Example



Classification Example

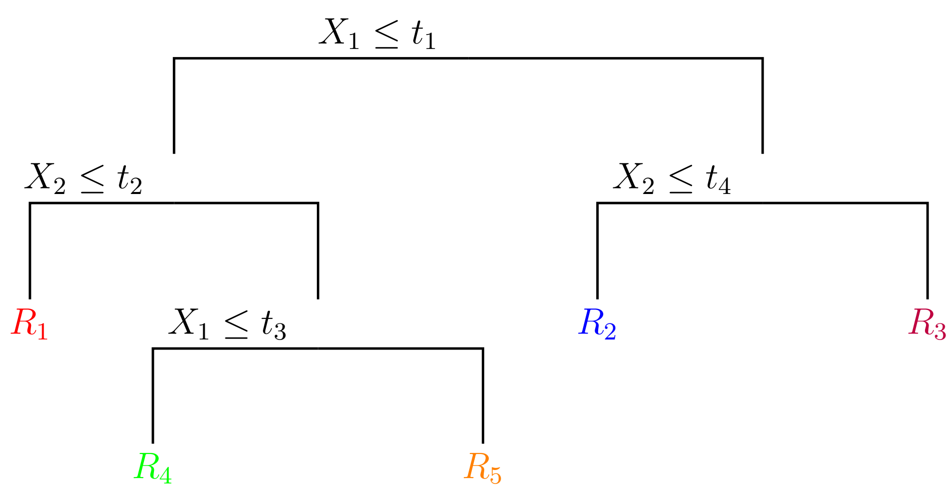


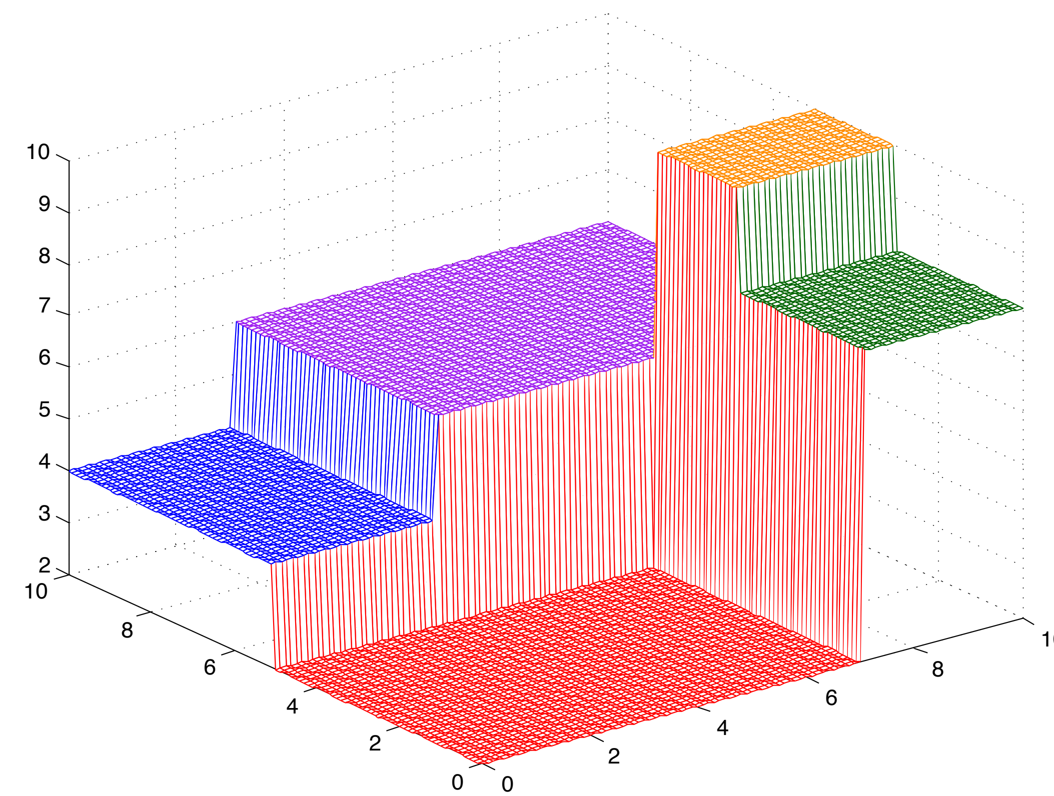
Classification Example



Decision Trees

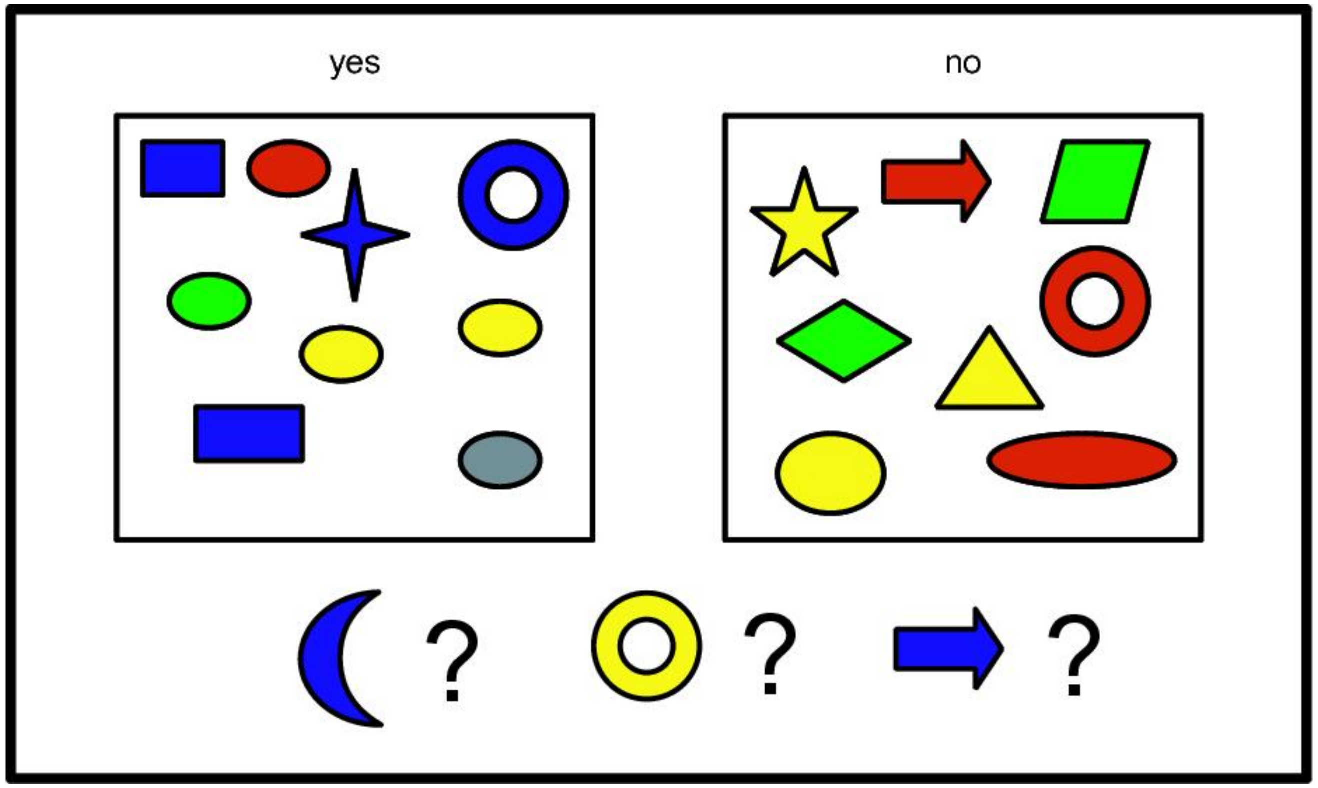
- A more general version of decision stumps are decision **trees:**

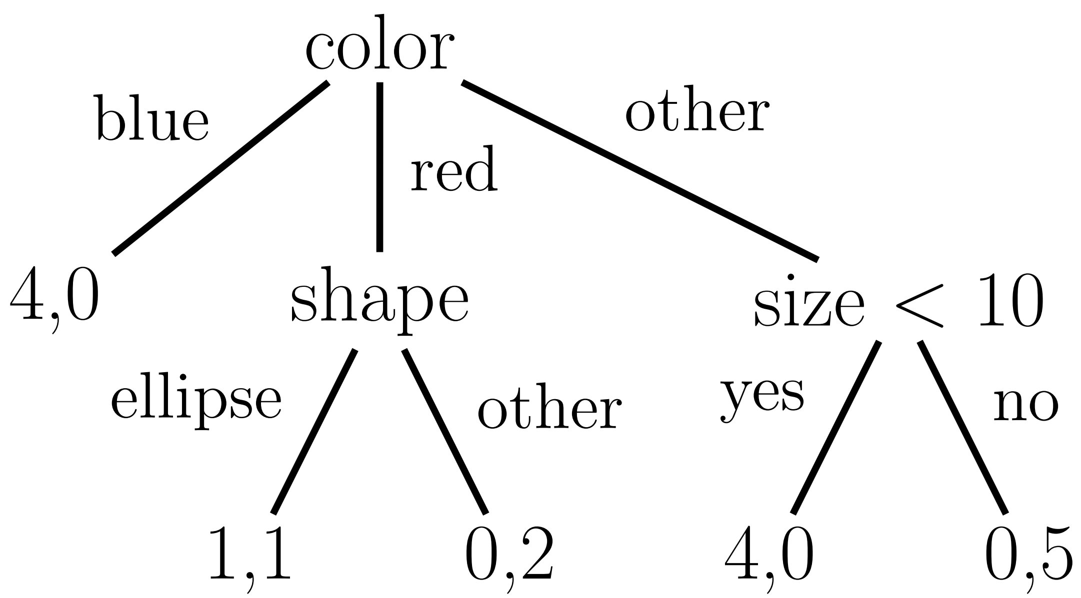




- At every node, a decision is made
- Can be used for classification and for regression (Classification And Regression Trees CART)

Decision Trees for Classification

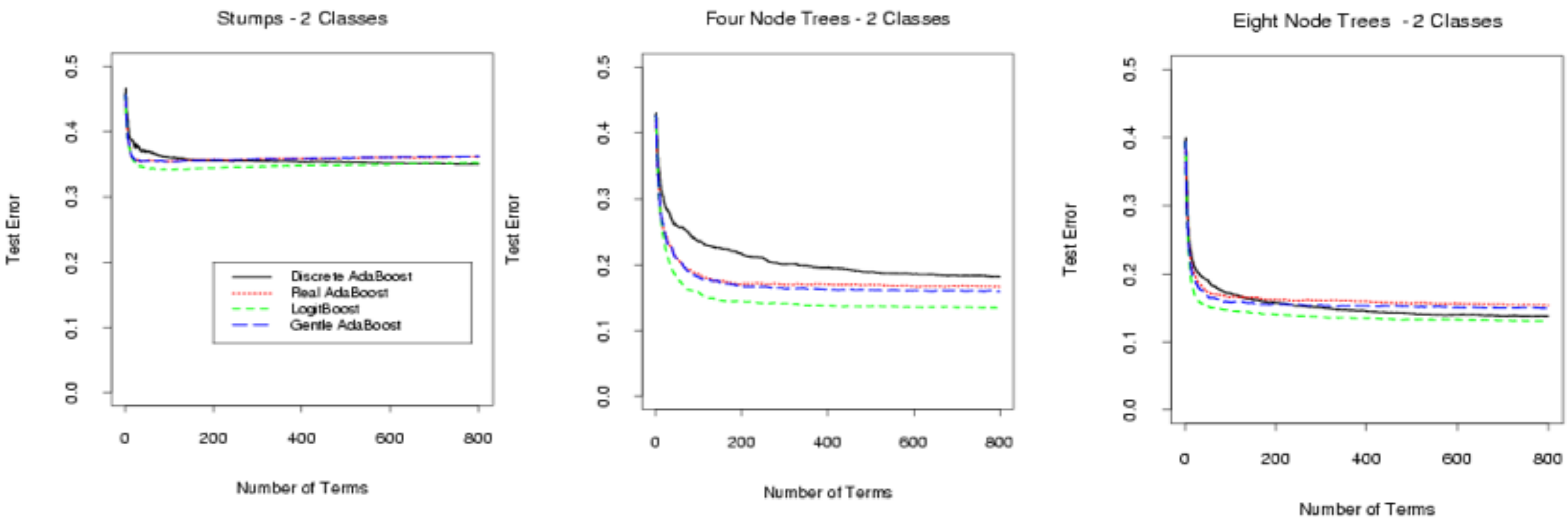




- Stores the distribution over class labels in each leaf (number of positives and negatives)
- With these, we can class label probabilities, e.g. $p(y = 1 \mid \mathbf{x}) = 1/2$ if we have a red ellipse

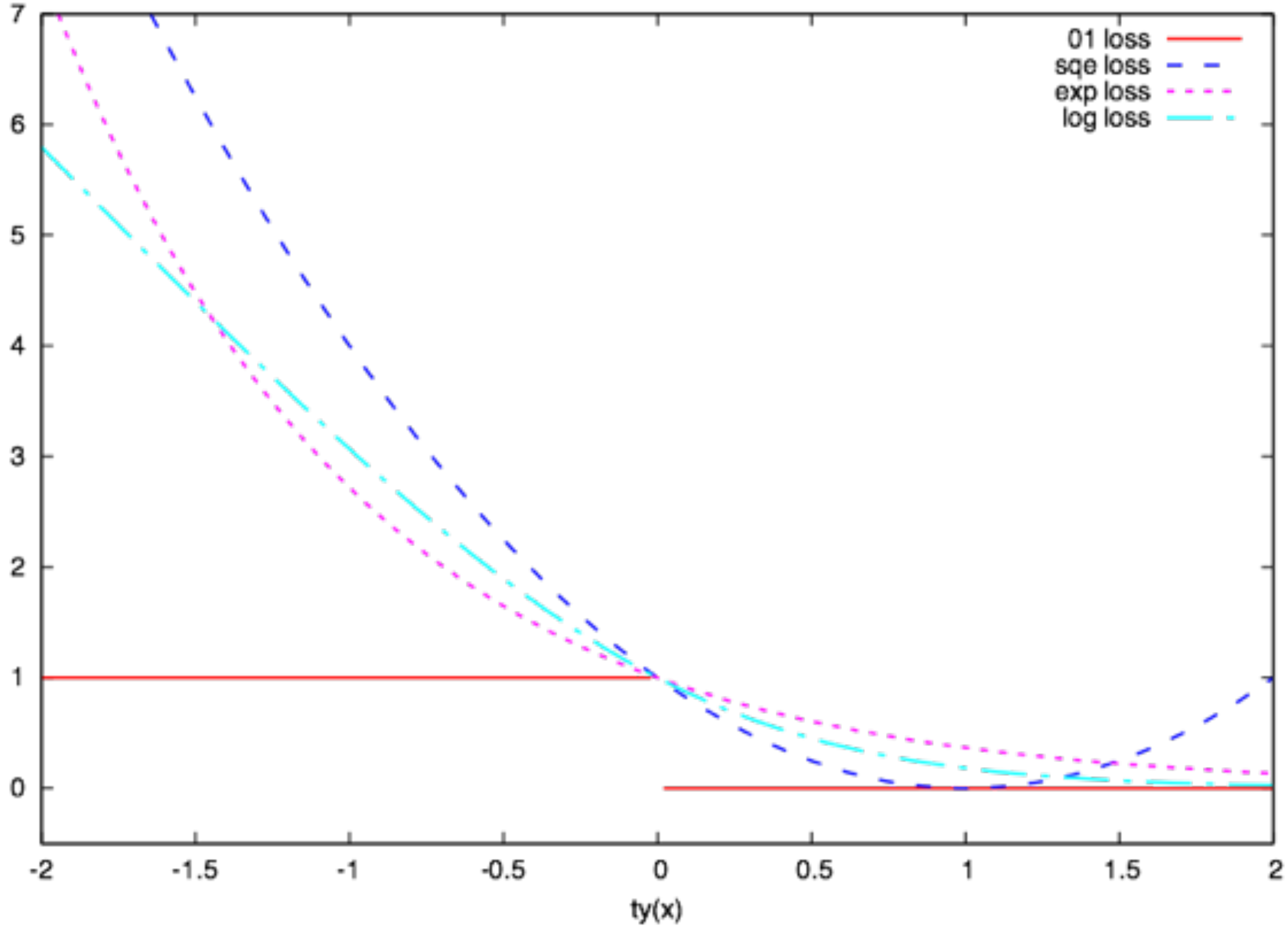
Different Weak Classifiers

- AdaBoost has been shown to perform very well, especially when using decision trees as weak classifiers



- However: the exponential loss weighs misclassified examples very high!

Using the Log-Loss



- The log-loss is defined as:

$$L(t, y(\mathbf{x})) = \log_2(1 + \exp(-2ty(\mathbf{x}))$$

- It penalizes misclassifications only **linearly**

The LogitBoost Algorithm

1. For $i = 1, \ldots, N$: $v_i \leftarrow 1/N \quad \pi_i \leftarrow 1/2$
2. For $m = 1, \ldots, M$

   Compute the working response $z_i = \dfrac{t_i - \pi_i}{\pi_i(1 - \pi_i)}$

   Compute the weights $v_i = \pi_i(1 - \pi_i)$

   Find ϕ_m that minimizes

$$\sum_{i=1}^{N} v_i (z_i - \phi(\mathbf{x}_i))^2$$

   Update $y(\mathbf{x}) \leftarrow y(\mathbf{x}) + \frac{1}{2}\phi_m(\mathbf{x})$ and $\pi_i \leftarrow \dfrac{1}{1 + \exp(-2y(\mathbf{x}_i))}$

3. Use the resulting classifier:

$$y(\mathbf{x}) = \operatorname{sgn} \sum_{m=1}^{M} \phi_m(\mathbf{x})$$

Weighted Least-Squares Regression

- Instead of a weak classifier, LogitBoost uses "weighted least-squares regression"
- This is very similar to standard least-squares regression:

$$E(\mathbf{w}) = \frac{1}{2}\sum_{i=1}^{N} v_i(\mathbf{w}^T \quad \mathbf{x}_i \quad - t_i)^2$$

- This results in a matrix $\hat{\Phi} = V^{1/2}\Phi$ where

$$V^{1/2} = \mathrm{diag}(\sqrt{v_1}, \ldots, \sqrt{v_N})$$

- The solution is

$$\mathbf{w} = (\hat{\Phi}^T\hat{\Phi})^{-1}\hat{\Phi}^T\mathbf{t}$$

Application of AdaBoost: Face Detection

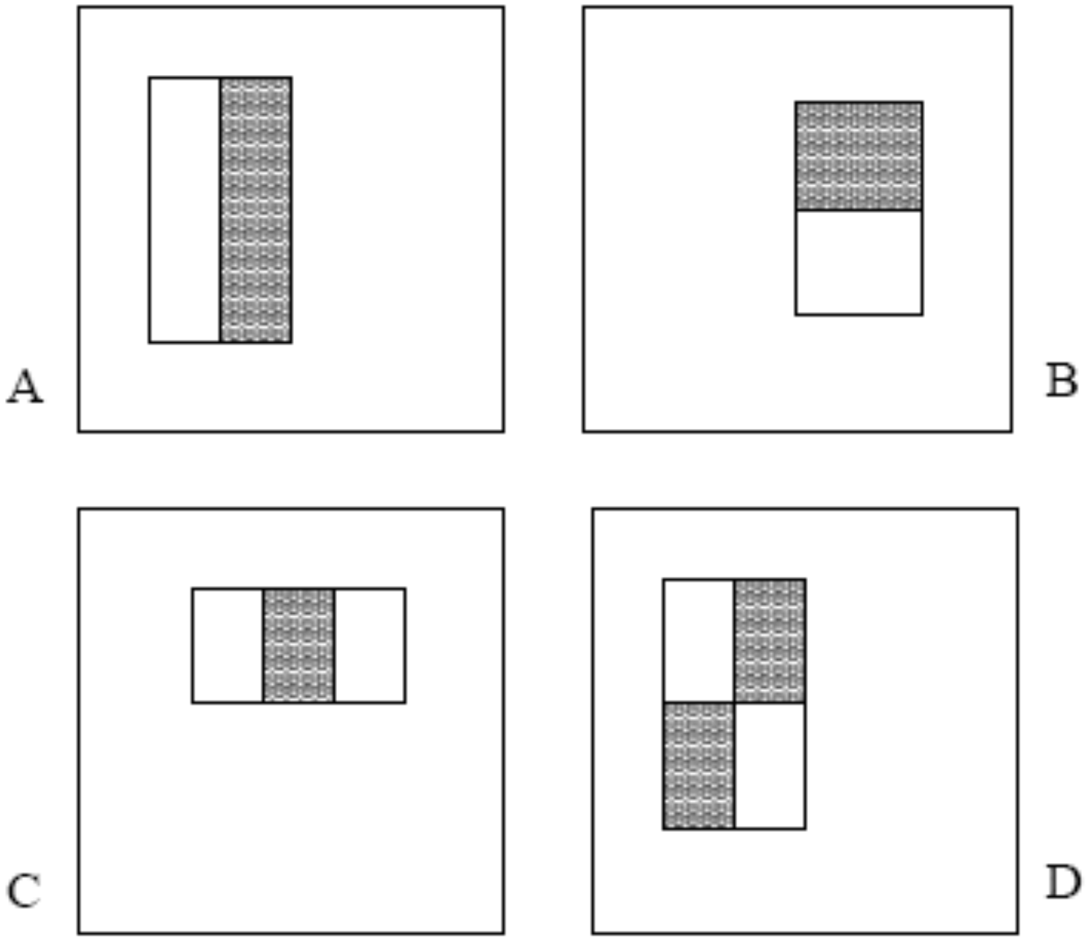
- The biggest impact of AdaBoost was made in face detection
- Idea: extract features (“Haar-like features”) and train AdaBoost, use a cascade of classifiers
- Features can be computed very efficiently
- Weak classifiers can be decision stumps or decision trees
- As inference in AdaBoost is fast, the face detector can run in **real-time**!

Haar-like Features

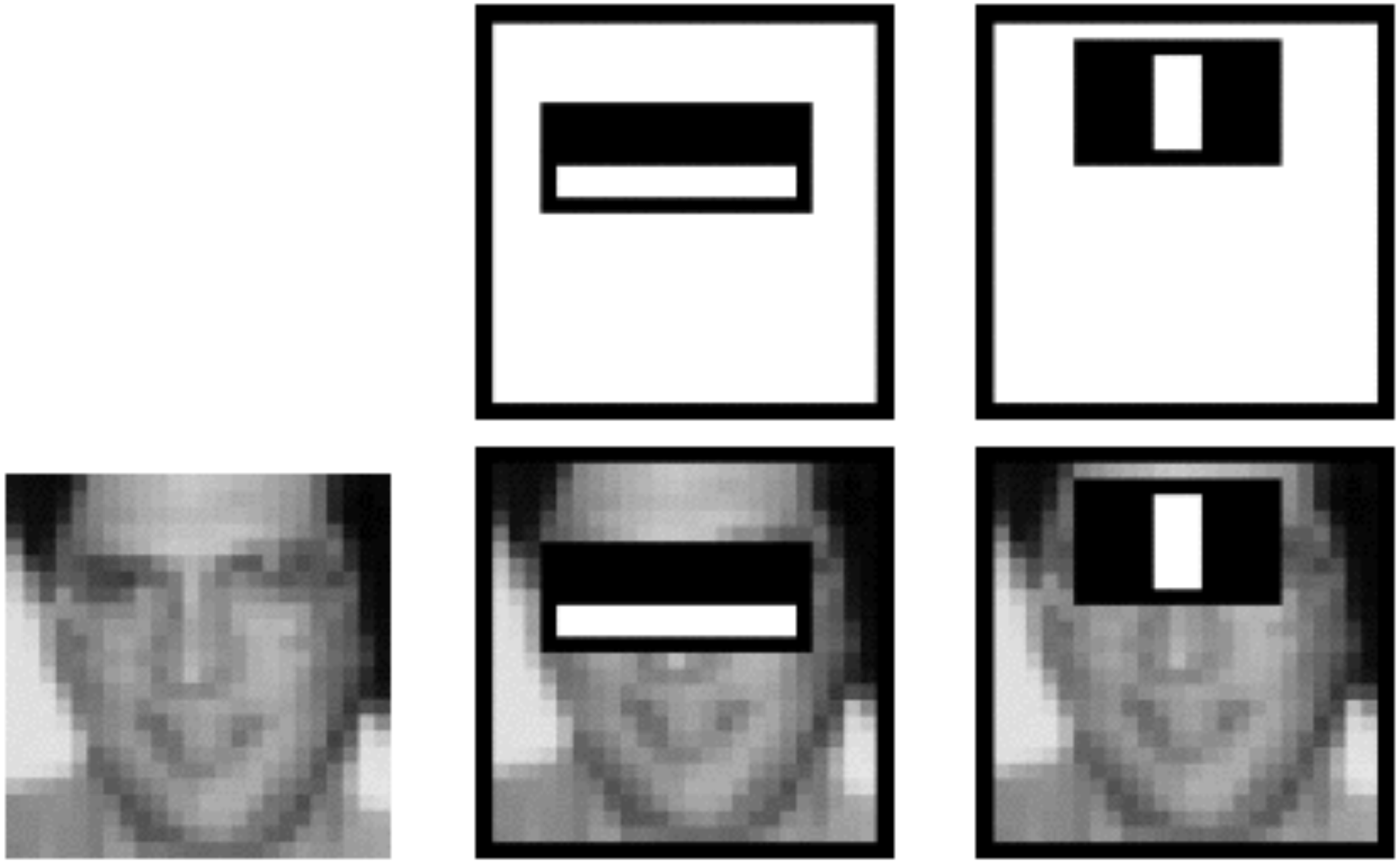
- Defined as difference of rectangular integral area:
  - The sum of the pixels which lie within the white rectangles are subtracted from the sum of pixels in the grey rectangles.

$$\left(\iint_{White} I(x,y)dxdy\right) - \left(\iint_{Grey} I(x,y)dxdy\right)$$

- One feature defined as:
  - Feature type: A,B,C or D
  - Feature position and size



Two First Classifiers Selected by AdaBoost



A classifier with only this two features can be trained to recognise 100% of the faces, with 40% of false positives

Results

Bagging

- So far: Boosting as an **ensemble** learning method, i.e.: a combination of (weak) learners
- A different way to combine classifiers is known as **bagging ("bootstrap aggregating")**
- **Idea:** sample M "bootstrap" data sets (sub sets) **with replacement** from the training set and train different models
- Overall classifier is then the **average** over all models:

$$\bar{y}(\mathbf{x}) = \frac{1}{M} \sum_{m=1}^{M} y_m(\mathbf{x})$$

Bagging

Bagging reduces the expected error. E.g. in regression:

$$y_m(\mathbf{x}) = h(\mathbf{x}) + \epsilon_m(\mathbf{x})$$

prediction ground truth error

- Expected error: $E_x[(y_m(\mathbf{x}) - h(\mathbf{x}))^2]$
- Average error over all (weak) learners:

$$E_{AV} = \frac{1}{M}\sum_{m=1}^{M} E_x[(y_m(\mathbf{x}) - h(\mathbf{x}))^2]$$

- Average error of committee:

$$E_{COM} = E_x\left[(\bar{y}(\mathbf{x}) - h(\mathbf{x}))^2\right]$$

Bagging

Bagging reduces the expected error. E.g. in regression:

$$y_m(\mathbf{x}) = h(\mathbf{x}) + \epsilon_m(\mathbf{x})$$

prediction ground truth error

- Expected error: $E_x[(y_m(\mathbf{x}) - h(\mathbf{x}))^2]$
- Average error over all weak learners (indep.):

$$E_{AV} = \frac{1}{M} \sum_{m=1}^{M} E_x[(y_m(\mathbf{x}) - h(\mathbf{x}))^2]$$

- Average error of committee:

$$E_{COM} = E_x\left[\left(\frac{1}{M} \sum_{m=1}^{M} y_m(\mathbf{x}) - h(\mathbf{x})\right)^2\right]$$

Bagging

Bagging reduces the expected error. E.g. in regression: $y_m(\mathbf{x}) = h(\mathbf{x}) + \epsilon_m(\mathbf{x})$

- Expected error: $E_x[(y_m(\mathbf{x}) - h(\mathbf{x}))^2]$
- Average error over all (weak) learners:

$$E_{AV} = \frac{1}{M} \sum_{m=1}^{M} E_x[(y_m(\mathbf{x}) - h(\mathbf{x}))^2]$$

- Average error of committee if learners are uncorrelated:

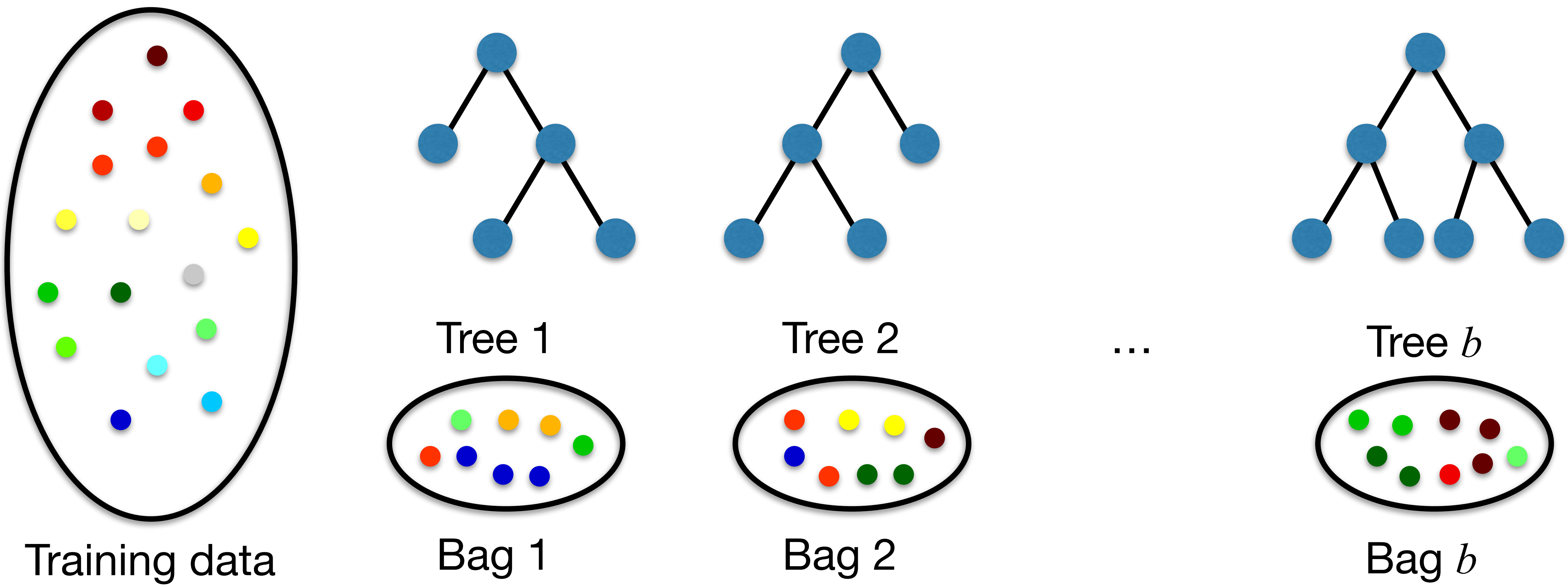
$$E_{COM} = \frac{1}{M} E_{AV}$$

Random Forests

Given: training set of size N $\{\mathbf{x}_1, \ldots, \mathbf{x}_N\}$ $\mathbf{x}_i \in \mathbb{R}^d$

1. Randomly sample $n \leq N$ elements from training set **with replacement (repetitions likely)**
2. Randomly select a subset of p features ($p<d$)
3. Pick from those the feature that produces the best **split** of the data
4. Perform the split and go back to 2.
5. If maximum tree depth is reached:
6. If number of trees M is reached then stop.
7. Else: go to 1. building a new tree.

Random Forests



- Each bag is a subset of the entire training data
- Repetitions are very likely, especially if $n=N$
- In contrast to boosting, classifiers are independent (can be trained in parallel)

Performance of Random Forests

The error rate depends on two main aspects:

- the **correlation** between any two trees:
  high correlation → high error rate
- the **strength** of each tree (low error per tree)
  higher strength → lower overall error rate

These values are mainly influenced by p:

- If p is low: correlation and strength are low
- If p is high: correlation and strength are high

There is usually an “optimal range” of p

Splitting Criterion

- **Aim**: split such that both data sub sets contain samples that are as **pure** as possible
- Possible impurity values:
  - misclassification error: let π be the prob of class 1 (binary classification), i.e. $\pi = P(y = 1|\Omega)$ data subset then use $\min(\pi, 1 - \pi)$
  - Gini index: $2\pi(1 - \pi)$
  - Deviance: $-\pi \log \pi - (1 - \pi) \log(1 - \pi)$
  - For regression trees we can use the mean-squared error

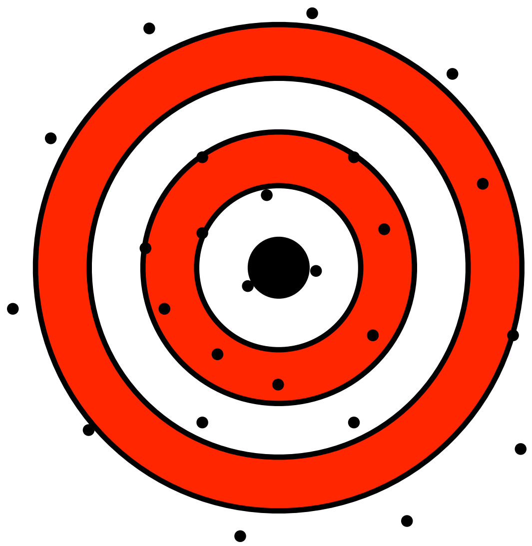
Properties of Random Forests

- They reduce the **variance** of the classification estimate, by training several trees on randomly sampled subsets of the data ("**bagging**")
- They tend to give **uncorrelated** trees by randomly sampling the features (splits)
- They can **not overfit**! One can use as many trees as required
- Only restriction is memory
- Random Forests have very good accuracy and are widely used, e.g. for body pose recognition

Bias and Variance

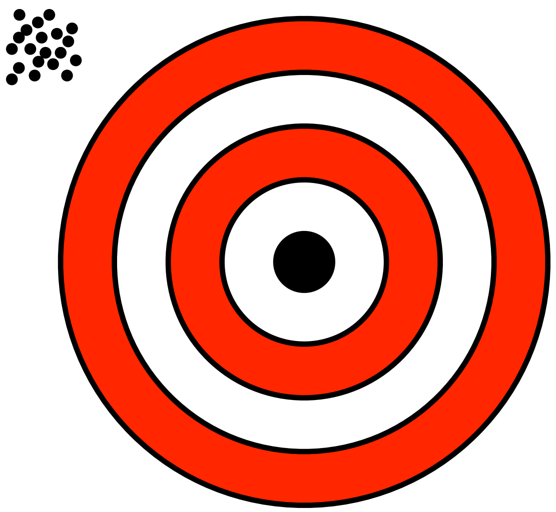
Consider training on a sub-set plus prediction as one “trial”:

Comparing with ground truth gives usually one of these situations (**“bias-variance-tradeoff”**):



high variance, low bias

“overfitting”



high bias, low variance

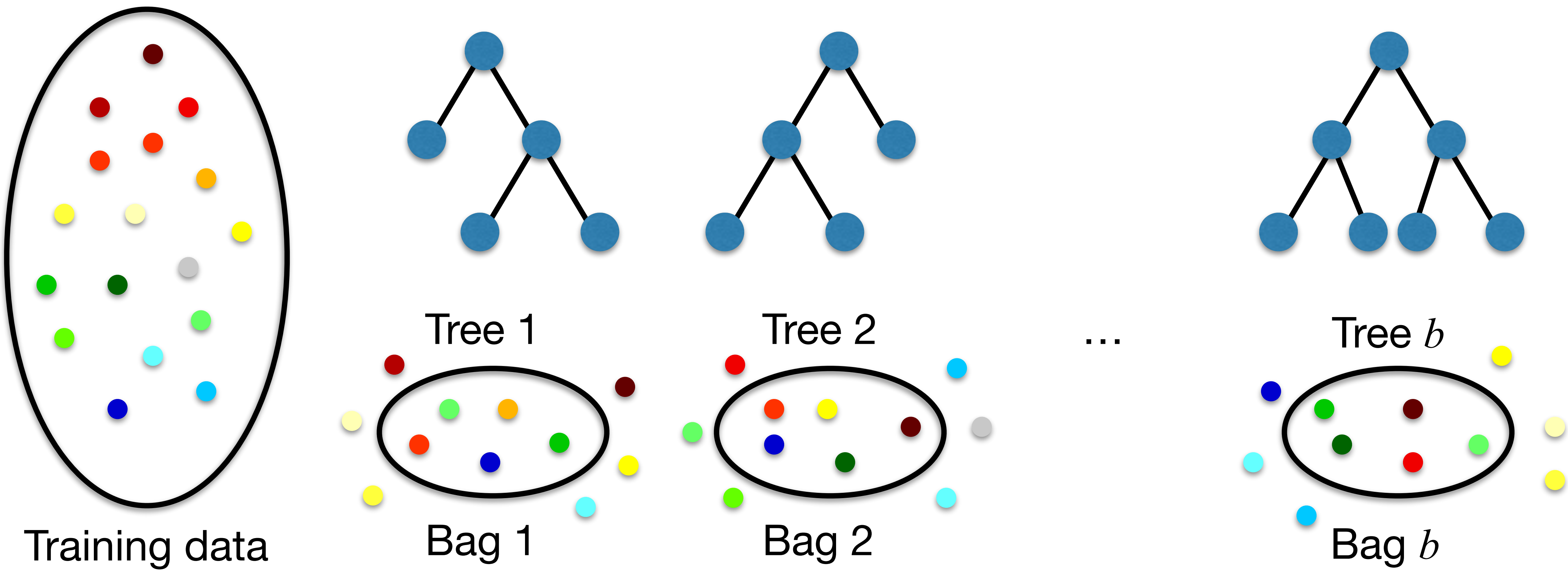
“underfitting”

Advantages of Random Forests

- One of the best classifiers in general
- Runs very **efficiently** on large data sets
- Can handle thousands of **feature dimensions**
- Can provide **importance** of variables
- Can deal with missing data
- Implicitly generates **proximities** of pairs of data samples, useful e.g. for clustering
- Can be extended to unlabeled data

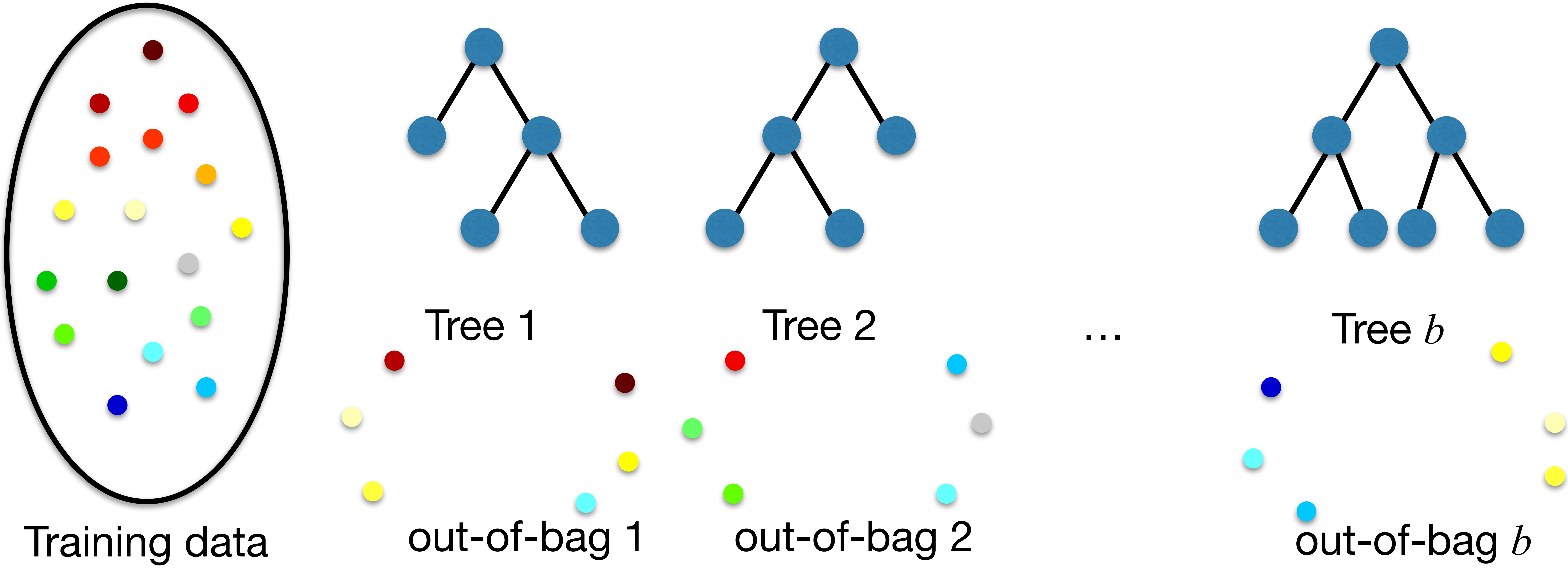
Out-of-Bag (OOB) Error

- All samples that are not used to train a tree are called the **out-of-bag data**
- These samples can be used to evaluate the overall random forest **without** an additional validation set



Out-of-Bag (OOB) Error

- All samples that are not used to train a tree are called the **out-of-bag data**
- This is done by evaluating each tree with its own out-of-bag data



Variable Importance

Idea: rate variables (features) according to their potential to change the tree structure

Method:

1. compute **tree impurity** ι_m (sum of node impurities of leaf nodes per tree) for each tree $m=1,\dots,M$
2. for all features $j=1,\dots,d$: **permute** the jth feature value in the out-of-bag data
3. compute tree impurity of the **permuted** data ι_{jm}
4. compute the **difference** of tree impurity:

$$\delta_{mj} = \iota_{mj} - \iota_m$$

Variable Importance

Idea: rate variables (features) according to their potential to change the tree structure

Method:

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3. compute tree impurity of the **permuted** data ι_{jm}
4. compute the **difference** of tree impurity
5. variable importance is: $$\frac{\bar{\delta}_j}{\sqrt{\frac{1}{M}\sum_m(\delta_{mj}-\bar{\delta}_m)^2}}$$

mean

standard deviation

Summary

- Boosting uses **weak** classifiers and turns them into a **strong** one (arbitrarily small training error!)
- AdaBoost minimizes the **exponential** loss
- To be more robust against outliers, we can use **LogitBoost**
- Face detection can be done with Boosting
- Bagging reduces the overall committee error
- Random Forests are an example of bagging with a very good performance