# LEC 8: Classification trees and ensemble learning

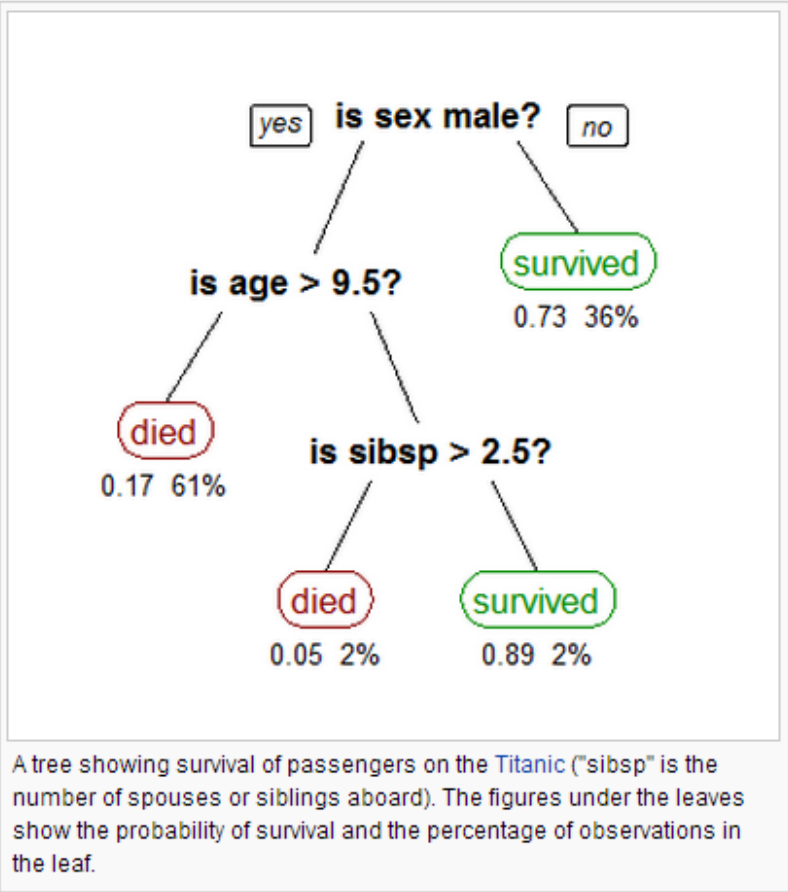
Dr. Guangliang Chen

April 21, 2016

# Outline

- Classification trees
- Ensemble learning
  - Bagging
  - Random forest
  - Boosting
- Summary

# What is a classification tree?

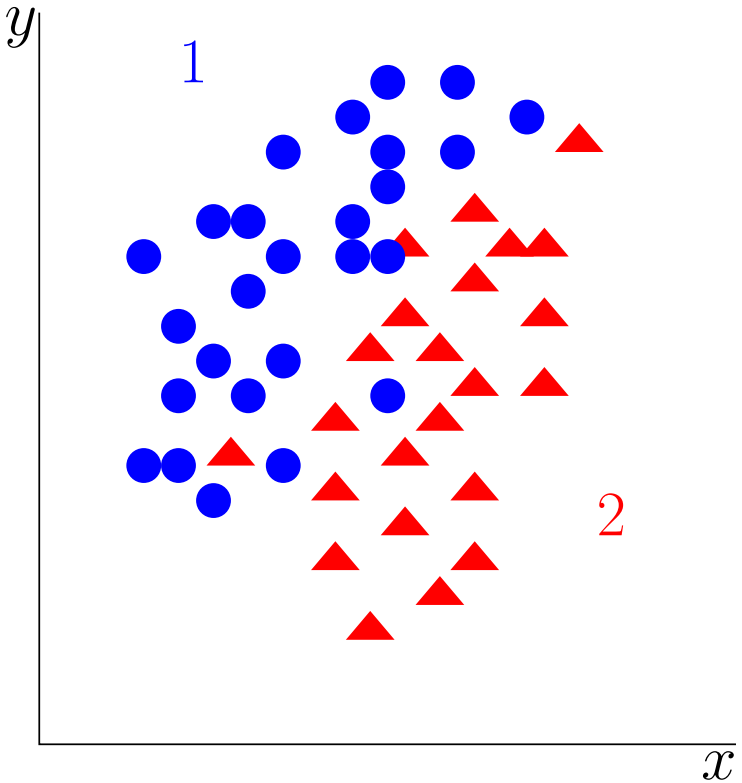


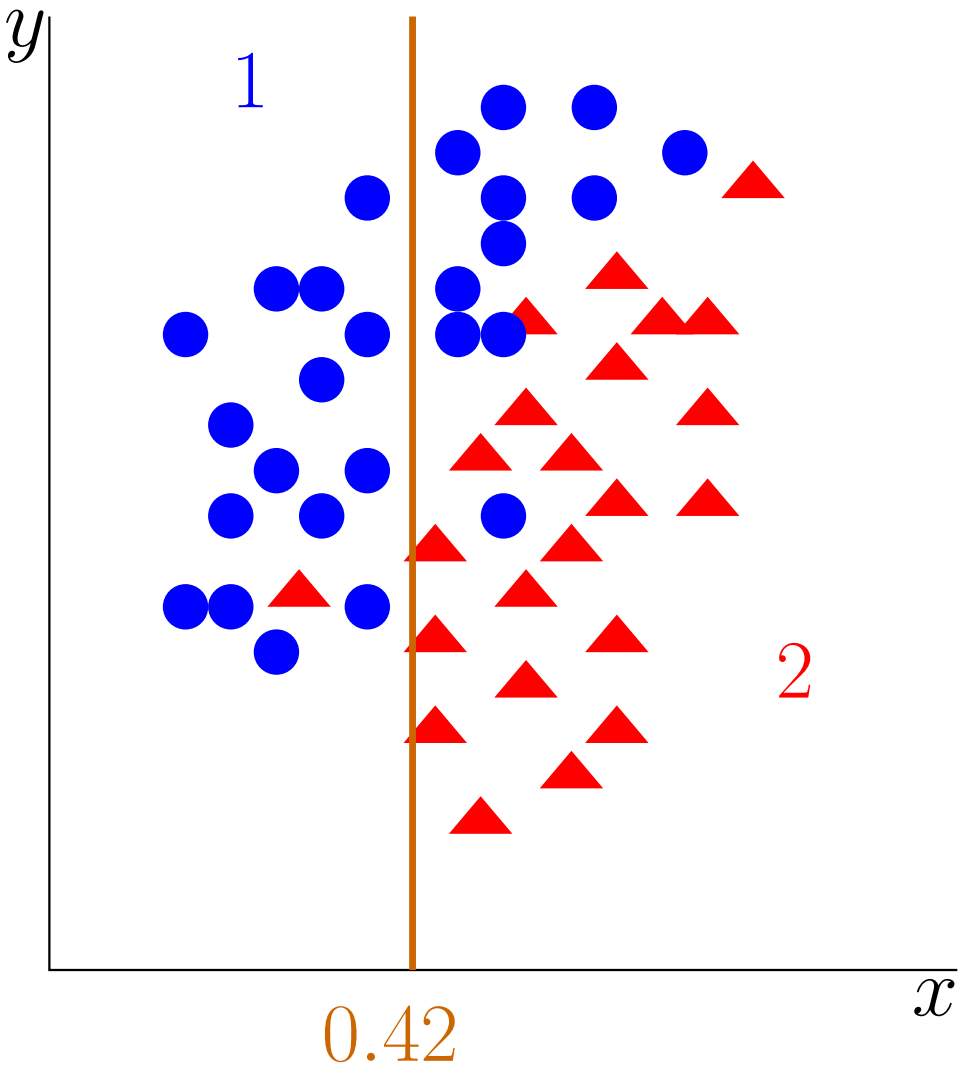

A tree showing survival of passengers on the Titanic ("sibsp" is the number of spouses or siblings aboard). The figures under the leaves show the probability of survival and the percentage of observations in the leaf.

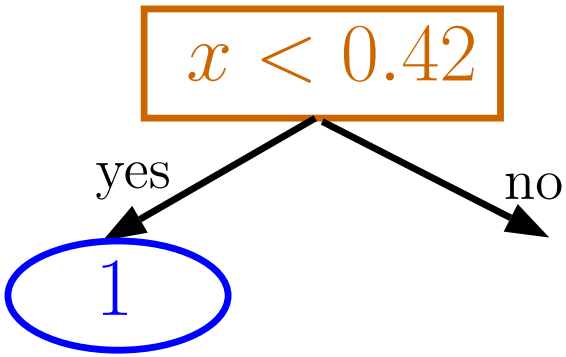
- The tree is grown using training data, by recursive splitting.
- Each internal node represents a query on one of the variables.
- The terminal nodes are the decision nodes, typically dominated by one of the classes.
- New observations are classified in the respective terminal nodes by using majority vote.

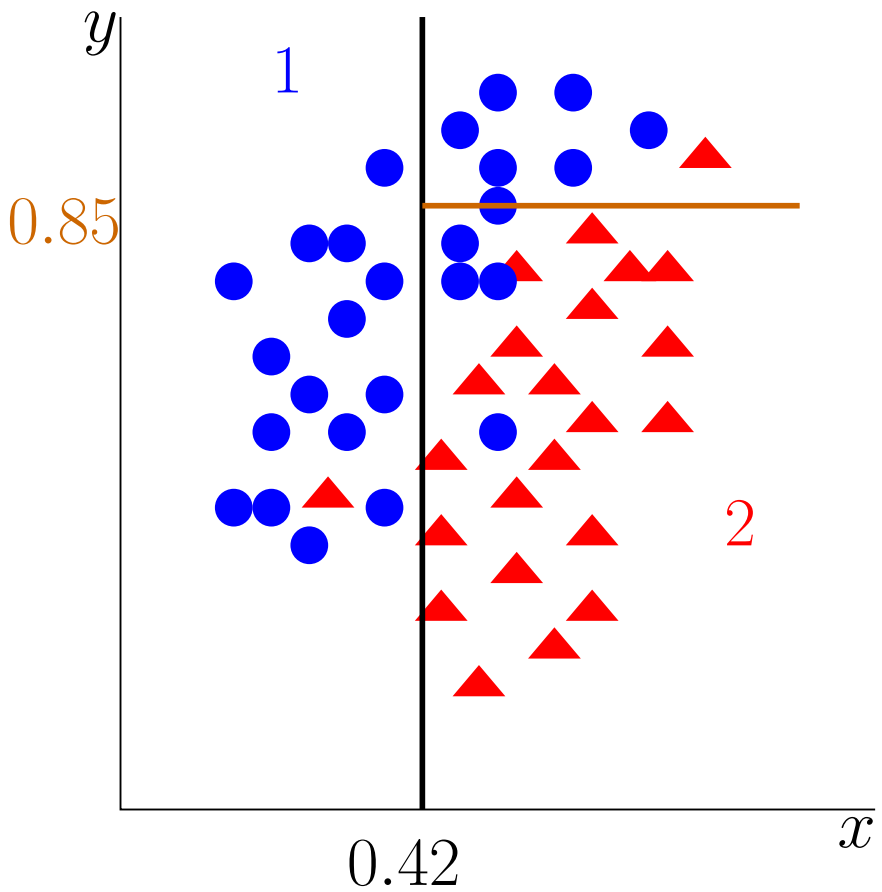
# Demonstration of how to build a classification tree

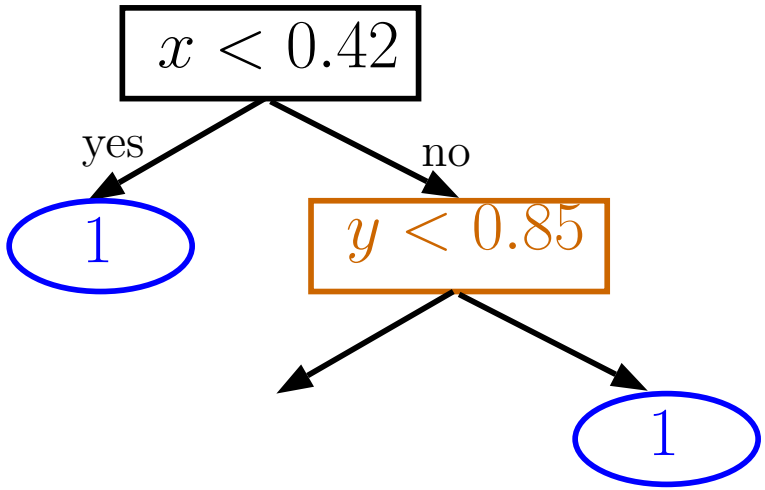
Consider the following training data.

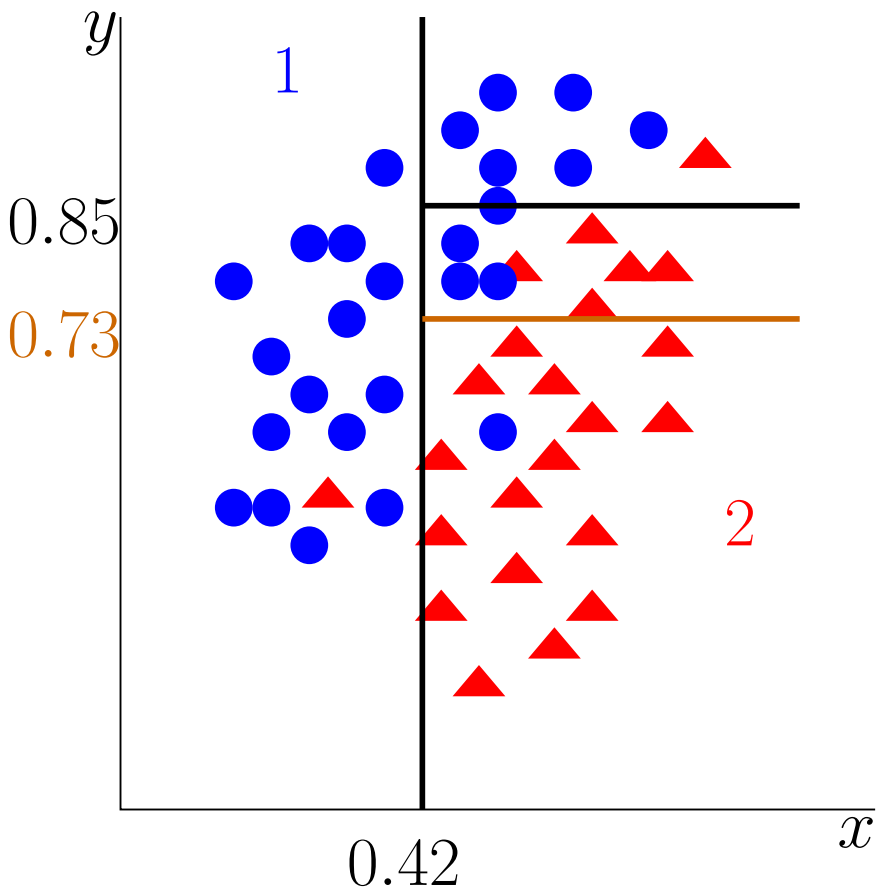


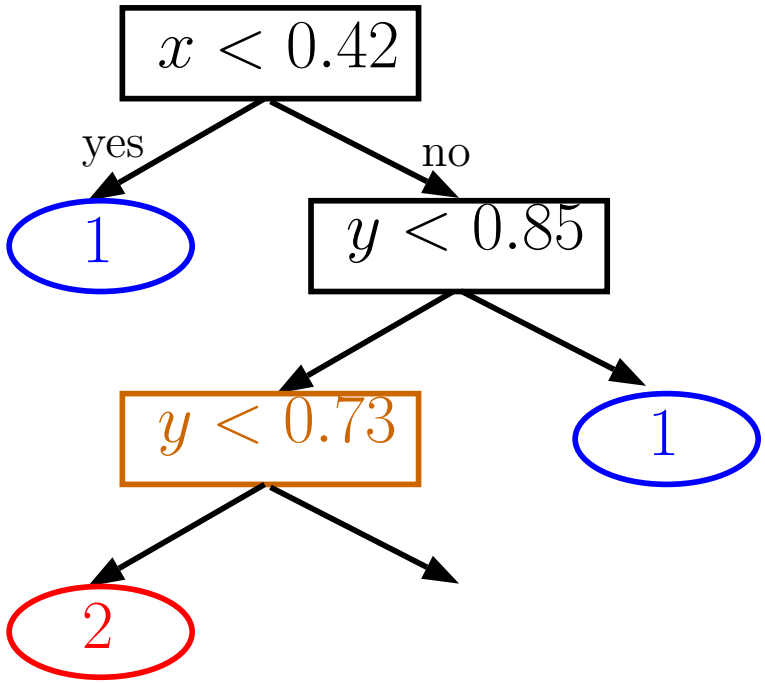

y
1
2
x
0.42

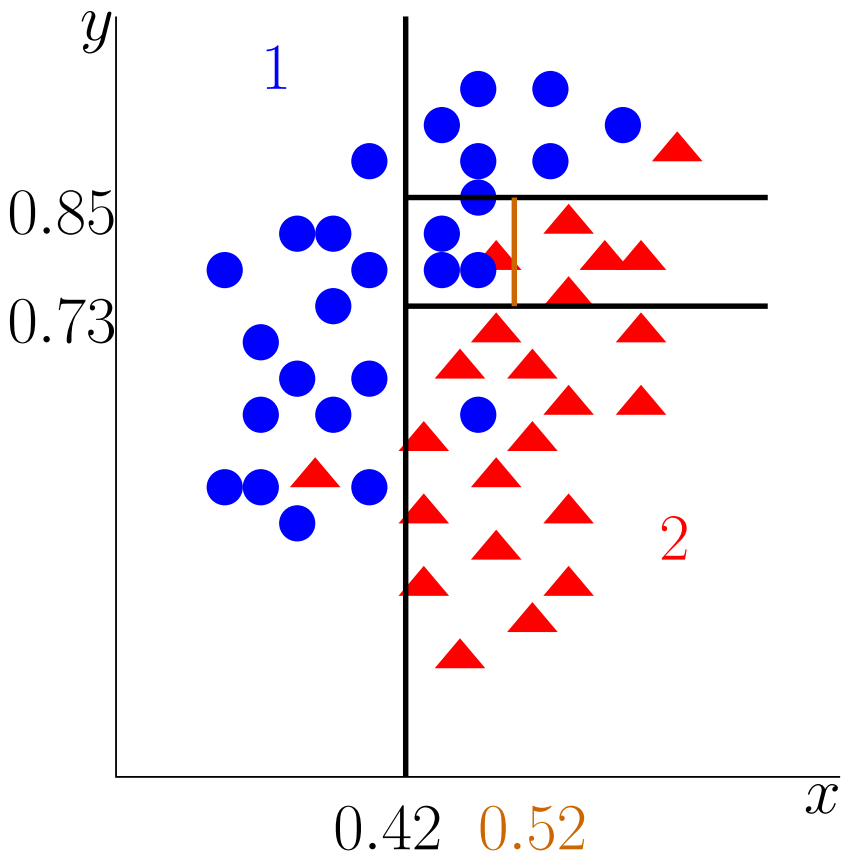

$x < 0.42$
yes
no
1

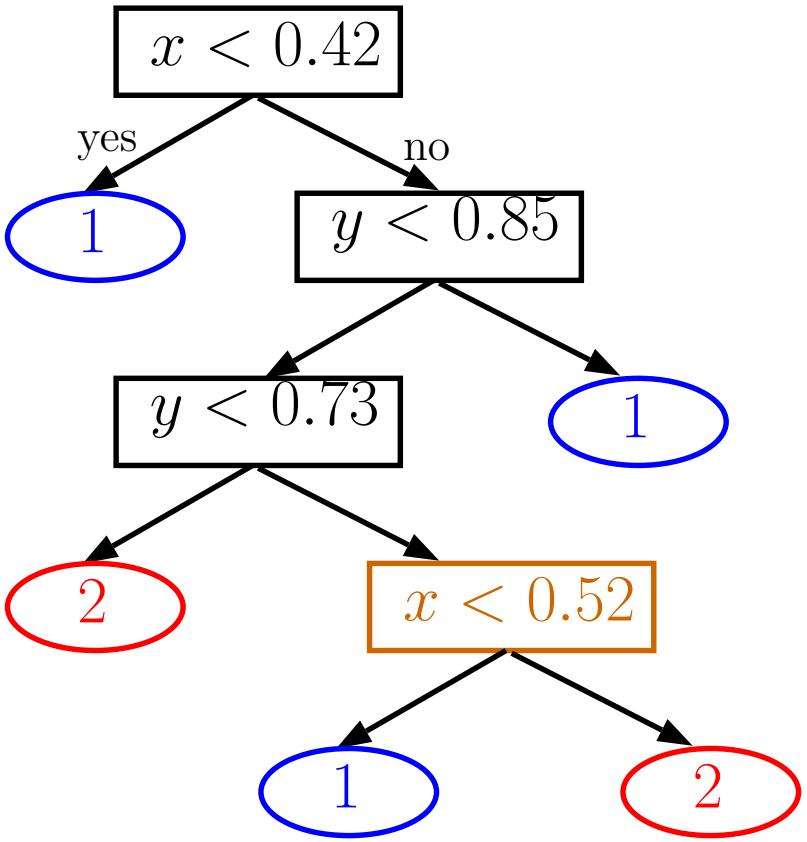

y
1
0.85
2
x
0.42

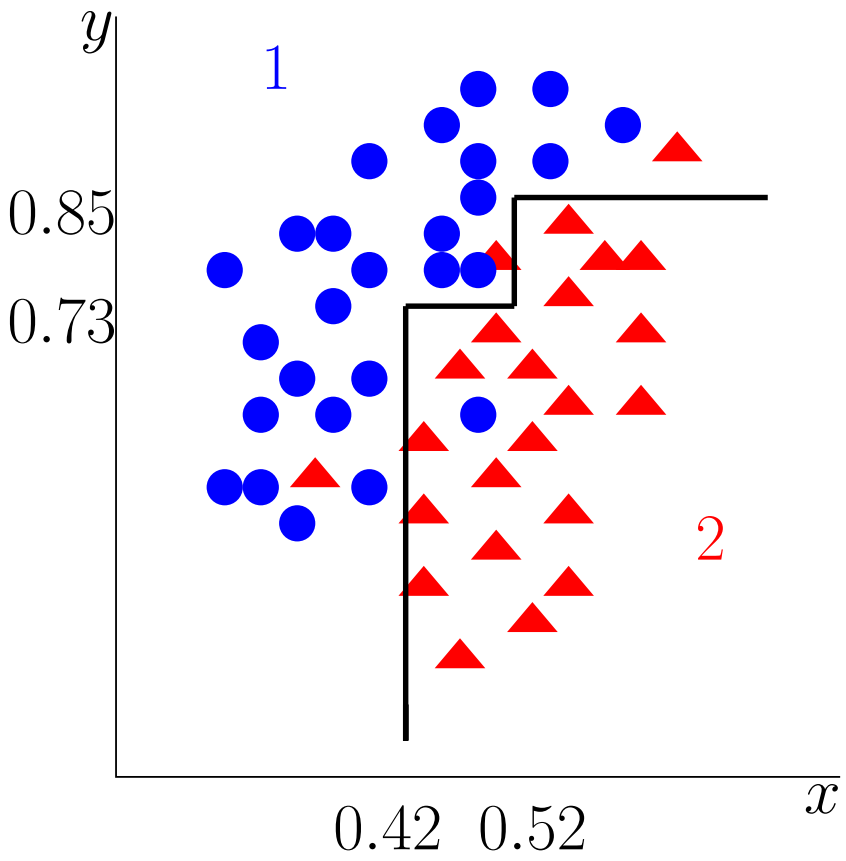

$x < 0.42$
yes
no
1
$y < 0.85$
1

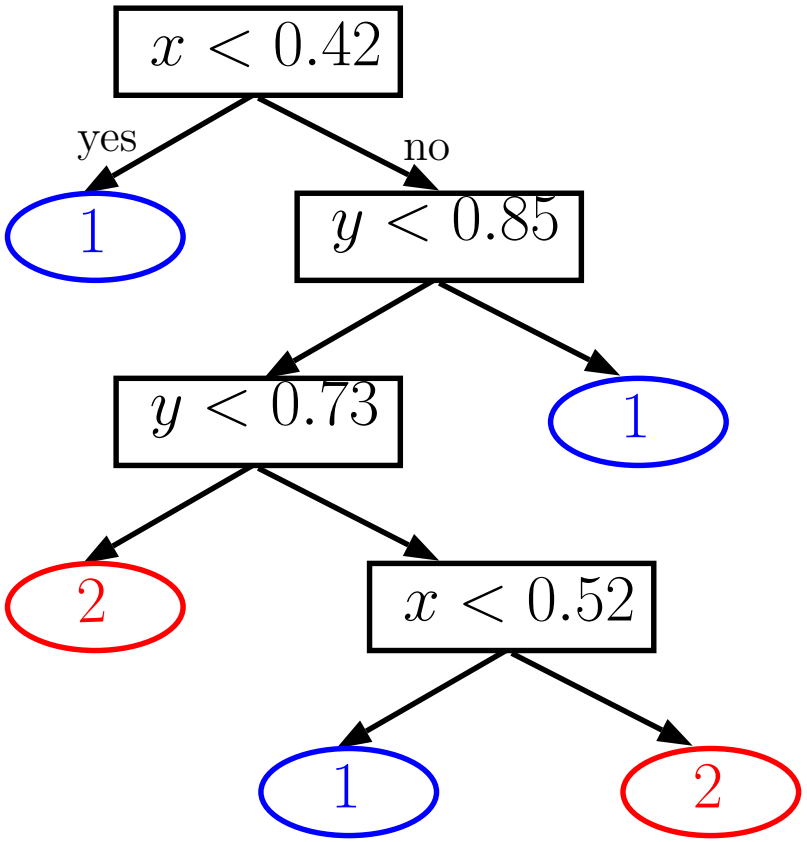

y
1
0.85
0.73
2
x
0.42

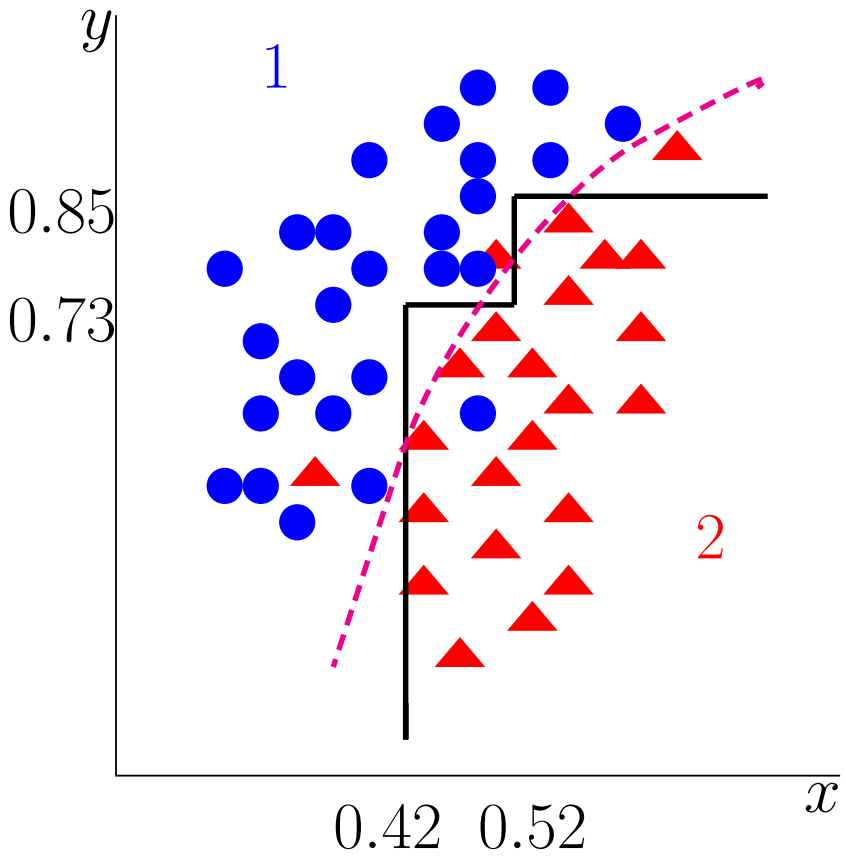

$x < 0.42$
yes
no
1
$y < 0.85$
$y < 0.73$
1
2

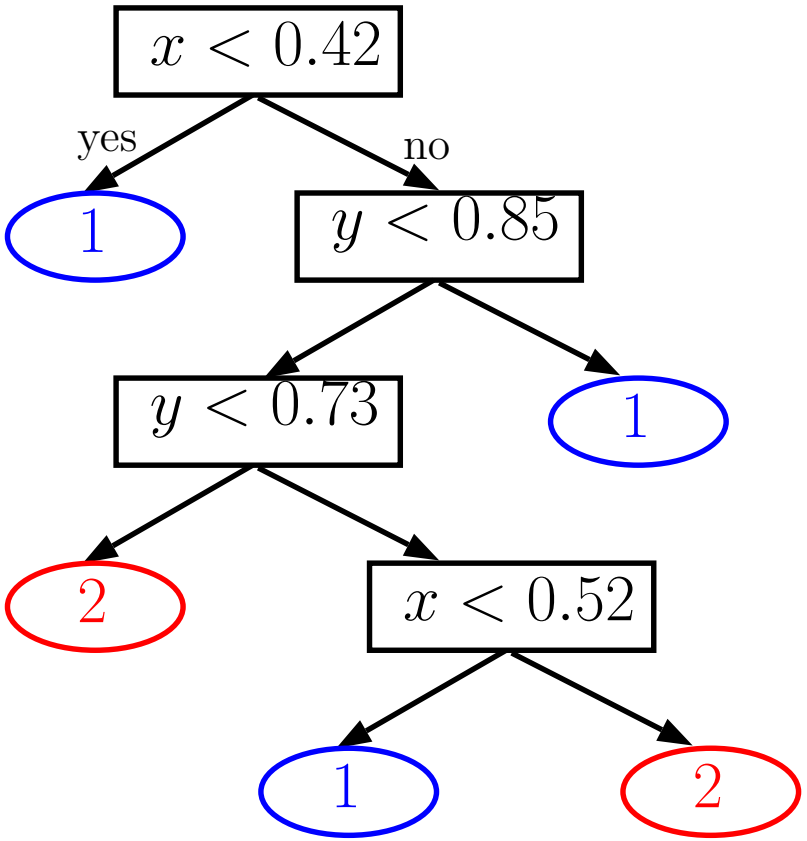

y
1
0.85
0.73
2
x
0.42
0.52


$x < 0.42$
yes
no
1
$y < 0.85$
$y < 0.73$
1
2
$x < 0.52$
1
2

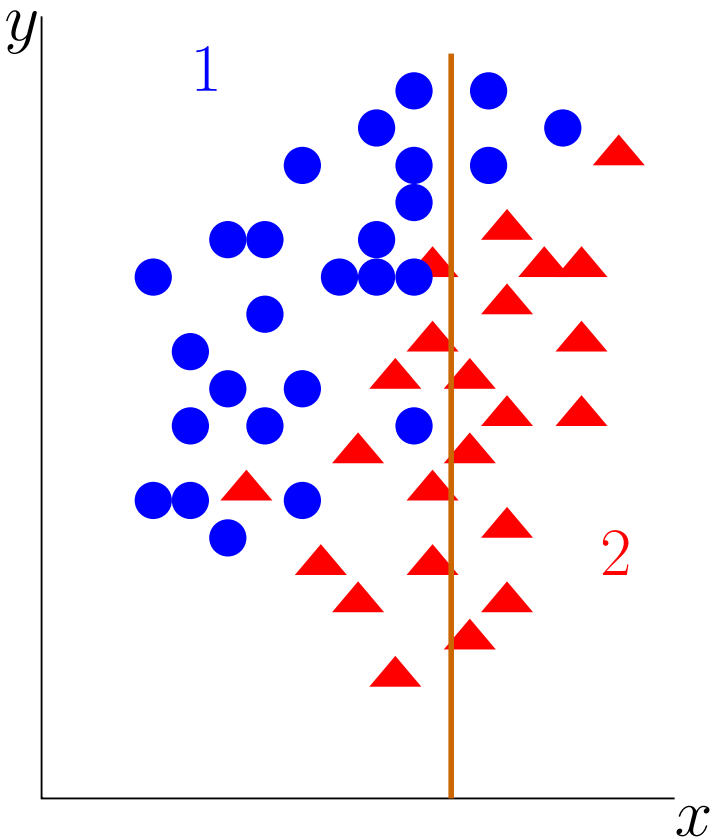

y
1
0.85
0.73
2
0.42
0.52
x


x < 0.42
yes
no
1
y < 0.85
y < 0.73
1
2
x < 0.52
1
2


y
1
0.85
0.73
2
x
0.42
0.52


$x < 0.42$
yes
no
1
$y < 0.85$
$y < 0.73$
1
2
$x < 0.52$
1
2

# Splitting criterion: Gini impurity score




Gini diversity index for a given split

$$n^{(\mathrm{L})} \sum_{i=1}^{k} p_i^{(\mathrm{L})}(1 - p_i^{(\mathrm{L})}) + n^{(\mathrm{R})} \sum_{i=1}^{k} p_i^{(\mathrm{R})}(1 - p_i^{(\mathrm{R})})$$

where

- $n^{(\mathrm{L})}$: number of observations in left region
- $p_1^{(\mathrm{L})}$: proportion of blue dots in left region
- $p_2^{(\mathrm{L})}$: proportion of red triangles in left region

(*The smaller the index, the better the split*)

# MATLAB function for classification trees

```
t = fitctree(trainX, trainLabels);

view(t, 'mode', 'graph') % to visualize the tree


pred = predict(t, testX);
```

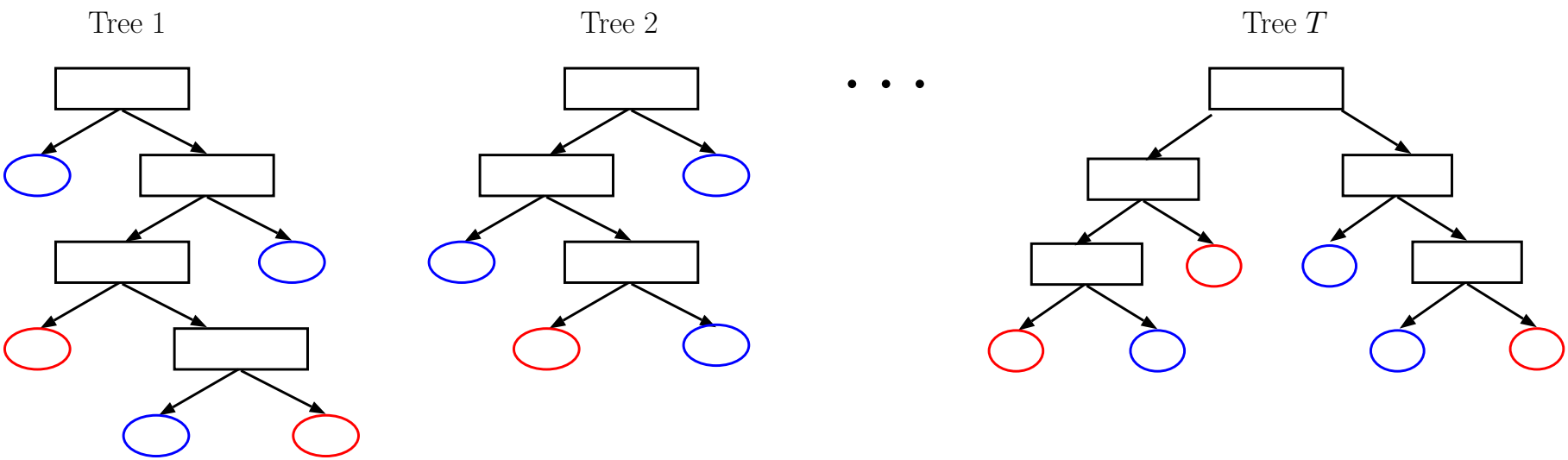
# Some remarks about classification trees

Classification trees are fast to build but considered as weak learners.

- The decision boundary is piecewise linear
- Unstable (if we change the data a little, the tree may change a lot)
- Prediction performance is often poor (due to high variance)
- No formal distributional assumptions (non-parametric)
- Works in the same way in multiclass settings
- Can handle large data sets
- Can handle categorical variables naturally

# Ensemble methods

Ensemble methods train many trees (or other kinds of weak classifiers) and combine their predictions to enhance the performance of a single weak learner:

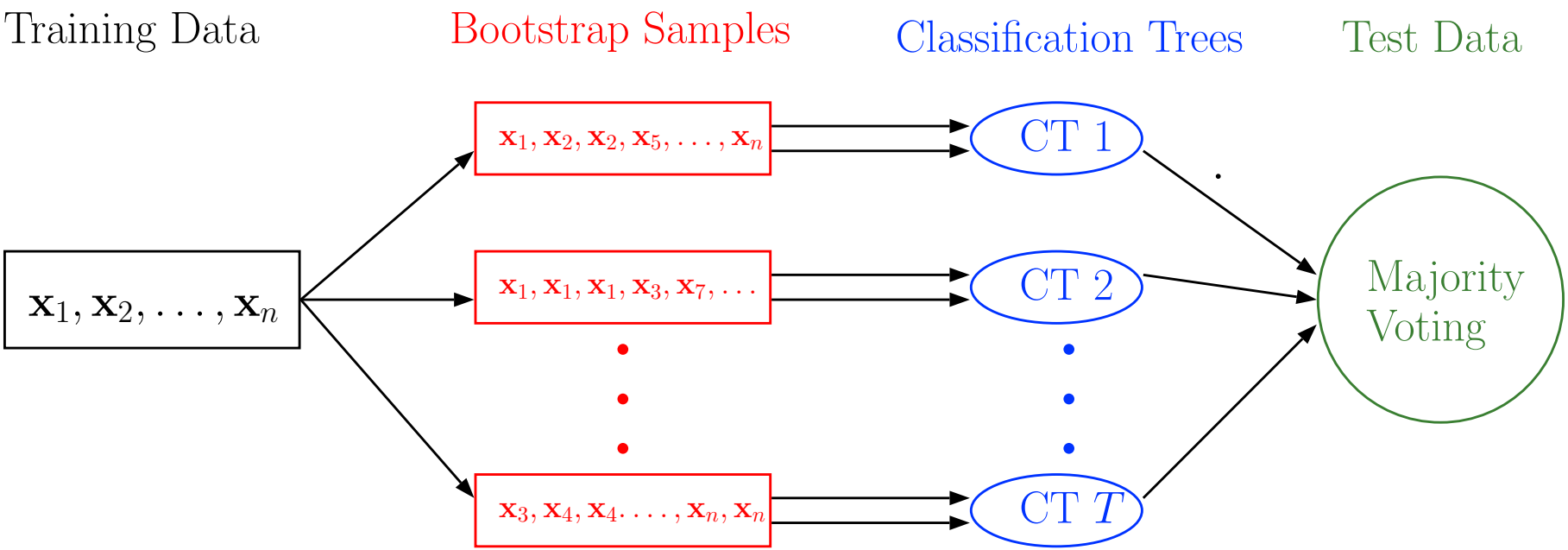


To be covered in this course:

- **Bagging (Bootstrap AGGregatING)**: build many trees independently from different bootstrap samples of the training data and then vote their predictions to get a final prediction
- **Random Forest**: a variant of bagging by allowing to use different subsets of variables at the nodes of any tree in the ensemble
- **Boosting**: build many trees adaptively and then add their predictions
  - AdaBoost (Adaptive Boosting)
  - GradientBoost (Gradient boosting)

# Bagging

**Idea**: build a classification tree on a separate **bootstrap sample** of the training data, i.e., a **random sample with replacement**, and then use majority vote.



# Out-of-bag

- Drawing $n$ out of $n$ observations with replacement omits on average **36.8%** of observations for each decision tree.
- We say that those samples left out by a tree are **out-of-bag (oob)** with respect to the tree.
- For each training example, we may vote the predictions of all the trees (for which the observation is oob) and compare with the true label to compute an average oob error.
- Such measure is an unbiased estimator of the true ensemble error and it does not require an independent validation dataset for evaluating the predictive power of the model.

# Some further comments on bagging

- Averaging many trees decreases the variance of the model, without increasing the bias (as long as the trees are not correlated)
- Bootstrap sampling is a way of de-correlating the trees (as simply training many trees on a single training set would give strongly correlated trees)
- The number of bootstrap samples/trees, $T$, is a free parameter. Typically, a few hundred to several thousand trees are used, depending on the size and nature of the training set.
- An optimal value of $T$ can be found using cross-validation, or by observing the out-of-bag error.

# MATLAB function for bagging

% train 50 trees with training data $X, y$ and make oob predictions in the meantime
**TB = TreeBagger(50, X, y, 'oobpred', 'on', 'NVarToSample', 'all')**;

% plot out-of-bag errors figure; plot(oobError(TB))
xlabel('number of grown trees')
ylabel('out-of-bag classification error')

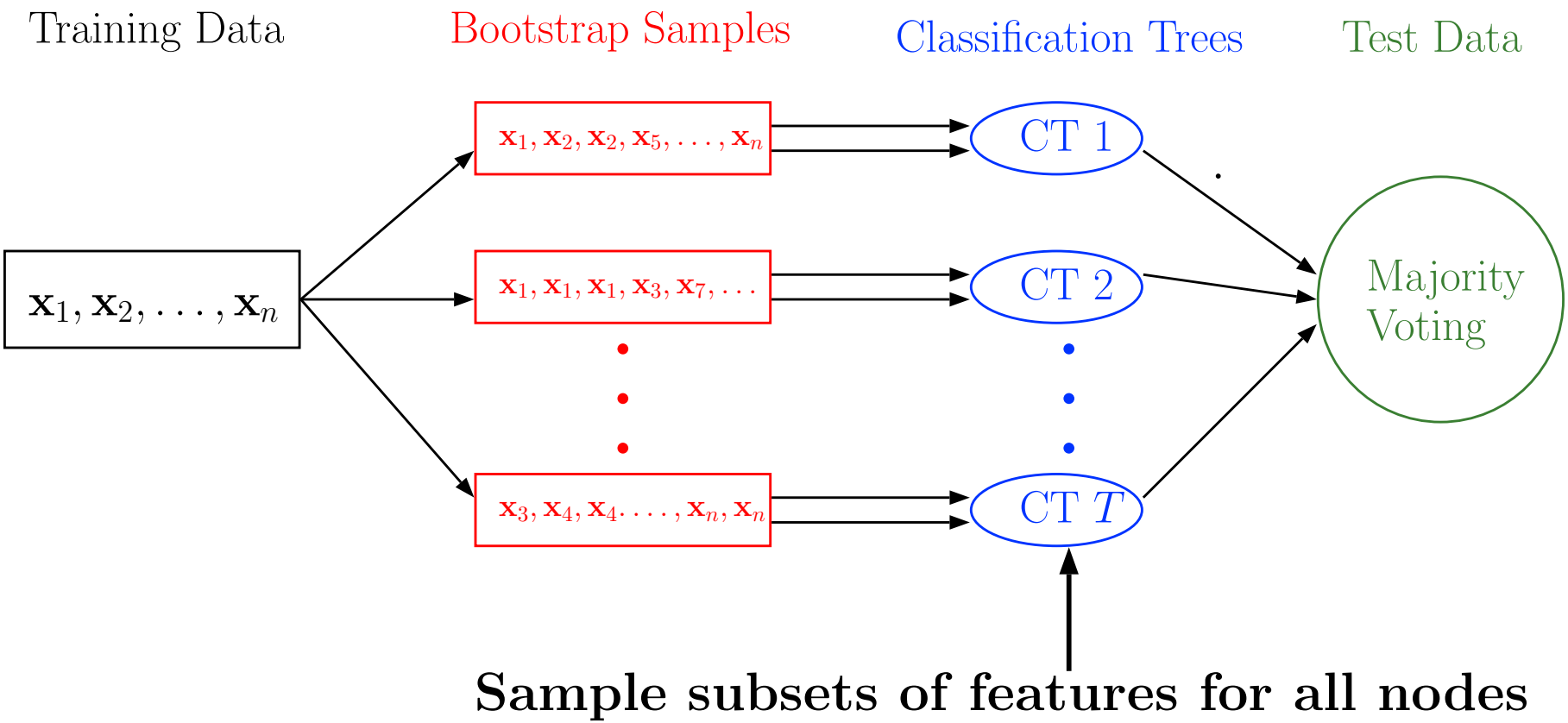
**pred = predict(TB, testX)**; % make prediction
**pred = cellfun(@str2num, pred)**; % convert string cell output to vector

# Random forest

Random forests improve bagging by **allowing every tree in the ensemble to randomly select predictors for its nodes**. This process is sometimes called "feature bagging".

The motivation is to further de-correlate the trees in bagging: If one or a few features are very strong predictors for the class label, these features will be selected in many of the trees, causing them to become correlated.

Typically, for a classification problem with $d$ features, $\sqrt{d}$ features (selected at random) are used in each split.


Training Data
Bootstrap Samples
Classification Trees
Test Data
$\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$
$\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_2, \mathbf{x}_5, \ldots, \mathbf{x}_n$
$\mathbf{x}_1, \mathbf{x}_1, \mathbf{x}_1, \mathbf{x}_3, \mathbf{x}_7, \ldots$
$\mathbf{x}_3, \mathbf{x}_4, \mathbf{x}_4. \ldots, \mathbf{x}_n, \mathbf{x}_n$
CT 1
CT 2
CT $T$
Majority Voting
Sample subsets of features for all nodes

# MATLAB function 1 for random forest

% train 50 trees with feature bagging + oob prediction
**TB = TreeBagger(50, X, y, 'oobpred', 'on', 'NVarToSample', 40)**;
% default value of 'NVarToSample' $= \sqrt{d}$, so you don't really need to specify this option

% make prediction
**pred = predict(TB, testX)**;
**pred = cellfun(@str2num, pred)**; % convert string cell output to vector

# MATLAB function 2 for random forest

```
% build a random forest of 50 trees for classification
ens = fitensemble(X, y, 'bag', 50, 'Tree', 'type', 'classification');

% or instead
temp = templateTree('NumVariablesToSample', sqrt(d));
ens = fitensemble(X,y,'bag',50,temp,'type','classification');


% make predictions on test data
pred = predict(ens, testX);
```

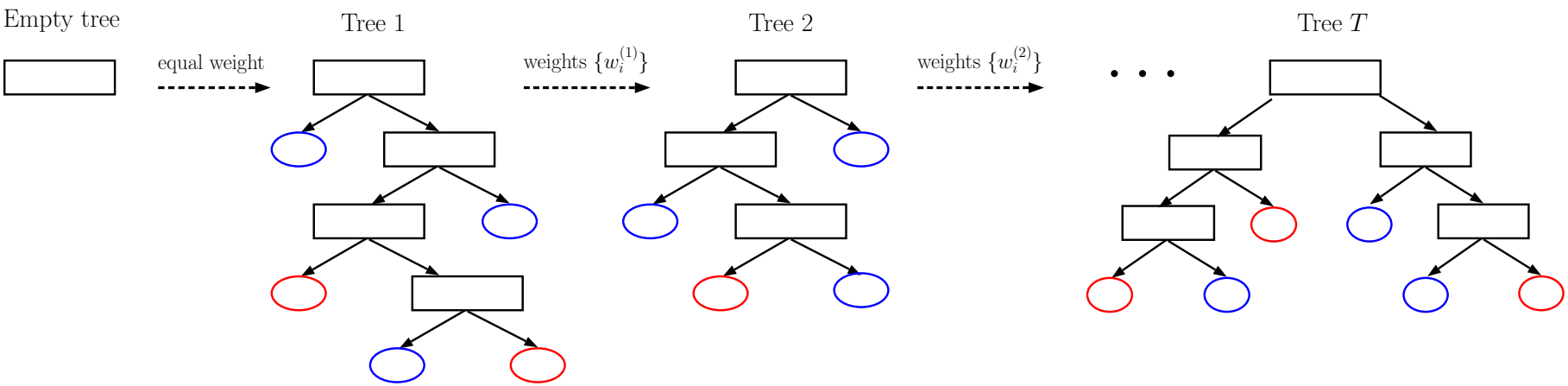
## Python function for random forest

See documentation at

`http://scikit-learn.org/stable/modules/generated/sklearn.ensemble.RandomForestClassifier.html`

# AdaBoost (Adaptive Boosting)

**Main idea**: build tree classifiers sequentially by" focusing more attention" on training errors made by the preceding trees and then add their predictions.




One way to realize this idea is to **reweight the training data** for each new tree based on the training error of the previous trees.

# How to choose weights

Initially (for the first tree in the ensemble), all training examples have an equal weight, i.e., $w_i^{(0)} = \frac{1}{n}, \forall\, i$.

For any subsequent tree $t > 1$,

- Compute the training error by first $t-1$ trees, denoted as $\epsilon_t$
- Choose $\alpha_t = \log \frac{1-\epsilon_t}{\epsilon_t}$
- Modify the weights of the misclassified points by $w_i^{(t)} = w_i^{(t-1)} \cdot \exp(\alpha_t)$ (no change for the correctly classified points)
- Renormalize all $w_i^{(t)}$ to have a sum of 1.

# How to use weights

Consider a weighted training set $(\mathbf{x}_i, y_i, w_i^{(t)}), 1 \le i \le n, t \ge 1$. In all calculations (wherever used), every training point $\mathbf{x}_i$ will count as "$w_i^{(t)}$ points".

For example, when computing the Gini impurity for a candidate split

$$n^{(\mathrm{L})} \sum_{j=1}^{k} p_j^{(\mathrm{L})}(1 - p_j^{(\mathrm{L})}) + n^{(\mathrm{R})} \sum_{j=1}^{k} p_j^{(\mathrm{R})}(1 - p_j^{(\mathrm{R})})$$

we will use instead

$$n^{(\mathrm{L})} = \sum_{i \in \text{left node}} w_i^{(t)} \qquad \text{and} \quad p_j^{(\mathrm{L})} = \frac{1}{n^{(\mathrm{L})}} \sum_{i \in \text{class } j \cap \text{left node}} w_i^{(t)}$$

# How to combine the trees

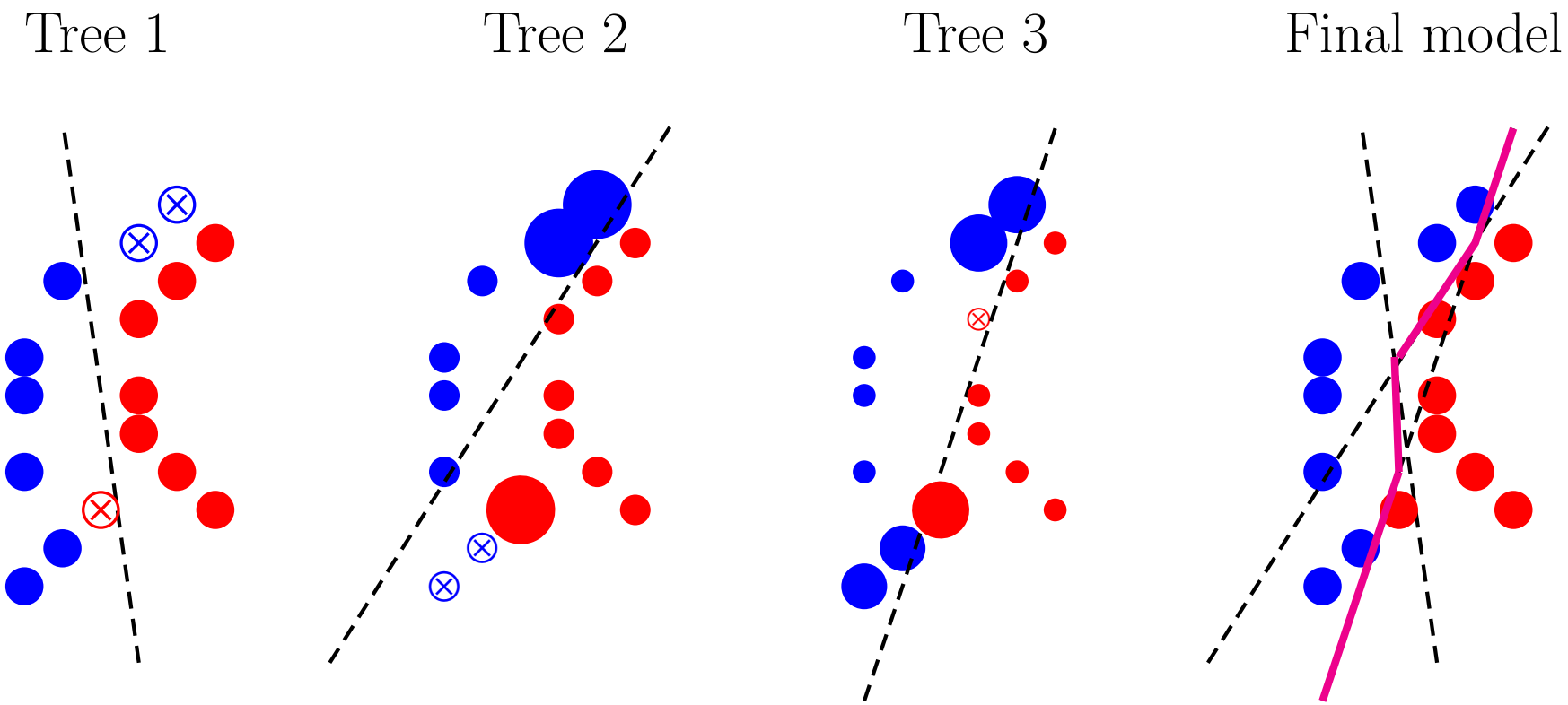
The final prediction is made based on the learned function

$$f(\mathbf{x}) = \sum_{t=1}^{T} \alpha_t C_t(\mathbf{x})$$

by voting with weights $\alpha_t = \log \frac{1-\epsilon_t}{\epsilon_t}$ for the different trees:

$$j^* = \text{argmax}_j \sum_{t\,:\,C_t(\mathbf{x})=j} \alpha_t$$

# Demo: an ensemble of 3 boosted trees




Observe that no point was predicted wrong more than once!

# Some comments on AdaBoost

- Given any weak learner better than random guess (i.e., error rate $< 0.5$), AdaBoost can achieve an arbitrarily high accuracy on the training data.
- Excellent generalization performance
- Can handle many features easily
- In general, AdaBoost $\succ$ random forest $\succ$ bagging $\succ$ single tree
- Lots of variants since AdaBoost (first significant boosting method )
  - GradientBoost (to be covered in Ryan's final project presentation)
  - GentleBoost, LogitBoost, and many more

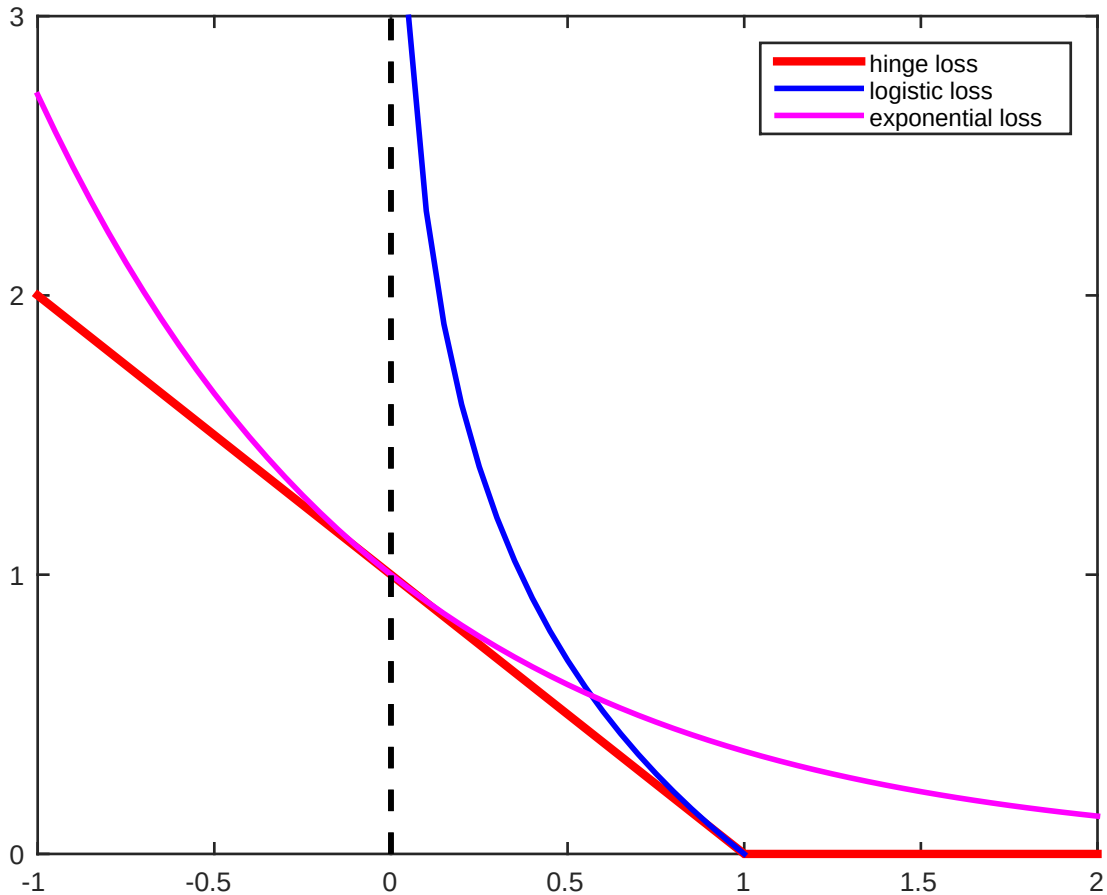
- It can be shown (see e.g. `https://en.wikipedia.org/wiki/AdaBoost`) that in the binary setting ($y_i = \pm 1$), AdaBoost builds an **additive logistic regression model of trees**

$$f(\mathbf{x}) = \log \frac{P(Y = 1 \mid \mathbf{x})}{P(Y = -1 \mid \mathbf{x})} = \sum_{t=1}^{T} \alpha_t C_t(\mathbf{x})$$

by using the **exponential loss**

$$L(y, f(\mathbf{x})) = e^{-y \cdot f(\mathbf{x})} = \begin{cases} \frac{1}{e}, & \text{if } y \cdot f(x) = 1; \\ e, & \text{if } y \cdot f(x) = -1 \end{cases}$$

In contrast, logistic regression trains an optimal linear combination of the *features* under the *logistic loss*.


hinge loss
logistic loss
exponential loss
3
2
1
0
-1
-0.5
0
0.5
1
1.5
2

# MATLAB function for AdaBoost

```
% build an ensemble of 50 trees by adaptive boosting
ens = fitensemble(X, y, 'AdaBoostM1', 50, 'Tree'); % for 2 classes
ens = fitensemble(X, y, 'AdaBoostM2', 50, 'Tree'); % for 3 or more classes


% make predictions on test data
pred = predict(ens, testX);
```

## Python function for AdaBoost

See documentation at

`http://scikit-learn.org/stable/modules/generated/sklearn.ensemble.AdaBoostClassifier.html`

## Exercise

Apply Bagging, Random Forest, and AdaBoost (with the same number of trees) to the digits 4 and 9 in the MNIST dataset and compare their performance.

# Summary

- Classification trees (weak learner)
- Ensemble methods
  - Independent trees: bagging, random forest
  - Adaptive trees: boosting such as AdaBoost (and GradientBoost)
- Many advantages:
  - Simple and fast
  - Can handle large data well (with automatic feature selection)
  - Excellent performance

# Optional HW6a (due Wed. noon, May 17)

This homework tests the ensemble methods on the MNIST digits. In all questions below report your results using both graphs and texts.

1. Apply bagging with 500 trees to the MNIST handwritten digits. Plot the out-of-bag error and use it to select a reasonable number of trees. Apply bagging again but with this size instead to the dataset. How does the corresponding test error compare with that you obtained with 500 trees?

2. Repeat Question 1 with random forest instead of bagging.

3. Repeat Question 1 with adaptive boosting instead of bagging.

## Midterm project 6: Ensemble learning

This project asks you to describe the ensemble methods and summarize the results obtained on the MNIST digits. You are also encouraged to try new options and compare with other relevant methods.