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Classification with PAM and Random Forest

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Two roads to classification

- **Given:** patient profiles already diagnosed by an expert.
- **Task:** infer a general rule to diagnose new patients.
- Basically, there are two ways to solve this task
 1. **model class probabilities**
QDA, LDA, ...
 2. **model class boundaries** directly
Optimal Separating Hyperplanes, Random Forest

What's the problem?

In classification you have to trade off

- overfitting versus underfitting
- bias versus variance.

Curse of dimensionality! In 12'000 dimensions even linear methods are very complex! High variance!

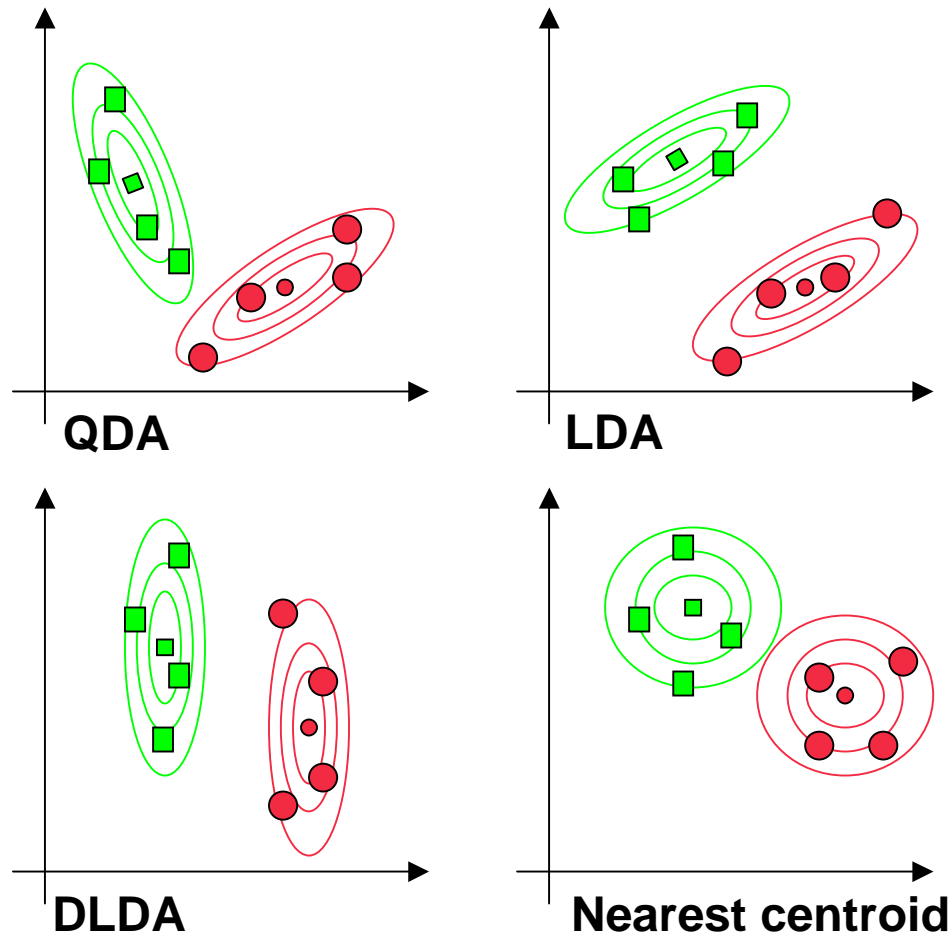
Simplify your models

Discriminant analysis and gene selection

Comparing Gaussian likelihoods

- **Assumption:** each group of patients is well described by a normal density.
- **Training:** estimate mean and covariance matrix for each group.
- **Prediction:** assign new patient to group with higher likelihood.
- **Constraints** on covariance structure lead to different forms of discriminant analysis.

Discriminant analysis in a nutshell



Characterize each class by **mean** and **covariance structure**.

1. **Quadratic D.A.**
different COVs
2. **Linear D.A.**
requires same COVs.
3. **Diagonal linear D.A.**
same diagonal COVs.
4. **Nearest centroids**
forces COVs to $\sigma^2 I$.

Discriminant analysis in a nutshell

Choose k that maximizes the **linear discriminant function**

$$\delta_k(x) = x^t \Sigma^{-1} \mu_k - \frac{1}{2} \mu_k^t \Sigma^{-1} \mu_k + \log \pi_k$$

The given data

Covariance matrix:
same for all groups

Group centroid:
one for each group

Prior class probability

For **DLDA**: Choose k that minimizes

$$\delta_k(x) = \sum_g \frac{(x_g - (\mu_k)_g)^2}{\sigma_g^2} - 2 \log \pi_k$$

variance of gene i

Feature selection

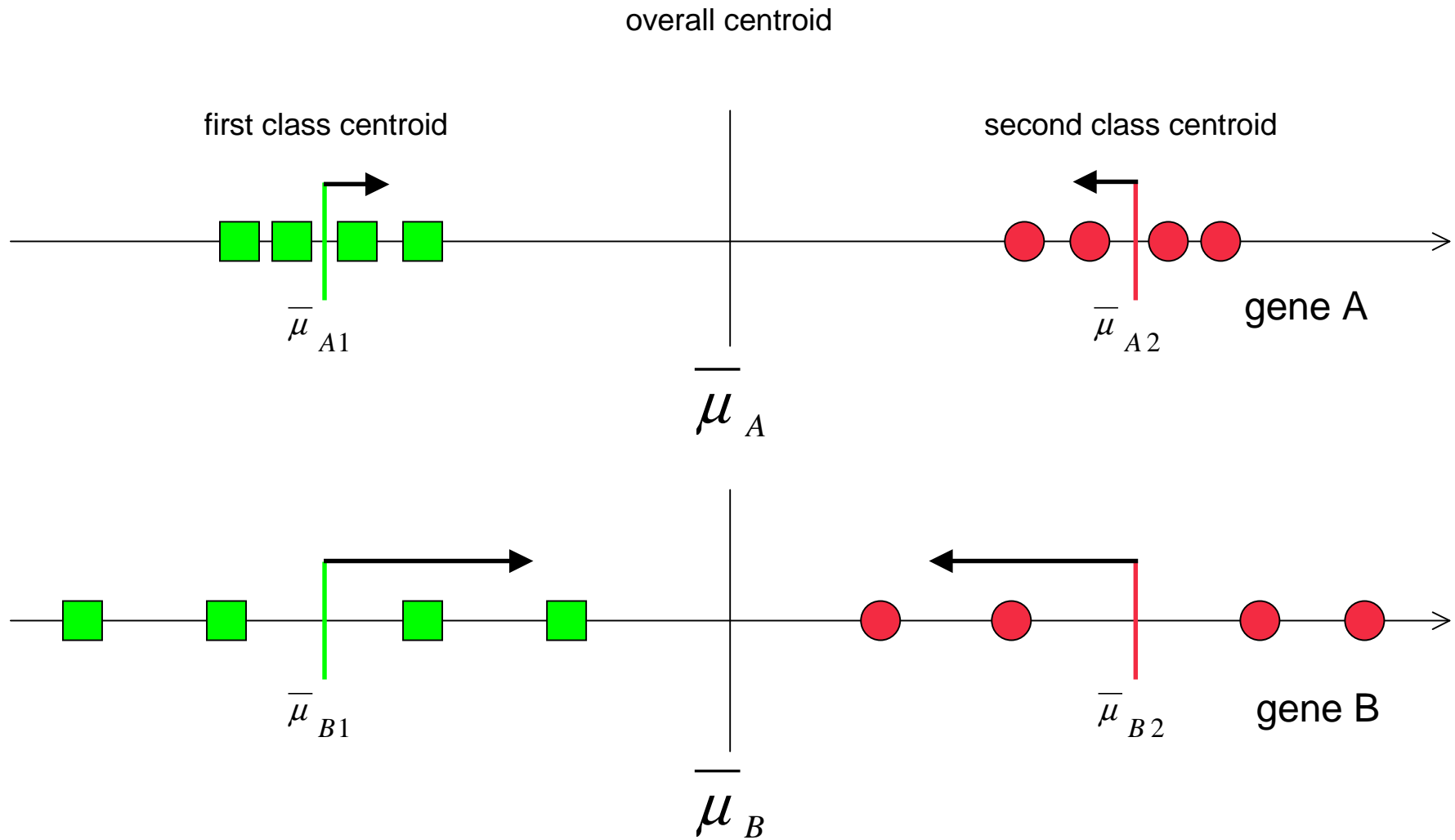
Next simplification:

Base the classification only on a small number of genes.

Feature selection: Find the **most discriminative genes**.

1. **Filter**: Rank genes according to discriminative power by t-statistic, Wilcoxon, ...
Use only the first k genes for classification. Discrete, hard thresholding.
2. **Shrinkage**: Continuously shrink genes until only a few have influence on classification.
Example: **Nearest Shrunken Centroids**.

Shrunken Centroids



Nearest Shrunken Centroids

The difference between the **group centroid** for gene i and class k and the **overall centroid** can be written as follows:

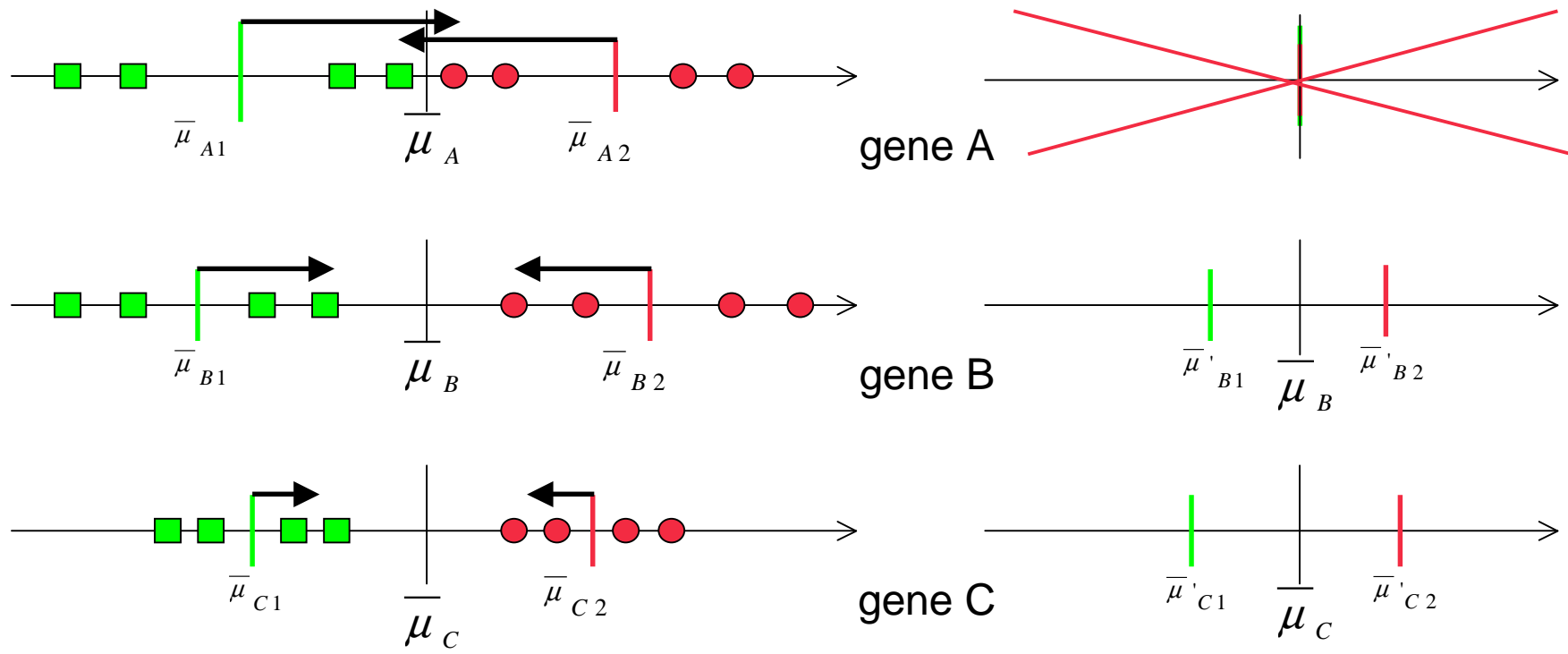
$$\bar{\mu}_{gk} - \bar{\mu}_g = \sqrt{1/n_k + 1/n} \cdot (s_g + s_0) \cdot d_{gk}$$

where s_i is the pooled within-class standard deviation of gene i and s_0 is an offset to guard against genes with low expression levels.

Shrinkage: Each d_{gk} is reduced by Δ in absolute value, until it reaches zero. Genes with $d_{gk}=0$ for all classes do not contribute to the classification.

(Tibshirani et al., 2002)

Shrunken Centroids



$$\delta_k \left(\begin{pmatrix} x_B^* \\ x_C^* \end{pmatrix} \right) = \frac{(x_B^* - \bar{\mu}'_{Bk})^2}{(s_B + s_0)^2} + \frac{(x_C^* - \bar{\mu}'_{Ck})^2}{(s_C + s_0)^2} - 2 \log \pi_k$$

Shortcomings of filter and shrinkage methods

- Filter and Shrinkage work only on **single genes**.
They don't find interactions between groups of genes.
- Filter and Shrinkage methods are only **heuristics**.
Search for best subset is infeasible for more than 30 genes.

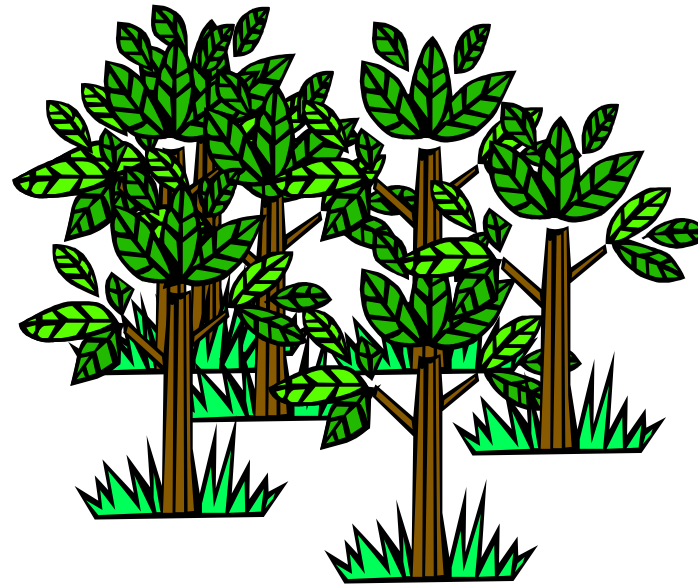
Random Forest

Random Forest

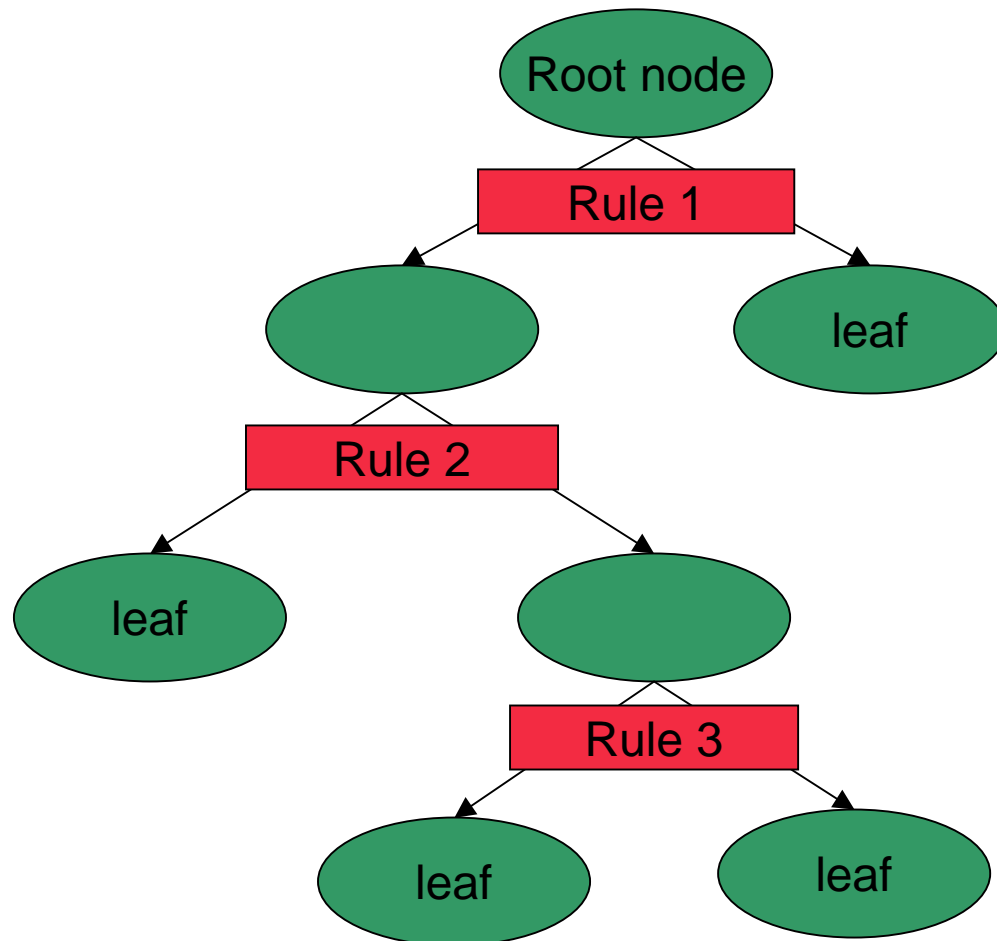
- Growing one tree



- Growing many trees (a forest)

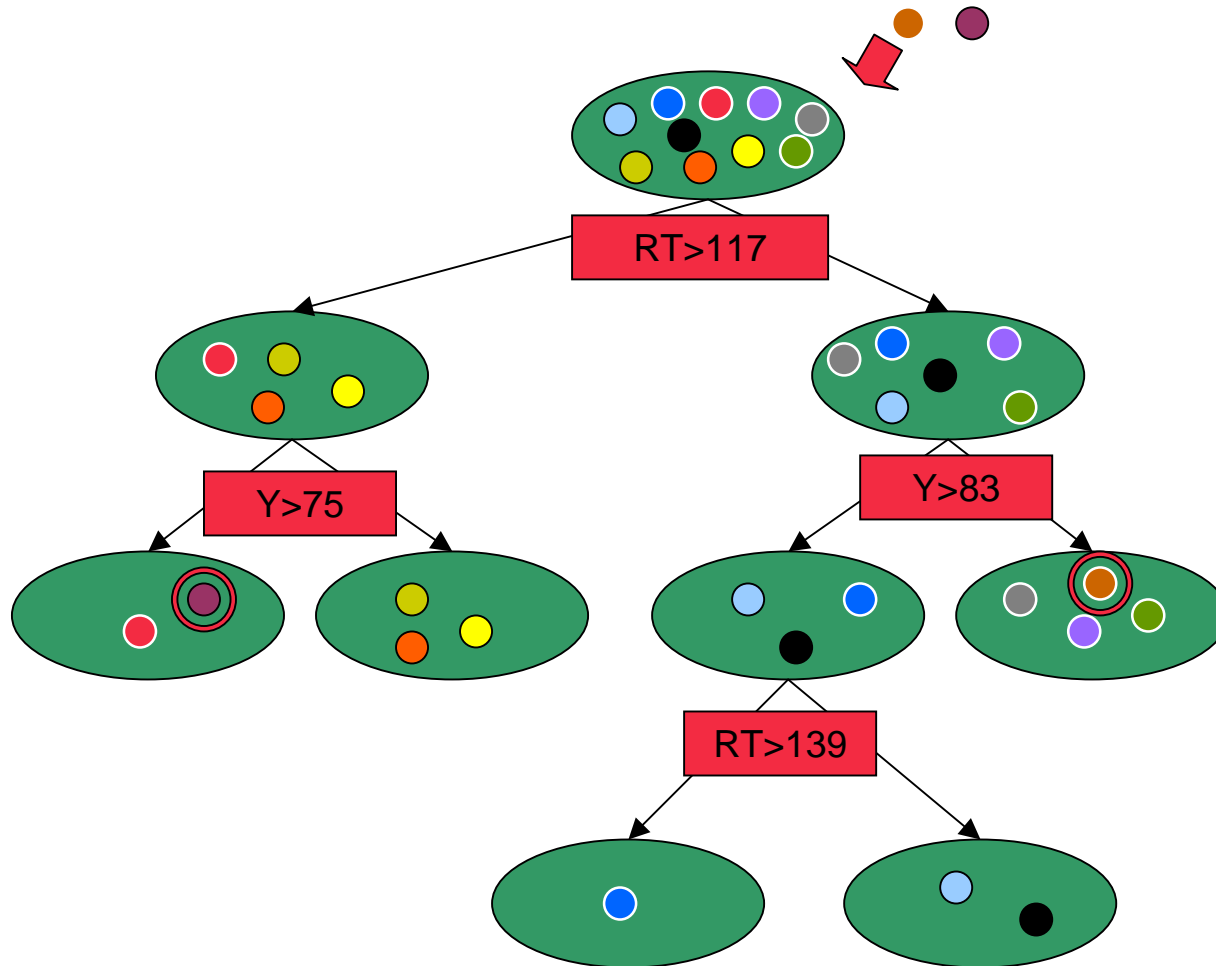


A binary tree for classification



- The root node contains all samples.
- Each node contains a fraction of samples.
- Each rule splits up the samples into two groups.
- Every rule is of the form
 - $X > t$ for continuous X
 - $X \in A$ for categorical XOnly one variable per rule.
- Each leaf should be more or less pure (contains only samples of one type).
- A new sample is run through the tree and one looks for the leaf it ends up.

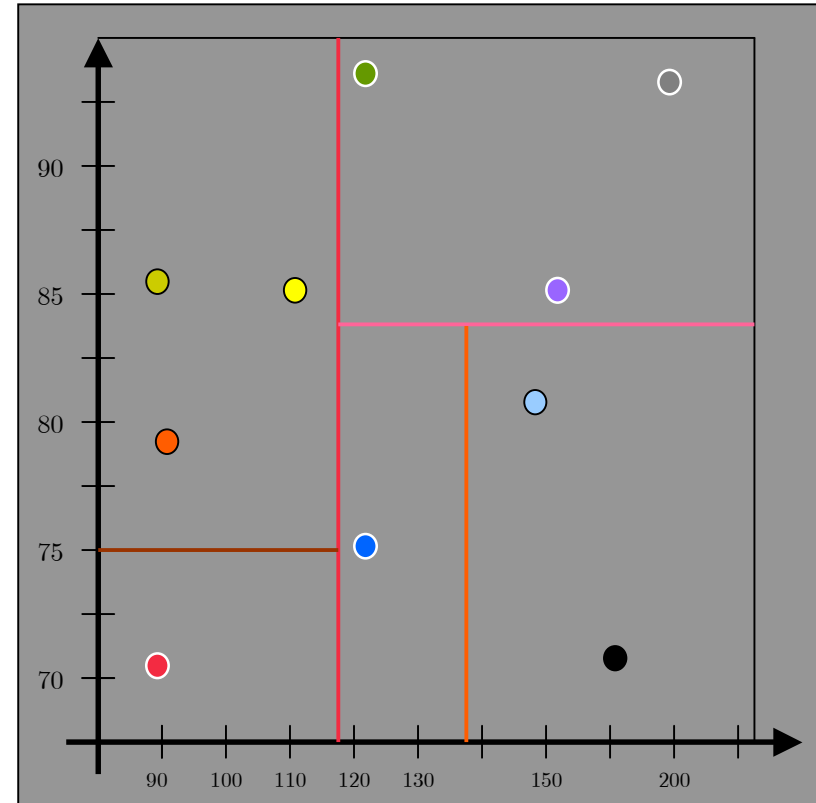
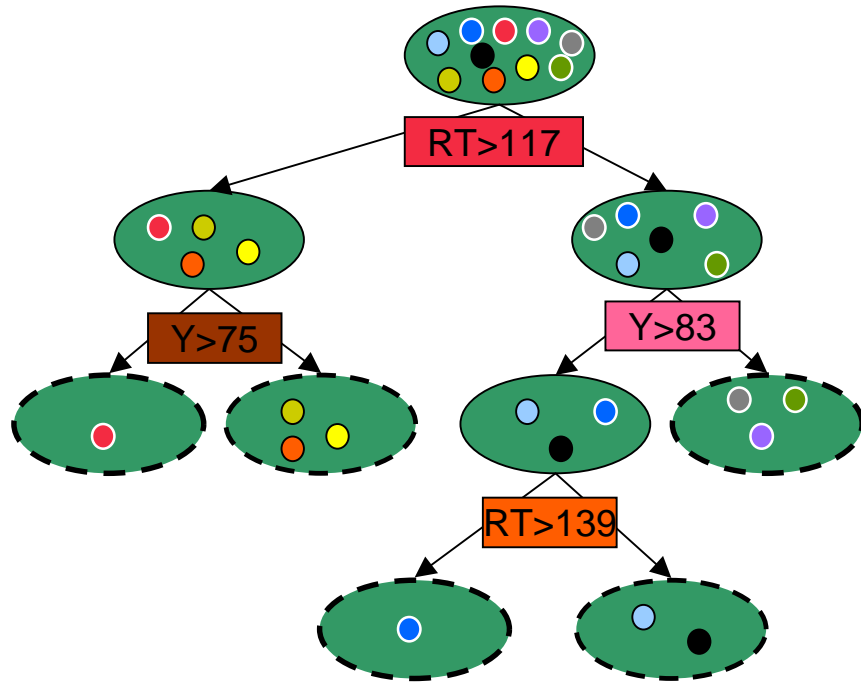
A binary tree – a classification example



Title	Year (Y)	Running time (RT)	Spielberg
Jaws	75	124	X
Duel	71	90	X
The Color Purple	85	154	X
Schindler's List	93	195	X
Jurassic Park	93	127	X
Back to the future	85	111	
The Godfather	72	175	
Das Boot	81	150	
Life of Brian	79	94	
Stand by me	86	89	

Hook	91	144	X
Harold and Maude	71	91	

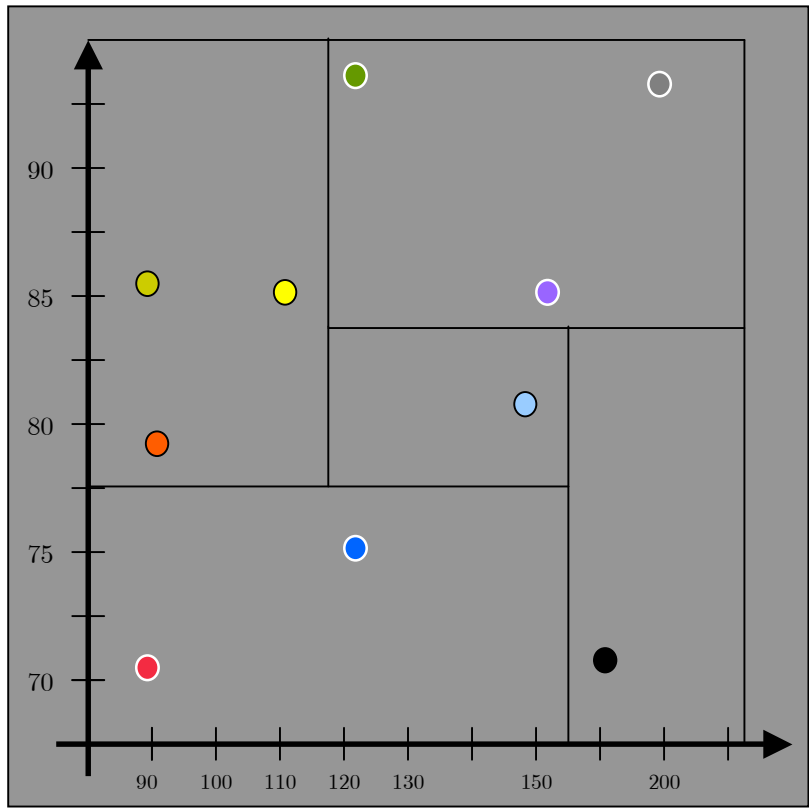
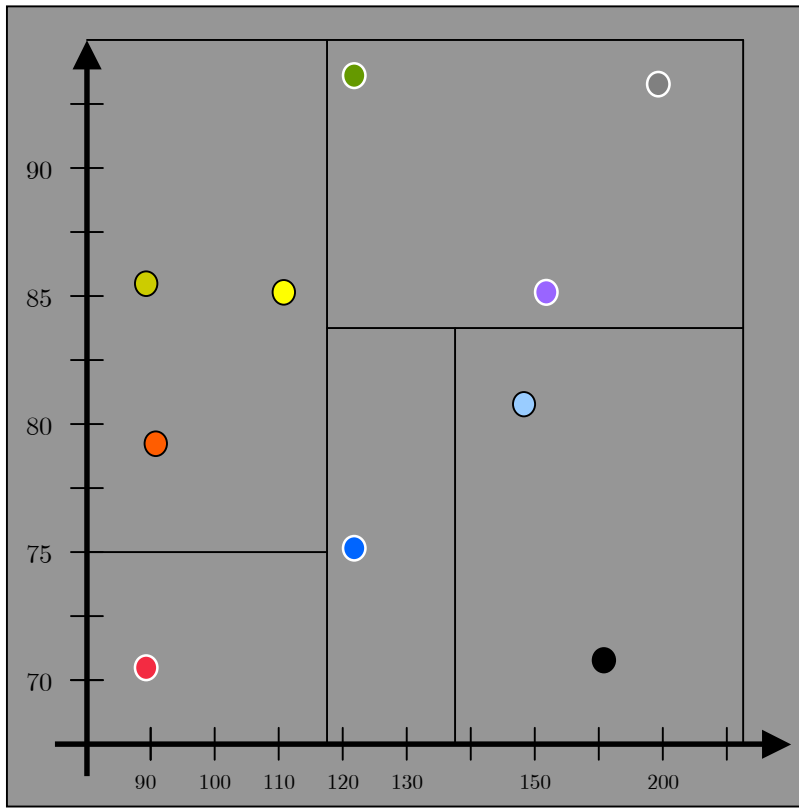
A binary tree – a classification example



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Not every partition can be achieved through a tree



How to construct a tree?

- Choose a good node/rule pair (x_i, t_i) for each split („Splitting rule“)
 - Which parameter should we choose?
 - Which threshold should we use?
- Decide how many nodes your tree should have („Split-stopping rule“, „pruning“).
- Assign a class to each leaf („Class assignment rule“).

Splitting rule

Impurity function $\Phi: [0,1]^k \rightarrow \mathfrak{R}$ (k : number of different classes)

A low impurity function is achievable.

Attributes:

- minimal for $(1,0,0,\dots,0)$ and all permutations.
- maximal for $(1/k,\dots,1/k)$
- is symmetric function
 $\Phi(p_1,\dots,p_n) = \Phi(\varphi(p_1),\dots,\varphi(p_n))$ for all permutations φ

There are various impurity functions: [entropy](#), [Gini index](#)

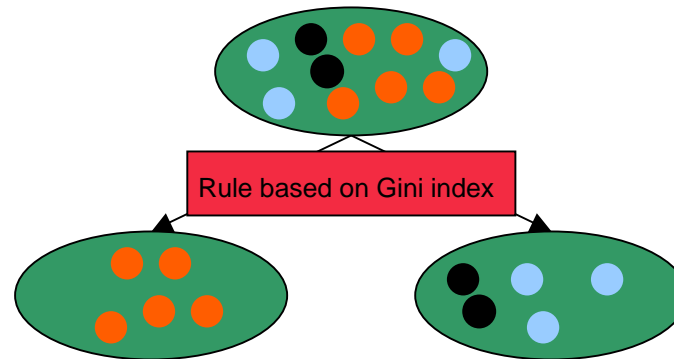
Gini index

Gini index $\Phi(p_1, \dots, p_k) = 1 - \sum p_i^2 = \sum p_i (1 - p_i) = \sum \sum p_i p_j$

Minimum 0

Maximum $1 - 1/k$

Gini index tries to separate the largest class from the rest.



Gini index for two classes:

$$\Phi(p_1, p_2) = 2p_1p_2$$

Using the impurity function

Define a function $i(v)$ (v is a node of the tree)

$$i(v) = \Phi(P(1|v), \dots, P(k|v)).$$

$P(j|v) :=$ probability that you are member of class j if you are in node v

If the probabilities for all classes are equal one has

$$i(v) = \Phi(n_1(v)/n(v), \dots, n_k(v)/n(v)).$$

$n(v) =$ all samples in node v

$n_j(v) =$ all samples of class j in node v

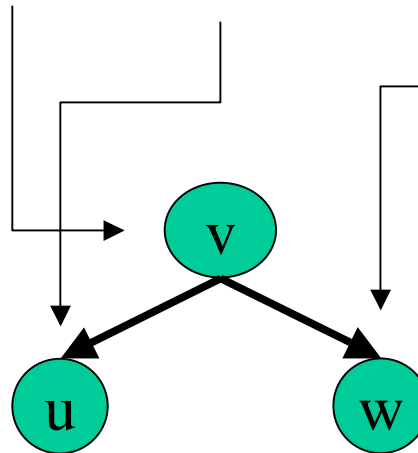
Two classes, Gini index, equal probability:

$$i(v) = \frac{2 n_1(v) n_2(v)}{n(v)^2}$$

Goodness of fit – decrease of impurity

Determine variable x and threshold t that maximizes the following term:

$$G = i(v) - (p_u i(u) + p_w i(w))$$



p_u = fraction of samples in node u
 p_w = fraction of samples in node w

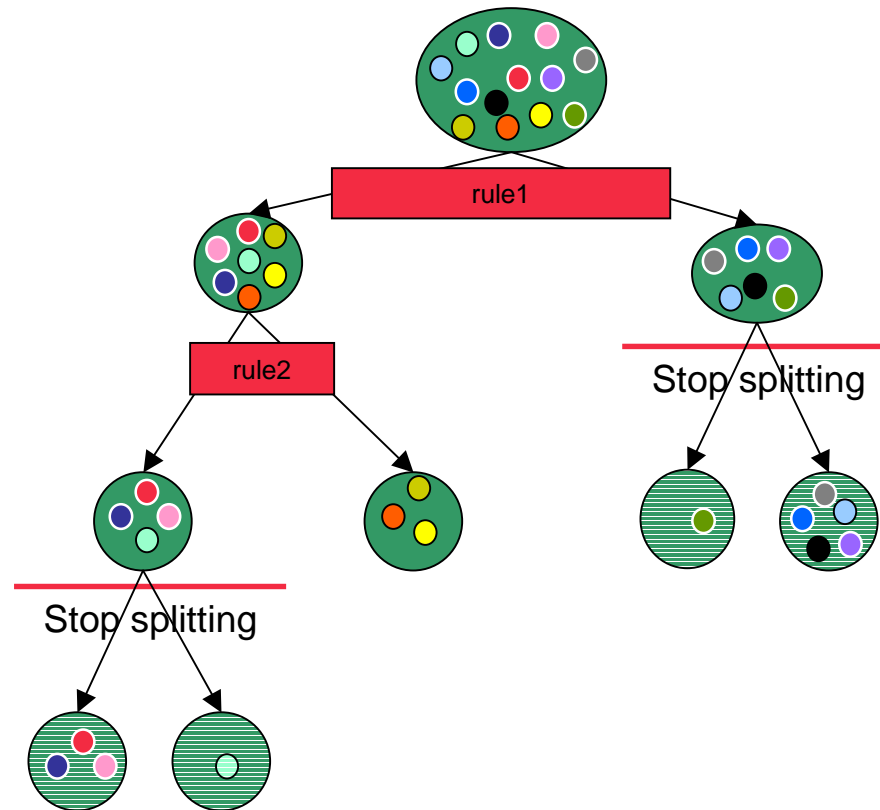
Because you have only a finite number of parameters and a finite number of values, you have to test a finite number of pairs.

Two classes, Gini index, equal probability:

$$G = \frac{2}{n(v)} \cdot \left(\frac{n_1(v)n_2(v)}{n(v)} - \frac{n_1(u)n_2(u)}{n(u)} - \frac{n_1(w)n_2(w)}{n(w)} \right)$$

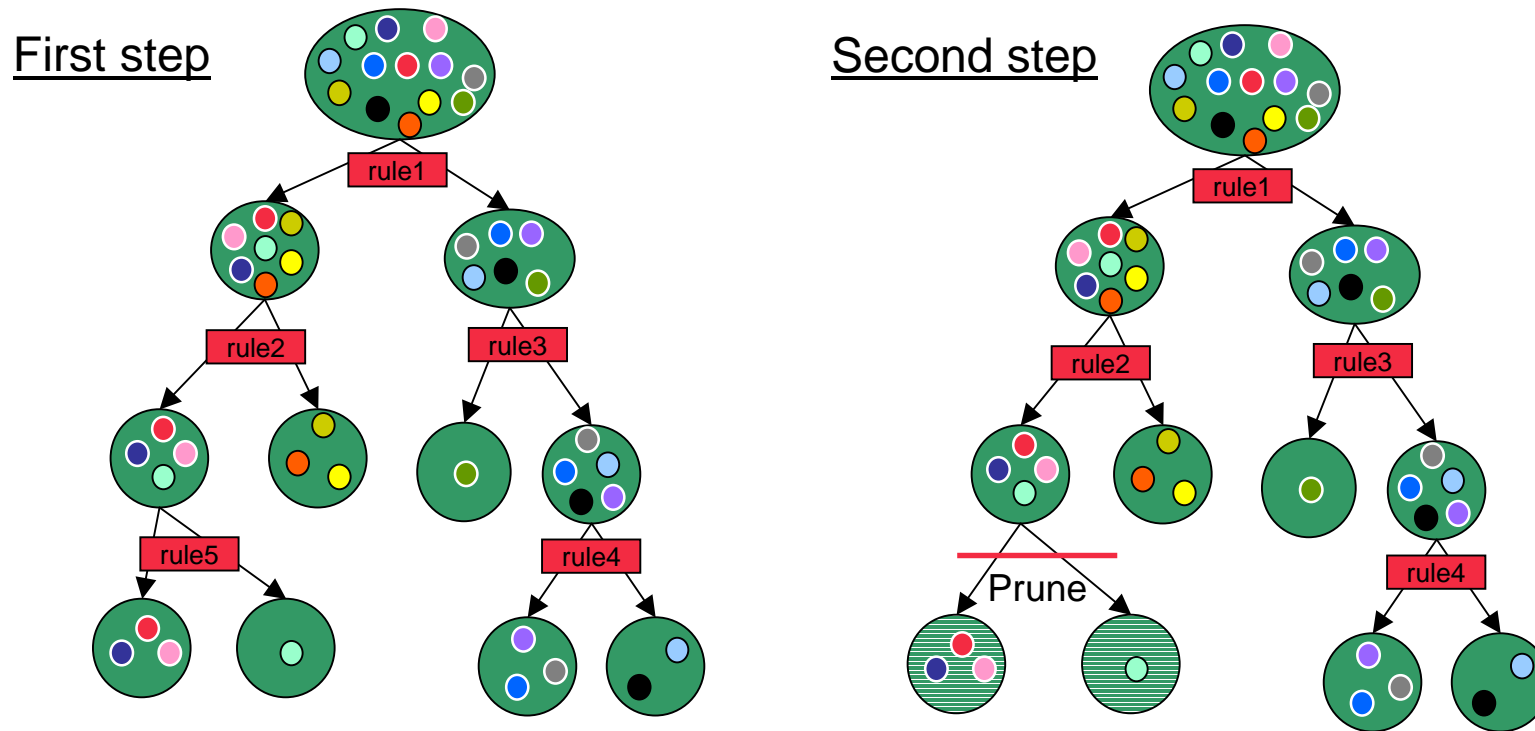
Stop splitting rules – stop decision

- Decide at each node if the node should be split further or not. Is there a high decrease in the Gini index?



Stop splitting rules - pruning

- First split until each node is pure or has a maximum number of elements, then prune the tree. Remove the splits with low decrease in the impurity function.



Advantages and Disadvantages for trees

- Advantages
 - At first sight good interpretation
 - Can cope with any data structure or type
 - Uses conditional information effectively
 - Invariant under transformations of the variables
- Disadvantages
 - not robust
 - classification performance is not that good
 - You have to do a variable selection
 - Variables can be hidden due to other variables

From the tree to the forest

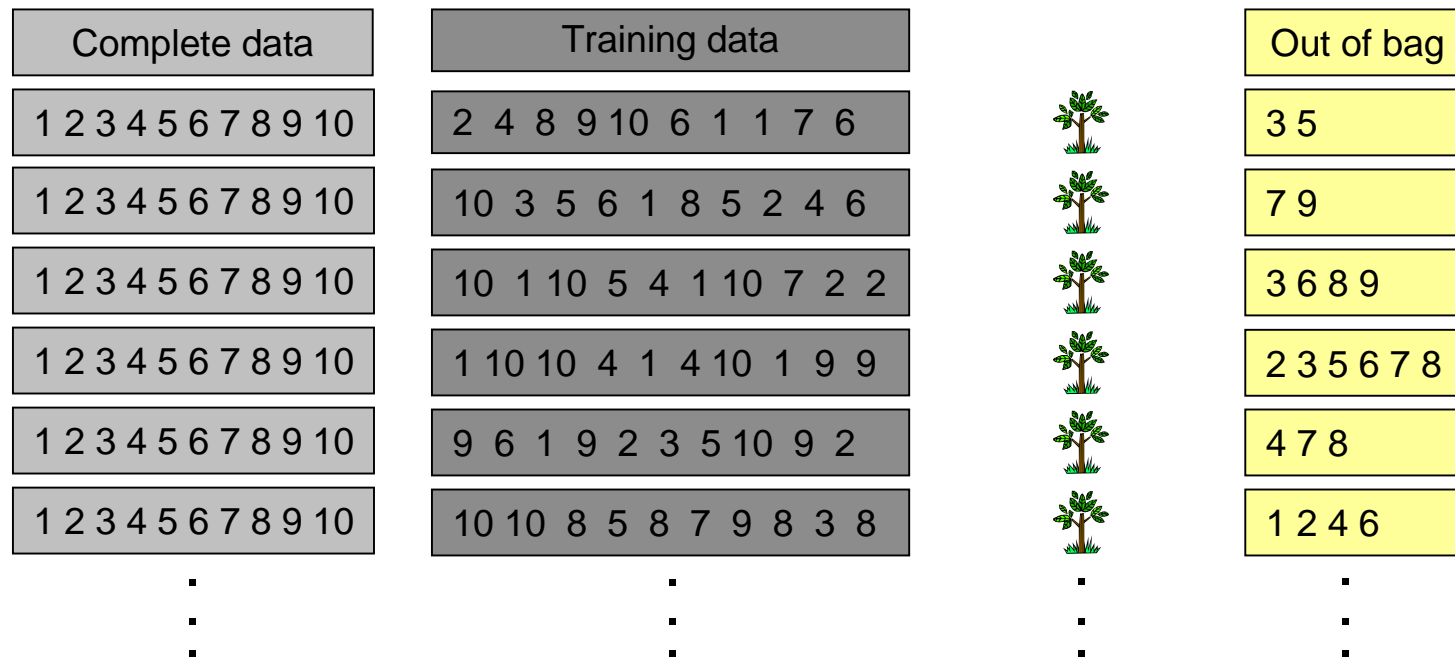
- **General idea:** combine collection of weak learners to construct a classification algorithm with better properties.
- **Here:** Construct a collection of trees and combine results of individual trees.

- Because the algorithm is deterministic, we have to introduce some kind of randomness. For each tree we will have two different sources of randomness:
 - random training set (bootstrap)
 - random variable selection

Bootstrap

- Complete data : K samples/patients
- Training data: draw K times with replacement from the data set
- Out of bag: sample that do not belong to the training set

Training data contains approximately 2/3 of the elements of the complete data set.

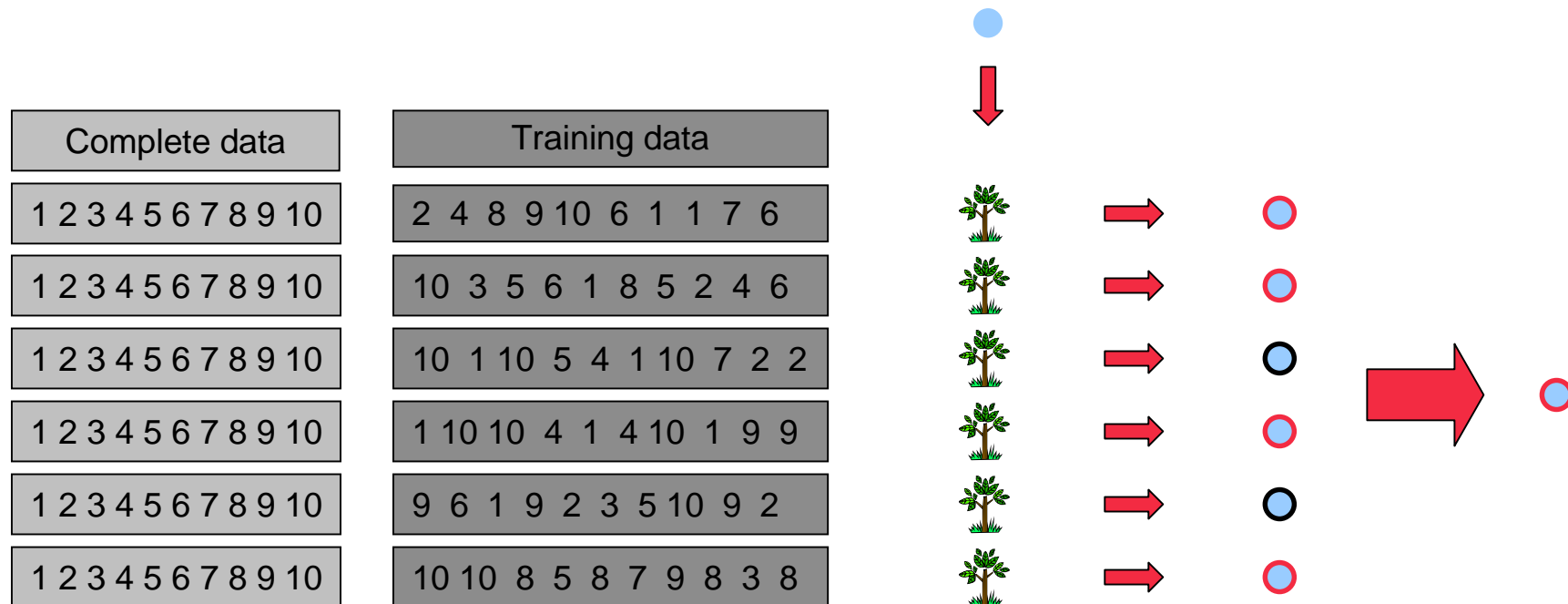


Random Forest – random variable selection

- Set the parameters **m** and **s**. These are the same for all nodes and all trees. Specify the number of trees you want to grow.
- For each tree:
 - Use bootstrap to get a training set T . You use only data from this set to build the tree!
 - For each node, first choose **m** parameters x_1, \dots, x_m at random.
 - Upon these parameters choose the best pair (x_i, t_i) .
 - Go on until each node contains elements of one class or consists of **s** elements.

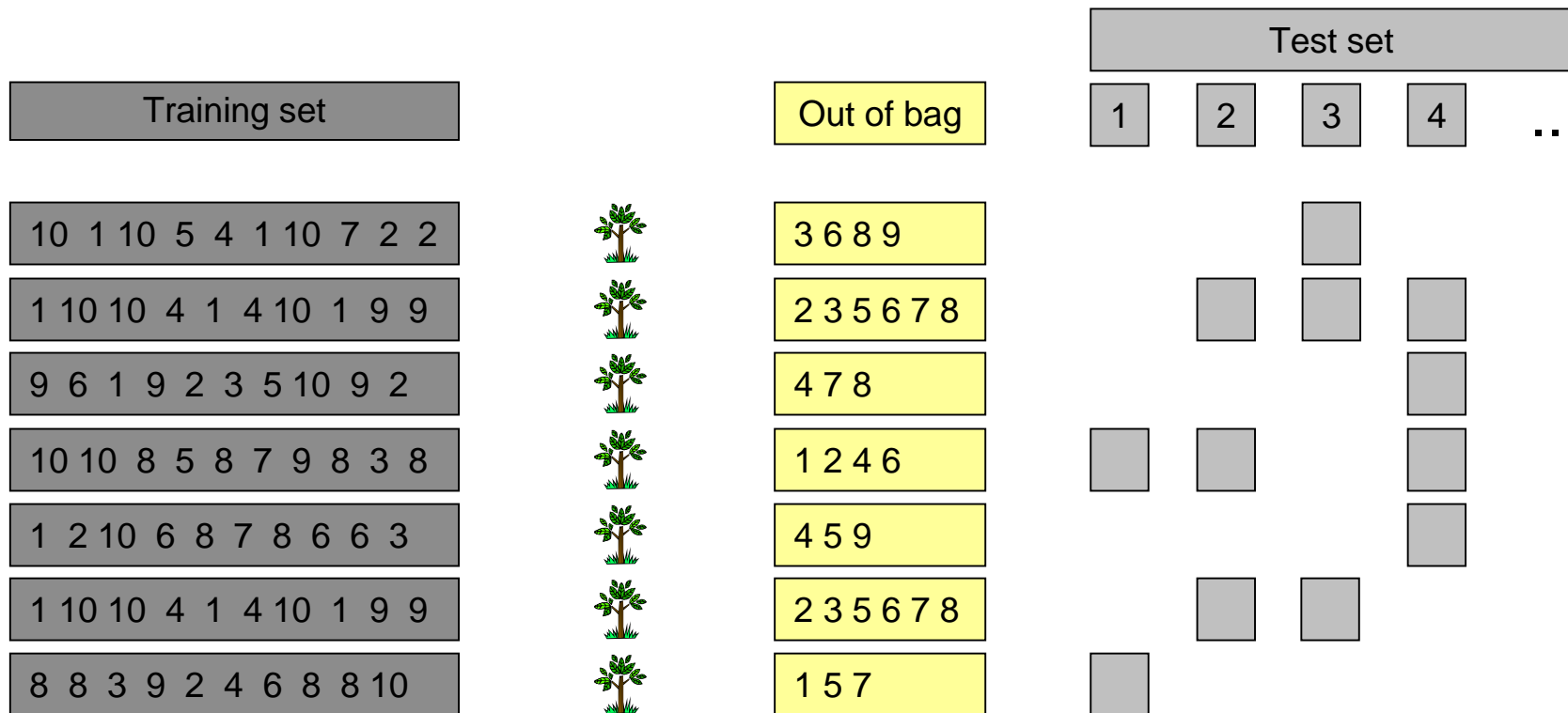
Random Forest

- Classification rule: First classify a new sample with each tree. In the end form a major vote.



Estimating the test error

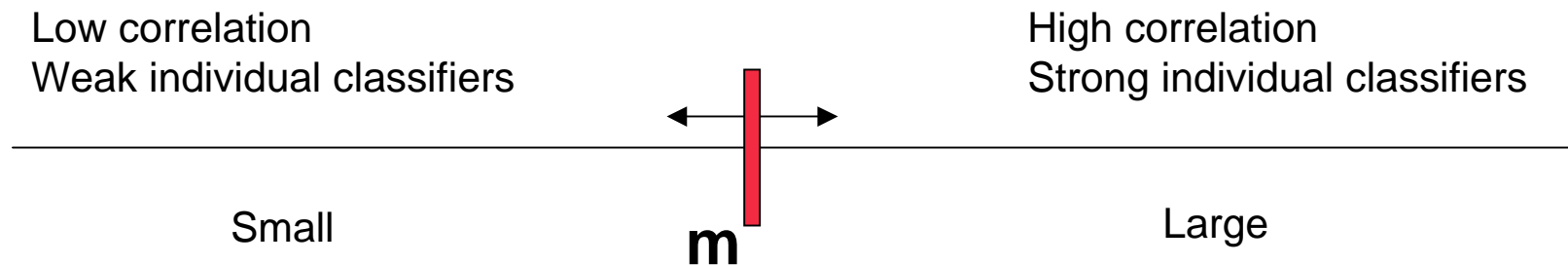
- For each sample x predict the class but use only the trees for which x belongs to the OOB set.
- Good estimate for the test error because the information provided by x was not used for building these trees.



Tradeoff correlation - prediction

The forest error rate depends on two things:

- The correlation between any two trees in the forest. Increasing the correlation increases the forest error rate.
- The strength of each individual tree in the forest. A tree with a low error rate is a strong classifier. Increasing the strength of the individual trees decreases the forest error rate.



Use the OOB error estimate to find a good parameter m .

Variable importance

Idea: Change the values of a parameter x and check whether the OOB error changes dramatically.

- For each parameter x do the following:
 - For each tree t of a forest permute the values of x for the samples that belong to the out-of-bag set.
 - Estimate the OOB error as before (the samples have new values for the parameter x).
 - Compare the OOB error of the samples with the original values to the OOB error of the samples with permuted values. This gives you an importance measure.

Literature

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Thank you

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