ETH
Eidgenössische Technische Hochschule Zürich
Swiss Federal Institute of Technology Zurich

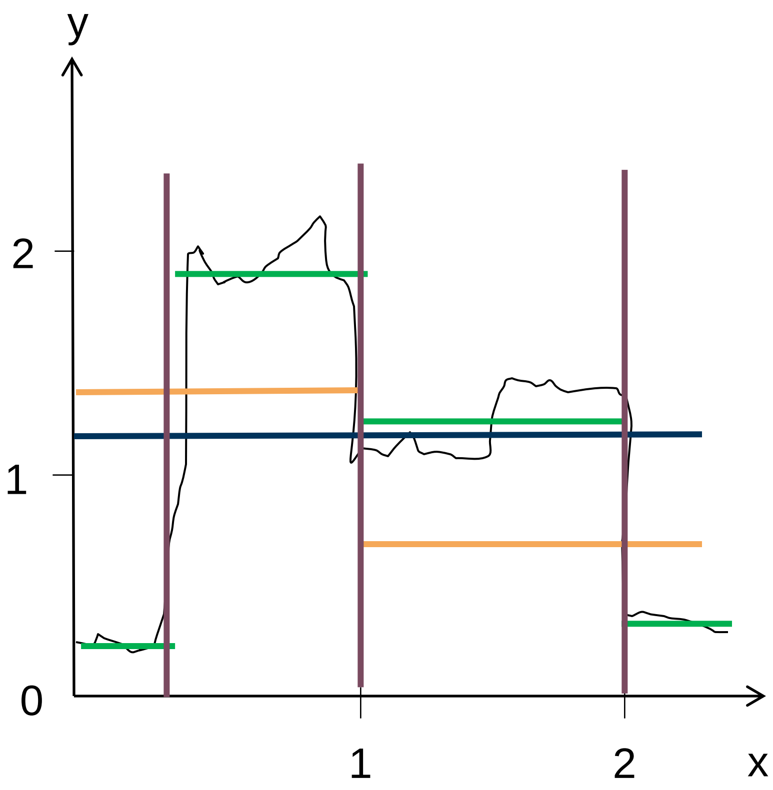
Trees

Applied Multivariate Statistics – Spring 2012

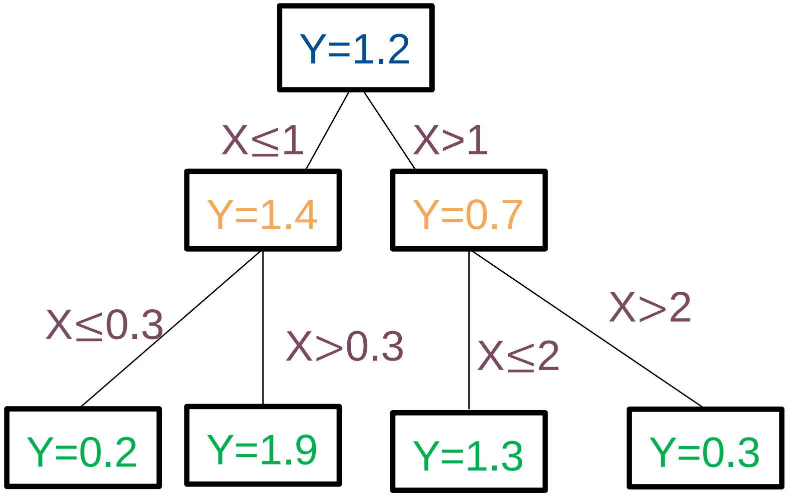
Overview

- Intuition for Trees
- Regression Trees
- Classification Trees

Idea of Trees: Regression Trees
Continuous response

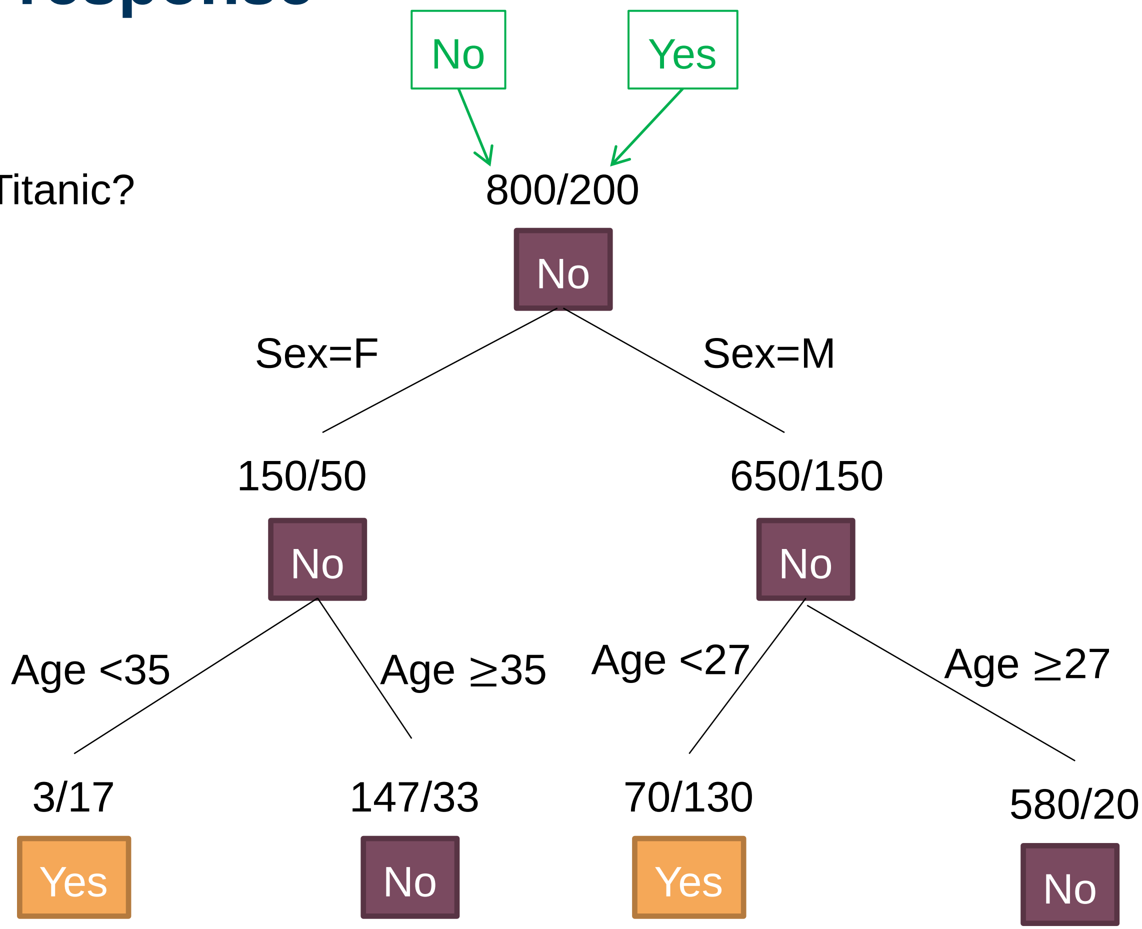


Binary Tree



Idea of Trees: Classification Tree
Discrete response

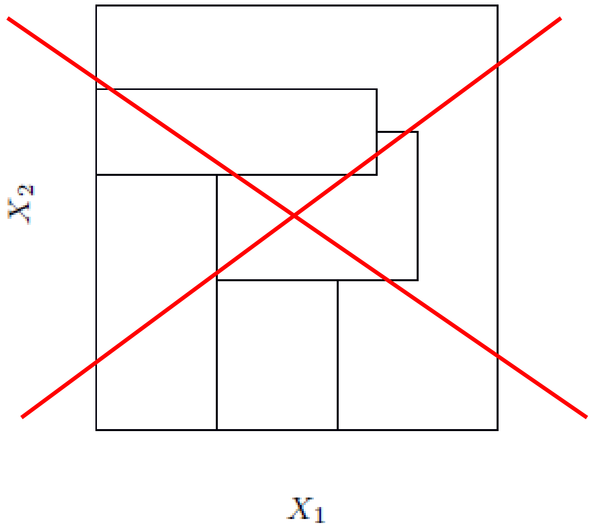
Survived in Titanic?

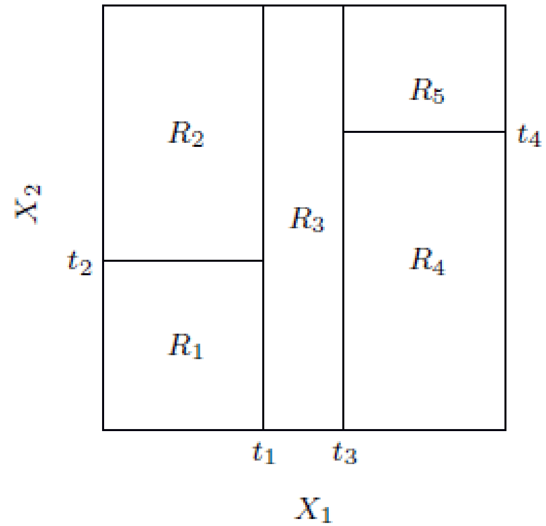


Missclassification rate:

- Total: (3+33+70+20) / 1000 = 0.126
- “Yes”-class: 53/200 = 0.26
- “No”-class: 73/800 = 0.09

Intuition of Trees: Recursive Partitioning



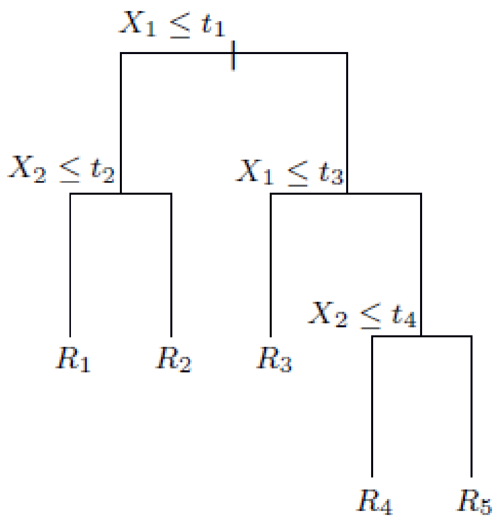


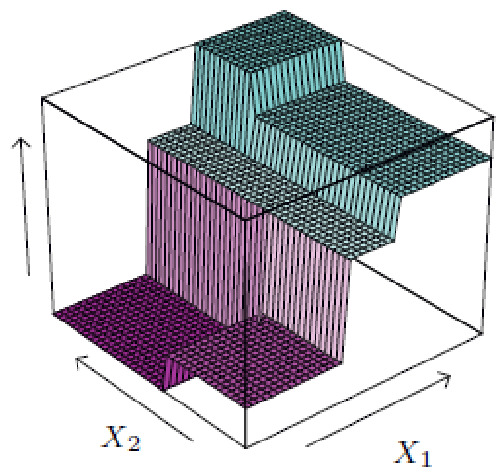
For simplicity:

Restrict to

recursive

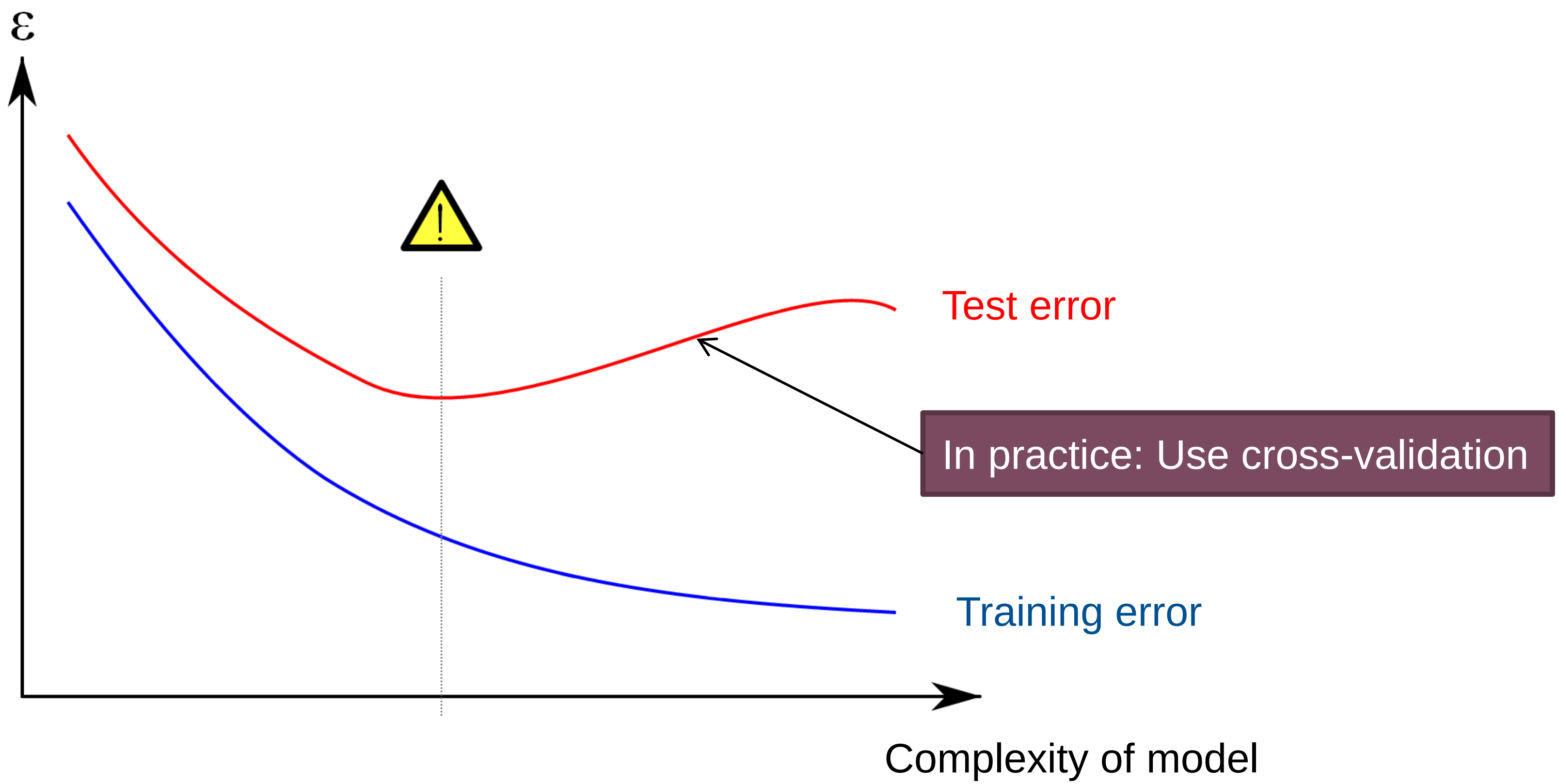
binary splits





Fighting overfitting: Cost-complexity pruning

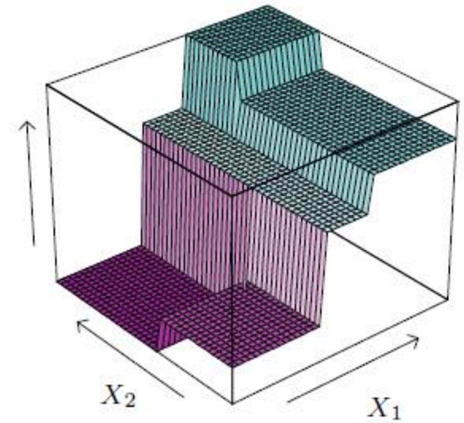
Overfitting: Fitting the training data **perfectly** might not be good for predicting future data



For trees:

1. Fit a very detailed model
2. Prune it using a complexity penalty to optimize cross-validation performance

Building Regression Trees 1/2



- Assume given partition of space $R_1, \ldots, R_M$

  Tree model: $f(x) = \sum_{m=1}^{M} c_m I(x \in R_m)$

- Goal is to minimize sum of squared residuals:

$$\sum (y_i - f(x_i)^2)$$

- Solution: Average of data points in every region

$$\hat{c}_m = \text{ave}(y_i | x_i \in R_m)$$

Building Regression Trees 2/2

- Finding the best binary partition is computationally infeasible
- Use greedy approach: For variable j and split point s define the two generated regions:

$$R_1(j,s) = \{X|X_j \le s\} \text{ and } R_2(j,s) = \{X|X_j > s\}$$

- Choose splitting variable j and split point s that solve:

$$\min_{j,\, s}\left[\min_{c_1} \sum_{x_i \in R_1(j,s)} (y_i - c_1)^2 + \min_{c_2} \sum_{x_i \in R_2(j,s)} (y_i - c_2)^2\right]$$

inner minimization is solved by

$$\hat{c}_1 = \text{ave}(y_i|x_i \in R_1(j,s)) \text{ and } \hat{c}_2 = \text{ave}(y_i|x_i \in R_2(j,s))$$

- Repeat splitting process on each of the two resulting regions

Pruning Regression Trees

- Stop splitting when some minimal node size (= nmb. of samples per node) is reached (e.g. 5)
- Then, cut back the tree again ("pruning") to optimize the cost-complexity criterion:

$$N_m = \#\{x_i \in R_m\},$$

$$\hat{c}_m = \frac{1}{N_m} \sum_{x_i \in R_m} y_i,$$

$$Q_m(T) = \frac{1}{N_m} \sum_{x_i \in R_m} (y_i - \hat{c}_m)^2$$

"Impurity measure"

$$C_\alpha(T) = \underbrace{\sum_{m=1}^{|T|} N_m Q_m(T)}_{\text{Goodness of fit}} + \underbrace{\alpha|T|}_{\text{Complexity}}$$

- Tuning parameter α is chosen by cross-validation

Classification Trees

- Regression Tree:
  Quality of split measured by “Squared error”
- Classification Tree:
  Quality of split measured by general “Impurity measure”

Classification Trees: Impurity Measures

- Proportion of class k observations in node m:

$$\hat{p}_{mk} = \frac{1}{N_m} \sum_{x_i \in R_m} I(y_i = k)$$

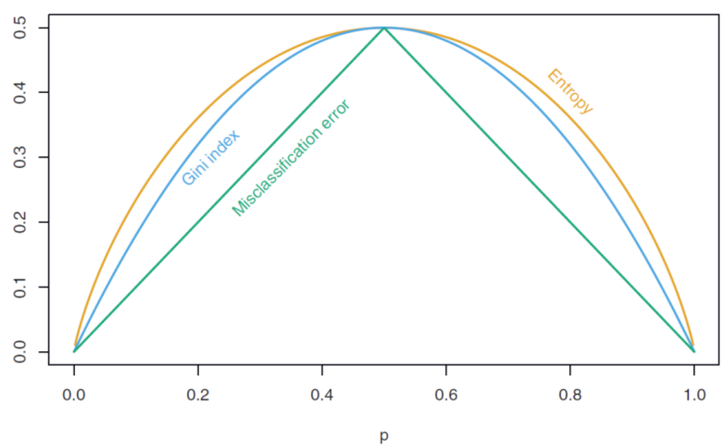
- Define majority class in node m: k(m)
- Common impurity measures $Q_m(T)$:

Misclassification error: $\frac{1}{N_m} \sum_{i \in R_m} I(y_i \neq k(m)) = 1 - \hat{p}_{mk(m)}$

Gini index: $\sum_{k \neq k'} \hat{p}_{mk} \hat{p}_{mk'} = \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk})$

Cross-entropy or deviance: $-\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}.$

- For just two classes:



Example: Gini Index

Side effects after treatment? 100 persons, 50 with and 50 without side effects:

50 / 50 (No / Yes)

Split on sex

50 / 50

M: 30 / 40, Gini = 0.49

F: 20 / 10, Gini = 0.44

Total Gini = 0.49 + 0.44 =
= 0.93

Split on age

50 / 50

old: 10 / 50, Gini = 0.27

young: 40 / 0, Gini = 0

Total Gini = 0.27 + 0 =
= 0.27

0.27 < 0.93, therefore:

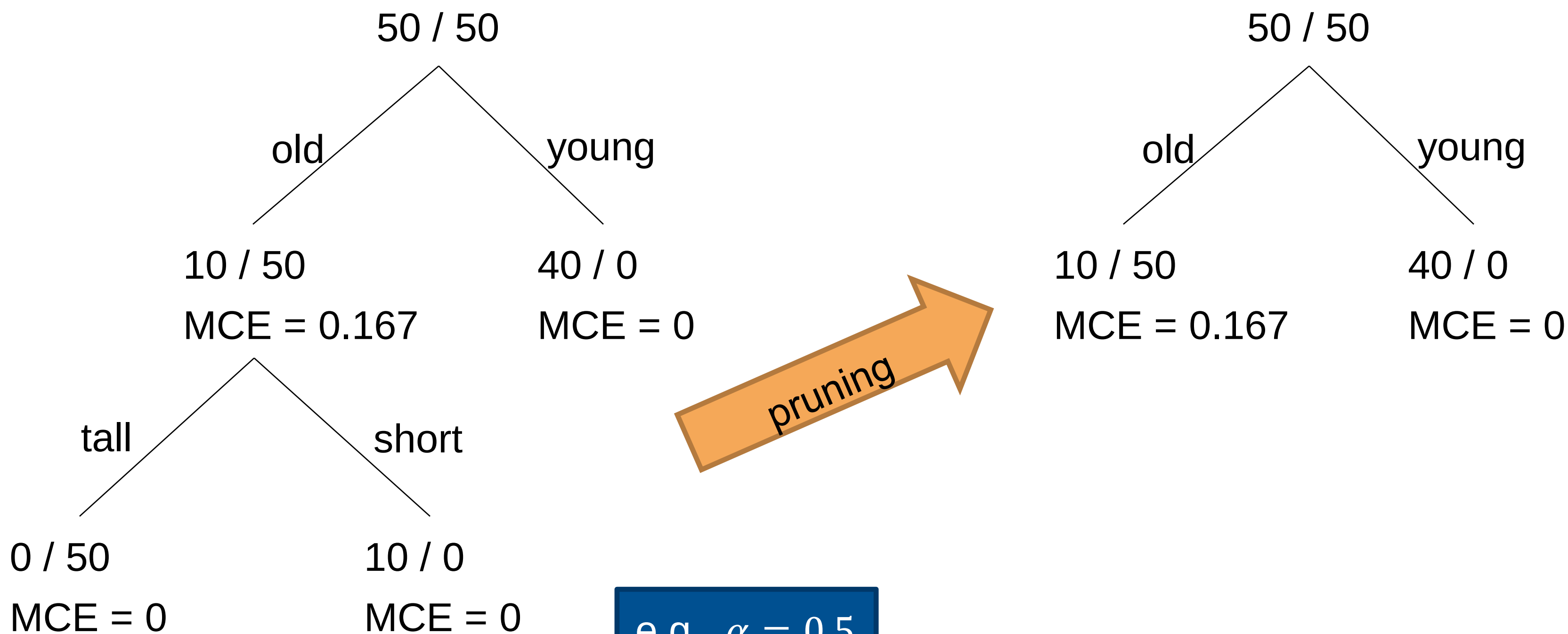
Choose split on age

Classification Trees: Impurity Measures

- Usually:
  - Gini Index used for building
  - Misclassification error used for pruning

Example: Pruning using Misclass. Error (MCE)

$$C_\alpha(T) = \sum_{m=1}^{|T|} N_m Q_m(T) + \alpha|T|$$



e.g., $\alpha = 0.5$

$C_\alpha(T) = 50 * 0 + 10 * 0 + 40 * 0 + 0.5 * 3 =$
$= 1.5$

Smaller $C_\alpha(T)$, therefore don't prune

$C_\alpha(T) = 60 * 0.167 + 40 * 0 + 0.5 * 2 =$
$= 11.0$

Trees in R

- Function “rpart” (recursive partitioning) in package “rpart” together with “print”, “plot”, “text”
- ***Function “rpart” automatically prunes using optimal α based on 10-fold CV***
- Functions “plotcp” and “printcp” for cost-complexity information
- Function “prune” for manual pruning

Concepts to know

- Trees as recursive partitionings
- Concept of cost-complexity pruning
- Impurity measures

R functions to know

- From package “rpart”: “rpart”, “print”, “plot”, “text”, “plotcp”, “printcp”, “prune”