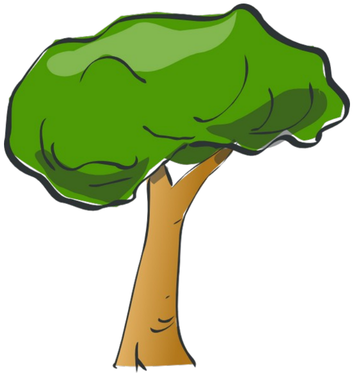
R-course:
Machine Learning using R

Decision trees

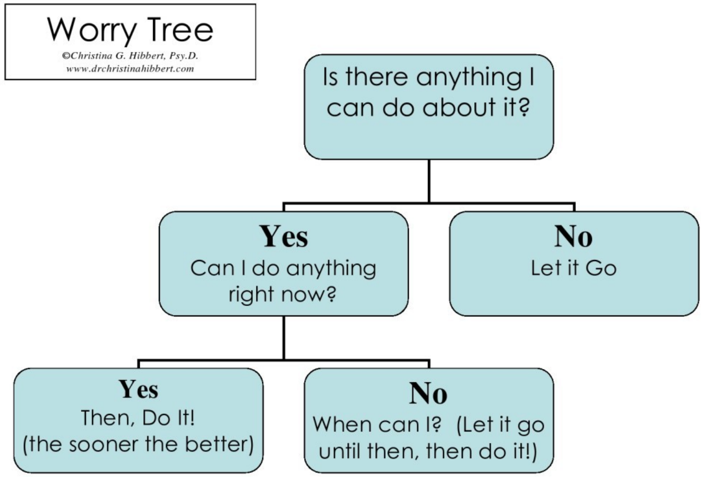


Yannick Rothacher

Zürich, 2021

What is a decision tree?

- Generally speaking, a **decision tree** is a diagram, which helps us determining a course of action (e.g. "should I worry?")



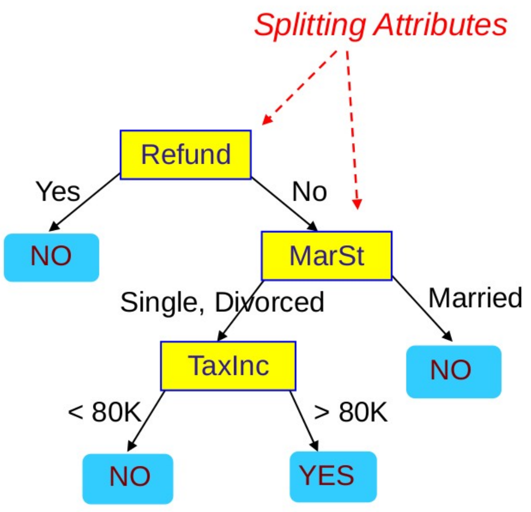
- We can use decision trees for **classification** or **regression**
  - Such trees are the result of what is referred to as **recursive partitioning**
- Let's look at an example of a decision tree used for **classification**...

Decision tree – classification

- We want to predict whether a person will cheat in his/her tax declaration based on some training data
- "**Cheat**" is the target variable (two levels: yes/no)
- The generated decision tree uses the three independent variables to model whether someone will cheat or not:

Tid	Refund (categorical)	Marital Status (categorical)	Taxable Income (continuous)	Cheat (class)
1	Yes	Single	125K	**No**
2	No	Married	100K	**No**
3	No	Single	70K	**No**
4	Yes	Married	120K	**No**
5	No	Divorced	95K	**Yes**
6	No	Married	60K	**No**
7	Yes	Divorced	220K	**No**
8	No	Single	85K	**Yes**
9	No	Married	75K	**No**
10	No	Single	90K	**Yes**

Training Data

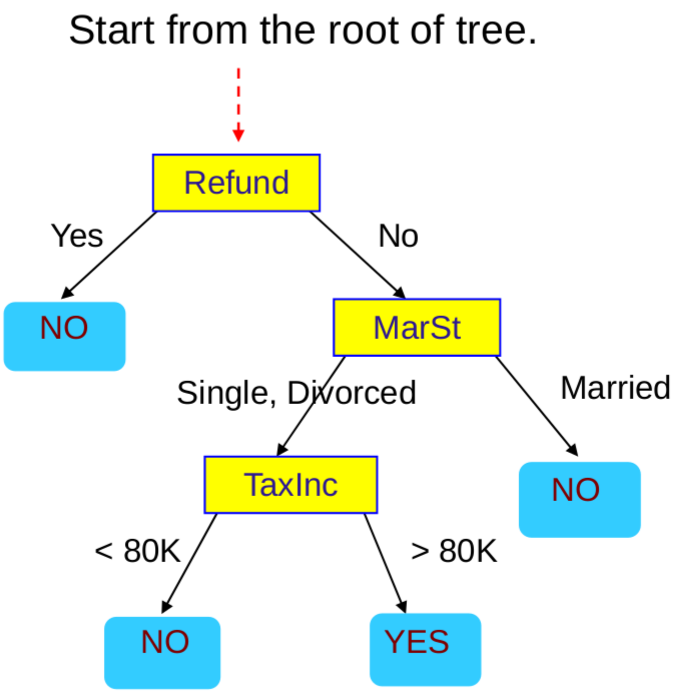


Model: Decision Tree

Source: Introduction to Data Mining, Pang-Ning Tan, Michael Steinbach, Vipin Kumar, Published by Addison Wesley.

Decision tree – classification

- Use the generated tree to predict outcome of a **new observation**
- Work through the tree for prediction:



Test Data

Refund	Marital Status	Taxable Income	Cheat
No	Married	80K	?

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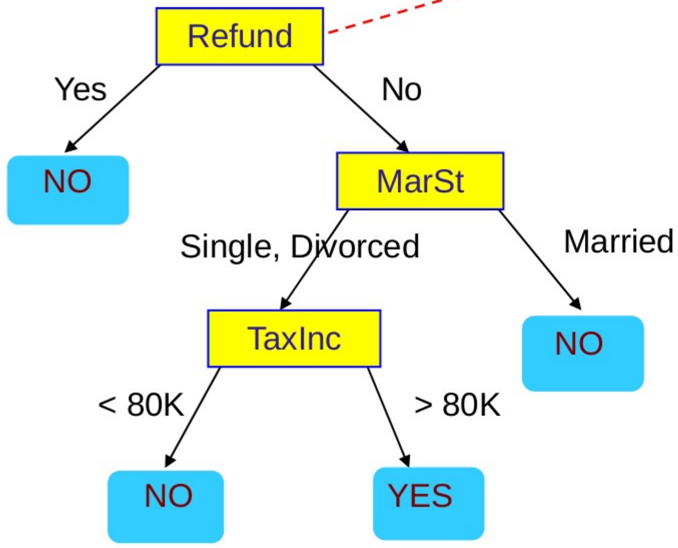

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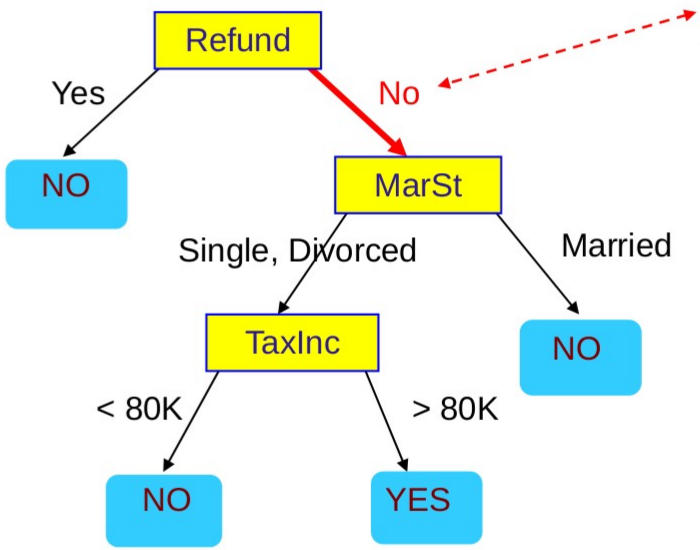

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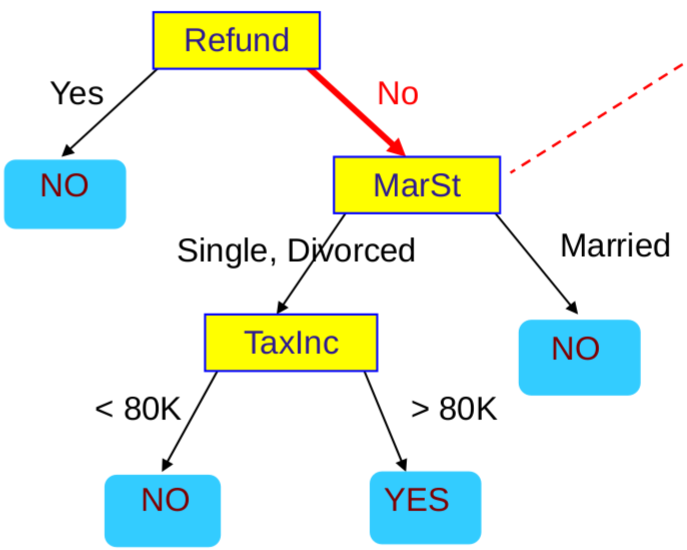

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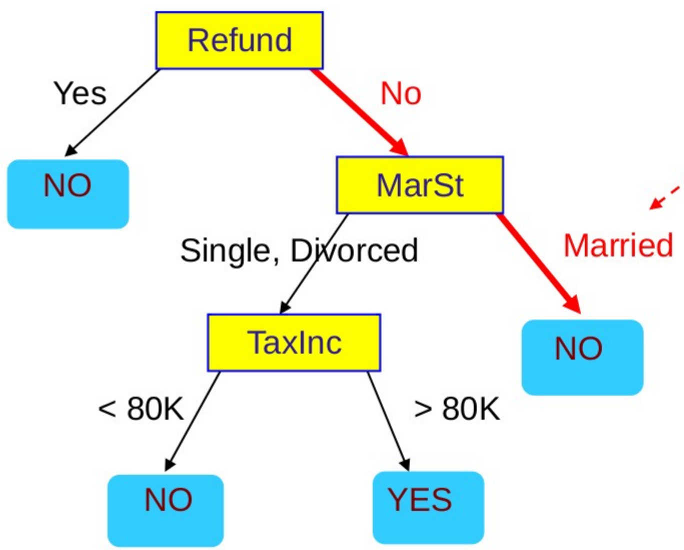

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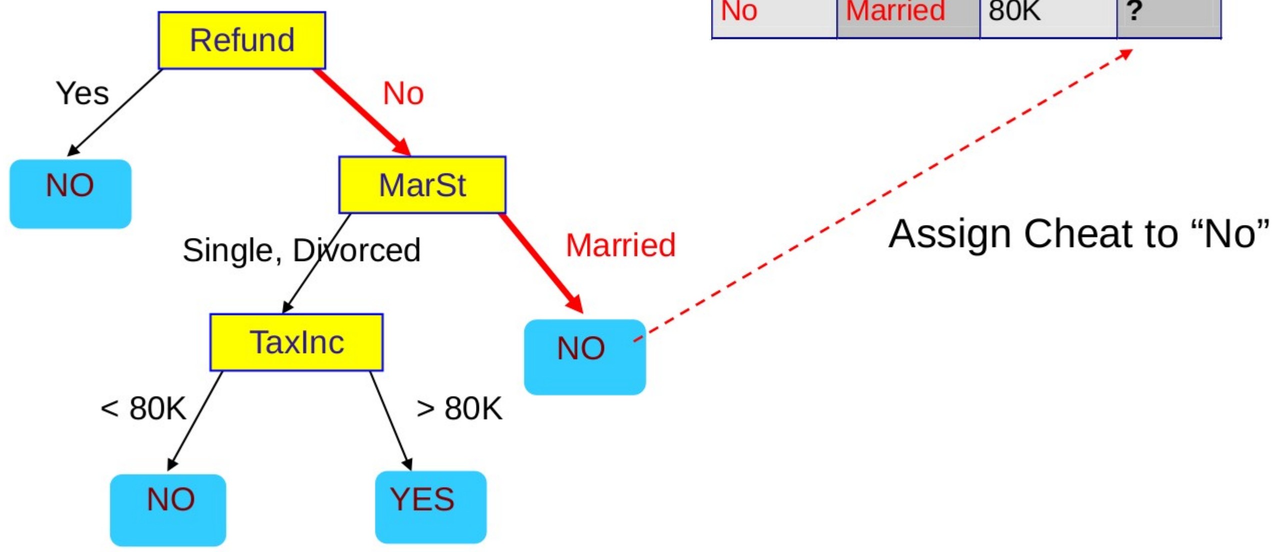

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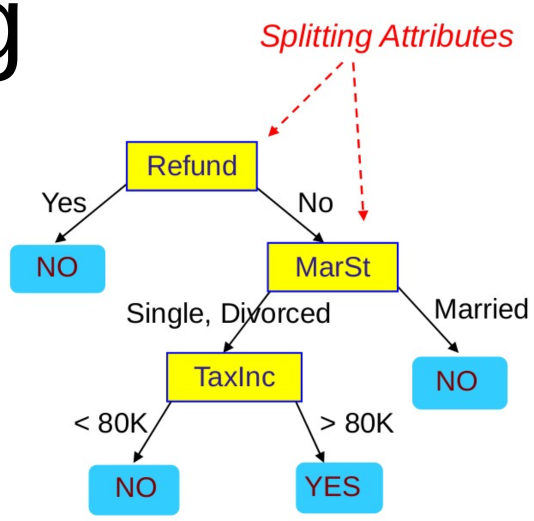
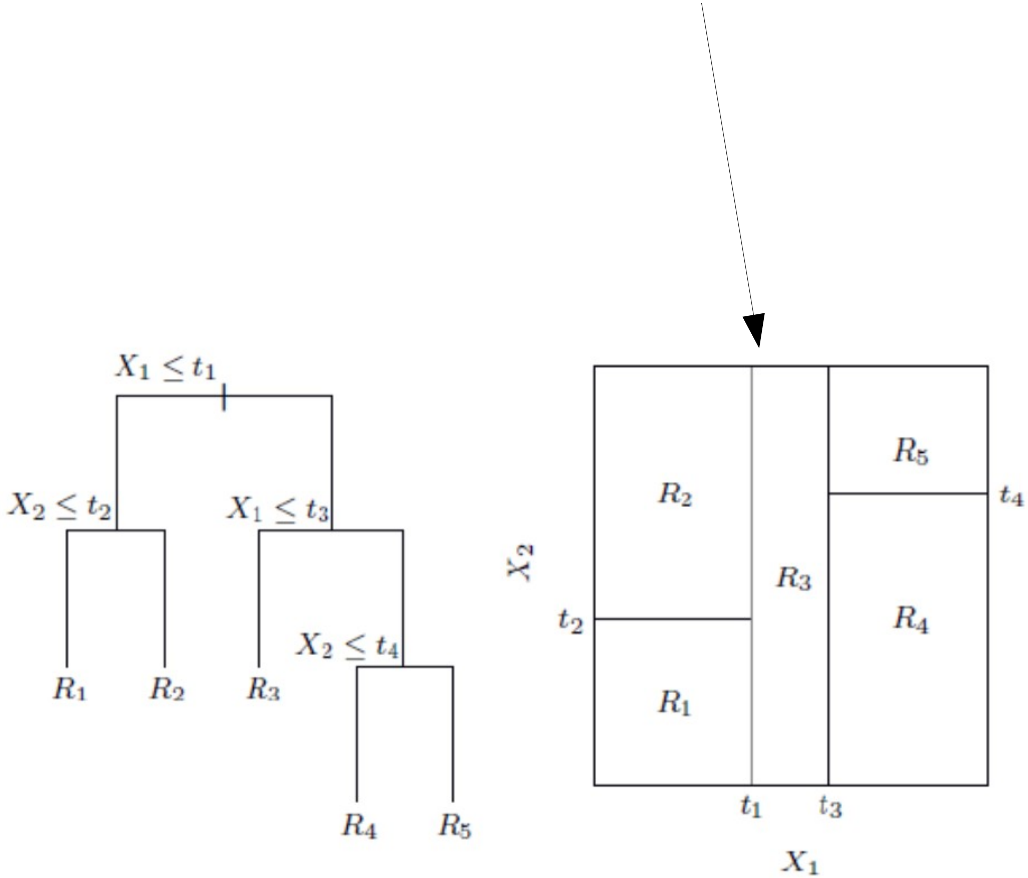
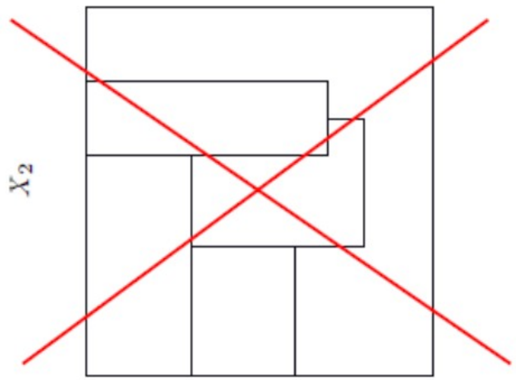
Decision tree – partitioning



Model: Decision Tree

- A classic decision tree splits the data at each node based on **one dependent variable**
- For the case of only **two dependent variables** we can visualize this in a 2D-coordinate system:





Only straight lines!

Decision tree – partitioning

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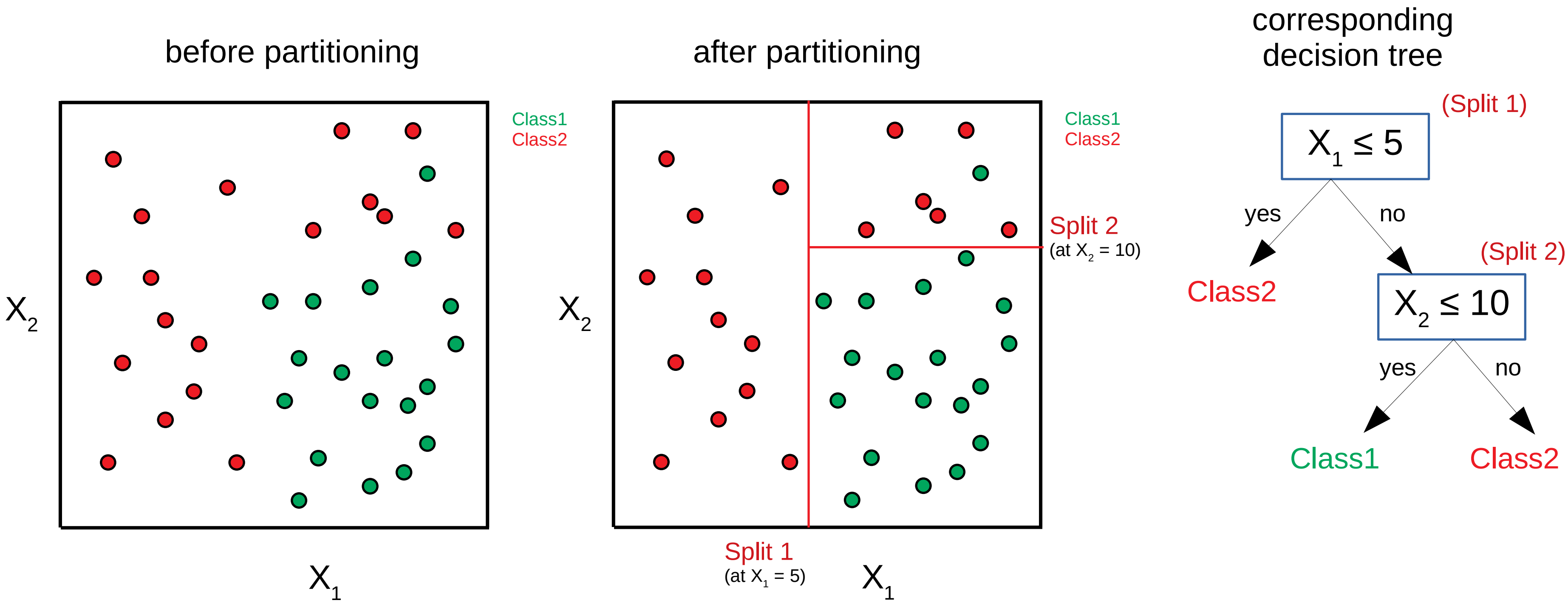

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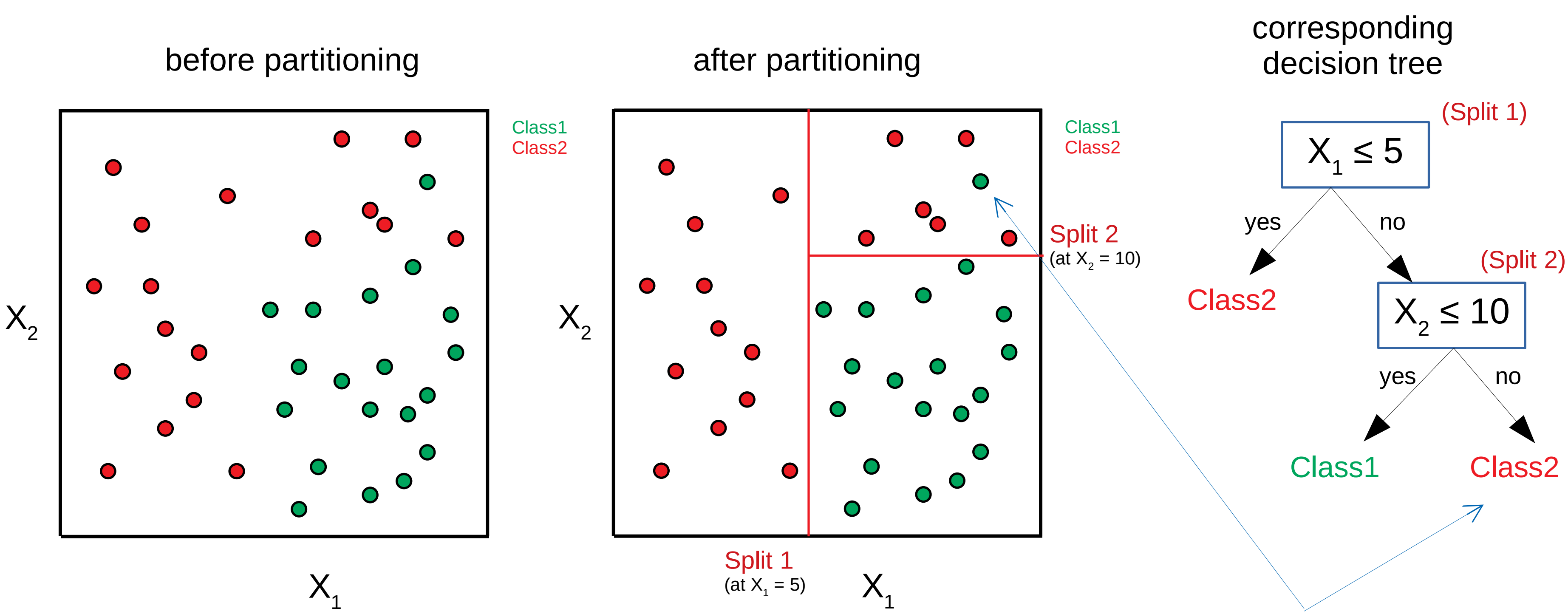
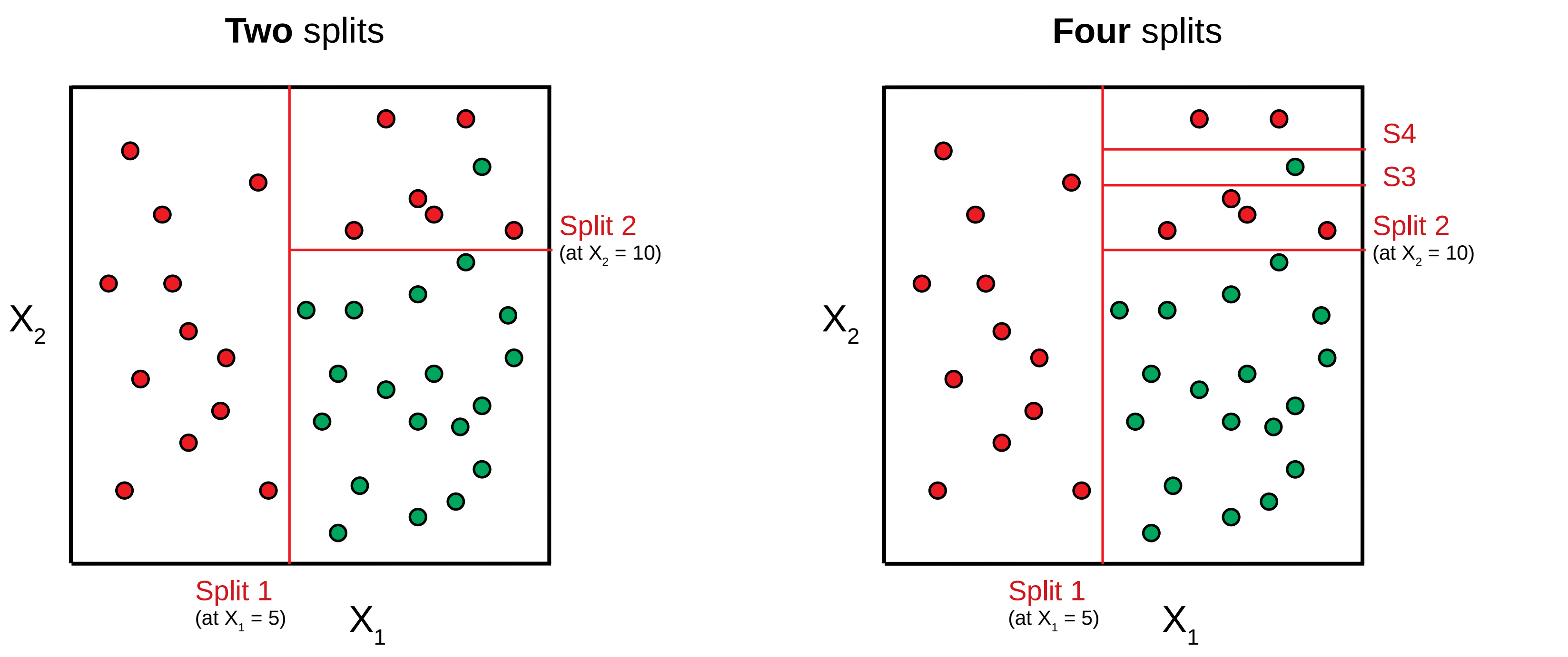


This partition is not **pure**!
-> we can use the majority vote for prediction (6 vs. 1)

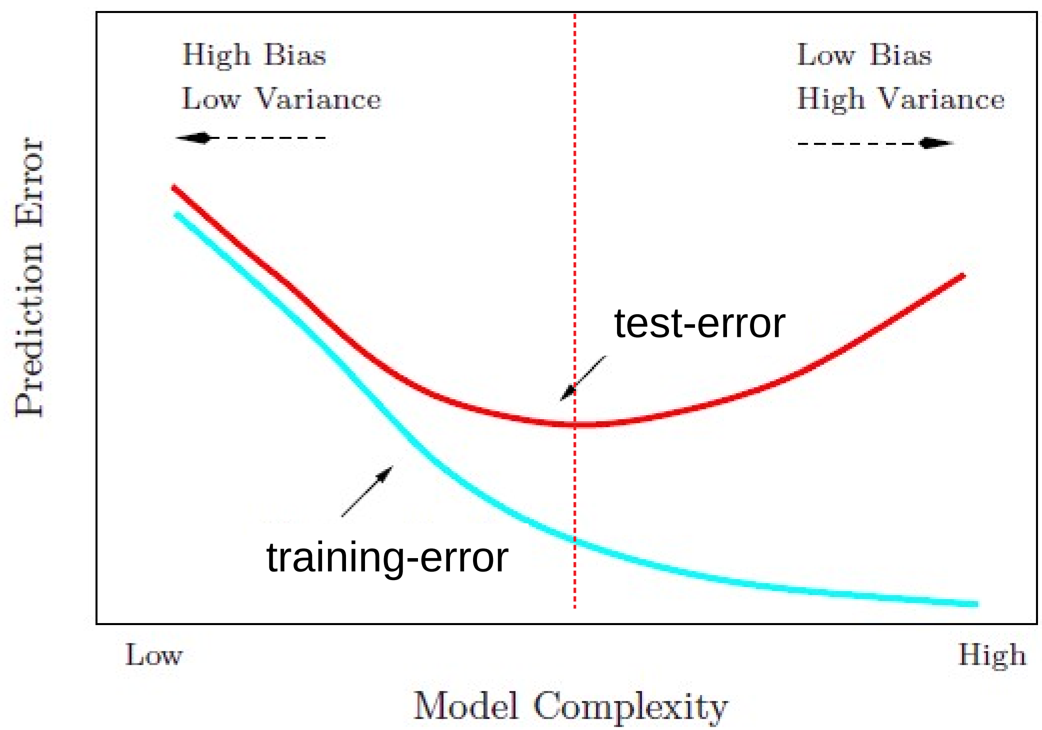
Decision trees – over- and underfitting

- How **deep** should a tree be allowed to grow?
  - We can always grow a tree until there are only pure partitions left (right figure below)
  - Same problem of **over- and underfitting** like with the KNN-classifier!
- Which one of the trees below is better?



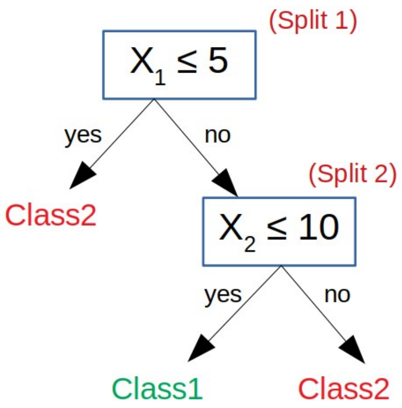
Recap: Test-error

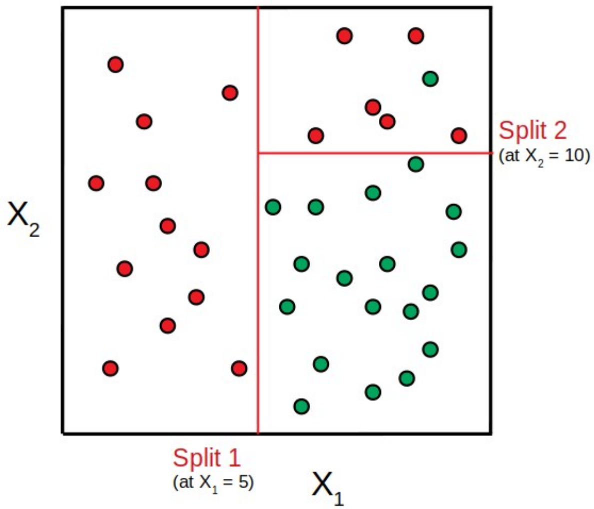
- Like in the case of the KNN-classifier we want to minimize the **test-error**
- Evaluation methods like e.g. **cross-validation** can of course also be applied to decision trees
  - Prevent **over-fitting**: Fully grown trees can be "**pruned**" (cut shorter) depending on whether a branch improves the fit to data evaluated by cross-validation



How are the partitions generated?

- Building a decision tree from scratch involves the following two questions at each node:
  - Which variable should be used for the next split?
  - Where along the chosen variable should we split?
- How can we decide what the **best variable** and **split-location** is?
- We will look at two different methods to solve these questions
  - 1) classic partitioning based on **impurity measure** (e.g. Gini-index)
  - 2) bias-free partitioning based on **significance tests**





Classification trees – impurity measure

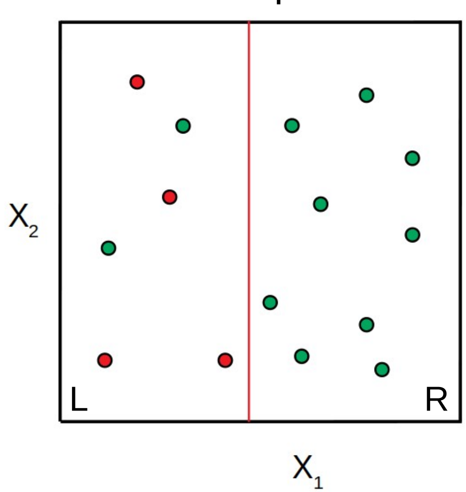
- **Main idea**: Try to find the split, which reduces the **impurity** of the data the most
  - How can we measure "impurity"?
- The Gini index is one of the most common impurity measures

$$Gini = 1 - \sum_{i}^{C} p_i^2$$

Entropy is another common impurity measure

$$Entropy = -\sum_{i}^{C} p_i \log_2(p_i)$$

Example



$\text{Gini}_{\text{root}}$ = 1 – ($(11/15)^2$ + $(4/15)^2$) = **0.391**

Gini_{L} = 1 – ($(2/6)^2$ + $(4/6)^2$) = **0.444**

Gini_{R} = 1 – ($(0/9)^2$ + $(9/9)^2$) = **0**

Gini-reduction (weighted by number of observations in each partition):

Gini_decrease = $\text{Gini}_{\text{root}}$ – (6/15)*Gini_{L} – (9/15)*Gini_{R}

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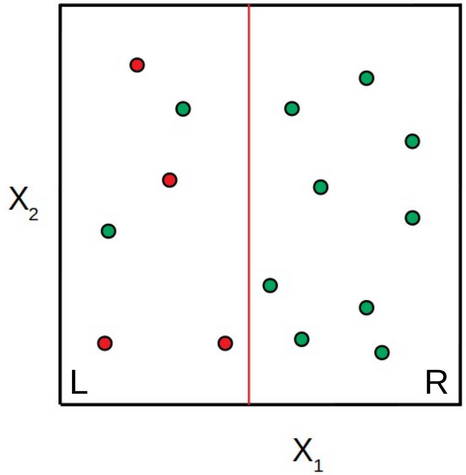

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Gini-reduction (weighted by number of observations in each partition):

$Gini\_decrease = Gini_{root} – (6/15)*Gini_{L} – (9/15)*Gini_{R}$

→ Choose the split with the largest Gini-reduction

Partition algorithm (impurity measure based)

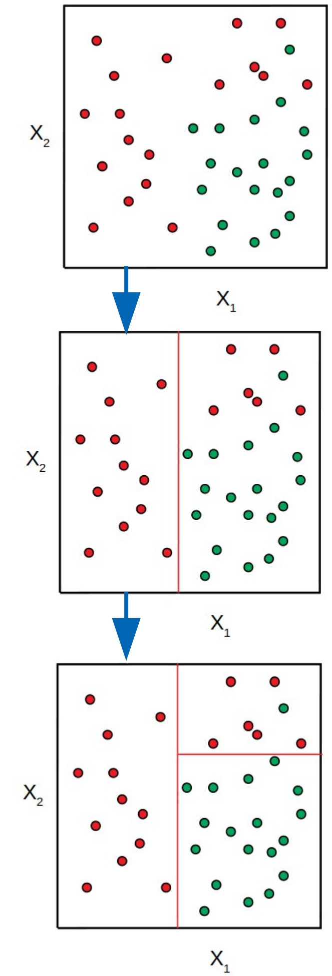
$$Gini = 1 - \sum_{i}^{C} p_i^2$$

- Start with a **single region** (encompassing all data)
- Iterate through the following steps:

For each region **R**
    For each variable $\mathbf{x}_i$ in **R**
        For each possible split $\mathbf{s}_i$ of $\mathbf{x}_i$
            Record impurity decrease

→ Choose ($\mathbf{x}_i$, $\mathbf{s}_i$) which gives maximum impurity decrease

→ Replace **R** with $\mathbf{R}_R$ and $\mathbf{R}_L$

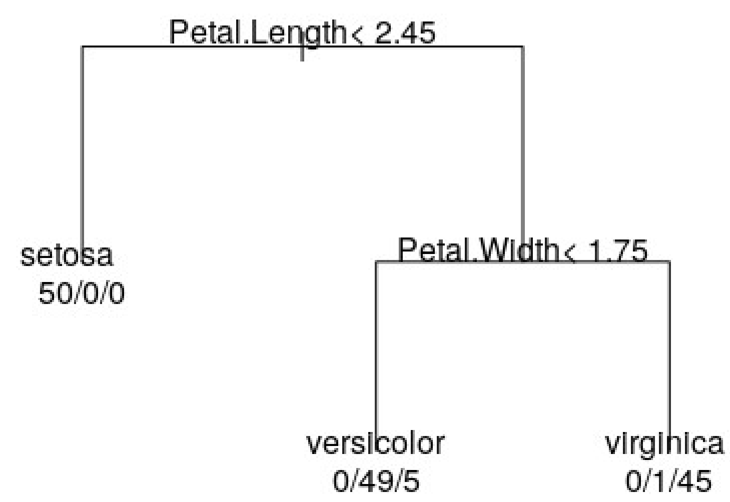


- Stop splitting either based on a **stopping rule** or when there is no more impurity reduction possible
  - Stopping rule example: Stop splitting when a branch contains less than a certain percentage of the data

Decision tree in R – rpart

- **rpart** is an R-package to fit decision trees (impurity measure based)
- Here an example of fitting a (classification) tree to the "Iris" data set:

```
library(rpart)
tree.iris <- rpart(Species ~., data=iris)  # default uses Gini-index
plot(tree.iris, margin = 0.1)
text(tree.iris, use.n = T)
# Predict training data (use type = 'prob' to get probabilities):
pred.tree <- predict(tree.iris, iris, type = 'class')
# Confusion matrix:
(confT <- table(pred.tree, iris$Species))
pred.tree    setosa versicolor virginica
  setosa         50          0         0
  versicolor      0         49         5
  virginica       0          1        45
# Training-error:
diag(confT) <- 0
missCount <- sum(confT)
(trainErr <- missCount/nrow(iris))
[1] 0.04
```



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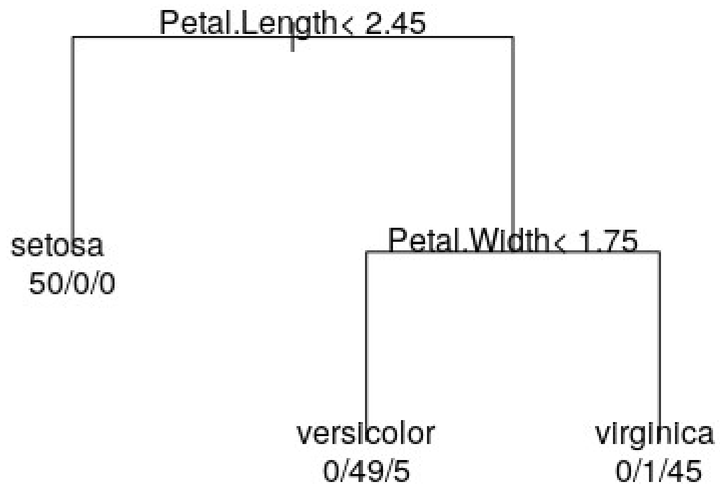
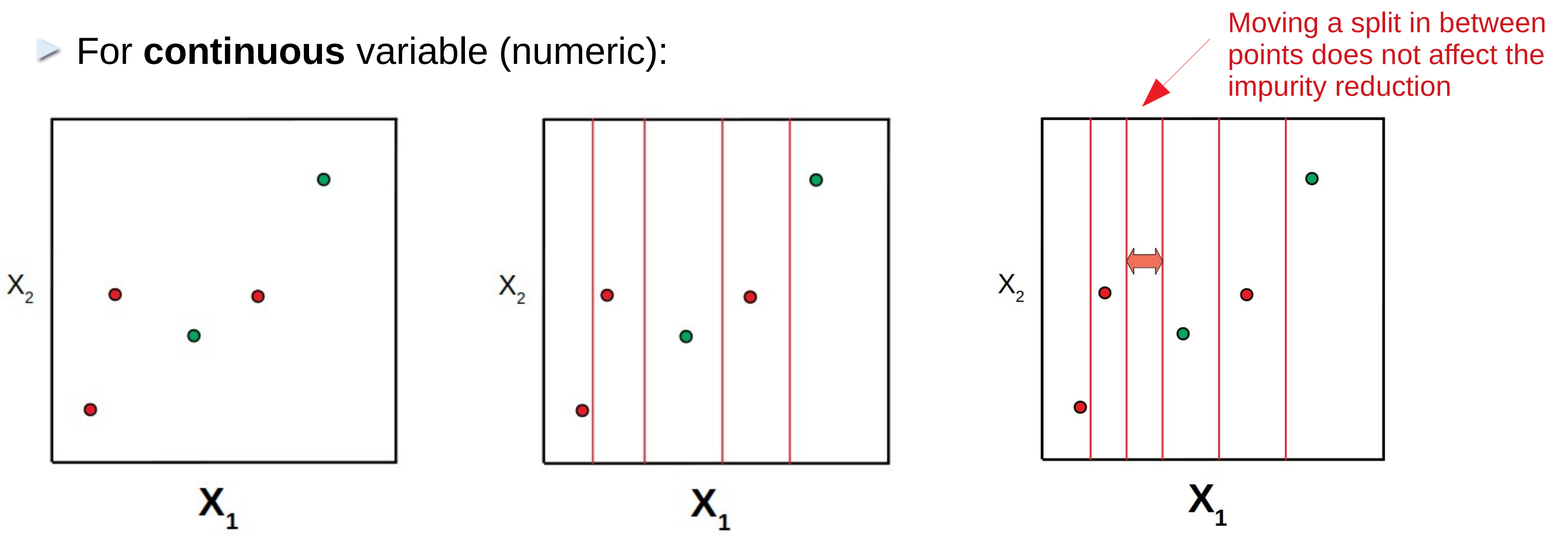


Problems with rpart

- Using an impurity measure based approach to select splits suffers from an **inherent bias** in certain cases
  - This bias is related to the **number of splits** that are possible for each variable
- How many splits are there per variable?
  - For **continuous** variable (numeric):



  - For the five data points above, there are only **four meaningful** splits possible (along X_1)
- What about **other types** of variables?

Problems with rpart

- We can also include **categorical variables** (factors) as predictors in a decision tree

- How many splits are possible for factors?

  - E.g. **two**-level factor (levels: a,b)
    a | b split1

  - E.g. **four**-level factor (levels: a,b,c,d):
    a | b,c,d split1
    b | a,c,d split2
    c | a,b,d split3
    d | a,b,c split4
    a,b | c,d split5
    a,c | b,d split6
    a,d | b,c split7

  - **k**-level factor: $\boxed{number\ of\ splits = 2^{(k-1)} - 1}$ → 10-levels: 511 splits

categorical categorical continuous class

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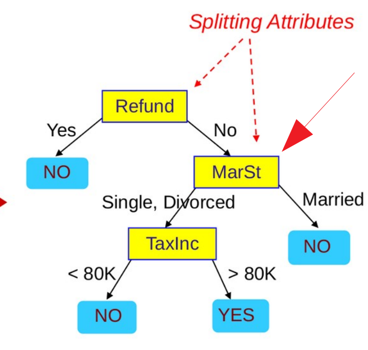

Model: Decision Tree

Source: Tan, Steinbach, Kumar

- With increasing number of levels we can apply an **exponentially growing** number of splits

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d | a,b,c split4
ab | c,d split5
ac | b,d split6
ad | b,c split7

- The difference in numbers of splits between continuous variables, factors with few levels and factors with many levels creates an issue of **multiple comparisons**

- Multiple comparisons problem in decision trees:
  - Even if there is **no real relation** between predictors and the target variable, under certain circumstances multi-level factors will be preferably selected for splitting compared to numerical variables or factors with few levels because they get **more "chances"** to reach a high impurity-decrease (even if this decrease is only achieved by pure luck)
  - More chances in the sense that more splits can be evaluated (more chances to get lucky)
  - Ideally, we **do not want** our decision trees to be biased in their variable selection

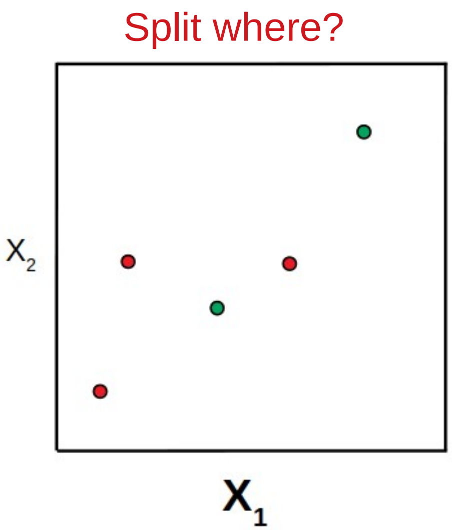
Bias-free partitioning

- **Bias-free partitioning** has been proposed to solve this problem (e.g. see Hothorn et al. 2006)
  - Main idea: Use significance tests instead of impurity measures to select variable and next split

- How does it work?
  - The selection process is more clearly separated into

    1) Choosing the next splitting **variable** and

    2) Choosing the splitting **location** along the chosen variable



Bias-free partitioning

- Choosing the next splitting variable:
  - Test for **each variable** whether it has a **significant association** with the target variable (e.g. think of correlation test for numerical variables and of ANOVA for categorical variables). Collect the associated p-values (can be compared between tests)
  - If no variable shows a significant p-value stop splitting (integrated **stopping rule**)
  - Otherwise choose the variable with the **lowest p-value** for the next split

Bias-free partitioning

Actual implementation uses special permutation tests (called "**conditional inference tests**") that are available for all types of variables.

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  - Otherwise choose the variable with the **lowest p-value** for the next split
- Choosing the next splitting location:
  - Calculate for each possible split (along the chosen variable) a **test-statistic** (expressing the difference between the created partitions, *could also use impurity measure*) and select split with the highest test-statistic
- Using this approach, there is **no bias** in the selection of different variable-types

Bias-free partitioning in R

- "party" is an R-package which includes functions to fit bias-free (significance test based) decision trees (**ctree**()-function)
- Fitting a classification tree to the "Iris" data set

```
library(party)
ctree.iris <- ctree(Species ~., data=iris)  # fit tree
plot(ctree.iris)
pred.ctree <- predict(ctree.iris, newdata=iris, type='response')
(confT <- table(pred.ctree, iris$Species))  # Confusion matrix
```

```
pred.ctree   setosa versicolor virginica
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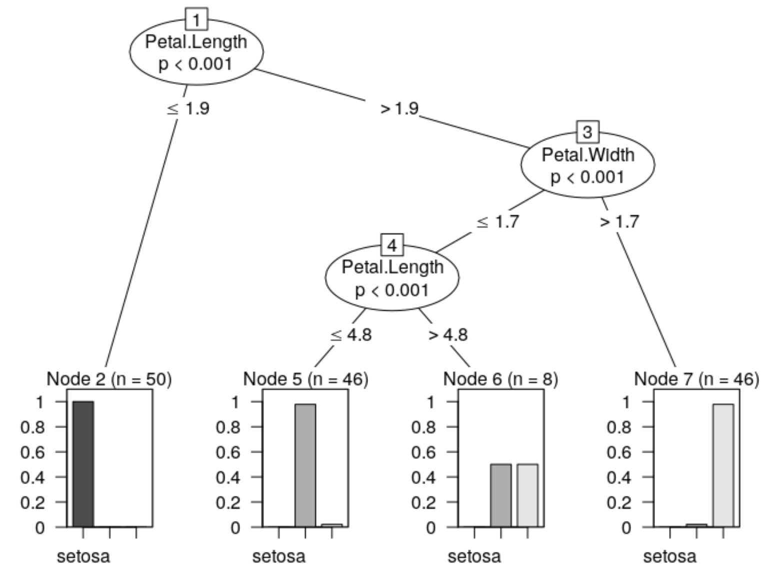
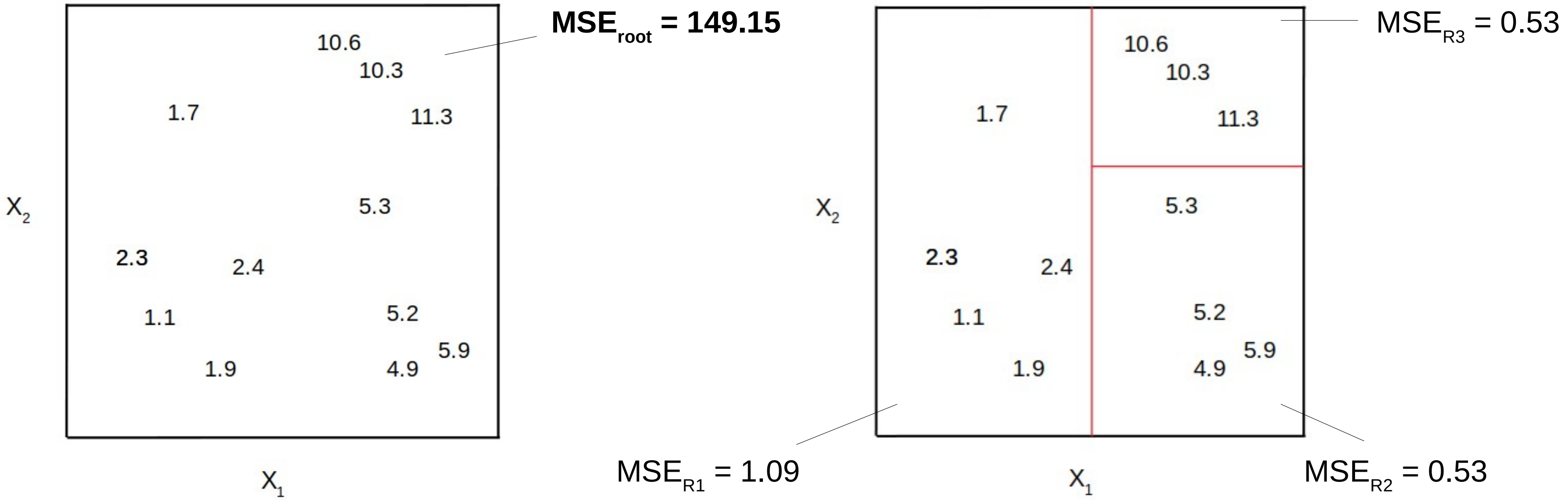


Decision trees for regression

- Decision trees can be used for classification (categorical target variable) and for **regression** (numerical target variable)
- The general principle behind building the tree structure does not change
  - E.g. use **mean squared error** as "impurity measure" instead of Gini-index

$$MSE = \frac{1}{n}\sum_{i}^{n}(x_i - \bar{x})^2$$

  - We try to find the splits which best reduce the mean squared error
- With **ctree** we can fit a bias-free regression tree (again based on significance tests)



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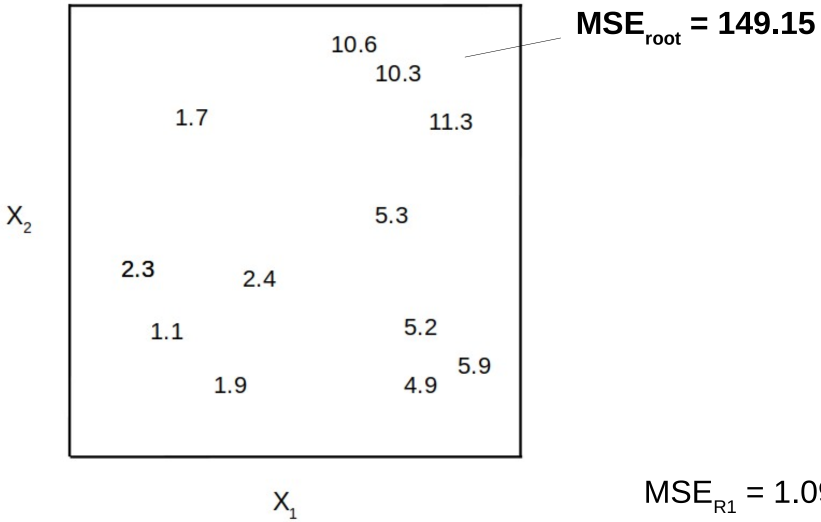
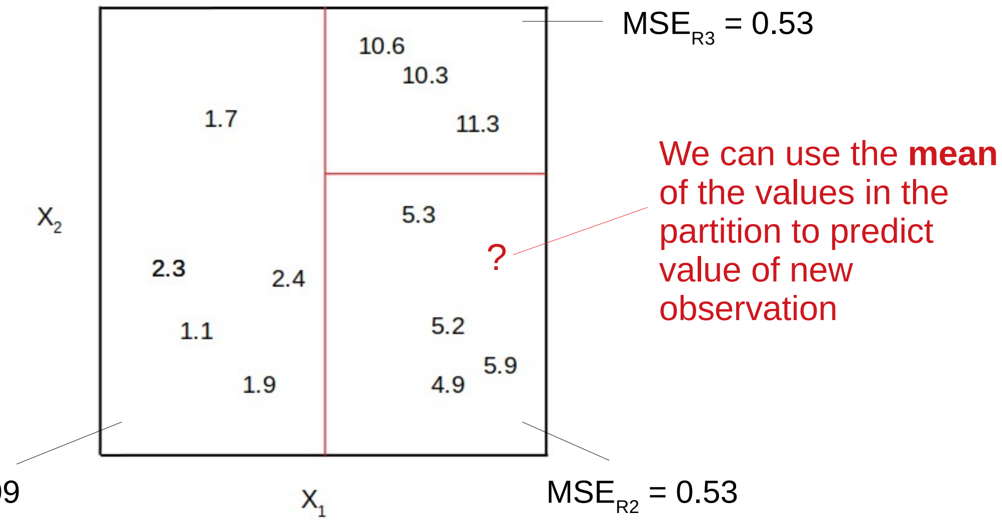
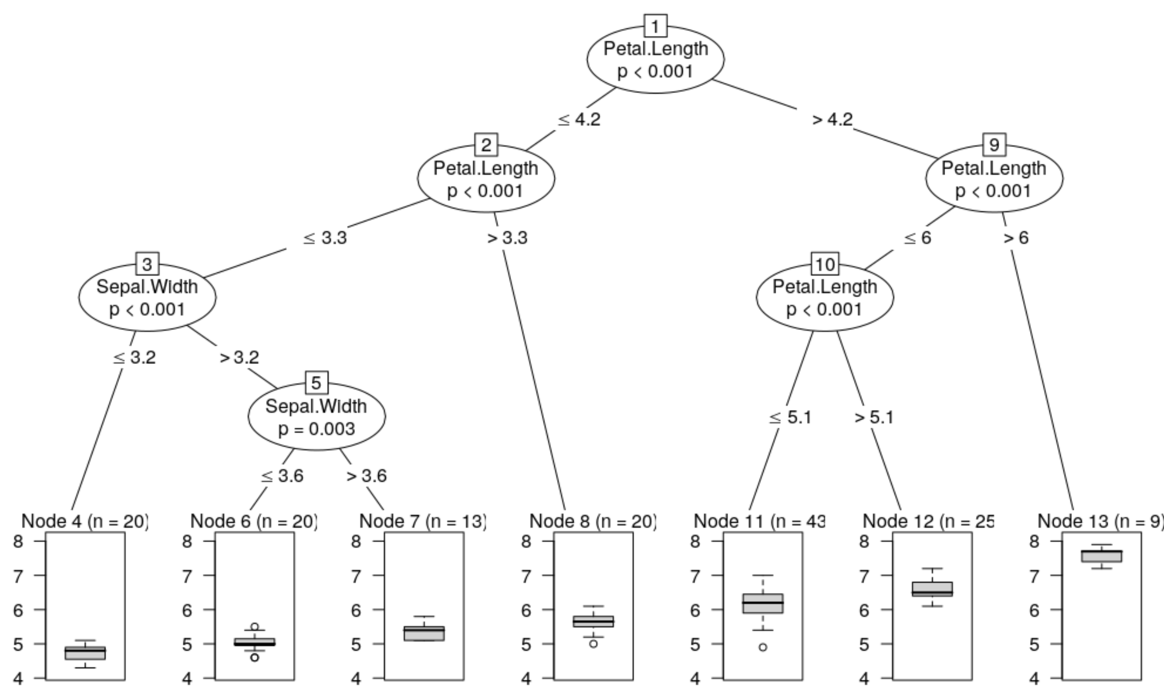




Regression tree in R

- Example of fitting a regression tree to the "Iris" data using ctree()

```
library(party)
ctree.iris <- ctree(Sepal.Length ~., data=iris)  # fit regression tree
plot(ctree.iris)
# Get the predicted values (for training data):
pred.ctree <- predict(ctree.iris, iris, type='response')
```



Decision trees – Summary

- Advantages of decision trees:
  - Good interpretability
  - No assumptions regarding distributions
  - Robust to outliers
  - Can capture non-linear structures and complex interactions
  - Low bias in prediction with sufficient depth
- Disadvantages:
  - Single trees are instable (small changes in data can give different-looking tree, especially if underlying pattern is complex)
  - In case of not pruned rpart-trees: Tend to overfit
  - Needs a lot of data to capture linear structures

Caution: In case of different types of predictor variables use algorithm with bias-free variable selection (ctree in R)

Further reading

- Strobl, C., Malley, J., & Tutz, G. (2009). **An introduction to recursive partitioning: Rationale, application, and characteristics of classification and regression trees, bagging, and Random Forests**. *Psychological Methods*, 14 (4), 323–348. doi: 10.1037/a0016973