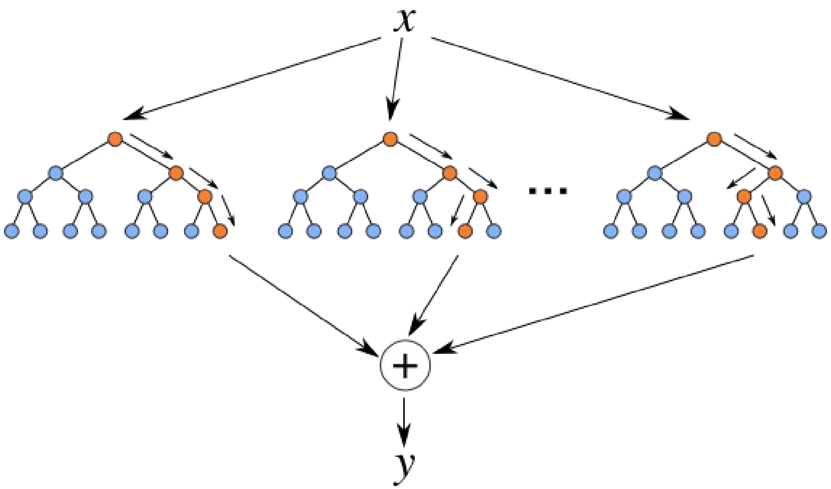
R-course:

Machine Learning using R

Random Forest

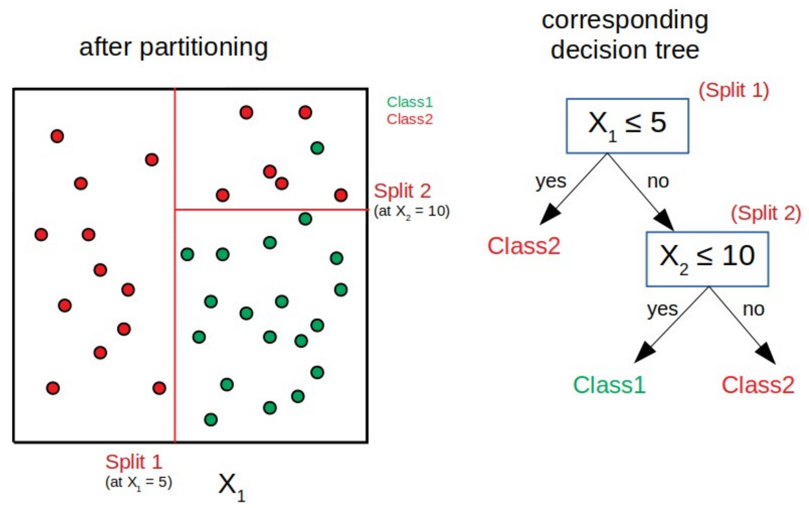


Yannick Rothacher

Zürich, 2021

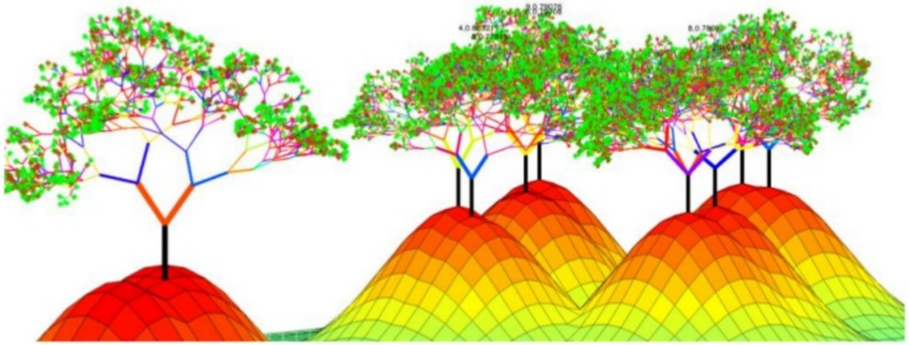
Recap: Decision trees

- Last lecture we saw how decision trees can be used for **classification** and **regression**
- Looked at the different methods for **variable** and **split selection** in rpart() and ctree() function
- One advantage of decision trees is their **good interpretability**
- **However**: If trees are allowed to grow deep they show large variability and low bias (overfitting the data)
- What can be done to prevent overfitting?



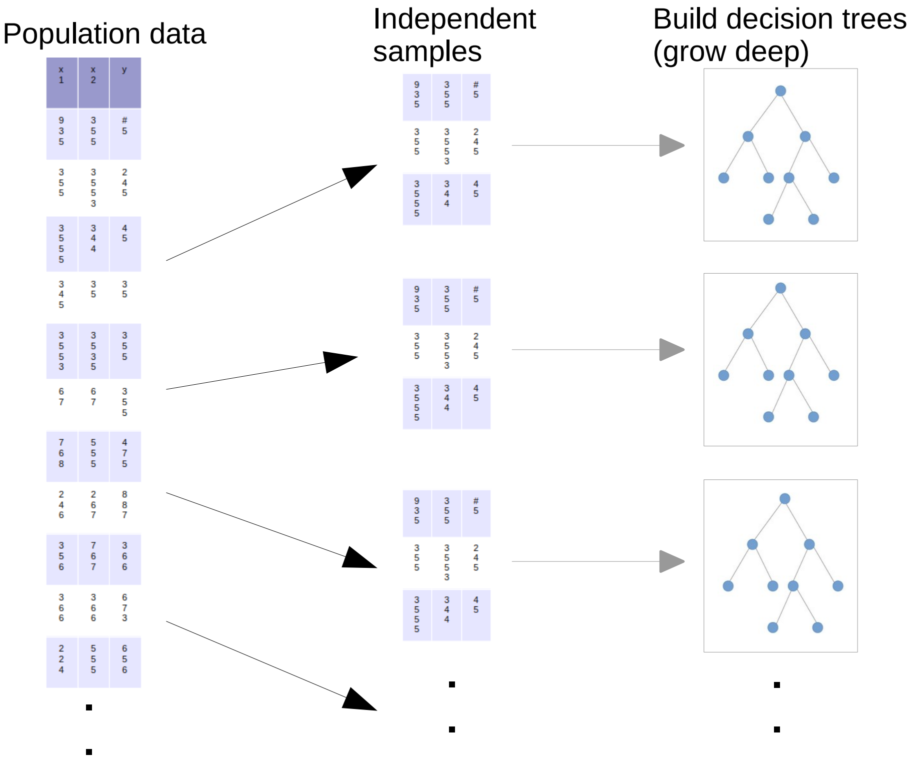
Ensemble methods

- Why not combine multiple classifiers to improve prediction?
- Given some training data and a test-observation:
  - You could apply multiple, different classifiers to the data (logistic regression, **KNN**, **decision tree**, neural network, …) and incorporate each classifier's prediction into your final prediction of the test observation (e.g. majority vote)
- **Ensemble methods** are based on a similar intuition: Combine multiple (simple) classifiers of the same type to improve performance
- With regard to decision trees there are two ensemble methods, which are mostly applied:
  - Bagging
  - Random Forest



Ensemble methods: Bagging

- **Bagging** (bootstrap aggregating) is an ensemble method typically applied to decision trees (but can be applied to all classifiers)
- Main idea: Fully grown decision trees have **low bias** but **high variance**...
  - ...it would be nice to have multiple independent samples from the same population to **reduce variance** by taking the mean of prediction



Population data

x1	x2	y
935	355	#5
355	3553	245
3555	344	45
345	35	35
3553	3535	355
67	67	355
768	555	475
246	267	887
356	767	366
366	366	673
224	555	656

Independent samples

935	355	#5
355	3553	245
3555	344	45

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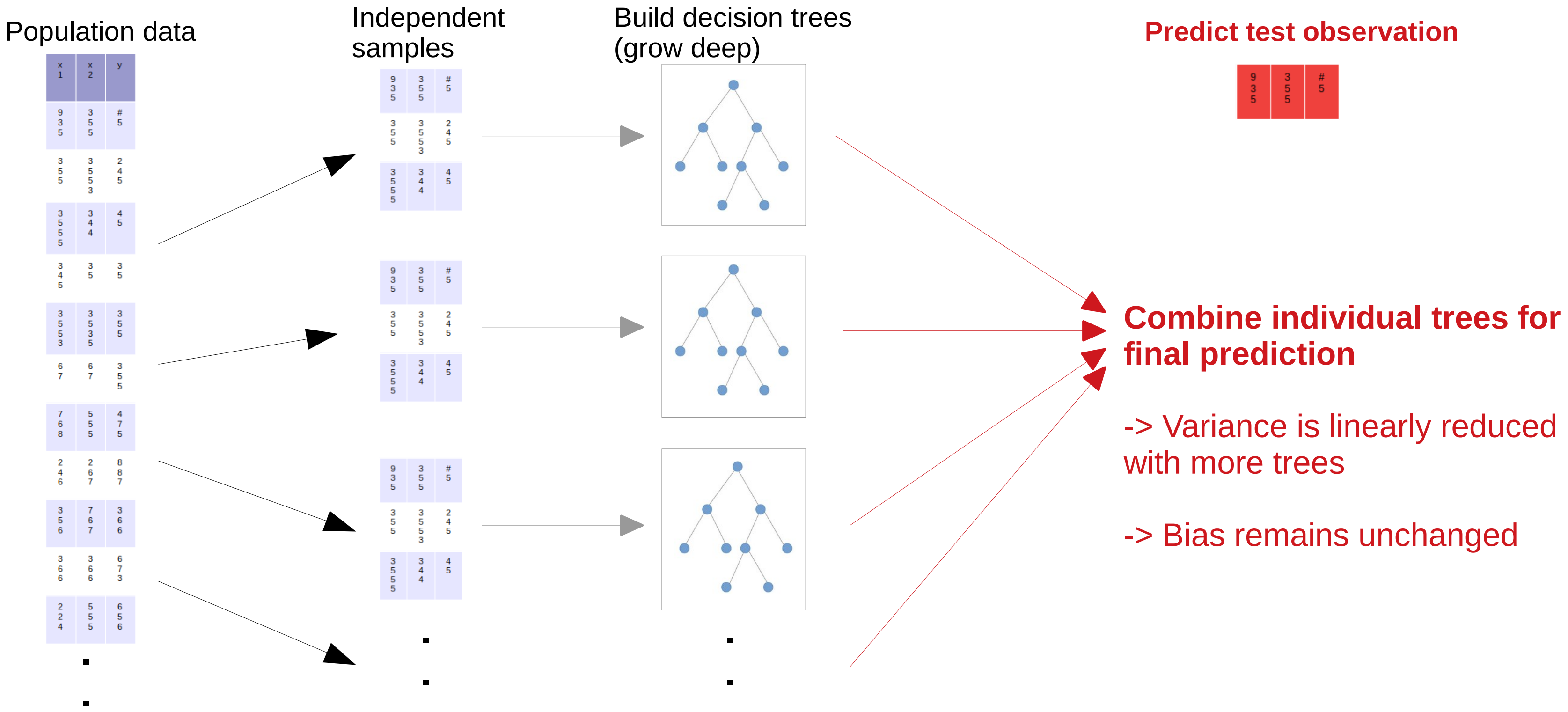

Population data

Independent samples

Build decision trees (grow deep)

Predict test observation

Combine individual trees for final prediction

-> Variance is linearly reduced with more trees

-> Bias remains unchanged

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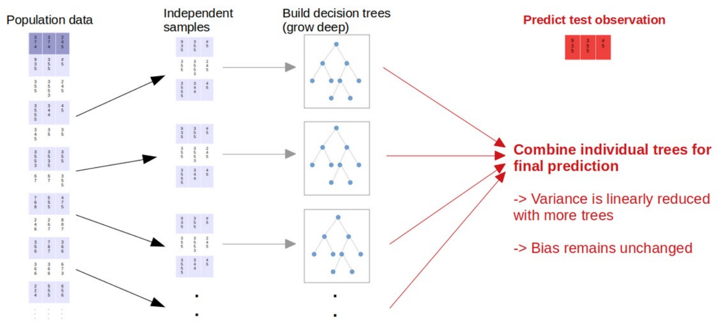
- By averaging the individual trees the variance of the estimation is reduced



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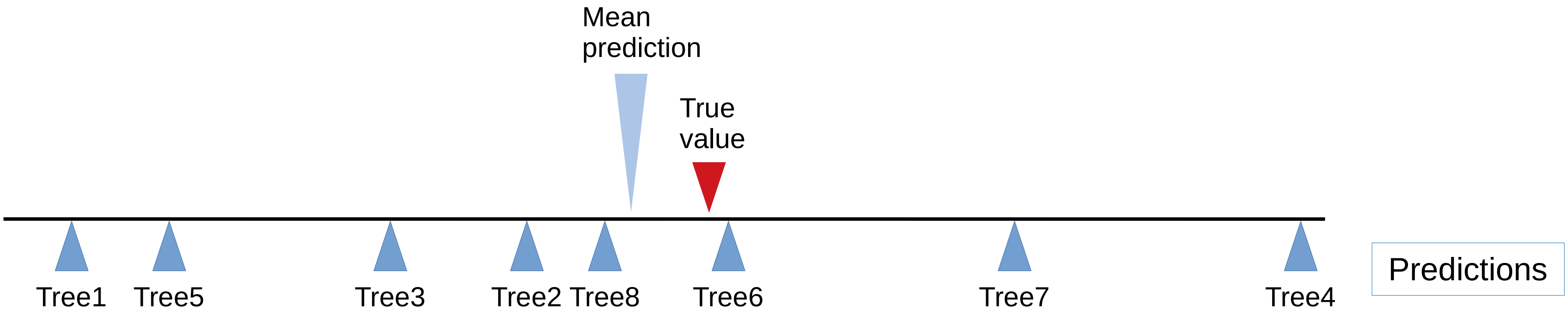

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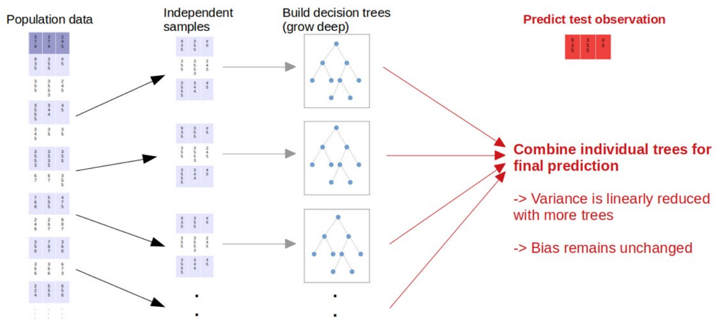
- By averaging the individual trees the variance of the estimation is reduced
- **However**: In reality we usually only have **one training sample** from the population



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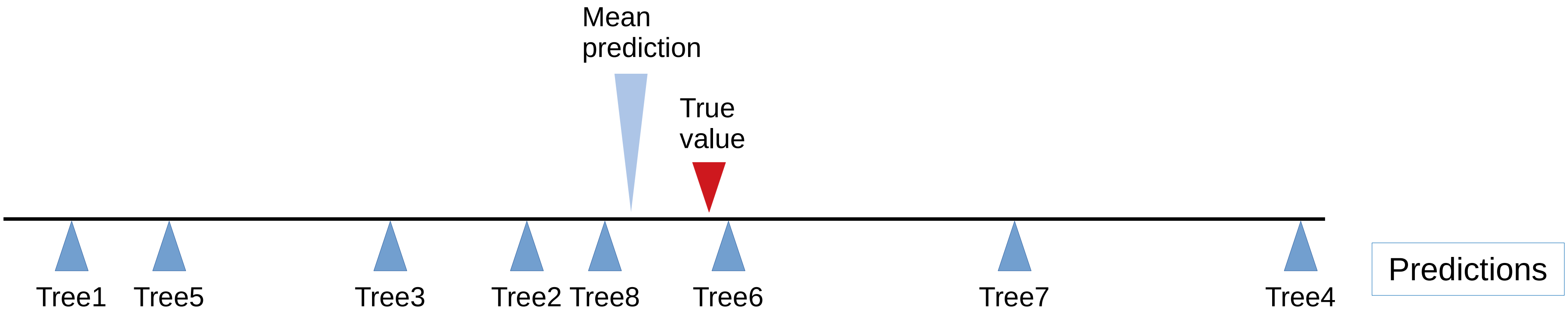


Mean prediction

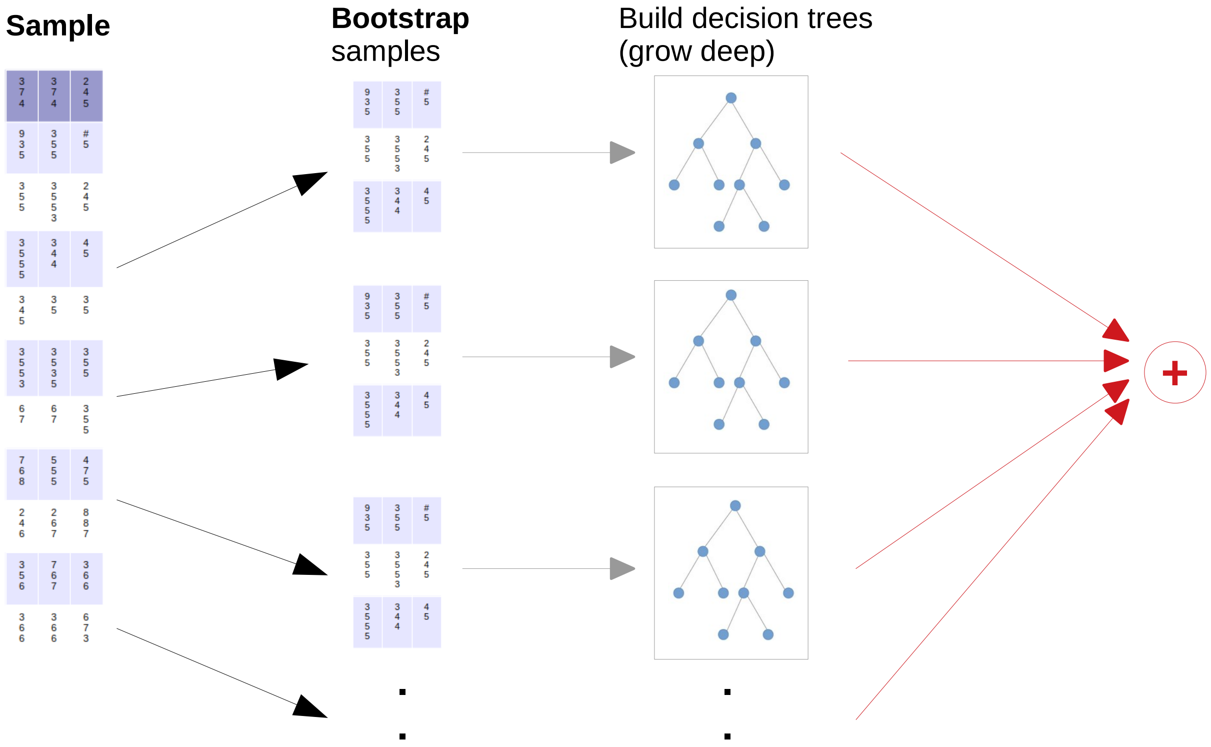
True value

Tree1 Tree5 Tree3 Tree2 Tree8 Tree6 Tree7 Tree4

Predictions

Ensemble methods: Bagging

- In reality we usually only have only **one sample** from the population
  - Solution: We now take **bootstrap samples** from our training data
  - Grow deep decision trees on bootstrap samples and combine the trees for prediction



Sample

Bootstrap samples

Build decision trees (grow deep)

Ensemble methods: Bagging

- In reality we usually only have only **one sample** from the population
  - Solution: We now take **bootstrap samples** from our training data (originally suggested by Breiman 1996)
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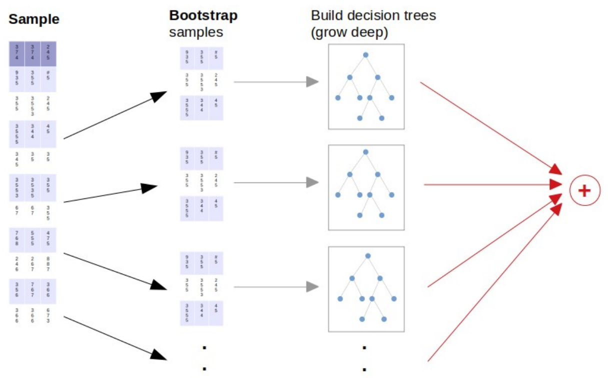
- Bootstrap samples are samples drawn with replacement:



Original data

4	5	22	3	99	67	43	1	21	2

Bootstrap samples (same size as original data)

3	5	67	5	43	67	21	2	99	3
2	4	4	67	21	1	1	67	99	3
5	5	21	99	1	2	22	99	67	5

.
.

Breiman L: Bagging Predictors. Machine Learning 1996, 24(2):123-140.

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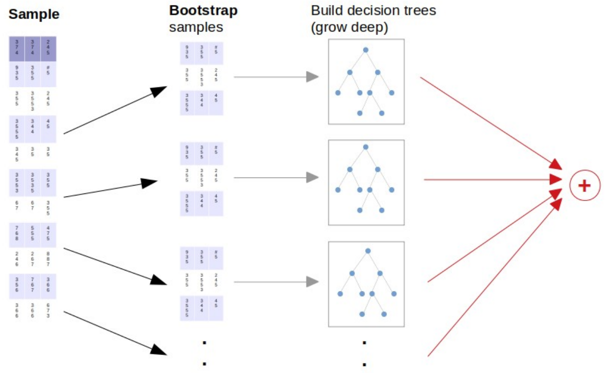

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Same observation can appear multiple times!

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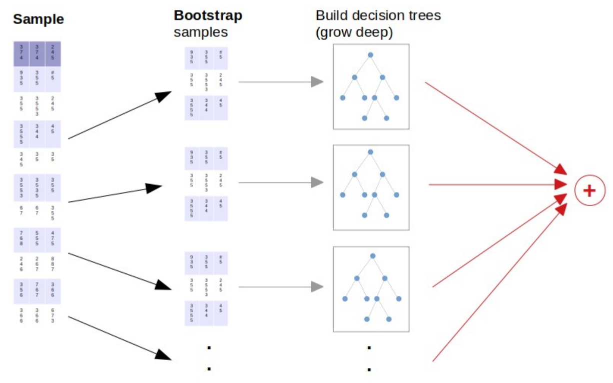
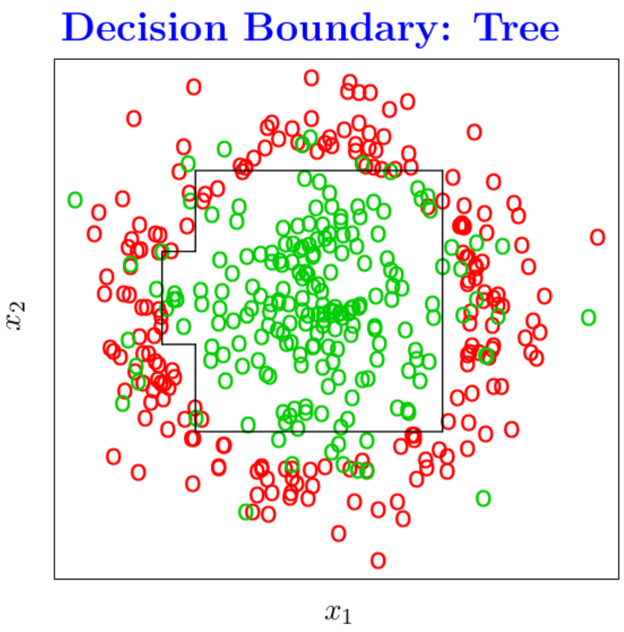


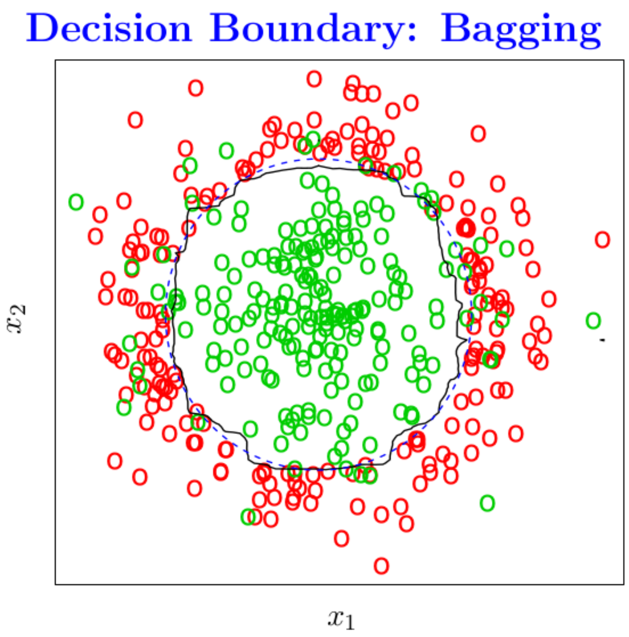
Bagging shows better performance than one decision tree applied to original data (why?)

Note: Individual bootstrap samples are not independent!

-> Variance is only reduced sublinearly

Ensemble methods: Bagging

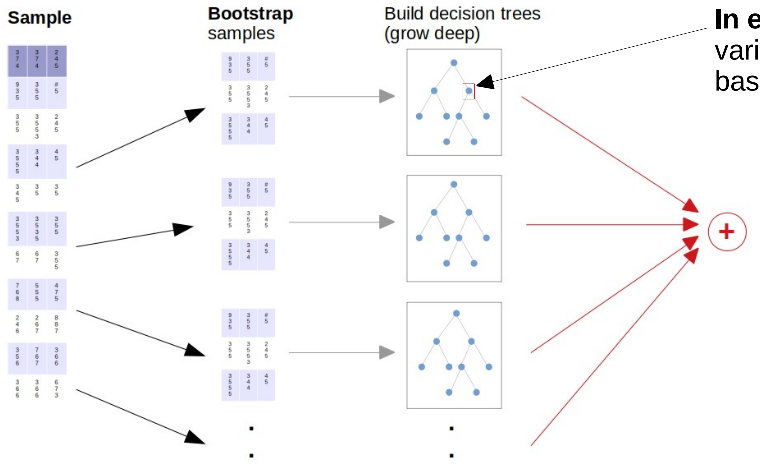

Decision Boundary: Tree


Decision Boundary: Bagging

Quelle: Ji Zhu, University of Michigan

Ensemble methods: Random Forest

- **Random forest** is an extension of bagging
  - Main idea: Do not only sample from the data but also from the **variables**, which are used for splitting
- In random forest the trees are generated in the following way
  - Generate bootstrap samples from original data (same like bagging)
  - Build a decision tree on each bootstrap sample, but...
  - ... at each node of a decision tree, **randomly select k variables**, which are evaluated for splitting. Choose the best split (using only the k variables).



In each node: Sample k variables, choose best split based on them

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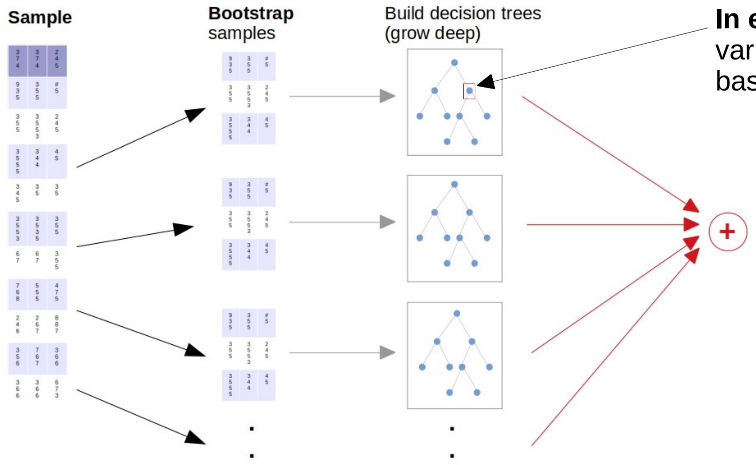
Can also use **sub-samples** instead of bootstrap samples. Bootstrap sampling can also induce bias in variable selection.

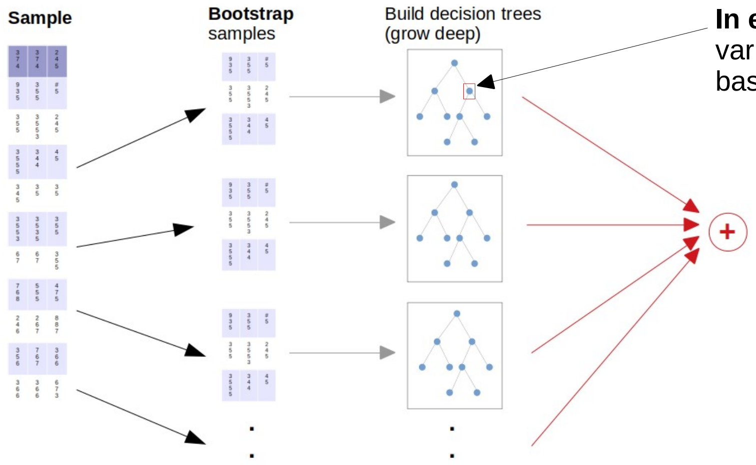


In each node: Sample k variables, choose best split based on them

Bias of bootstap sampling in RF:
Strobl, C., Boulesteix, A., Zeileis, A. et al. Bias in random forest variable importance measures: Illustrations, sources and a solution. BMC Bioinformatics 8, 25 (2007)

Ensemble methods: Random Forest

- What is the point of sampling the variables?
  - Sampling variables de-correlates the individual trees, makes them more diverse (this increases variance reduction)
  - **Intuition**: By restricting the variable selection at each node, some variables are incorporated in the analysis which might otherwise never be considered
  - This can reveal interactions in the data, which would otherwise not be detected



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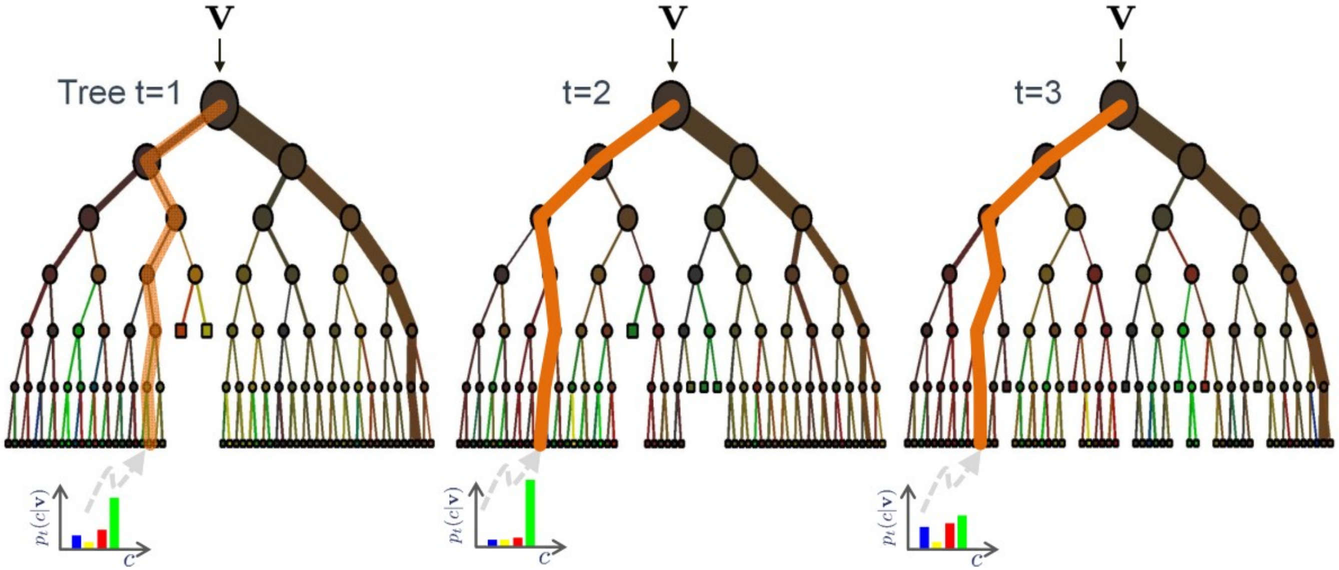
Ensemble methods: Random Forest

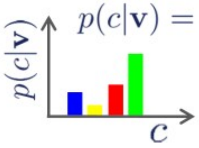
- Prediction of a new observation same like in bagging:
  - Run observation through all trees and incorporate each tree's prediction in the final prediction (e.g. majority vote for classification or mean for regression)
- Example of aggregating the tree's results for **classification**:



Source: Microsoft

Winner category: Category that was predicted most often (green)

Average probability:



$$p(c|\mathbf{v}) = \frac{1}{T}\sum_{t}^{T} p_t(c|\mathbf{v})$$

Random Forest in R

- We will use the **cforest()** function from the package "party" (unbiased variable selection)

```
library(party)
cfor_ctr <- cforest_unbiased(ntree = 500, mtry = 2)
(rf.iris <- cforest(Species~., data = iris, controls = cfor_ctr))
       Random Forest using Conditional Inference Trees


Number of trees:  500


Response:  Species
Inputs:  Sepal.Length, Sepal.Width, Petal.Length, Petal.Width
Number of observations:  150
# honest cross classification (OOB-error)
(confT <- table(iris$Species, predict(rf.iris, OOB = TRUE)))
             setosa versicolor virginica
  setosa         50          0         0
  versicolor      0         47         3
  virginica       0          4        46
diag(confT) <- 0
sum(confT)/nrow(iris)
[1] 0.04666667
varimp(rf.iris)
Sepal.Length  Sepal.Width Petal.Length  Petal.Width
 0.051127273  0.002109091  0.314800000  0.264909091
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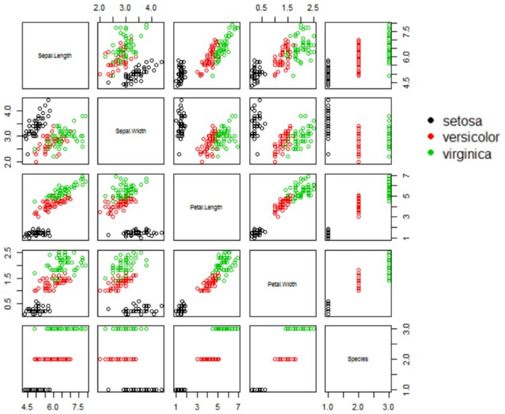

Random Forest in R

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Define the options/parameters for random forest

ntree: How many trees are grown?

mtry: How many variables are sampled at each node?

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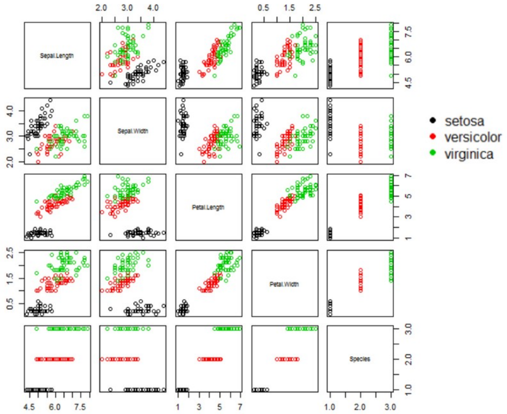
What is OOB? ...

What is varimp? ...



Out-of-bag error (OOB)

- Random Forest comes with its own integrated evaluation tool!
- Each tree is fitted to a bootstrap sample (or sub-sample) of original data
  - Thus, every tree in the forest has only seen a part of the data
- To calculate the **OOB-error**:
  - Predict each observation in the data using only the trees, which have not seen the observation when they were generated

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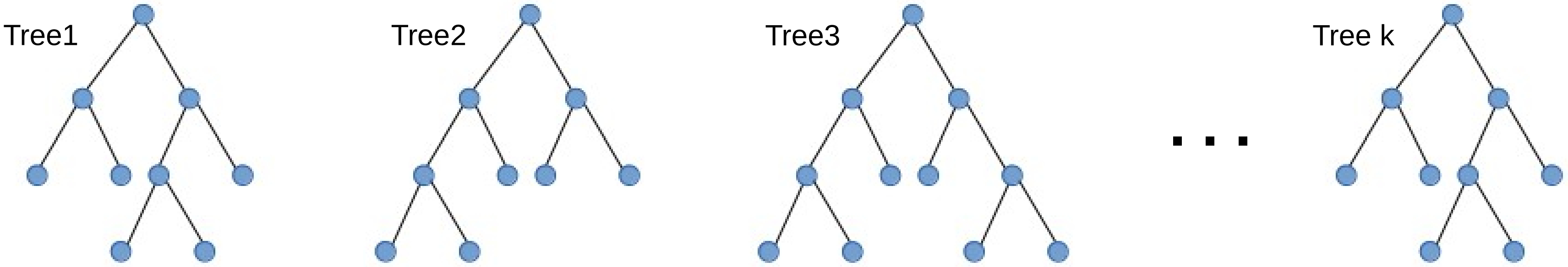
e.g. observation #24:

x1	x2	x3	y
23.4	66.3	2	A



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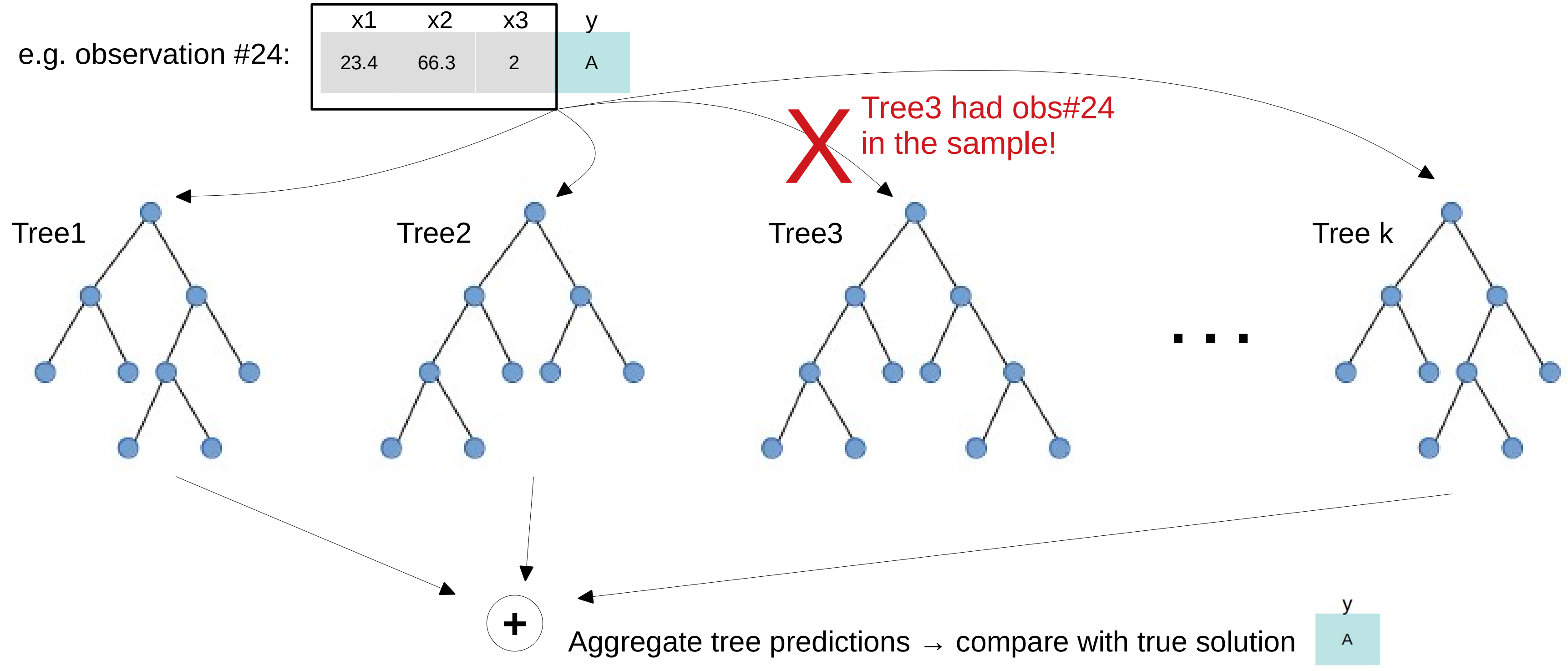

e.g. observation #24:

x1	x2	x3	y
23.4	66.3	2	A

Tree3 had obs#24 in the sample!

Aggregate tree predictions → compare with true solution

y
A

Out-of-bag error (OOB)

- Create OOB confusion table to look at the OOB-performance (see R-code slide)
- Use predict()-function and set OOB=TRUE, give no "newdata" argument

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rf.iris <- cforest(Species~., data = iris, controls =
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(confT <- table(iris$Species, predict(rf.iris, OOB = TRUE)))
             setosa versicolor virginica
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diag(confT) <- 0
sum(confT)/nrow(iris)
[1] 0.04666667
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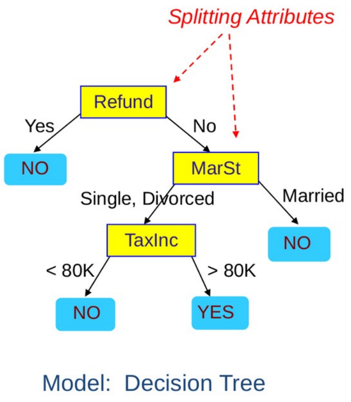
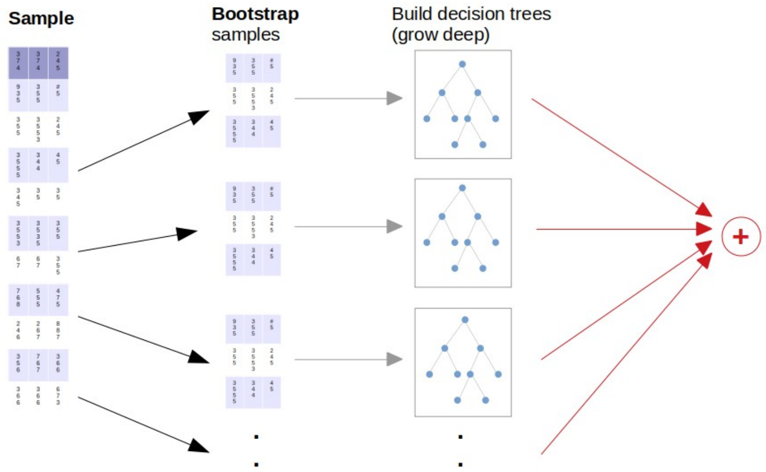
Interpretability of Random Forest

- One advantage of decision trees are their good interpretability
  - Can easily track how each variable affects the prediction
- In Random Forest we somewhat lose the interpretability
  - Difficult to track how each variable is active in each of the e.g. 500 trees…
- How can we assess which variables are **important** for prediction?

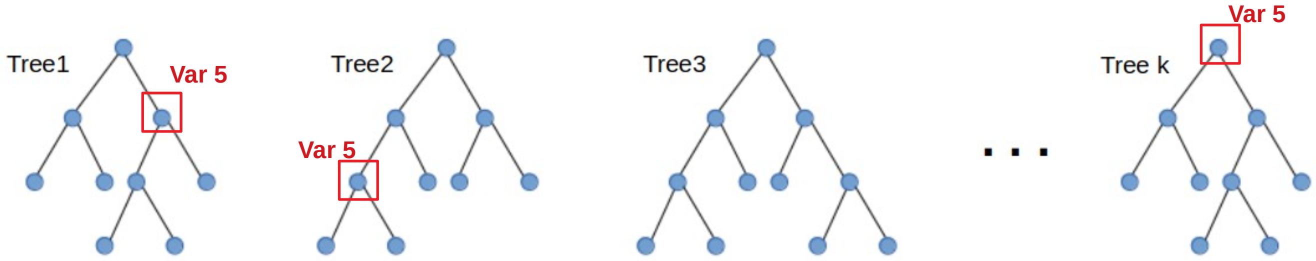


vs.



Variable importance in RF

- How could variable importance be **scored**?
  - Simple idea: Count the number of times a variable is chosen for splitting throughout all trees
- Two more elaborate approaches:
- **Variable importance 1**: Average score improvement at splits
  - For each node where variable x was used for splitting, record the achieved improvement in the splitting score (e.g. Gini-index -> **Gini-importance score**)
  - Variable x's importance 1 score is the average of all score improvements (can be weighted with the number of data points in each node)



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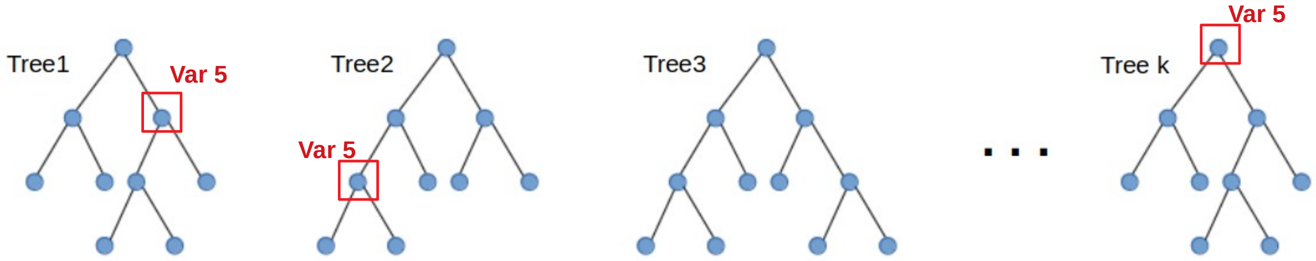
Caution: Gini-Importance is biased if different types of variables are present



Variable importance in RF

- **Variable importance 2**: Permutation importance
- **Permutation importance** is a very intuitive importance score
- Main idea: Mix up the values of variable x to break up any meaningful relation between x and the target variable (permutation)
  - Check how much the performance (usually the OOB-error) drops after permutation of x

Original data

Predictor 1	Predictor 2	Predictor 3	Target var
X1	**X2**	**X3**	**Y**
2.3	33.1	67	**A**
5.1	35.8	70.3	**B**
3.3	34.0	96	**A**
2.8	37.7	85	**C**
1.3	38.3	84.9	**A**

→ Calculate **OOB-error**

vs.

X1 permuted

Predictor 1	Predictor 2	Predictor 3	Target var
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1.3	37.7	85	**C**
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→ Calculate **OOB-error**

Permutation importance:
Difference in OOB-error

With stronger relation between x1 and target variable, the more should the OOB-error grow

Variable importance with R

- To calculate the variable importance after fitting a Random Forest use the **varimp()**-function (default is permutation importance score)

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rf.iris <- cforest(Species~., data = iris, controls = cfor_ctr)
varimp(rf.iris)
Sepal.Length  Sepal.Width Petal.Length  Petal.Width
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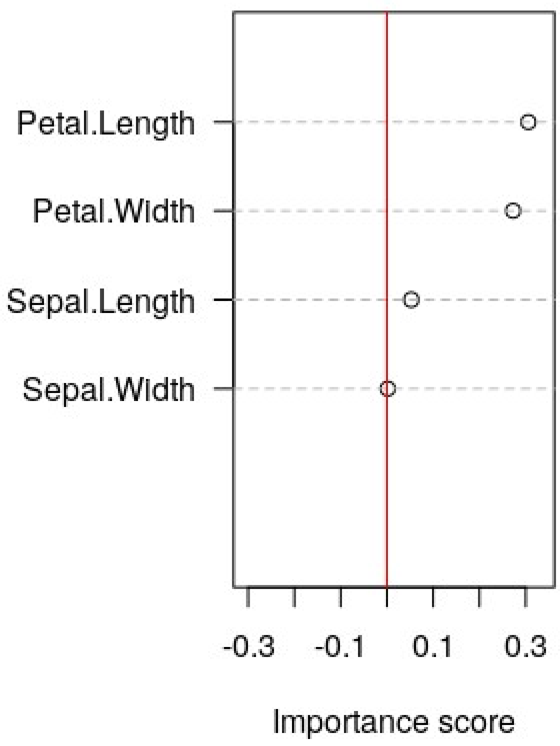
# Function to plot importance scores nicely
implot <- function(rf.fit){
  par(mar=c(9,9,9,9))
  scores <- sort(varimp(rf.fit))
  plot(x = scores, y = 1:length(scores) ,
       xlim=c(-max(scores), max(scores)*1.1),
       ylim=c(-1,(length(scores)+1)),
       yaxt='n', ylab='', xlab='Importance score')
  axis(2, at=1:length(scores), labels = names(scores), las=1)
  abline(h=1:length(scores), lty=2, col='grey')
  abline(v=0, col='red')
}

implot(rf.iris)
```



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Permutation importance scores can also be negative! → Why?

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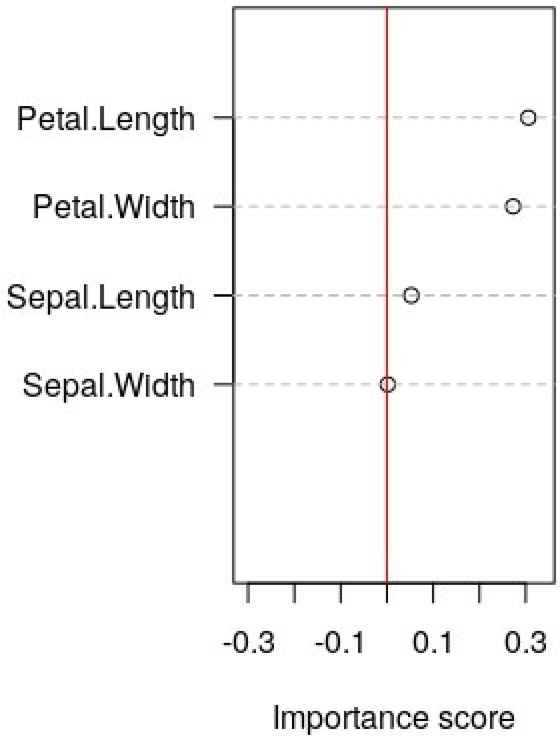
implot(rf.iris)
```

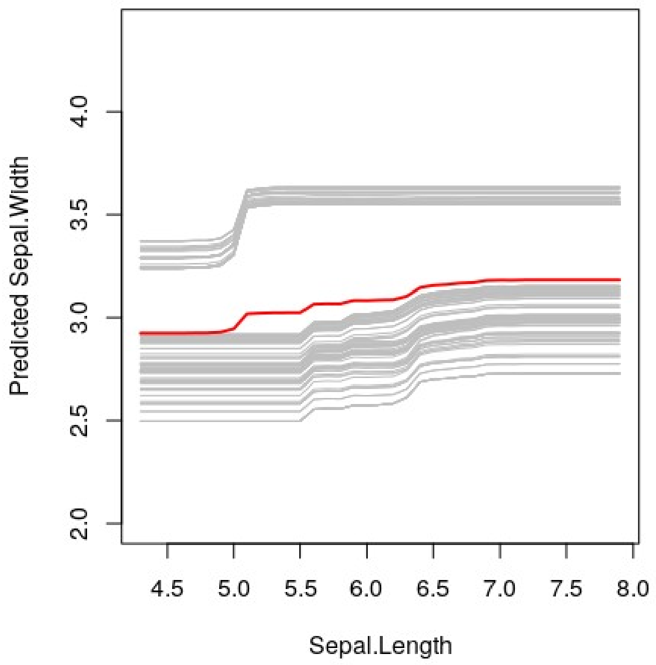


Because importance scores are based on random permutation we should fix the random seed when calculating them

Dependency plots in Random Forest

- Dependency plots are another method to "bring light" into what is happening in the forest
- Main idea: See how the prediction of the target variable changes when only **one predictor** is shifted in its value
- Example of **partial dependency plot** on RF-regression on the iris data (target variable: Sepal.width):

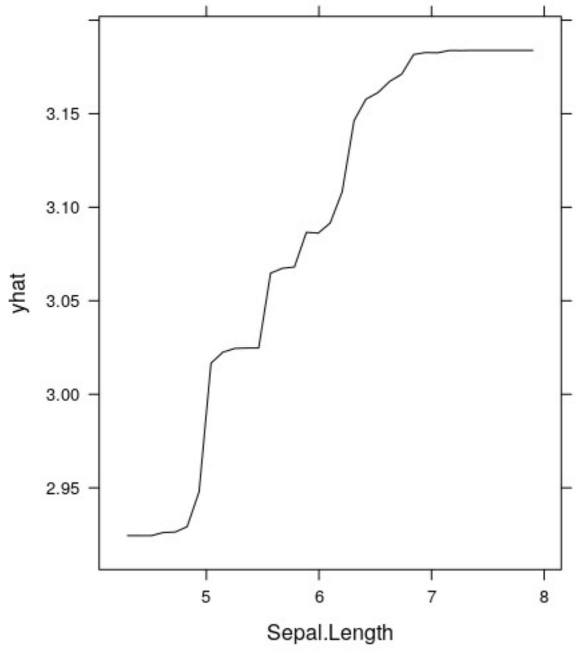
```
cfor_ctr <- cforest_unbiased(ntree = 500, mtry = 2)
rf.SepWid <- cforest(Sepal.Width~., data = iris, controls = cfor_ctr)
steps <- seq(min(iris$Sepal.Length), max(iris$Sepal.Length), by = 0.1)
predic <- matrix(NA, nrow=nrow(iris), ncol = length(steps))
for (i in 1:nrow(iris)){
  obs <- iris[i,]
  obs$Sepal.Width <- NULL # Remove column
  for(s in 1:length(steps)){
    obs$Sepal.Length <- steps[s]
    predic[i,s] <- predict(rf.SepWid, newdata=obs)
  }
}
plot(NULL, xlim=c(min(iris$Sepal.Length), max(iris$Sepal.Length)),
     ylim=c(min(iris$Sepal.Width), max(iris$Sepal.Width)),
     xlab='Sepal.Length', ylab='Predicted Sepal.Width')
for(l in 1:nrow(predic)){
  lines(x = steps, y = predic[l,], col='grey')
}
lines(x=steps, y=apply(predic, 2, mean), col='red', lwd=2)
```



Partial dependency plots with "pdp"

- "**pdp**" is an R package to construct partial dependency plots
- Can be applied to different Machine Learning methods
  - Also works for Random Forests fitted with cforest()

```
cfor_ctr <- cforest_unbiased(ntree = 500, mtry = 2)
rf.SepWid <- cforest(Sepal.Width~., data = iris,
             controls = cfor_ctr)
#install.packages("pdp")
library(pdp)
partial(rf.SepWid, pred.var = "Sepal.Length", plot = TRUE)
```



- Meaning of curve (same like in previous slide):
  - Mean predicted Sepal.Width for varying Sepal.Length
    (averaged over all observed constellations of other co-predictors)

Summary Random Forest

- **Advantages:**
  - Random Forest is a very effective ML method (good performance in ML-competitions)
  - Is non-parametric, poses no assumption regarding distribution of variables or residuals
  - Comes with included performance evaluation (OOB-error)
  - Random Forest does not tend to overfit
  - Can handle thousands of input variables
  - Can handle lots of noise variables with only few relevant variables
  - We can derive variable importance measures
  - Random Forest can detect strong and local interactions
  - Is robust against outliers
  - It can handle imbalanced data (e.g. using stratified bootstrap sampling)
  - ...

Summary Random Forest

- **Disadvantages:**
  - Less interpretability, feeling of a "black box"
  - Can not extrapolate predictions beyond the range of training data well
  - Takes more time to train than e.g. decision tree

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. https://doi.org/10.1037/a0016973