# Random Forest for Classification Problems

Raphael, Arkadiusz and Burak

Uni Bonn

January 16, 2020

# Overview

# Decision Tree: Example

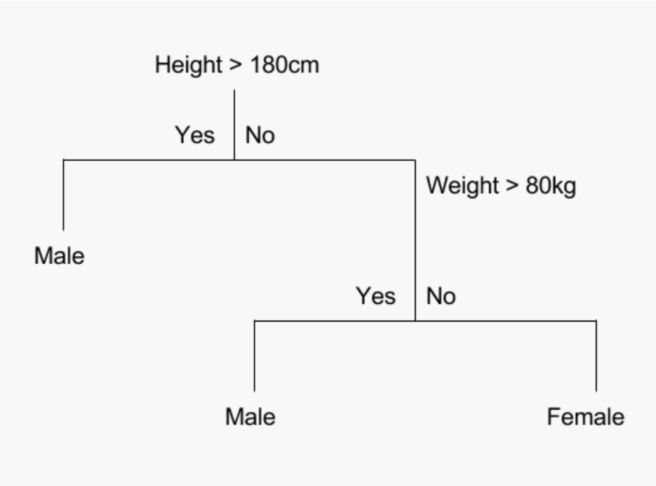


Figure: Source:[3]

# Decision Tree: Tree Building Process

A tree is grown starting from the root node by repeatedly using the following steps on each node (also called binary splitting) [1]:

(i) **Find best split $s$ for each feature $X_m$:** For each feature $X_m$, there exist $K-1$-many potiential splits whereas $K$ is the number of different values for the respective feature. Evaluate each value $X_{m,i}$ at the current node $t$ as a candidate split point (for $x \in X_m$, if $x \leq X_{m,i} = s$, then $x$ goes to left child node $t_L$ else to right child node $t_R$). The best split point is the one that maximize the splitting criterion $\Delta i(s,t)$ the most when the node is split according to it. The different splitting criteria will be covered in the next chapter.

(ii) **Find the nodes best split:** Among the best splits for each feature from Step (i) find the one $s^*$, which maximizes the splitting criterion $\Delta i(s,t)$.

(iii) **Satisfy stopping criterion:** Split the node $t$ using best node split $s^*$ from Step (ii) and repeat from Step (i) until stopping criterion is satisfied.

# Decision Tree: Purity Measures

## Gini Measure

$$i(t) = \sum_{c \in C} p(c|t)(1 - p(c|t)) = 1 - \sum_{c \in C} p_c^2 \tag{1}$$

## Information Entropy

$$i(t) = \sum_{c \in C} p(c|t) log(p(c|t)) \tag{2}$$

# Bias Variance Trade-off

## The Expected Generalization Error

$$y = f(x) + \epsilon \text{ and } \epsilon \sim \mathcal{N}(0, \sigma_\epsilon^2)$$
$$D = \{(x_1, y_1), (x_2, y_2), ..., (x_N, y_N)\}$$

The decomposition of a model's expected generalization error is

$$\boldsymbol{Err}(\hat{f}(x)) = \sigma_\epsilon^2 + [Bias(\hat{f}(x))]^2 + Var(\hat{f}(x))$$

$\sigma_\epsilon^2$ is irreducible and independent of the model.

Trade-off between bias and variance.

**Aim:** Decrease variance while keeping bias unincreased.

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# Bias-Variance Trade-off

## Illustration

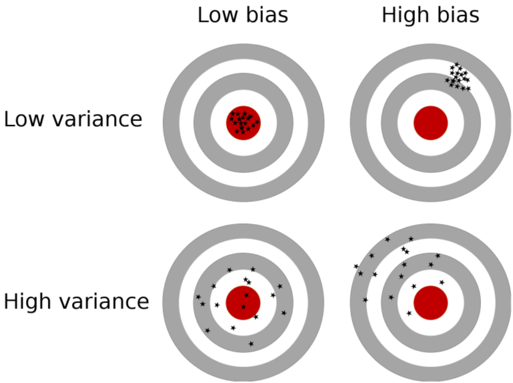


Figure: Illustration of bias-variance trade-off [5]

Decision trees generally have low bias and high variance [2].

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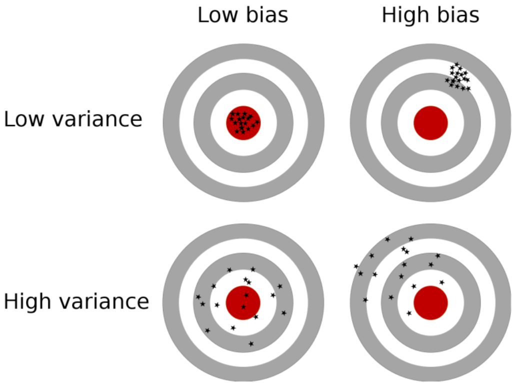


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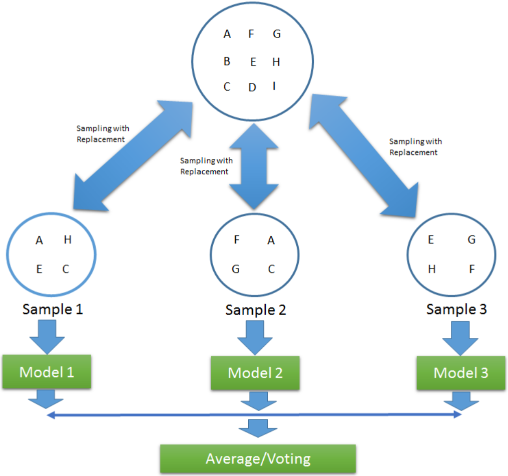
# Bagging

1. created for methods with high variance
2. reduces variance and gives better predictions
3. improvement of bagging: Random Forest



# Random Forest

An ensemble of randomly trained decision trees, so in other words random forest was defined by L. Breiman:

**Theorem**

*A random forest is a classifier consisting of a collection of tree-structured classifiers $\hat{T}_{\theta_b}(\mathbf{x}), b = 1, ..., B$ where the $\theta_b$ are independent identically distributed random vectors and each tree casts a unit vote for the most popular class at input $\mathbf{x}$ .*

Random Forest is an extension and improvement over bagging:

1. Like in bagging, multiple decision trees are built
2. Improvement: an injection of randomness is made

# Random Forest: randomness in the model

Two key concepts that makes decision forest "random" are:

1. Random sampling of training data points when building trees
2. Random subsets of features considered when splitting nodes. Recommended number of variables:
   a. For classification: $\lfloor \sqrt{n} \rfloor$
   b. For regression: $\lfloor \frac{n}{3} \rfloor$

# Random Forest: algorithm

**Algorithm 1:** Random Forest for Regression or Classification

1. For $b = 1$ to $B$:
   a. Draw a bootstrap sample $\theta_b$ of size N from the training data.
   b. Grow the Random Forest tree $T_{\theta_b}$ to the bootstrapped data, by recursively repeating the following steps for each terminal node of the tree, until the minimum node size $n_{min}$ is reached:
      i. Select $m$ variables at random from the $n$ variables
      ii. Pick the best variable/split-point among the $m$
      iii. Split the node into two daughter nodes
2. Output the ensemble of trees $\{T_{\theta_b}\}_1^B$

Section 2

# Mathematical Concept

# Mathematical Concept

Let $D = \{(x_1, y_1), (x_2, y_2), ..., (x_N, y_N)\}$ and
$T_{D,\theta}$ is a fully grown tree trained on set $D$ with using parameters $\theta$.
Random Forest estimate of an observation $x^*$ is

### Majority Voting

$$\boldsymbol{RF}_{D,\theta_1,\theta_2,...,\theta_B}(x^*) = \underset{c\in Y}{argmax} \sum_{b=1}^{B} 1(\hat{T}_b(x^*) = c)$$

### Soft Voting

$$\boldsymbol{RF}_{D,\theta_1,\theta_2,...,\theta_B}(x^*) = \underset{c\in Y}{argmax} \frac{1}{B} \sum_{b=1}^{B} \hat{p}_{D,\theta_b}(Y = c|X = x^*)$$

where $\hat{p}_{D,\theta_b}(Y = c|X = x^*)$ is the probability estimates of a tree.

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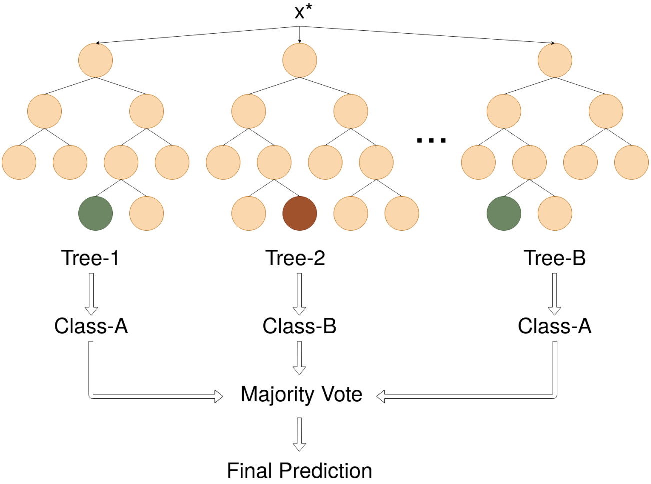

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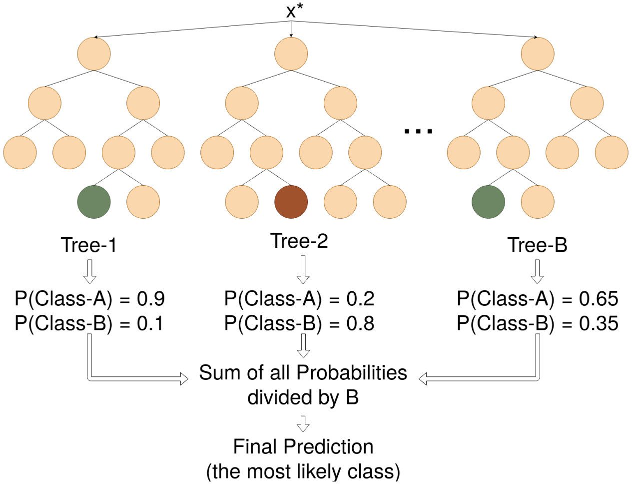

# Mathematical Concept

## The Expected Generalization Error of $\boldsymbol{T_{D,\theta}}$

Given $D = X \cup Y$,
the expected generalization error of $T_{D,\theta}$ is

$$\boldsymbol{Err}(T_{D,\theta}(X)) = \mathbb{E}_{X,Y}\{L(Y, T_{D,\theta}(X))\}$$

where $L(Y, T_{D,\theta}(X))$ is the loss function.

The decomposition of $\boldsymbol{Err}(T_{D,\theta})$ is

$$\boldsymbol{Err}(T_{D,\theta}(X)) = \boldsymbol{Err}(\phi_\beta(X)) + [Bias(T_{D,\theta}(X))]^2 + Var(T_{D,\theta}(X))$$

similarly

$$\boldsymbol{Err}(\boldsymbol{RF}_{D,\Theta}(X)) = \boldsymbol{Err}(\phi_\beta(X)) + [Bias(\boldsymbol{RF}_{D,\Theta}(X))]^2 + Var(\boldsymbol{RF}_{D,\Theta}(X))$$

where $\Theta = \{\theta_1, \theta_2, \ldots, \theta_B\}$.

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# Mathematical Concept

## Bayes Error

$$\boldsymbol{Err}(\boldsymbol{RF}_{D,\Theta}(X)) = \boldsymbol{Err}(\phi_\beta(X)) + [Bias(\boldsymbol{RF}_{D,\Theta}(X))]^2 + Var(\boldsymbol{RF}_{D,\Theta}(X))$$

Theoretically, there exists a model that minimizes the generalization error and can be derived analitically independent of the model [4].
Conditioning the expected generalization error on X gives:

$$\mathbb{E}_{X,Y}\{L(Y,\phi_\beta(X))\} = \mathbb{E}_X\{\mathbb{E}_{Y|X}\{L(Y,\phi_\beta(X))\}\}$$

Point-wise minimization of inner term yields:

$$\phi_\beta = \underset{c\in Y}{argmin}\ \mathbb{E}_{Y|X=x}\{L(Y,c)\}$$

Bayes Model $\phi_\beta$ is best attainable model.

$\boldsymbol{Err}(\phi_\beta(X))$ is the irreducible error.

**Result:** Ensembling has no effect on Bayes Error.

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$$[Bias(T_{D,\theta}(X))]^2 = (\phi_\beta(X) - \mathbb{E}_D\{T_{D,\theta}(X)\})^2$$

### $Bias^2$ of Random Forest

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We need $\mathbb{E}_{D,\Theta}\{\boldsymbol{RF}_{D,\Theta}(X))\}$.

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## Bias: The Expected Value of Random Forest

Random Forest Estimator for regression shares the same idea with soft-voting classification;

$$\boldsymbol{RF}_{D,\Theta}(X) = \frac{1}{B}\sum_{b=1}^{B} T_{D,\theta_b}(X)$$

Taking expectation gives;

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\mathbb{E}_{D,\Theta}\{\boldsymbol{RF}_{D,\Theta}(X)\} &= \mathbb{E}_{D,\Theta}\{\frac{1}{B}\sum_{b=1}^{B} T_{D,\theta_b}(X)\} \\
&= \frac{1}{B}\sum_{b=1}^{B} \mathbb{E}_{D,\theta_b}\{T_{D,\theta_b}(X)\} \\
&= \mu_{D,\hat{\theta}}(X)
\end{aligned}$$

where $\mu_{D,\hat{\theta}}(X)$ is the average prediction of all ensembled trees.

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For any two trees $T_{D,\theta'}$ and $T_{D,\theta''}$ trained with the same data $D$ and different growing parameters $\theta'$ and $\theta''$, we can define the correlation coefficient as follows

$$\rho(X) = \frac{\mathbb{E}_{D,\theta',\theta''}\{T_{D,\theta'}(X)T_{D,\theta''}(X)\} - \mu^2_{D,\theta}(X)}{\sigma^2_{D,\theta}(X)}$$

$\rho(X)$ is close to 1

- Highly correlated trees.
- Randomization has no significant effect.

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### Variance of Random Forest

$$\mathbb{V}_{D,\Theta}\{\boldsymbol{RF}_{D,\Theta}(X)\} = \rho(X)\sigma^2_{D,\theta}(X) + \frac{1-\rho(X)}{B}\sigma^2_{D,\theta}(X)$$

As $B \to \infty$, $\mathbb{V}\{\boldsymbol{RF}_{D,\Theta}(X)\}$ converges to $\rho(X)\sigma^2_{D,\theta}(X)$.

Due to randomization $\rho(X) < 1$

$$\implies \mathbb{V}\{\boldsymbol{RF}_{D,\Theta}(X)\} = \rho(x)\sigma^2_{D,\theta}(X) < \sigma^2_{D,\theta}(X) = \mathbb{V}\{T_{D,\theta}(X)\}.$$

**Result:**Ensembling trees decreases the variance.

$$\boldsymbol{Err}(\boldsymbol{RF}_{D,\Theta}(X)) = \boldsymbol{Err}(\phi_\beta(X)) + [Bias(\boldsymbol{RF}_{D,\Theta}(X))]^2 + Var(\boldsymbol{RF}_{D,\Theta}(X))$$

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# Mathematical Concept
## Variance Comparison

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# Mathematical Concept

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# Mathematical Concept

## Variance Comparison

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**Variance of Random Forest**

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**Result:** Ensembling trees decreases the variance.

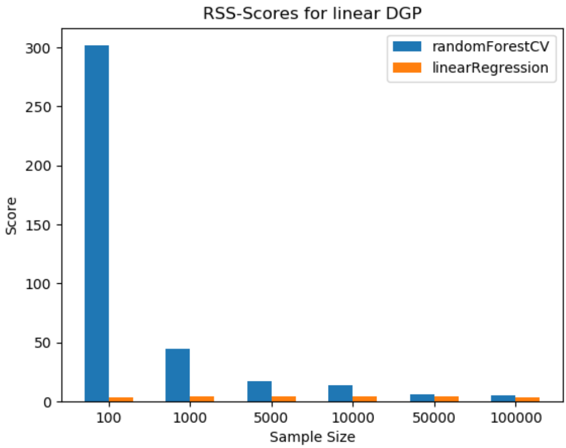
# Simulation Study: Linear DGP

The linear DGP generates the data tuples $(y, x_1, x_2, x_3)$ as follows:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \epsilon, \tag{3}$$

whereas $(\beta_0, \beta_1, \beta_2, \beta_3) = (0.3, 5, 10, 15)$, $x_1, x_2, x_3 \sim \mathcal{N}(0,\ 3)$, and $\epsilon \sim \mathcal{N}(0,\ 1)$.

# Decision Tree: Linear DGP Results



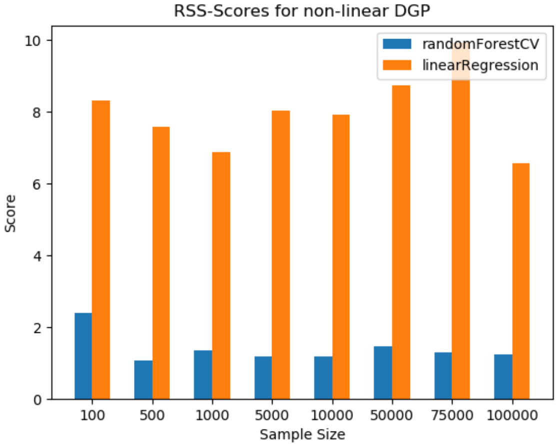
# Simulation Study: Non-Linear DGP

The non-linear DGP generates the data tuples $(y, x_1, x_2)$ as follows:

$$y = \beta_0 + \beta_1 \mathbb{1}(x_1 \geq 0, x_2 \geq 0) + \beta_2 \mathbb{1}(x_1 \geq 0, x_2 < 0) + \beta_3 \mathbb{1}(x_1 < 0) + \epsilon, \quad (4)$$

whereas $(\beta_0, \beta_1, \beta_2, \beta_3)$, $x_1, x_2$ and $\epsilon$ are the same as in the previous DGP.

# Simulation Study: Non-Linear DGP Results



# Real Data

**Data**: Titanic data
**Method used**:

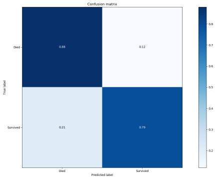
1. Random Forest
2. AdaBoost
3. Gradient Boosting Classifier

**Goal**: Given features of passengers predict which passengers survived the Titanic shipwreck

# Real Data: results

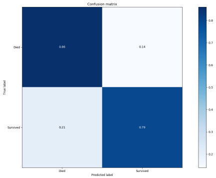
Random Forest

Accuracy: 84,32%



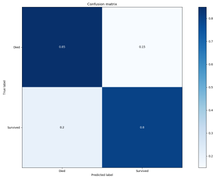

AdaBoost

Accuracy: 82.8%




Gradient Boosting

Accuracy: 82,8%



# The End

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