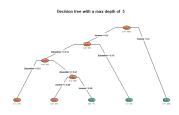
Wrap-up

Introduction

# Machine Learning for Official Statistics & SDGs Random Forest



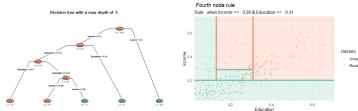
#### *Trees* are methods for classification or regression analysis.





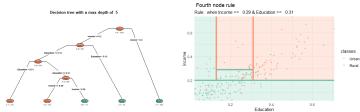
Education

Trees are methods for classification or regression analysis.



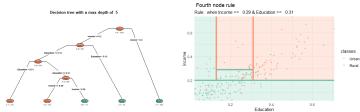
► Trees are based on recursive binary splits

*Trees* are methods for classification or regression analysis.



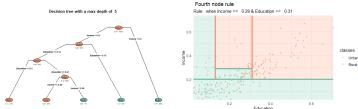
- ► Trees are based on recursive binary splits
- ► The structure is simple and corresponds to regions in the variable's space

Trees are methods for classification or regression analysis.

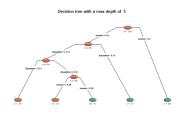


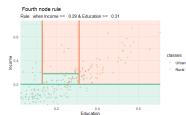
- ► Trees are based on recursive binary splits
- ► The structure is simple and corresponds to regions in the variable's space
- ► Each node is based on a the value of one variable and a threshold

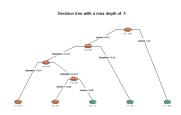
*Trees* are methods for classification or regression analysis.



- ► Trees are based on recursive binary splits
- ► The structure is simple and corresponds to regions in the variable's space
- ► Each node is based on a the value of one variable and a threshold
- ► Trees can be very detailed and prone to **over fitting**



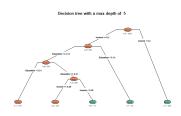






#### By structure:

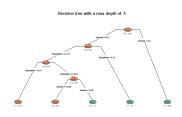
► Trees are splitting the variable's space into "rectangles"

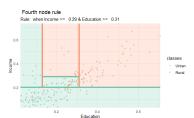




#### By structure:

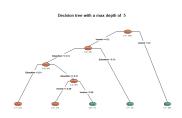
- ► Trees are splitting the variable's space into "rectangles"
- ► Predictions using a tree may not be very accurate

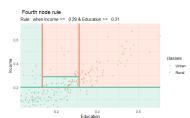




#### By structure:

- ► Trees are splitting the variable's space into "rectangles"
- ► Predictions using a tree may not be very accurate
- ► Trees are not robust to changes in the data





#### By structure:

- ► Trees are splitting the variable's space into "rectangles"
- ▶ Predictions using a tree may not be very accurate
- ► Trees are not robust to changes in the data
- ► Trees are prone to overfiting

The decision trees suffer from *high variance*:

The decision trees suffer from *high variance*:

► Take a sample and build a tree

The decision trees suffer from high variance:

- ► Take a sample and build a tree
- ▶ Divide the sample in two parts and build a tree on each part

## [ Problems with trees ]

The decision trees suffer from high variance:

- ► Take a sample and build a tree
- ➤ Divide the sample in two parts and build a tree on each part
- $\hookrightarrow$  The two trees will likely be very different

## [ EXAMPLE ON A SIMPLE TREE ]

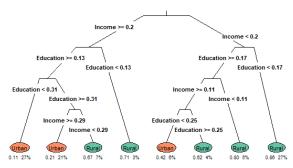
Wrap-up

## [ EXAMPLE ON A SIMPLE TREE ]

Introduction

#### Which tree do you trust?

#### Tree with all observations (max depth = 4)

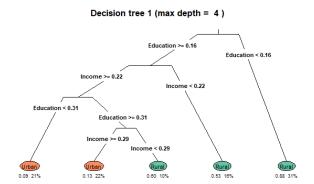


Tree using all observations

## [ EXAMPLE ON A SIMPLE TREE ]

Introduction

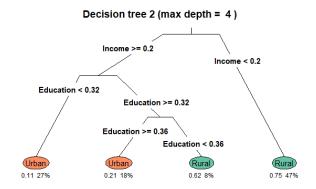
#### Which tree do you trust?



First tree with 50% of observations

Introduction

### Which tree do you trust?

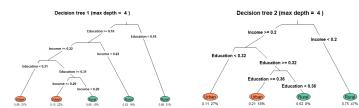


Second tree with 50% of observations

Introduction

Which tree do you trust?

Outcomes are different from one tree to another



## [ How to use trees? ]

Alternative to simple tree models:

Wrap-up

## [ How to use trees? ]

Introduction

Alternative to simple tree models:

► Aggregating the results of trees can help

## [ How to use trees? ]

Alternative to simple tree models:

- ► Aggregating the results of trees can help
- $\hookrightarrow$  "Bagging"

## [ How to use trees? ]

#### Alternative to simple tree models:

- ► Aggregating the results of trees can help
- → "Bagging"

Introduction

► Some trees may be too similar (correlated) and have to be "decorrelated" using random draws of the variable used

## [ HOW TO USE TREES? ]

#### Alternative to simple tree models:

- ► Aggregating the results of trees can help
- → "Bagging"

- ► Some trees may be too similar (correlated) and have to be "decorrelated" using random draws of the variable used
- $\hookrightarrow$  "Random forest"

## [ How to use trees? ]

#### Alternative to simple tree models:

- ► Aggregating the results of trees can help
- $\hookrightarrow$  "Bagging"

- ► Some trees may be too similar (correlated) and have to be "decorrelated" using random draws of the variable used
- $\hookrightarrow$  "Random forest"
  - ► Trees can be constructed *sequentially*

## [ How to use trees? ]

#### Alternative to simple tree models:

- ► Aggregating the results of trees can help
- $\hookrightarrow$  "Bagging"

- ► Some trees may be too similar (correlated) and have to be "decorrelated" using random draws of the variable used
- $\hookrightarrow$  "Random forest"
- ► Trees can be constructed *sequentially*
- $\hookrightarrow$  "Boosting"

Wrap-up

## [SOME SIMPLE MATHEMATICAL TRICKS]

Introduction

Aggregating the results of trees can help decrease the variance

Introduction

## [SOME SIMPLE MATHEMATICAL TRICKS]

Aggregating the results of trees can help decrease the variance

▶ Intuitively, if  $U_i$ , ...  $U_B$  are iid with variance  $\sigma^2$ , then the average of these variables has a lower variance

Introduction

## [SOME SIMPLE MATHEMATICAL TRICKS]

Aggregating the results of trees can help decrease the variance

▶ Intuitively, if  $U_i$ , ...  $U_B$  are iid with variance  $\sigma^2$ , then the average of these variables has a lower variance

$$Var\left(\frac{1}{B}\sum_{i=1}^{B}U_{i}\right) = \frac{\sigma^{2}}{B}$$

$$< \sigma^{2}$$

Aggregating the results of trees can help decrease the variance

▶ Intuitively, if  $U_i$ , . . .  $U_B$  are iid with variance  $\sigma^2$ , then the average of these variables has a lower variance

$$Var\left(\frac{1}{B}\sum_{i=1}^{B}U_{i}\right) = \frac{\sigma^{2}}{B}$$

$$< \sigma^{2}$$

► This is a simple principle that is used here

Bagging stands for Bootstrap Aggregating uses a simple logic:

1. Draw *B* bootstrapped samples from the original sample

- 1. Draw *B* bootstrapped samples from the original sample
- 2. Construct *B* trees, one on each sample

Introduction

- 1. Draw *B* bootstrapped samples from the original sample
- 2. Construct *B* trees, one on each sample
- 3. Average the result to get a prediction with a lower variance

Introduction

- 1. Draw *B* bootstrapped samples from the original sample
- 2. Construct *B* trees, one on each sample
- 3. Average the result to get a prediction with a lower variance

## [ BAGGING ]

Introduction

Bagging stands for Bootstrap Aggregating uses a simple logic:

- 1. Draw *B* bootstrapped samples from the original sample
- 2. Construct *B* trees, one on each sample
- 3. Average the result to get a prediction with a lower variance

In classification, we do not average but take the *majority vote* rule

# [ Bagging ]

Introduction

#### Bagging scheme:

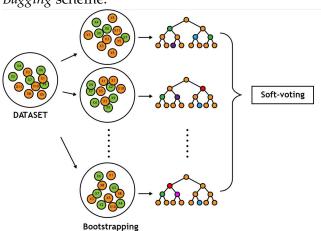


Image from igem.org

# [ THE PROBLEM WITH Bagging ]

Bootstrapped (Bagging) trees use the same set of variables

Wrap-up

# [ THE PROBLEM WITH Bagging ]

Introduction

Bootstrapped (Bagging) trees use the same set of variables

► Aggregating *correlated* trees will **not** decrease variance

# [ THE PROBLEM WITH Bagging ]

Introduction

Bootstrapped (Bagging) trees use the same set of variables

- ► Aggregating *correlated* trees will **not** decrease variance
- ▶ Intuitively, if  $U_i, ..., U_B$  are with variance  $\sigma^2$ , and cross-correlation  $\rho$ , then the average has a variance:

$$Var\left(\frac{1}{B}\sum_{i=1}^{B}U_{i}\right) = \rho \cdot \sigma^{2} + \frac{\sigma^{2}}{B}$$

Introduction

# [ THE PROBLEM WITH Bagging ]

Bootstrapped (*Bagging*) trees use the same set of variables

- ► Aggregating *correlated* trees will **not** decrease variance
- ▶ Intuitively, if  $U_i, ..., U_B$  are with variance  $\sigma^2$ , and **cross-correlation**  $\rho$ , then the average has a variance:

$$Var\left(\frac{1}{B}\sum_{i=1}^{B}U_{i}\right) = \rho \cdot \sigma^{2} + \frac{\sigma^{2}}{B}$$

ightharpoonup This could be "high" if  $\rho$  is "high"

# [ THE PROBLEM WITH Bagging ]

Bootstrapped (Bagging) trees use the same set of variables

- ► Aggregating *correlated* trees will **not** decrease variance
- ▶ Intuitively, if  $U_i$ , . . .  $U_B$  are with variance  $\sigma^2$ , and cross-correlation  $\rho$ , then the average has a variance:

$$Var\left(\frac{1}{B}\sum_{i=1}^{B}U_{i}\right) = \rho \cdot \sigma^{2} + \frac{\sigma^{2}}{B}$$

- ▶ This could be "high" if  $\rho$  is "high"
- → Random forest use a decorrelation algorithm by adding randomness in the set of variables used

Random forest use two mechanisms:

► Bootstrap aggregating (bagging)

Introduction

- ► Bootstrap aggregating (*bagging*)
- $\hookrightarrow$  Construct *B* trees, on *B* bootstrapped samples

Wrap-up

### [ RANDOM FOREST]

Introduction

- ► Bootstrap aggregating (*bagging*)
- $\hookrightarrow$  Construct *B* trees, on *B* bootstrapped samples
- ► **Random** selection of variables (*Feature sampling*)

Wrap-up

### [ RANDOM FOREST]

Introduction

- ► Bootstrap aggregating (*bagging*)
- $\hookrightarrow$  Construct *B* trees, on *B* bootstrapped samples
- ► **Random** selection of variables (*Feature sampling*)
- $\hookrightarrow$  At each node, randomly select only **m** variables

Introduction

- ► Bootstrap aggregating (*bagging*)
- $\hookrightarrow$  Construct *B* trees, on *B* bootstrapped samples
- ► **Random** selection of variables (*Feature sampling*)
- $\hookrightarrow$  At each node, randomly select only **m** variables
- ► The resulting predictor will have a lower variance

$$Var_{Random\ forest} = \rho \cdot \sigma^2 + \frac{\sigma^2}{B}$$

Introduction

#### Random forest use two mechanisms:

- ► Bootstrap aggregating (*bagging*)
- $\hookrightarrow$  Construct *B* trees, on *B* bootstrapped samples
- ► **Random** selection of variables (*Feature sampling*)
- $\hookrightarrow$  At each node, randomly select only **m** variables
- ► The resulting predictor will have a lower variance

$$Var_{Random\ forest} = \rho \cdot \sigma^2 + \frac{\sigma^2}{B}$$

Common practice (p = nb of variables):

Introduction

*Random forest* use two mechanisms:

- ► Bootstrap aggregating (*bagging*)
- $\hookrightarrow$  Construct *B* trees, on *B* bootstrapped samples
- ► **Random** selection of variables (*Feature sampling*)
- $\hookrightarrow$  At each node, randomly select only **m** variables
- ► The resulting predictor will have a lower variance

$$Var_{Random\ forest} = \rho \cdot \sigma^2 + \frac{\sigma^2}{B}$$

Common practice (p = nb of variables):

►  $m \approx \sqrt{p}$  in classification

Introduction

*Random forest* use two mechanisms:

- ► Bootstrap aggregating (*bagging*)
- $\hookrightarrow$  Construct *B* trees, on *B* bootstrapped samples
- ► **Random** selection of variables (*Feature sampling*)
- $\hookrightarrow$  At each node, randomly select only **m** variables
- ► The resulting predictor will have a lower variance

$$Var_{Random\ forest} = \rho \cdot \sigma^2 + \frac{\sigma^2}{B}$$

Common practice (p = nb of variables):

- ►  $m \approx \sqrt{p}$  in classification
- ►  $m \approx p/3$  in regression

Introduction

Random forest scheme:

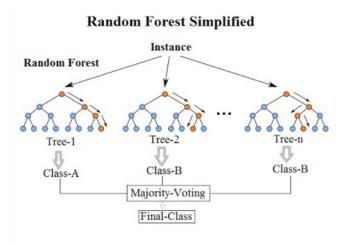


Image from Venkata Jagannath (wikimedia.org)

Introduction

Random forest are sensitive to several hyperparameters

Wrap-up

### [ OPTIMIZING RANDOM FOREST]

Introduction

*Random forest* are sensitive to several *hyperparameters* 

► All the parameters used to build a *tree* 

Wrap-up

### [ OPTIMIZING RANDOM FOREST]

Introduction

Random forest are sensitive to several hyperparameters

- ► All the parameters used to build a *tree* 
  - ► *Purity* criterion (Gini *vs* Entropy)

Boosting

Wrap-up

### [ OPTIMIZING RANDOM FOREST]

#### Random forest are sensitive to several hyperparameters

- ► All the parameters used to build a *tree* 
  - ► *Purity* criterion (Gini *vs* Entropy)
  - ► Tree *Depth*

#### *Random forest* are sensitive to several *hyperparameters*

- ► All the parameters used to build a *tree* 
  - ► *Purity* criterion (Gini *vs* Entropy)
  - ► Tree *Depth*

Introduction

► Complexity parameter Cp

Wrap-up

## [ OPTIMIZING RANDOM FOREST]

#### Random forest are sensitive to several hyperparameters

- ► All the parameters used to build a *tree* 
  - ► *Purity* criterion (Gini *vs* Entropy)
  - ► Tree *Depth*
  - ► *Complexity* parameter *Cp*
  - **▶** ...

#### Random forest are sensitive to several hyperparameters

- ► All the parameters used to build a *tree* 
  - ► *Purity* criterion (Gini *vs* Entropy)
  - ► Tree *Depth*
  - Complexity parameter Cp
  - ▶ ..

Introduction

▶ Parameters used to construct the *Forest* 

#### Random forest are sensitive to several hyperparameters

- ► All the parameters used to build a *tree* 
  - ► *Purity* criterion (Gini *vs* Entropy)
  - ► Tree *Depth*
  - ► *Complexity* parameter *Cp*
  - ▶ ..

- ▶ Parameters used to construct the *Forest* 
  - ► Number of variables *m* used in each node

#### Random forest are sensitive to several hyperparameters

- ► All the parameters used to build a *tree* 
  - ► *Purity* criterion (Gini *vs* Entropy)
  - ► Tree *Depth*
  - Complexity parameter Cp
  - ▶ ..

- ▶ Parameters used to construct the *Forest* 
  - ► Number of variables *m* used in each node
  - ► Number of trees

#### Random forest are sensitive to several hyperparameters

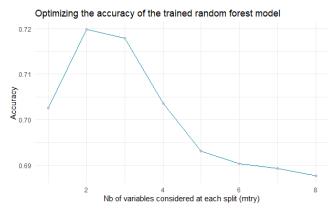
- ► All the parameters used to build a *tree* 
  - ► *Purity* criterion (Gini *vs* Entropy)
  - ► Tree *Depth*
  - ► *Complexity* parameter *Cp*
  - ▶ ..

- ▶ Parameters used to construct the *Forest* 
  - ▶ Number of variables *m* used in each node
  - ► Number of trees
  - ► Minimum number of observations per leaves

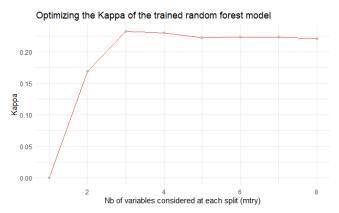
#### Random forest are sensitive to several hyperparameters

- ► All the parameters used to build a *tree* 
  - ► *Purity* criterion (Gini *vs* Entropy)
  - ► Tree *Depth*
  - ► *Complexity* parameter *Cp*
  - ▶ ..

- ▶ Parameters used to construct the *Forest* 
  - ▶ Number of variables *m* used in each node
  - ► Number of trees
  - ► Minimum number of observations per leaves
  - **>** ...



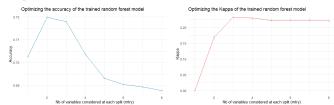
The impact of the number of variables (m) on accuracy



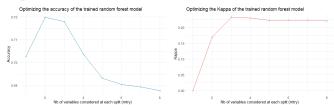
The impact of the number of variables (m) on kappa

The impact of the number of variables (*m*):

#### The impact of the number of variables (m):

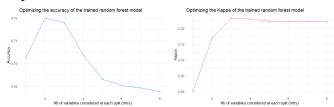


#### The impact of the number of variables (m):



Why are the curves decreasing after a threshold?

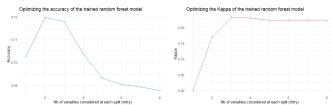
The impact of the number of variables (m):



Why are the curves decreasing after a threshold?

► The variance depends on  $\rho \cdot \sigma^2$ 

#### The impact of the number of variables (m):



Why are the curves decreasing after a threshold?

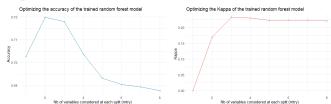
- ► The variance depends on  $\rho \cdot \sigma^2$
- $\hookrightarrow \textit{ Trees using similar variables are very similar (same predictions)}$

$$\nearrow m \Longrightarrow \rho \nearrow$$

Introduction

### [ RANDOM FOREST ON AN EXAMPLE]

#### The impact of the number of variables (m):



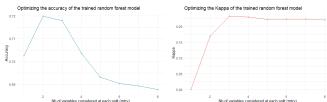
Why are the curves decreasing after a threshold?

- ► The variance depends on  $\rho \cdot \sigma^2$
- $\hookrightarrow$  Trees using similar variables are very similar (same predictions)  $\nearrow m \Longrightarrow \rho \nearrow$ 
  - ▶ Optimum for 3 (out of 7) regressors only at each node

Introduction

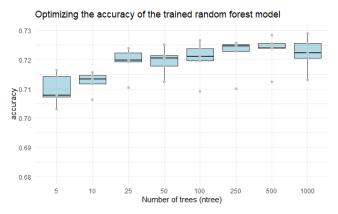
### [ RANDOM FOREST ON AN EXAMPLE]

#### The impact of the number of variables (m):

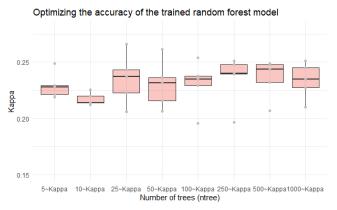


Why are the curves decreasing after a threshold?

- ► The variance depends on  $\rho \cdot \sigma^2$
- $\hookrightarrow$  Trees using similar variables are very similar (same predictions)  $\nearrow$   $m \Longrightarrow \rho \nearrow$ 
  - ▶ Optimum for 3 (out of 7) regressors only at each node
- $\hookrightarrow$  Rule of thumb:  $m \approx \sqrt{p}$



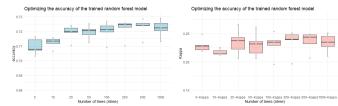
The impact of the number of trees on accuracy



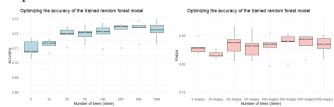
The impact of the number of trees on kappa

The impact of the number of trees:

#### The impact of the number of trees:



#### The impact of the number of trees:

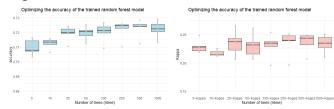


▶ No clear optimum → Moderate number of trees is OK

Introduction

# [ RANDOM FOREST ON AN EXAMPLE]

#### The impact of the number of trees:

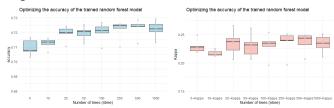


- ightharpoonup No clear optimum  $\hookrightarrow$  Moderate number of trees is OK
- ► The variance depends on  $\frac{\sigma^2}{B}$   $\nearrow B \Longrightarrow \frac{\sigma^2}{B} \searrow$

Introduction

# [ RANDOM FOREST ON AN EXAMPLE]

#### The impact of the number of trees:



- ▶ No clear optimum 

  Moderate number of trees is OK
- ► The variance depends on  $\frac{\sigma^2}{B}$   $\nearrow B \Longrightarrow \frac{\sigma^2}{B} \searrow$
- → More tree reduces variance (up-to a certain point)

### [IMPROVEMENTS]

### [IMPROVEMENTS]

Trees can also grow differently:

► Random Forest grow *independently* 

### [ IMPROVEMENTS]

- ► Random Forest grow *independently*
- ► "Vote" or average of the outcome from leaves

### [ IMPROVEMENTS]

- ► Random Forest grow *independently*
- ► "Vote" or average of the outcome from leaves
- ► Trees can be constructed *sequentially*

## [IMPROVEMENTS]

- ► Random Forest grow *independently*
- ► "Vote" or average of the outcome from leaves
- ► Trees can be constructed *sequentially*
- $\hookrightarrow$  "Boosting"

Boosting helps construct trees sequentially

Boosting helps construct trees sequentially

► Based on weak learners

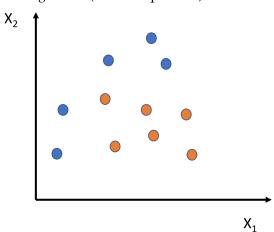
Boosting helps construct trees sequentially

- ► Based on weak learners

#### Boosting helps construct trees sequentially

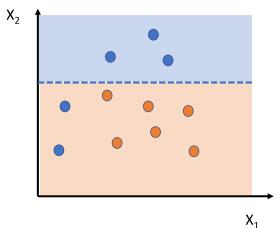
- ▶ Based on weak learners
- - ightharpoonup "Mistakes" at tree nb t are overweighed for tree nb t+1

*Boosting* a tree (iterative process)



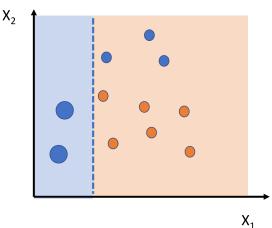
Two classes of observations: Orange and blue

#### *Boosting* a tree (iterative process)



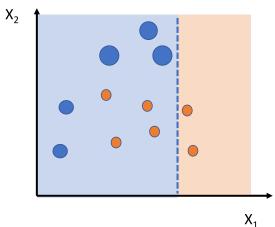
First weak learner

#### *Boosting* a tree (iterative process)



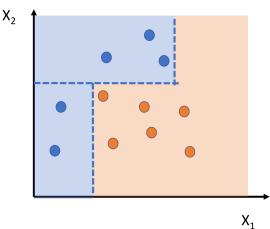
Second weak learner. Misclassification overweighed

#### *Boosting* a tree (iterative process)



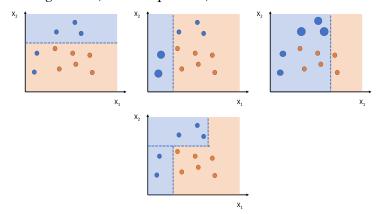
Third weak learner. New misclassification overweighed

*Boosting* a tree (iterative process)



Combining weak learners.

#### *Boosting* a tree (iterative process)



Combining weak learners. Classification tree completed

#### Boosting has several features

► Extremely powerful

- ► Extremely powerful
- ► Based on simple trees (weak learners)

Introduction

- ► Extremely powerful
- ► Based on simple trees (weak learners)
- ► The "weight" placed on "mistakes" is important

Introduction

- ► Extremely powerful
- ► Based on simple trees (weak learners)
- ► The "weight" placed on "mistakes" is important
- → Several choices gradient boosting

Introduction

- ► Extremely powerful
- ► Based on simple trees (weak learners)
- ► The "weight" placed on "mistakes" is important
- Several choices gradient boosting
- ► Sequential procedure (no parallel computation)

Introduction

- ► Extremely powerful
- ► Based on simple trees (weak learners)
- ► The "weight" placed on "mistakes" is important
- → Several choices gradient boosting
- ► Sequential procedure (no parallel computation)
- $\hookrightarrow$  Xgboosting

► Random forest are simple and easy to interpret

- Random forest are simple and easy to interpret
- Random forest use two mechanisms: bagging + (random) feature selection

- ► Random forest are simple and easy to interpret
- Random forest use two mechanisms: bagging + (random) feature selection
  - ► Bootstrap aggregating (*bagging*)

- ► Random forest are simple and easy to interpret
- ► *Random forest* use two mechanisms: bagging + (random) feature selection
  - ► Bootstrap aggregating (*bagging*)
  - $\hookrightarrow$  Construct *B* trees, on *B* bootstrapped samples

- ► Random forest are simple and easy to interpret
- ► *Random forest* use two mechanisms: bagging + (random) feature selection
  - ► Bootstrap aggregating (*bagging*)
  - $\hookrightarrow$  Construct *B* trees, on *B* bootstrapped samples
  - ► **Random** selection of variables (*Feature sampling*)

- ► Random forest are simple and easy to interpret
- ► *Random forest* use two mechanisms: bagging + (random) feature selection
  - ► Bootstrap aggregating (*bagging*)
  - $\hookrightarrow$  Construct *B* trees, on *B* bootstrapped samples
  - ► **Random** selection of variables (*Feature sampling*)
  - $\hookrightarrow$  At each node, randomly select only **m** variables

- ► Random forest are simple and easy to interpret
- ► *Random forest* use two mechanisms: *bagging* + (random) feature selection
  - Bootstrap aggregating (bagging)
  - $\hookrightarrow$  Construct *B* trees, on *B* bootstrapped samples
  - ► **Random** selection of variables (*Feature sampling*)
  - $\hookrightarrow$  At each node, randomly select only **m** variables
  - ► The resulting predictor will have a lower variance

$$Var_{Random\ forest} = \rho \cdot \sigma^2 + \frac{\sigma^2}{B}$$

Introduction

- ► Random forest are simple and easy to interpret
- Random forest use two mechanisms: bagging + (random) feature selection
  - Bootstrap aggregating (bagging)
  - $\hookrightarrow$  Construct *B* trees, on *B* bootstrapped samples
  - ► **Random** selection of variables (*Feature sampling*)
  - $\hookrightarrow$  At each node, randomly select only **m** variables
  - ► The resulting predictor will have a lower variance

$$Var_{Random forest} = \rho \cdot \sigma^2 + \frac{\sigma^2}{B}$$

► Many variations in random forest exist (boosting, gradient boosting, Xgboosting)

- ► Random forest are simple and easy to interpret
- ► *Random forest* use two mechanisms: bagging + (random) feature selection
  - ► Bootstrap aggregating (*bagging*)
  - $\hookrightarrow$  Construct *B* trees, on *B* bootstrapped samples
  - ► **Random** selection of variables (*Feature sampling*)
  - $\hookrightarrow$  At each node, randomly select only **m** variables
  - ► The resulting predictor will have a lower variance

$$Var_{Random\ forest} = \rho \cdot \sigma^2 + \frac{\sigma^2}{B}$$

- ► Many variations in random forest exist (boosting, gradient boosting, Xgboosting)
- ➤ Several parameters to adjust: Nb of trees, nb of variables in each node, minimum number of obs. in leaves/nodes, tree complexity, stopping rules, etc.

- ► Random forest are simple and easy to interpret
- ► *Random forest* use two mechanisms: *bagging* + (random) feature selection
  - ► Bootstrap aggregating (*bagging*)
  - $\hookrightarrow$  Construct *B* trees, on *B* bootstrapped samples
  - ► **Random** selection of variables (*Feature sampling*)
  - $\hookrightarrow$  At each node, randomly select only **m** variables
  - ► The resulting predictor will have a lower variance

$$Var_{Random\ forest} = \rho \cdot \sigma^2 + \frac{\sigma^2}{B}$$

- ► Many variations in random forest exist (boosting, gradient boosting, Xgboosting)
- ► Several parameters to adjust: Nb of trees, nb of variables in each node, minimum number of obs. in leaves/nodes, tree complexity, stopping rules, etc.
- ► Implemented in many software!