Machine Learning for Official Statistics and SDGs

Fourth Live Lecture (Webinar): Starts in **15** minutes

Christophe Bontemps, UN SIAP



Machine Learning for Official Statistics and SDGs

Fourth Live Lecture (Webinar): Starts in **10** minutes

Christophe Bontemps, UN SIAP



Wrap-up

Machine Learning for Official Statistics and SDGs

Fourth Live Lecture (Webinar): Starts in **5** minutes

Christophe Bontemps, UN SIAP



Bagging

Machine Learning for Official Statistics and SDGs

Tree-based methods:

From Trees to (random) Forest



► Introduction

- Introduction
- ► Lecture "From Trees to Forest"

- ► Introduction
- ▶ Lecture "From Trees to Forest"
- ► Q&A

- ► Introduction
- ► Lecture "From Trees to Forest"
- ► Q&A
- ► Next week

Trees are methods for classification or regression analysis.

Trees are based on recursive binary splits

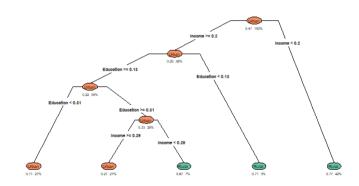
- Trees are based on recursive binary splits
- ▶ The structure is simple and corresponds to regions in the variable's space

- 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 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

Let us see how this tree is constructed:

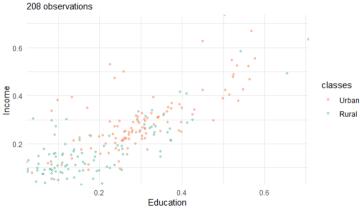
Decision tree with a max depth of 5



4 nodes leading to final leaves \hookrightarrow Depth = 5

The problem is a 2D space

Position of Rural and Urban households in (Education, Income) space



Random Forest

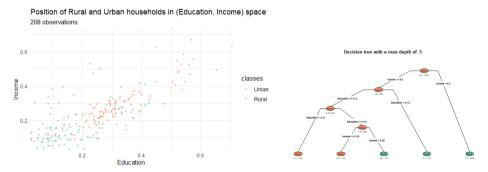
Boosting

Wrap-up

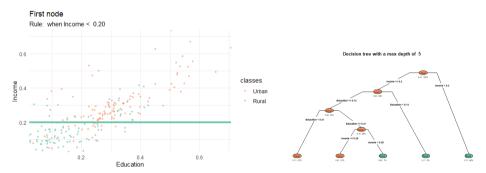
[EXAMPLE ON A SIMPLE TREE]

The problem with trees

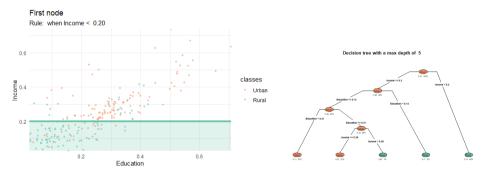
Introduction



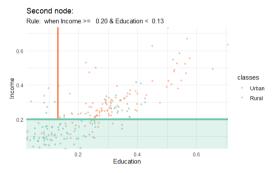
How to split the (Education, Income) space?

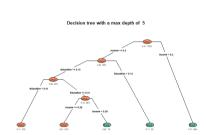


The first boundary decision line

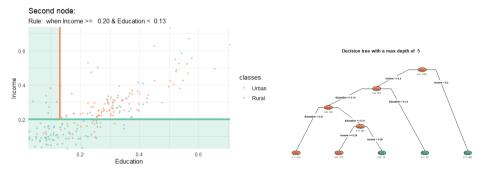


The space below the line is classified as rural

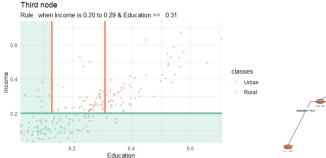




Second boundary decision line

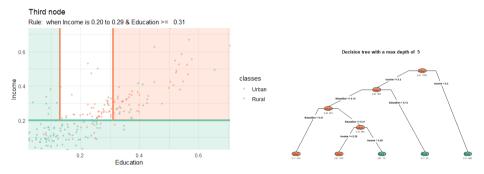


The space on the left of the line is classified as rural

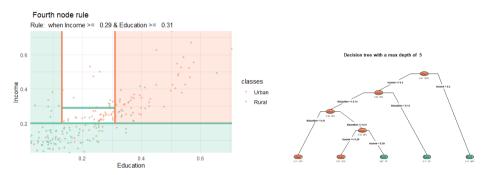


Decision tree with a max depth of 5

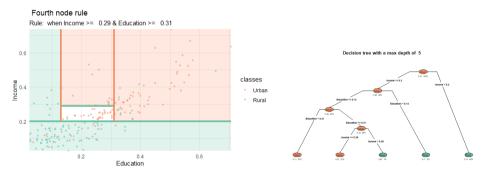
Third boundary decision line



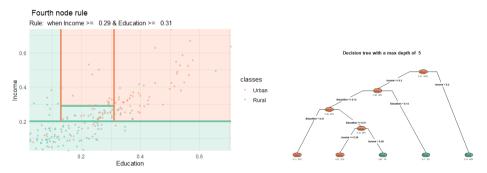
The space on the right of the line is classified as Urban



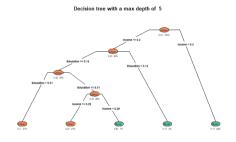
Fourth boundary decision line

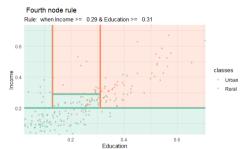


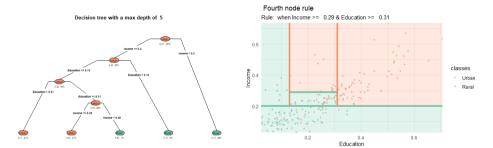
The space above the line is classified as Urban



Finally, the remaining space is classified as rural

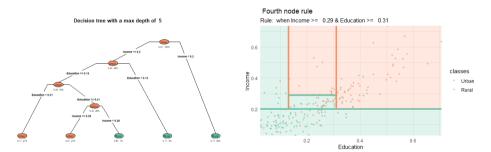






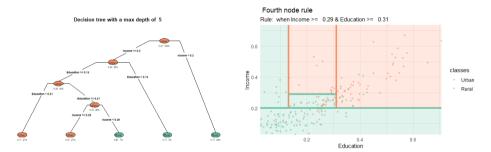
By structure:

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



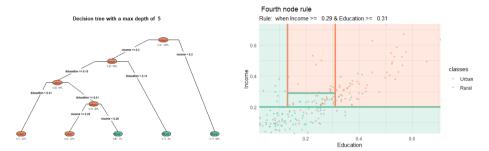
By structure:

- ► 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 some data and build a tree

The decision trees suffer from *high variance*:

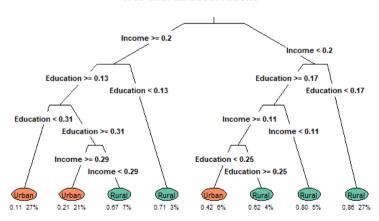
- ► Take some data and build a tree
- ▶ Divide the observations in two samples and build a tree on each

The decision trees suffer from *high variance*:

- ► Take some data and build a tree
- Divide the observations in two samples and build a tree on each
- \hookrightarrow The two trees will likely be very different

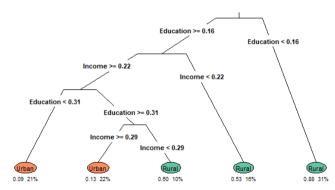
Which tree do you trust?

Tree with all observations



Which tree do you trust?

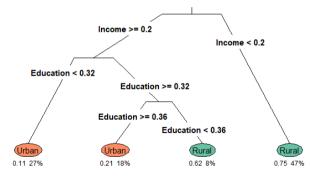
Decision tree 1 (first half sample)



First tree with 50% of observations

Which tree do you trust?

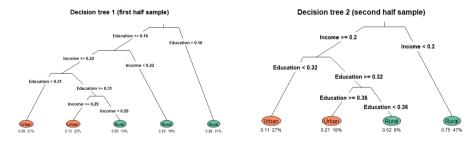
Decision tree 2 (second half sample)



Second tree with 50% of observations

Which tree do you trust?

Outcomes are different from one tree to another



[HOW TO USE TREES?]

Alternative to simple tree models:

► Aggregating the results of trees can help

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

- 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

- 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
- → "Random forest"

- 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"
- Trees can be constructed sequentially

[HOW TO USE TREES?]

- 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"
- Trees can be constructed sequentially
- → "Boosting"

[BAGGING]

[BAGGING]

Bagging stands for Bootstrap Aggregating uses a simple logic:

1. Draw ${\it B}$ bootstrapped samples from the original sample

[BAGGING]

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

[BAGGING]

- 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]

- 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]

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:

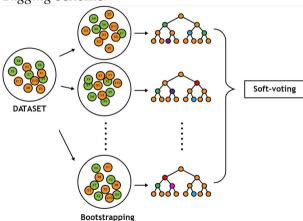


Image from igem.org

Aggregating the results of trees can help decrease the variance

Aggregating the results of trees can help decrease the variance

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

Introduction

Aggregating the results of trees can help decrease the variance

▶ Intuitively, if U_i , . . . U_B are iid with variance σ^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 $U_i, \dots U_B$ are iid with variance σ^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

Boosting

Wrap-up

[Bagging]

Introduction

Bagging scheme:

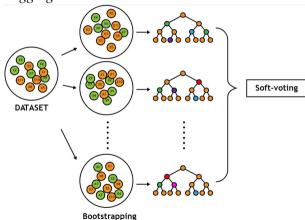


Image from igem.org

Bootstrapped (Bagging) trees use the same set of variables

Bootstrapped (Bagging) trees use the same set of variables

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

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 σ^2 , and cross-correlation ρ , then the average has a variance:

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

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 σ^2 , and cross-correlation ρ , 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 ρ is "high"

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 σ^2 , and cross-correlation ρ , 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 ρ 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) of trees → Forest

- ▶ Bootstrap aggregating (bagging) of trees → Forest
- \hookrightarrow Construct *B* trees, on *B* bootstrapped samples

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

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

Introduction

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

[RANDOM FOREST]

Introduction

Random forest use two mechanisms:

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

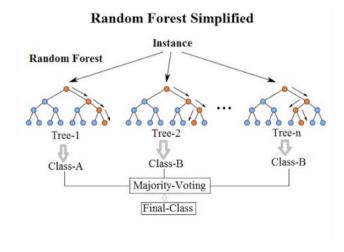
$$Var_{Random\ forest} = \rho \cdot \sigma^2 + \frac{\sigma^2}{B}$$

Common practice (p = nb of variables):

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

[RANDOM FOREST]

Random forest scheme:



Random forest are sensitive to several hyperparameters

▶ All the parameters used to build a *tree*

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

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

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

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

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

- ▶ 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*
 - **▶** ...

Introduction

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

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*
 - **>** ...

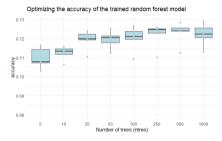
Introduction

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

- ▶ 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 (**B**)
 - ► Minimum number of observations per leaves
 - **▶** ...

The impact of the number of trees:

The impact of the number of trees:



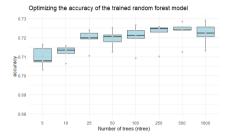
The impact of the number of trees:



→ Moderate number of trees is OK

The impact of the number of trees:

Introduction



- → Moderate number of trees is OK
- ► The variance depends on $\frac{\sigma^2}{B}$ $\nearrow B \Longrightarrow \frac{\sigma^2}{B} \searrow$

The impact of the number of trees:

Introduction



- → 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*

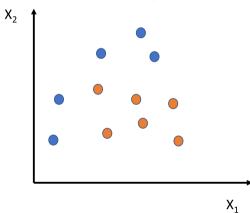
Boosting helps construct trees sequentially

- ► Based on *weak learners*
- → Very simple trees grow on previous "mistakes"

Boosting helps construct trees sequentially

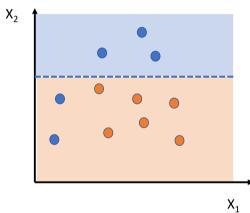
- Based on weak learners
- → Very simple trees grow on previous "mistakes"
- ightharpoonup "Mistakes" at stage t are overweighed for stage t+1

Boosting a tree (iterative process)



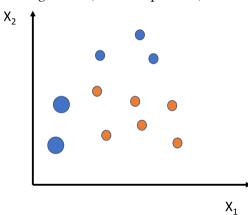
Two classes of observations: Orange and blue

Boosting a tree (iterative process)



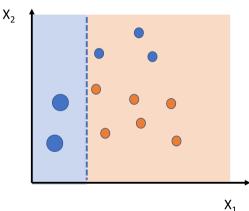
First weak learner

Boosting a tree (iterative process)



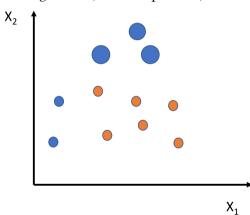
Misclassification overweighed

Boosting a tree (iterative process)



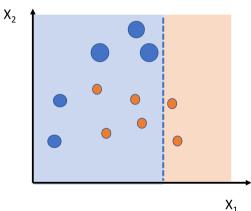
Second weak learner with misclassification overweighed

Boosting a tree (iterative process)



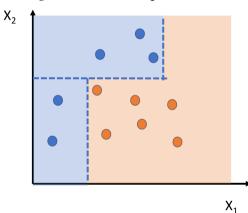
New misclassification overweighed

Boosting a tree (iterative process)



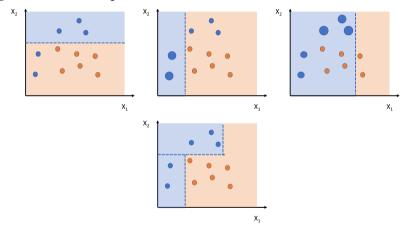
Third weak learner with new misclassification overweighed

Boosting a tree (iterative process)



Combining weak learners.

Boosting a tree (iterative process)



Combining weak learners creates an efficient tree

Boosting has several features

Extremely powerful

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

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

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

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

- 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:

- ▶ Random forest are simple and easy to interpret
- ► *Random forest* use two mechanisms:
 - ► Bootstrap aggregating (*bagging*) of trees → **Forest**

- ▶ Random forest are simple and easy to interpret
- ► *Random forest* use two mechanisms:
 - ▶ Bootstrap aggregating (*bagging*) of trees \rightarrow **Forest**
 - \hookrightarrow Construct **B** trees, on **B** bootstrapped samples

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

Introduction

- Random forest are simple and easy to interpret
- ▶ *Random forest* use two mechanisms:
 - ▶ Bootstrap aggregating (*bagging*) of trees \rightarrow **Forest**
 - \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

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

Introduction

- Random forest are simple and easy to interpret
- ► *Random forest* use two mechanisms:
 - ► Bootstrap aggregating (*bagging*) of trees → Forest
 - \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

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

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

Introduction

- Random forest are simple and easy to interpret
- ▶ *Random forest* use two mechanisms:
 - ► Bootstrap aggregating (*bagging*) of trees → Forest
 - \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

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

- 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:
 - ▶ Bootstrap aggregating (*bagging*) of trees \rightarrow **Forest**
 - \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

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

- ▶ 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!

[Q&A]

Write your questions in the chat

▶ Module 5: "*Advanced Methods*" (SVM, K-Means, Neural Networks) is open

- ▶ Module 5: "*Advanced Methods*" (SVM, K-Means, Neural Networks) is open
- ► The personal data-based ML project is worth a try! (Module 4)

- ▶ Module 5: "*Advanced Methods*" (SVM, K-Means, Neural Networks) is open
- ▶ The personal data-based ML project is worth a try! (Module 4)
- Next Thursday, webinar on:

"The Ethical Considerations of ML for Research and Statistical Purposes" with **Alice Toms**

(Centre for Applied Data Ethics, UK Statistics Authority)

- ▶ Module 5: "*Advanced Methods*" (SVM, K-Means, Neural Networks) is open
- ▶ The personal data-based ML project is worth a try! (Module 4)
- Next Thursday, webinar on:

"The Ethical Considerations of ML for Research and Statistical Purposes" with

Alice Toms

(Centre for Applied Data Ethics, UK Statistics Authority)

Enjoy the activities proposed - Last module opens soon.

- ▶ Module 5: "*Advanced Methods*" (SVM, K-Means, Neural Networks) is open
- The personal data-based ML project is worth a try! (Module 4)
- Next Thursday, webinar on:

"The Ethical Considerations of ML for Research and Statistical Purposes" with **Alice Toms**

(Centre for Applied Data Ethics, UK Statistics Authority)

- Enjoy the activities proposed Last module opens soon.
- Continue to post on the forums

- ▶ Module 5: "*Advanced Methods*" (SVM, K-Means, Neural Networks) is open
- The personal data-based ML project is worth a try! (Module 4)
- Next Thursday, webinar on:

"The Ethical Considerations of ML for Research and Statistical Purposes" with **Alice Toms**

(Centre for Applied Data Ethics, UK Statistics Authority)

- Enjoy the activities proposed Last module opens soon.
- Continue to post on the forums

Have a nice week and a happy learning!