



Institut de Mathématiques de Toulouse, INSA Toulouse

# CART, Random Forests, Boosting

Data Mining  
October 2021

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# Outline

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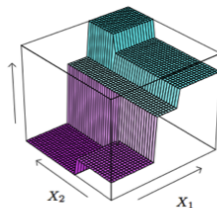
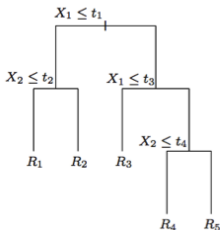
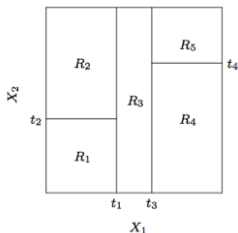
- Classification And Regression Trees (CART)
- Bagging
- Random Forests
- Boosting

# Classification And Regression Trees

## Introduction

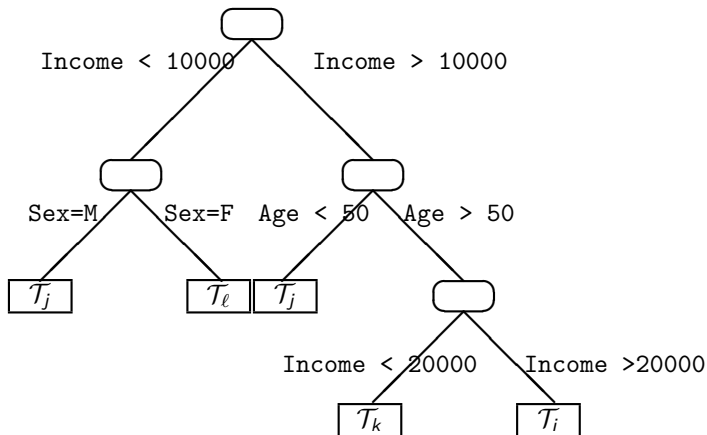
- Classification and regression trees (**CART**) : Breiman et al. (1984)
- $X^j$  explanatory variables (quantitative or qualitative)
- $Y$  qualitative with  $m$  modalities  $\{\mathcal{T}_\ell; \ell = 1 \dots, m\}$  : **classification tree**
- $Y$  quantitative : **regression tree**
- **Objective** : construction of a binary **decision tree** easy to interpret
- No assumption on the model : non parametric procedure.

# Example of binary regression tree



Source : Hastie, Tibshirani, Friedman (2019), "The elements of statistical learning"

## Example of binary classification tree



# Principles for constructing a tree

- Recursive binary split
  - Split a region in two, then split subregions in two, then ...
- Splits are defined by one variable
  - Very easy numerically :  $p$  optimizations in 1-dimension
- Clustering idea
  - Find a split that give the most homogeneous groups

## Definitions

- Determine an *iterative* sequence of *nodes*
- *Root* : initial note : the whole sample
- *Leaf* : Terminal node
- *Node* : choice of one *variable* and one *division* to proceed to a dichotomie
- *Division* : threshold value or group of modalities

## Rules

- We have to choose :
  - 1 Criterion for the “best” division among all *admissibles* ones (partition based on the values of one variable)
  - 2 Rules for a terminal node : *leaf*
  - 3 Rules to assign a leaf to a class  $\mathcal{T}_\ell$  or one value for  $Y$
- *Admissible* divisions : descendants  $\neq \emptyset$
- $X^j$  real or ordinal with  $c_j$  possible values :  $(c_j - 1)$  possible divisions
- $X^j$  nominal :  $2^{(c_j-1)} - 1$  possible divisions
- Heterogeneity function  $D_\kappa$  of one node



# Division criterion

## Optimal division

- Notations
  - $\kappa$  : a node
  - $\kappa_L$  and  $\kappa_R$  the two son nodes
- The algorithm retains the division which minimizes

$$D_{\kappa_L} + D_{\kappa_R}$$

- For each node  $\kappa$  in the construction of the tree :

$$\max_{\{ \text{Divisions of } X^j : j=1,p \}} D_{\kappa} - (D_{\kappa_L} + D_{\kappa_R})$$

# Stopping rule and affectation

## Leaf and affectation

- A **Node** is a **terminal** node or a **leaf**, if it is :
  - **Homogeneous**
  - **Number** of observations below some **threshold**
- **Affectation**
  - **$Y$  quantitative** : the value is the **mean of the observations in the leaf**
  - **$Y$  qualitative** : each leaf is affected to one class  $\mathcal{T}_\ell$  of  $Y$  by a majority vote.

# Constructing regression trees

For a given region (node)  $\kappa$  with size  $|\kappa|$ , define the **heterogeneity** by :

$$D_{\kappa} = \sum_{i \in \kappa} (y_i - \bar{y}_{\kappa})^2 = |\kappa| \frac{1}{|\kappa|} \sum_{i \in \kappa} (y_i - \bar{y}_{\kappa})^2$$

## Splitting procedure

For a variable  $x_j$ , and a split candidate  $t$ , define left and right subregions

$$\kappa_L(t, j) = \{x_j \leq t\}, \quad \kappa_R(t, j) = \{x_j > t\}.$$

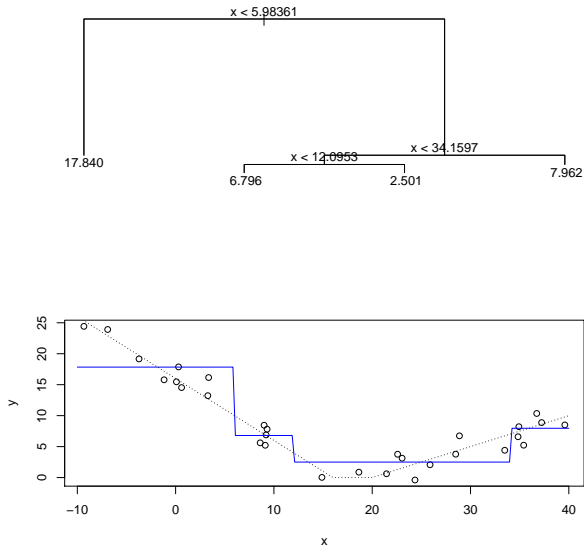
Find  $(j, t)$  in order to minimize the intra-class variance

$$J(j, t) = D_{\kappa_L(t, j)} + D_{\kappa_R(t, j)},$$

or equiv. to maximize the decrease in heterogeneity (inter-class variance)

$$D_{\kappa} - J(j, t)$$

## Illustration in 1 dimension



# Constructing classification trees

This is the same procedure, with specific notions of heterogeneity

## Heterogeneity measures in classification

$p_{\kappa}^{\ell}$  : proportion of the class  $\mathcal{T}_{\ell}$  of  $\mathcal{Y}$  in the node  $\kappa$ .

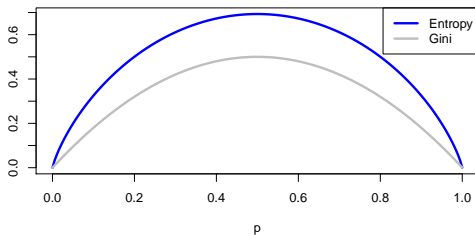
- Shannon Entropy

$$E_{\kappa} = - \sum_{\ell=1}^m p_{\kappa}^{\ell} \log(p_{\kappa}^{\ell}) \quad \Rightarrow \quad D_{\kappa} = -|\kappa| \sum_{\ell=1}^m p_{\kappa}^{\ell} \log(p_{\kappa}^{\ell})$$

Maximal in  $(\frac{1}{m}, \dots, \frac{1}{m})$ , minimal in  $(1, 0, \dots, 0), \dots, (0, \dots, 0, 1)$   
(by continuity, we assume that  $0 \log(0) = 0$ )

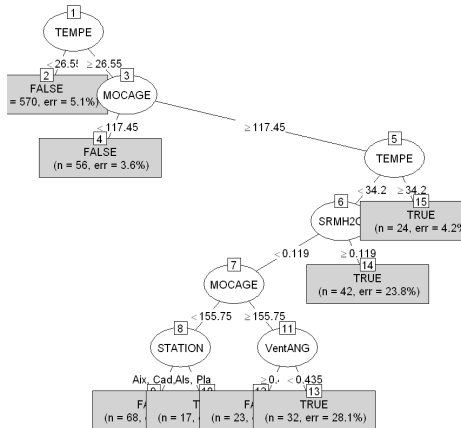
- Gini concentration :  $D_{\kappa} = |\kappa| \sum_{\ell=1}^m p_{\kappa}^{\ell} (1 - p_{\kappa}^{\ell})$

## Illustration with two classes ( $m = 2$ )



**FIGURE** – Heterogeneity criteria for classification. Both are minimal for  $p = 0$  or  $p = 1$ , and maximal for  $p = 1/2$ .

# Example for Ozone data



*Ozone : Classification tree pruned by cross-validation*

# Stopping rule, pruning, optimal tree

- We need a tradeoff between maximal tree (overfits) and the constant tree (too rough)
- There exists a nice theory to find an optimal tree, minimizing prediction error penalized by complexity (number of leaves)
- When aggregating trees (random forest), simpler procedures are often preferred (see why after), e.g. fixing the number of leaves



# Pruning and optimal tree

## Pruning : notations

- We look for a **parcimonious** tree
- **Complexity** of a tree :  $K_A$  = numbers of leaves in  $A$
- Adjustment error of  $A$  :

$$D(A) = \sum_{\kappa=1}^{K_A} D_{\kappa}$$

$D_{\kappa}$  : heterogeneity of leaf  $\kappa$

## Sequence of embedded trees

- Adjustment error **penalized** by the **complexity** :

$$Crit_{\gamma}(A) = D(A) + \gamma \times K_A$$

- When  $\gamma = 0$  :  $A_{\max}$  (maximal tree) minimizes  $Crit_{\gamma}(A)$
- When  $\gamma$  increases, the division of  $A_H$ , for which the improvement of  $D$  is smaller than  $\gamma$ , is cancelled ; **hence**
  - two leaves are gathered (**pruned**)
  - there father node becomes a **terminal** node
  - $A_K$  becomes  $A_{K-1}$ .
- After **iteration** of this process, we get a sequence of trees :

$$A_{\max} \supset A_K \supset A_{K-1} \supset \cdots A_1$$

# Optimal tree

## Algorithm to select the optimal tree

- Maximal tree  $A_{\max}$
- Imbedded sequence  $A_{\max}, A_K \dots A_1$  associated with an increasing sequence of values  $\gamma_K \leq \dots \leq \gamma_1$
- V-fold cross validation error :  
  **for**  $v = 1, \dots, V$  **do**
  - Estimation of the sequence of trees associated to  $(\gamma_K)$  with all the folds except  $v$
  - Estimation of the error with the fold  $v$ .

### EndFor

- Sequence of the mean of these errors for each value of  $\gamma_K, \dots, \gamma_1$
- $\gamma_{\text{Opt}}$  optimal value for the tuning parameter minimizing the mean of the errors
- Tree associated to  $\gamma_{\text{Opt}}$  in  $A_K \dots A_1$

## Advantages

- **Trees** are easy to interpret
- **Efficient algorithms** to find the pruned trees
- Tolerant to **missing data**

⇒ Success of CART for practical applications

## Warnings

- **Variable selection** : the selected tree only depends on few explanatory variables, trees are often (wrongly) interpreted as a variable selection procedure
- **High instability** of the trees : not robust to the learning sample, curse of dimensionality ..
- **Prediction accuracy** of a tree is often poor compared to other procedures

⇒ **Aggregation of trees : bagging, random forests**

# Outline

- Classification And Regression Trees (CART)
- Bagging
- Random Forests
- Boosting

## Introduction

- Combination or **aggregation** of models (almost) without **overfitting**
- **Bagging** is for **bootstrap<sup>(\*)</sup>** **aggregating** : Breiman, 1996
- **Random forests** : Breiman, 2001
- Allows to aggregate any modelisation method
- **Efficient** methods : Fernandez-Delgado et al. (2014), *Kaggle*

(\*) *bootstrap = sampling with replacement*

- **Bagging** is appropriate for unstable algorithms, with small bias and high variance (CART)

# Bagging - Principle

## Bootstrap AGGREGatING

- **Variance reduction** : by aggregating independent predictions
  - Aggregation : average (regression), majority vote (classification)
- **Bootstrap trick** : get new data from themselves by resampling !
  - Caution : new data remain (slightly) dependent on the initial ones

# Bagging - Introductory example

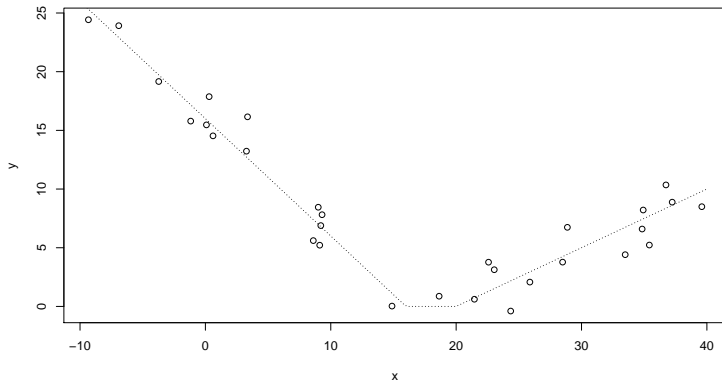


FIGURE – Original data



## Bagging - Introductory example

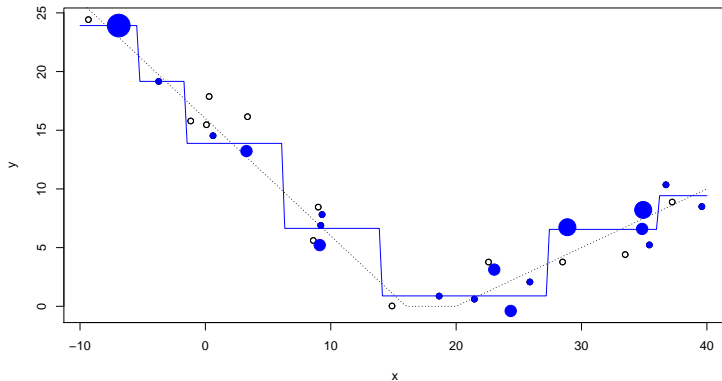
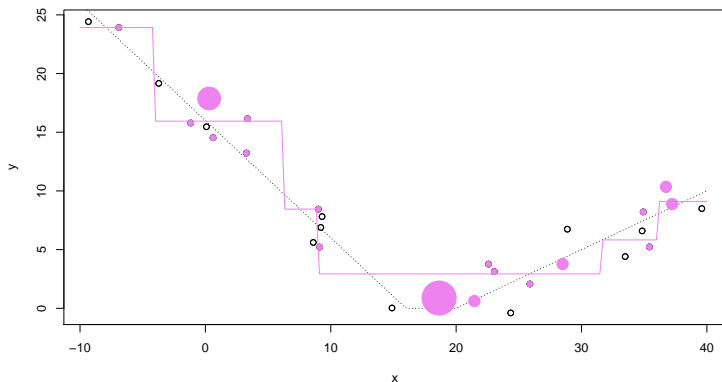


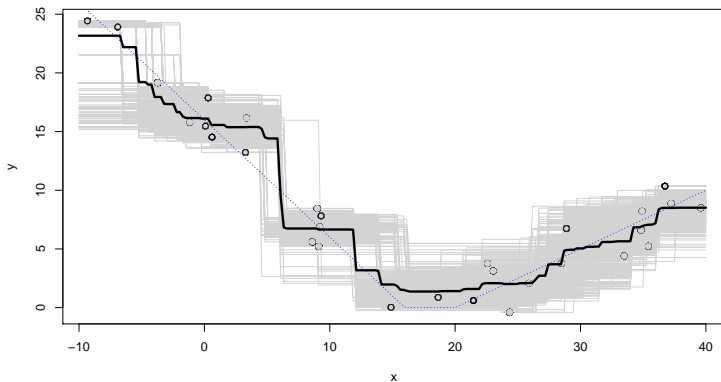
FIGURE – Bootstrap sample  $n^o1$  (in blue), and corresp. prediction with tree. The point size is proportional to the number of replicates.

## Bagging - Introductory example



**FIGURE** – Bootstrap sample  $n=2$  (in violet), and corresp. prediction with tree. The point size is proportional to the number of replicates.

# Bagging - Introductory example



**FIGURE** – 500 bootstrap samples (grey), corresp. predictions with tree, and their average (bold line).

# Bagging - Pause

Physical experiment !

Experiment yourself the bootstrap procedure by resampling “by hand”

**Question** : Choose a number between 1 and  $N$  (number of participants). What is the probability that your number does not appear in the bootstrap sample ?

# Bagging - Out-Of-Bag data

## Out-Of-Bag (OOB) data

For each bootstrap sample :

- Let  $U_1^*, \dots, U_N^*$  be random variables representing the bootstrapped indices. The probability that a given data  $z_i$  is not chosen is :

$$\mathbb{P}\left(z_{U_1^*} \neq z_i, \dots, z_{U_N^*} \neq z_i\right) = \left(1 - \frac{1}{N}\right)^N \xrightarrow{N \rightarrow +\infty} e^{-1} \approx 0.367$$

- The non-chosen data are called **Out-Of-Bag (OOB)**. They can be used **as a test set inside the bootstrap loop**

The **OOB error** is obtained by averaging prediction errors over OOB data

## Bagging - Out-Of-Bag data

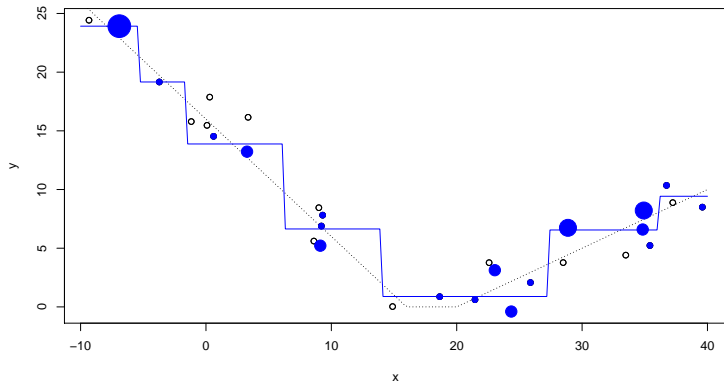


FIGURE – Residuals for the OOB bootstrap sample  $n^o1$  (red bars).

## Bagging - Out-Of-Bag data

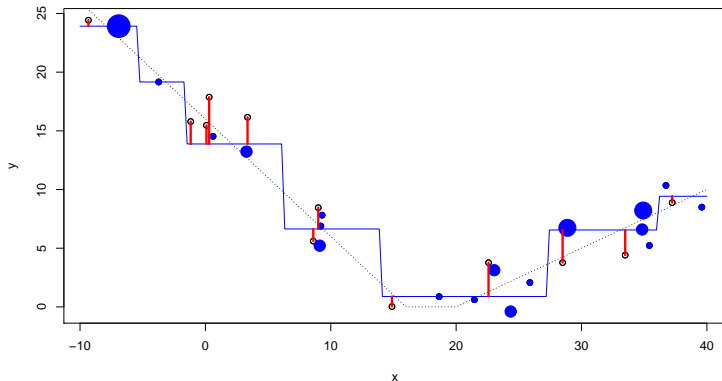


FIGURE – Residuals for the OOB bootstrap sample  $n^o1$  (red bars).

## Bagging - Out-Of-Bag data

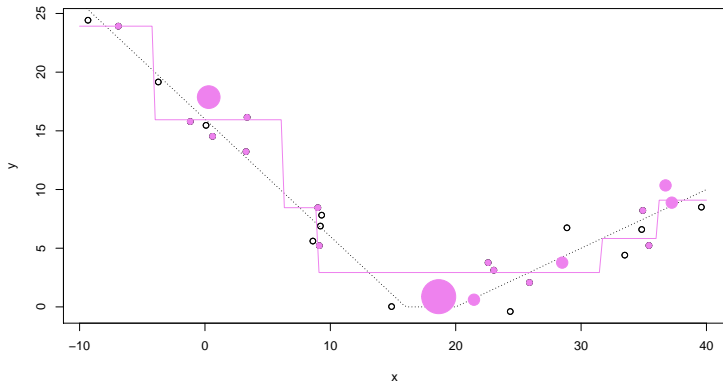


FIGURE – Residuals for the OOB bootstrap sample  $n^{o2}$  (red bars).



## Bagging - Out-Of-Bag data

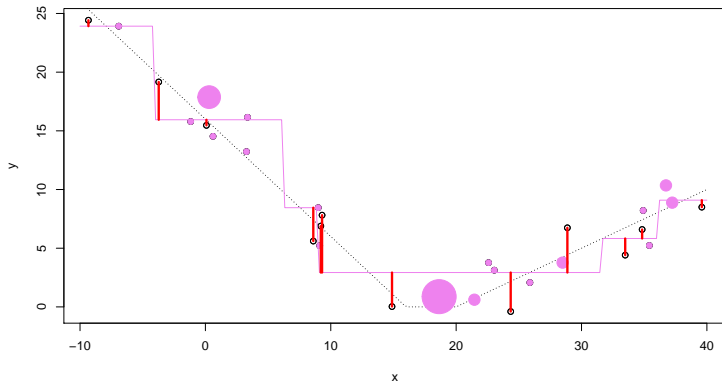


FIGURE – Residuals for the OOB bootstrap sample  $n^{o2}$  (red bars).

# Bagging - Theory

## Framework and notations

- Let  $Y$  a quantitative or qualitative variable to explain
- $X^1, \dots, X^p$  the explanatory variables
- $f(\mathbf{x})$  a model function of  $\mathbf{x} = \{x^1, \dots, x^p\} \in \mathbb{R}^p$
- $\mathbf{z} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$  learning sample with distribution  $F$  and size  $n$ 
  - $\hat{f}_{\mathbf{z}}$  : predictor associated to the sample  $\mathbf{z}$  with  $f(\cdot) = E_F(\hat{f}_{\mathbf{z}})$
  - $B$  independent samples  $\{\mathbf{z}_b\}_{b=1, B}$
  - $Y$  quantitative :  $\hat{f}_B(\cdot) = \frac{1}{B} \sum_{b=1}^B \hat{f}_{\mathbf{z}_b}(\cdot)$  (mean)
  - $Y$  qualitative :  $\hat{f}_B(\cdot) = \arg \max_j \text{card} \left\{ b \mid \hat{f}_{\mathbf{z}_b}(\cdot) = j \right\}$  (majority vote)
- **Principle** : Take the mean of independent predictions to reduce the variance
- $B$  independent samples replaced by  $B$  bootstrap replications

## Bagging : algorithm

- Let  $\mathbf{x}_0$  to point where we want to predict and
- $\mathbf{z} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$  a learning sample
- **For**  $b = 1$  **to**  $B$ 
  - Generate a bootstrap sample  $\mathbf{z}_b^*$  (with size  $m_n \leq n$ )
  - Estimate  $\hat{f}_{\mathbf{z}_b}(\mathbf{x}_0)$  with the bootstrap sample
- **Compute the mean** estimation  $\hat{f}_B(\mathbf{x}_0) = \frac{1}{B} \sum_{b=1}^B \hat{f}_{\mathbf{z}_b}(\mathbf{x}_0)$   
or the result of the **majoritary vote**

- The  $B$  bootstrap samples are built on the same learning sample  $\mathbf{z} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$  :  
 $\implies$  the estimators  $\hat{f}_{\mathbf{z}_b}(\mathbf{x}_0)$  are **not independent**
- Regression case : If  $\text{Corr}(\hat{f}_{\mathbf{z}_b}(\mathbf{x}_0), \hat{f}_{\mathbf{z}_{b'}}(\mathbf{x}_0)) = \rho(x_0)$ ,

$$\begin{aligned} E(\hat{f}_B(\mathbf{x}_0)) &= f(\mathbf{x}_0) \\ \text{Var}(\hat{f}_B(\mathbf{x}_0)) &= \rho(x_0)\text{Var}(\hat{f}_b(\mathbf{x}_0)) + \frac{(1 - \rho(x_0))}{B}\text{Var}(\hat{f}_b(\mathbf{x}_0)) \\ &\rightarrow \rho(x_0)\text{Var}(\hat{f}_b(\mathbf{x}_0)) \text{ as } B \rightarrow +\infty \end{aligned}$$

$\implies$  Importance to find **low correlated predictors**  $(\hat{f}_b(\mathbf{x}_0))_{1 \leq b \leq B}$  .  
 $\hookrightarrow$  **Random forests**

## Bagging : practical use

- *Bootstrap out-of-bag* estimation of the prediction error : control of the **quality** and avoid **overfitting**
- **CART** to build a sequence of **binary trees**
- Three pruning **strategies** are possible :
  - 1 keep a **whole tree** for each of the samples
  - 2 tree with at most  **$q$  leaves**
  - 3 whole tree **pruned** by cross-validation
- **First strategy** compromise between computations and prediction accuracy : small **bias** for each tree and reduced **variance** by aggregation

### Bagging : limitations

- Computation time and control of the error
- Storage of all the models to aggregate
- **Black box** model

# Outline

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# Random forests

## Random forests : principle

- **Random forests** means initially any aggregation method for classification or regression trees
- Now, it refers to the **Random input** method introduced by Breiman and Cutler (2005)  
<http://www.stat.berkeley.edu/users/breiman/RandomForests/>
- Improvement of the **bagging** of binary trees
- Variance of  $B$  correlated variables :  $\rho\sigma^2 + \frac{1-\rho}{B}\sigma^2$
- Add a **randomisation** to get more **independent** trees
- **Random** choice of variables
- **Interesting** in high dimension



## Random forests : algorithm

- Let  $\mathbf{x}_0$  the point where we want to predict,  
 $\mathbf{z} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$  a learning sample.
- **for**  $b = 1$  **to**  $B$ 
  - Generate a bootstrap sample  $\mathbf{z}_b^*$
  - Estimate a tree with randomization of the variables : for each **node**,  
**random sample** of  $m < p$  **predictors** to built the subdivision
- **Compute** the **mean** estimation  $\hat{f}_B(\mathbf{x}_0) = \frac{1}{B} \sum_{b=1}^B \hat{f}_{\mathbf{z}_b}(\mathbf{x}_0)$   
or the majority **vote**

## Random forests : utilisation

- **Pruning** : tree with  $q$  leaves, or complete tree,
- **Random selection** of  $m$  predictors :  $m = \sqrt{p}$  for classification,  $\frac{p}{3}$  for regression.
- Small  $m$  increases the **variability** of each tree but reduces the correlation between them : Each **model** is less accurate but **aggregation** is performing
- Iterative computation of the **out-of-bag** error.
- Good accuracy, easily implementable, parallelisable but **not easy to interpret**

## To help interpretation

- Index of importance for each variable

# Interpretation - Variable importance

How can we quantify the importance of a variable  $X^j$  in random forest ?

## Decrease in heterogeneity

Average the decrease of heterogeneity when  $X^j$  is chosen as a split.

- Mean Decrease Accuracy
- Mean Decrease Gini

## Permutation of variables

Compute the OOB error for the subsample of OOB data.

Compare with the OOB error when permuting at random the values of the variable  $X^j$  in the learning sample (but keeping the output  $Y$  unchanged).

## Example on ozone data

```
> library(randomForest)
> rf.reg <- randomForest(O3obs ~, data = datappr, xtest = datestr[, -2],
  ytest = datestr[, "O3obs"], ntree = 500, do.trace = 50, importance = TRUE)
```

Tree	Out -of	- bag	Test	set
	MSE	%Var(y)	MSE	%Var(y)
50	697.9	40.77	568.5	36.75
100	689.5	40.28	555.9	35.93
150	683.8	39.95	563.2	36.41
200	685.4	40.04	561	36.27
250	678.2	39.62	564.2	36.47
300	675.1	39.44	569.2	36.79
350	676.8	39.54	572.8	37.02
400	674.3	39.39	571.4	36.93
450	673.9	39.37	571.5	36.94
500	674.3	39.39	569.6	36.82

```
> round(importance(rf.reg), 2)
```

	%IncMSE	IncNodePurity
JOUR	1.98	11011.79
MOCAGE	41.46	388657.27
TEMPE	51.73	409018.57
STATION	21.73	75350.42
VentMOD	12.95	91387.20
VentANG	18.81	124908.37
SRMH2O	16.76	114463.05
LN02	7.73	84152.34
LNO	10.04	74387.32

#### Details (from R help file of function importance)

“The first measure [%IncMSE] is computed from permuting OOB data : For each tree, the prediction error on the out-of-bag portion of the data is recorded (error rate for classification, MSE for regression). Then the same is done after permuting each predictor variable. The difference between the two are then averaged over all trees, and normalized by the standard deviation of the differences.

The second measure [IncNodePurity] is the total decrease in node impurities from splitting on the variable, averaged over all trees. For classification, the node impurity is measured by the Gini index. For regression, it is measured by residual sum of squares.”

rf.reg

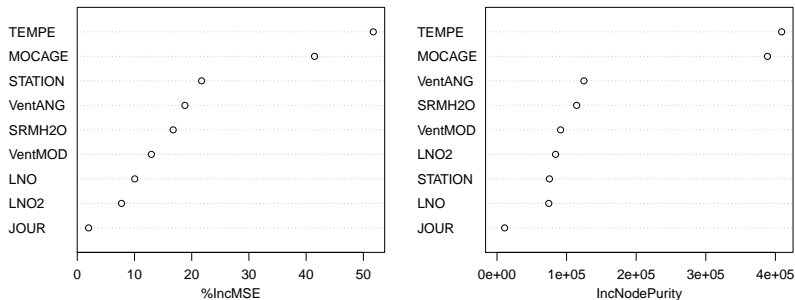


FIGURE – Variable importance plot, returned by the R function `importance`

## Other possible applications

- Proximity or similarity between observations
- Anomaly detection with IsolationForest
- Imputation of missing data with missForest
- Survival analysis with survival forest
- ...

# Outline

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# Boosting principle

## Boosting : principle

- Improve the performances of a **weak classifier** (Schapire, 1990 ; Freund and Schapire, 1996)
- **AdaBoost** (**Adaptative boosting**) prediction of a binary variable
- Reduction of the **variance** but also the **bias**
- Aggregation of a family of **recurrent** models : *Each **model** is an **adaptive** version of the previous one giving more **weight**, in the next estimate, to the **badly adjusted** observations*
- **Variants** : **type** of variable to predict (binary,  $k$  classes, real), **loss function**

# Basic algorithm

## AdaBoost

- AdaBoost is a boosting method to combine several binary classifiers  $f_1, \dots, f_k$  with values in  $\{-1, 1\}$ .
- $\mathbf{z} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$  a learning sample,  $y_i \in \{-1, 1\}$ .
- The aim is to minimize the empirical risk for the exponential loss function over linear combination of the classifiers

$$\hat{f} = \underset{f \in \text{span}(f_1, \dots, f_k)}{\text{argmin}} \left\{ \frac{1}{n} \sum_{i=1}^n \exp(-y_i f(\mathbf{x}_i)) \right\}.$$

# AdaBoost

- To approximate the solution, Adaboost computes a sequence of functions  $\hat{f}_m$  for  $m = 0, \dots, M$  with

$$\begin{aligned}\hat{f}_0 &= 0 \\ \hat{f}_m &= \hat{f}_{m-1} + \beta_m f_{j_m}\end{aligned}$$

where  $(\beta_m, j_m)$  minimizes the empirical risk

$$\operatorname{argmin}_{\beta \in \mathbb{R}, j=1, \dots, p} \left\{ \frac{1}{n} \sum_{i=1}^n \exp(-y_i(\hat{f}_{m-1}(\mathbf{x}_i) + \beta f_j(\mathbf{x}_i))) \right\}.$$

- The final classification rule is given by

$$\hat{f} = \operatorname{sign}(\hat{f}_M).$$

# AdaBoost

- We denote

$$w_i^{(m)} = \frac{1}{n} \exp(-y_i \hat{f}_{m-1}(\mathbf{x}_i))$$

- We assume that for all  $j = 1, \dots, k$ ,

$$\widehat{\mathcal{E}}_m(j) = \frac{\sum_{i=1}^n w_i^{(m)} \mathbb{1}_{f_j(\mathbf{x}_i) \neq y_i}}{\sum_{i=1}^n w_i^{(m)}} \in ]0, 1[.$$

- Then, we have :

$$j_m = \underset{j=1, \dots, k}{\operatorname{argmin}} \widehat{\mathcal{E}}_m(j),$$

and

$$\beta_m = \frac{1}{2} \log \left( \frac{1 - \widehat{\mathcal{E}}_m(j_m)}{\widehat{\mathcal{E}}_m(j_m)} \right).$$

# AdaBoost

## AdaBoost algorithm

- $w_i^{(1)} = 1/n$  for  $i = 1, \dots, n$ .
- For  $m = 1, \dots, M$

$$j_m = \operatorname{argmin}_{j=1,\dots,p} \widehat{\mathcal{E}}_m(j), \beta_m = \frac{1}{2} \log \left( \frac{1 - \widehat{\mathcal{E}}_m(j_m)}{\widehat{\mathcal{E}}_m(j_m)} \right).$$

$$\begin{aligned} w_i^{(m+1)} &= w_i^{(m)} \exp(-y_i \beta_m f_{j_m}(\mathbf{x}_i)) \text{ for } i = 1, \dots, n \\ &= \frac{1}{n} \exp(-y_i \hat{f}_{m-1}(\mathbf{x}_i)) \exp(-y_i \beta_m f_{j_m}(\mathbf{x}_i)) \\ &= \frac{1}{n} \exp(-y_i \hat{f}_m(\mathbf{x}_i)) \end{aligned}$$

- $\hat{f}_M(x) = \sum_{m=1}^M \beta_m f_{j_m}(x)$ .
- $\hat{f} = \operatorname{sign}(\hat{f}_M)$ .

# Gradient Boosting Models

## GBM : Principle 1

- Gradient Boosting Models (Friedman, 2002-2009)
- In the case of a **differentiable** loss function
- **Principle** :
  - Construct a **sequence** of models in such a way that at each **step**, each **model** added to the **linear combination**, appears as a **step** towards a **better solution**
  - This **step** is done in the direction of the **gradient** of the **loss function** approximated by a **regression tree**

## GBM : Principle 2

- Previous **Adaptative model** (AdaBoost) :

$$f_m(\mathbf{x}) = f_{m-1}(\mathbf{x}) + \beta_m f_{j_m}(\mathbf{x})$$

- Transformed in a **gradient descent**

$$f_m(\mathbf{x}_i) = f_{m-1}(\mathbf{x}_i) - \gamma_m \frac{\partial l(y_i, f_{m-1}(\mathbf{x}_i))}{\partial f_{m-1}(\mathbf{x}_i)}.$$

- Search for a **best step in the descent**  $\gamma$  :

$$\min_{\gamma} \sum_{i=1}^n \left[ l \left( y_i, f_{m-1}(\mathbf{x}_i) - \gamma \frac{\partial l(y_i, f_{m-1}(\mathbf{x}_i))}{\partial f_{m-1}(\mathbf{x}_i)} \right) \right].$$

## GBM in regression : algorithm

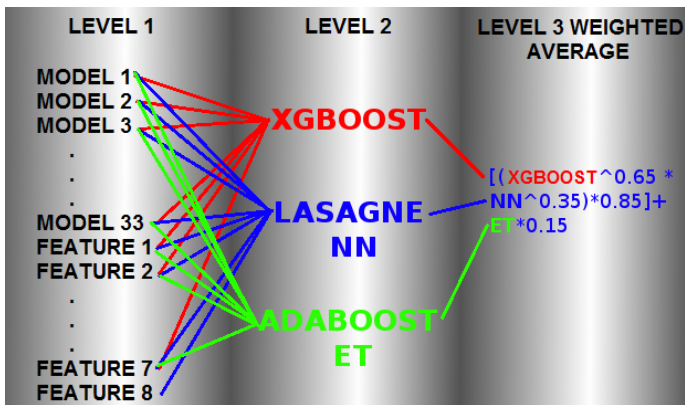
- Let  $\mathbf{x}_0$  the point where we want to predict
- Initialize  $\hat{f}_0 = \arg \min_{\gamma} \sum_{i=1}^n l(y_i, \gamma)$
- **For**  $m = 1$  **to**  $M$ 
  - Compute  $r_{m,i} = - \left[ \frac{\partial l(y_i, f(\mathbf{x}_i))}{\partial f(\mathbf{x}_i)} \right]_{f=f_{m-1}} ; \quad i = 1, \dots, n$
  - Adjust a regression tree  $\delta_m$  to  $(\mathbf{x}_i, r_{m,i})$
  - Calculate  $\gamma_m = \arg \min_{\gamma} \sum_{i=1}^n l(y_i, f_{m-1}(\mathbf{x}_i) + \gamma \delta_m(\mathbf{x}_i))$
  - Update :  $\hat{f}_m(\mathbf{x}) = \hat{f}_{m-1}(\mathbf{x}) + \gamma_m \delta_m(\mathbf{x})$
- **Result** :  $\hat{f}_M(\mathbf{x}_0)$



# Extreme gradient boosting

## XGBoost : motivation

- **Algorithm** introduced by Chen et Guestrin (2016)
- Additional **Penalization** to control overfitting
- **Problem** : number of parameters to optimize
- Implementation **tips** for parallelisation
- **Environments** : R (caret), Python, Julia, GPU, *Amazon Web Service*, Spark...
- **Winning solutions** for *Kaggle* competitions



*Kaggle : Identify people who have a high degree of Psychopathy based on Twitter usage*

## XGBoost : penalization

- Loss function  $L$  penalized version of  $l$

$$L(f) = \sum_{i=1}^n l(f(\mathbf{x}_i), y_i) + \sum_{m=1}^M \Omega(\delta_m)$$

$$\Omega(\delta) = \alpha|\delta| + \beta\|\mathbf{w}\|^2$$

- $|\delta|$  number of leaves in the tree  $\delta$
- $\mathbf{w}$  vector of values assigned to each leaf
- $\Omega$  Mix of  $l_1$  and  $l_2$  penalization

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