Introduction to machine learning
Non Parametric Regression/Classification
Decision Tree/ Bagging/ Random Forest/ Extra Trees

Mathilde Mougeot

ensIIE & ENS Paris-Saclay, France

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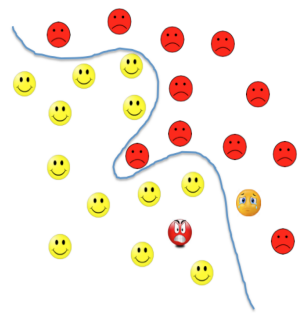
Leo Breiman.

Decision Trees & Ensemble methods

Outline

Regression & Classification Trees



Regression Tree

Boston Housing Data.The original data are $n = 506$ observations on $p = 14$ variables,

medv	median value, being the target variable
crim	per capita crime rate by town
zn	proportion of residential land zoned for lots over 25,000 sq.ft
indus	proportion of non-retail business acres per town
chas	Charles River dummy variable (= 1 if tract bounds river ; 0 otherwise)
nox	nitric oxides concentration (parts per 10 million)
rm	average number of rooms per dwelling
age	proportion of owner-occupied units built prior to 1940
dis	weighted distances to five Boston employment centres
rad	index of accessibility to radial highways
tax	full-value property-tax rate per USD 10,000
ptratio	pupil-teacher ratio by town
b	$1000(B - 0.63)^2$ where B is the proportion of blacks by town
lstat	percentage of lower status of the population
medv	median value of owner-occupied homes in USD 1000's

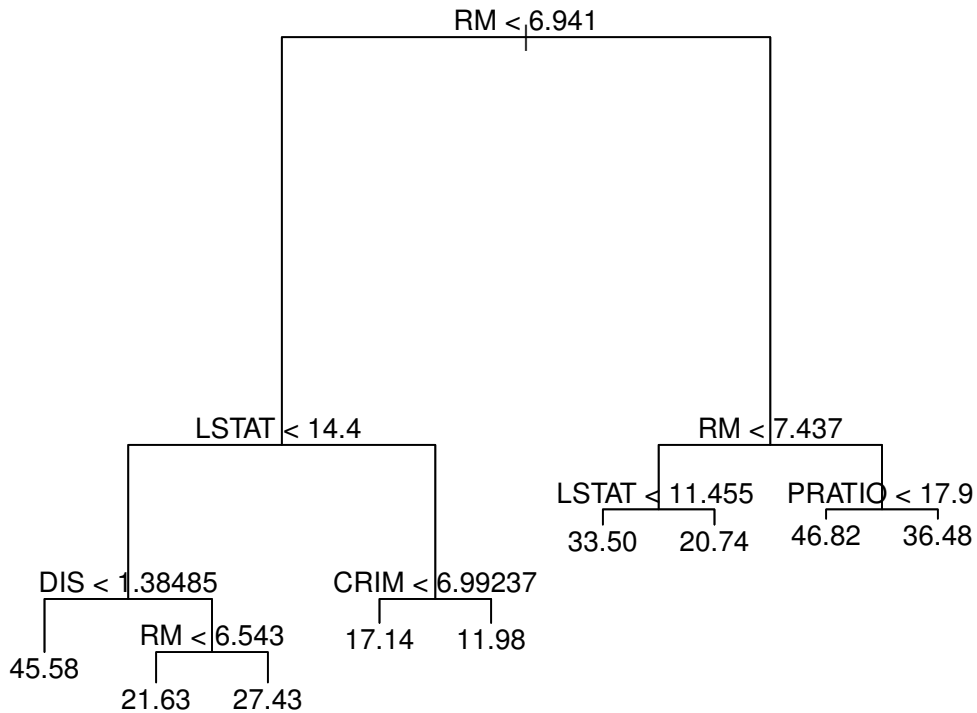
Boston Housing Data

Raw data :

n	crim	zn	indus	chas	nox	rm	age	dis	rad	tax	ptratio	b	lstat	medv
1	0.006	18	2.3	0	0.53	6.57	65.2	4.09	1	296	15.3	396.9	4.9	24.0
2	0.027	0	7.0	0	0.46	6.42	78.9	4.96	2	242	17.8	396.9	9.1	21.6
3	0.027	0	7.0	0	0.46	7.18	61.1	4.96	2	242	17.8	392.8	4.0	34.7
4	0.032	0	2.1	0	0.45	6.99	45.8	6.06	3	222	18.7	394.6	2.9	33.4
5	0.069	0	2.1	0	0.45	7.14	54.2	6.06	3	222	18.7	396.9	5.3	36.2
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...

Regression Tree. Boston Housing Data

Application : Prediction of the prize of an house in Boston given several co-variables.

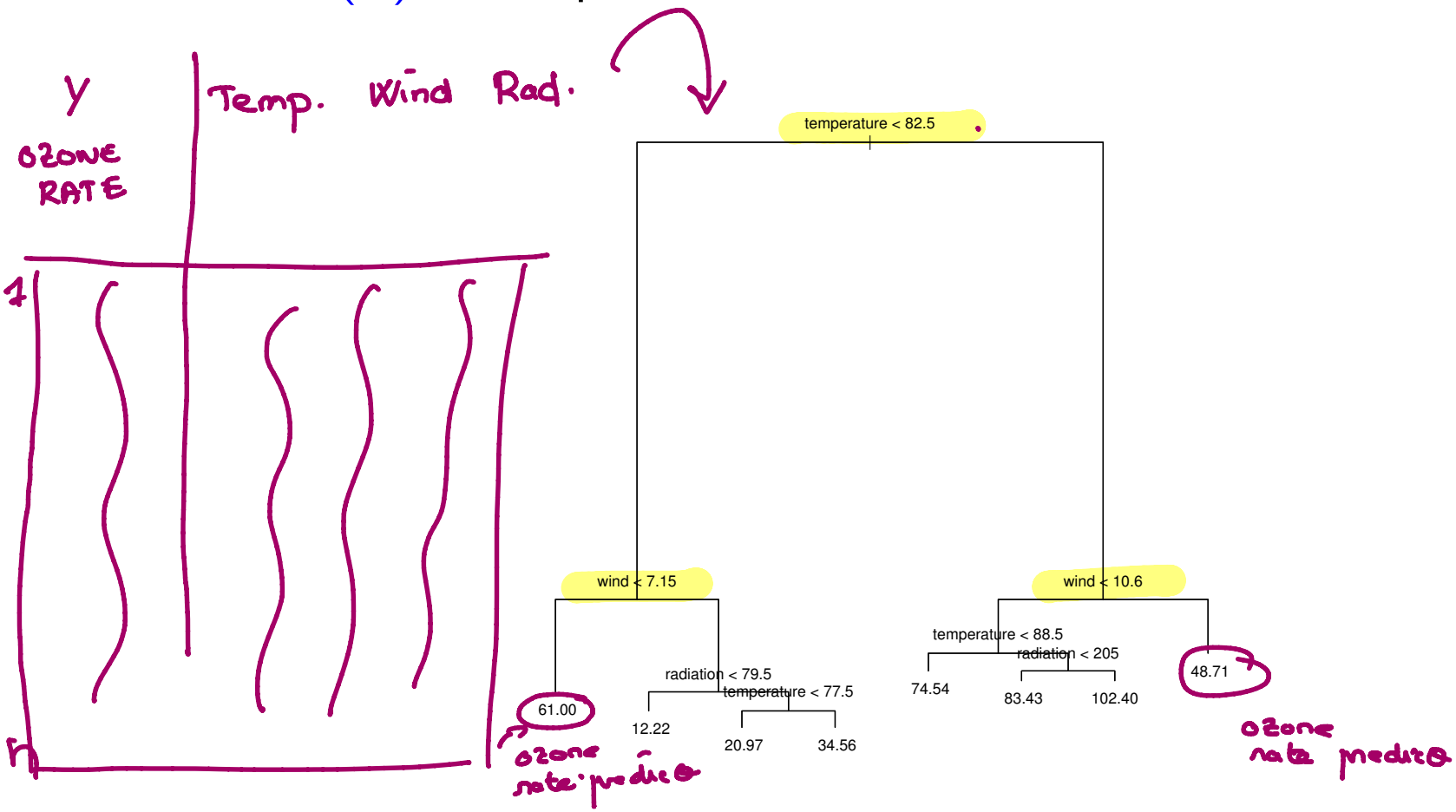


Regression Tree.

Application : Prediction of the ozone rate given several co-variables

Target variable (Y) : ozone rate.

Co-Variables (X) : Temperature, Wind, radiation rate



Classification Tree

Application : Coronary Heart Disease (variable CHD $\{0, 1\}$)

Co-Variables :

chd	response, coronary heart disease
sbp	systolic blood pressure
tobacco	cumulative tobacco (kg)
ldl	low density lipoprotein cholesterol
adiposity	
famhist	family history of heart disease (Present, Absent)
typea	type-A behavior
obesity	
alcohol	current alcohol consumption
age	age at onset

$Y = \{0, 1\}$.

Classification tree.

Application : Coronary Heart Disease (variable CHD $\{0, 1\}$)

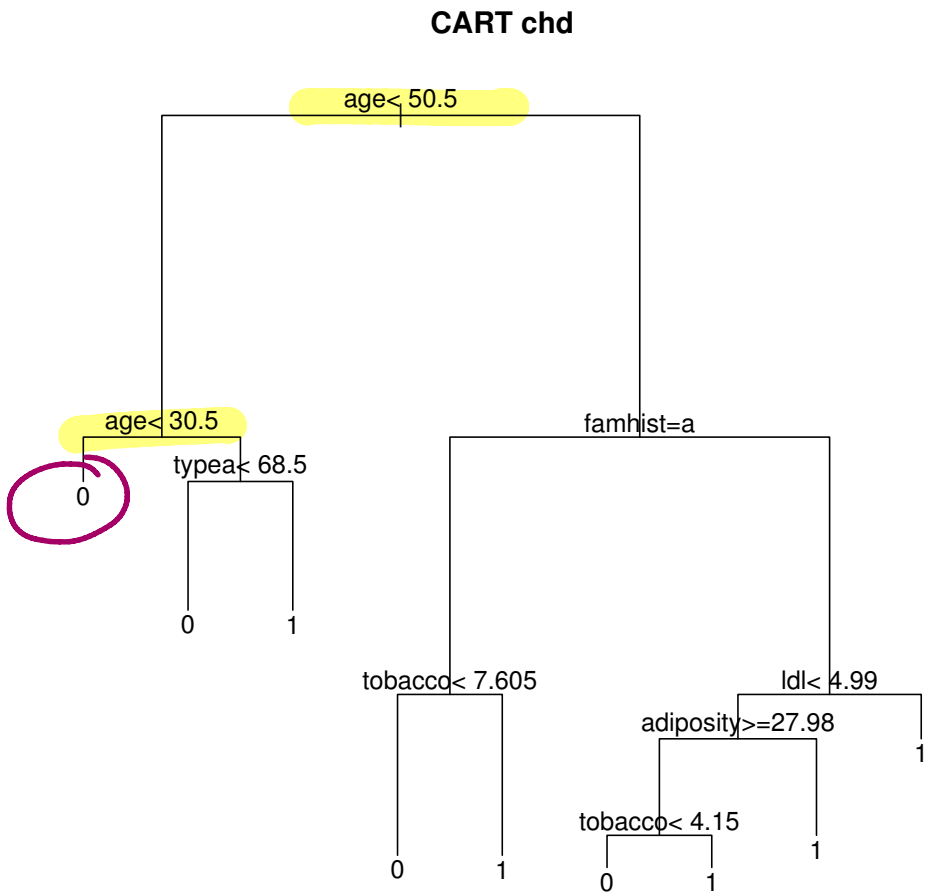
The data :

obs	sbp	tobacco	ldl	adiposity	famhist	typea	obesity	alcohol	age	chd
1	160	12.00	5.73	23.11	Present	49	25.30	97.20	52	1
2	144	0.01	4.41	28.61	Absent	55	28.87	2.06	63	1
3	118	0.08	3.48	32.28	Present	52	29.14	3.81	46	0
4	170	7.50	6.41	38.03	Present	51	31.99	24.26	58	1
5	134	13.60	3.50	27.78	Present	60	25.99	57.34	49	1
6	132	6.20	6.47	36.21	Present	62	30.77	14.14	45	0
7	142	4.05	3.38	16.20	Absent	59	20.81	2.62	38	0
8	114	4.08	4.59	14.60	Present	62	23.11	6.72	58	1
9	114	0.00	3.83	19.40	Present	49	24.86	2.49	29	0
10	132	0.00	5.80	30.96	Present	69	30.11	0.00	53	1

Classification tree.

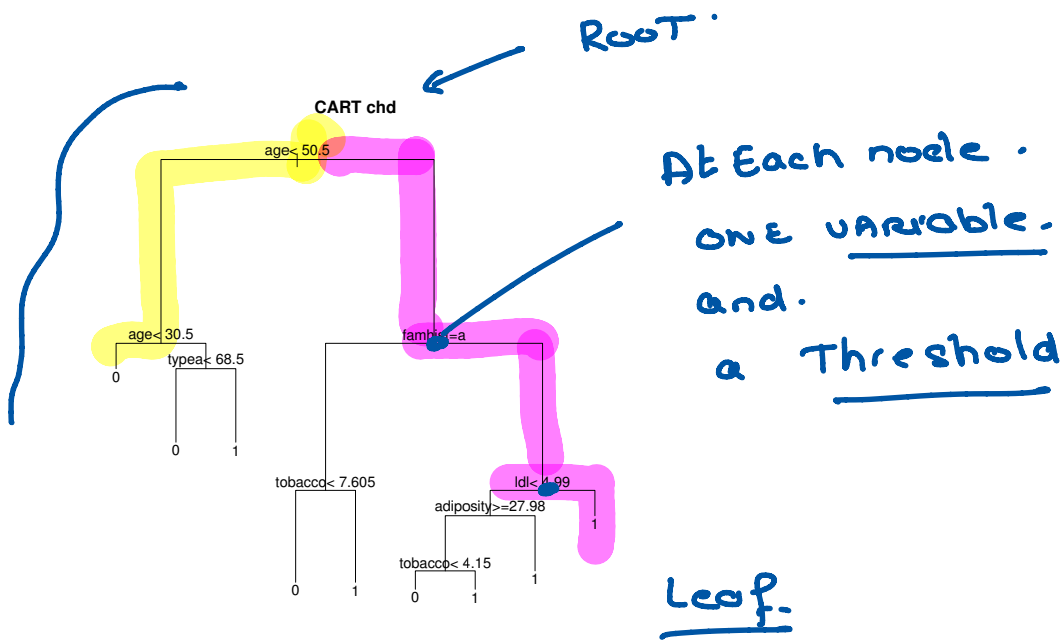
Application : Coronary Heart Disease (variable CHD $\{0, 1\}$)

Decision tree :



Decision tree

Some vocabulary



- Root : first node of the tree
- leaf : terminal node
- Rule between the root and a leaf
- Regions : spaces

Decision Trees

Leo Breiman, Friedman, Olshen 1984

Decision tree is a method which splits the input space in a set of rectangularly domains, in which a **constant model** is adjusted.

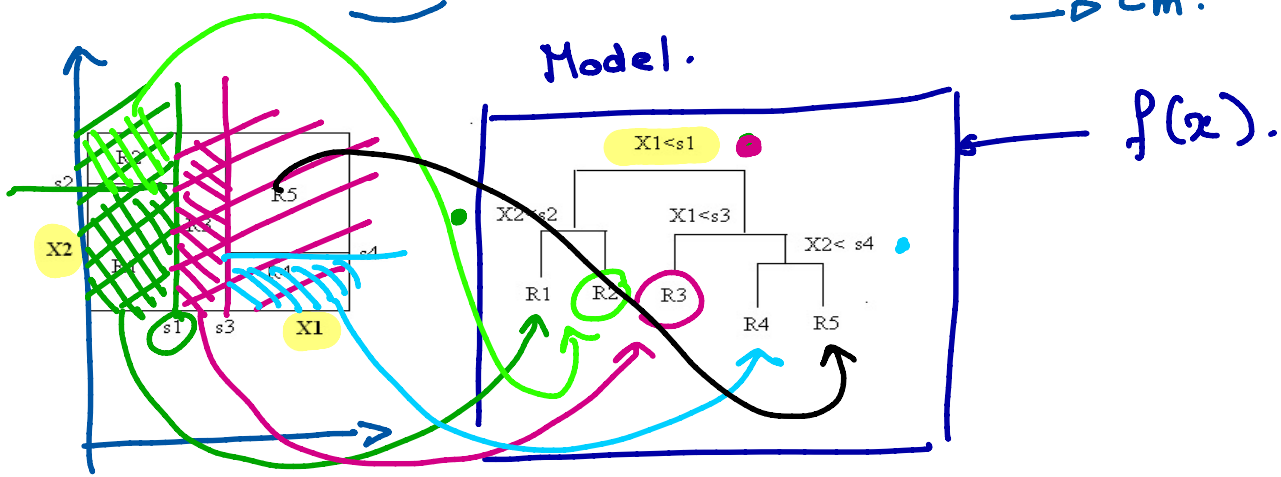
$\rightarrow$ The global regression function is given by

$$f(x) = \sum_{m=1}^{M} c_m 1_{x \in \mathcal{R}_m}$$

c_m is a modality for each region $\mathcal{R}_m$

For each region R_m $\rightarrow c_m$.

$y \quad x_1 \quad x_2$



CART = Classification And Regression Tree.

Classification And Regression Tree, Arbres de Décision

- Y : target variable
  - Qualitative : Classification Tres
  - Quantitative : Regression Tree
  - The same approach let to study regression or classification problems

- X^j : covariables, $1 \leq j \leq p$ qualitatives ou quantitatives

CART belongs to the Non Parametric method family

No assumption is made on the data distribution

$\rightarrow$ The method builds a binary tree

Outline

Regression trees

- The optimization problem is NP-hard.
- A greedy algorithm is used ('greedy' : algorithme glouton) :

Recursive construction :

- Recursive splits are computed regarding a set of given data (the data of the Training set),
  using
- Nodes
  - The Decision criteria at each node involves only one variable
  - and one threshold (for the selected variable)

Definition of the regions

Regarding the type (quantitative or qualitative) of each explanatory variable :

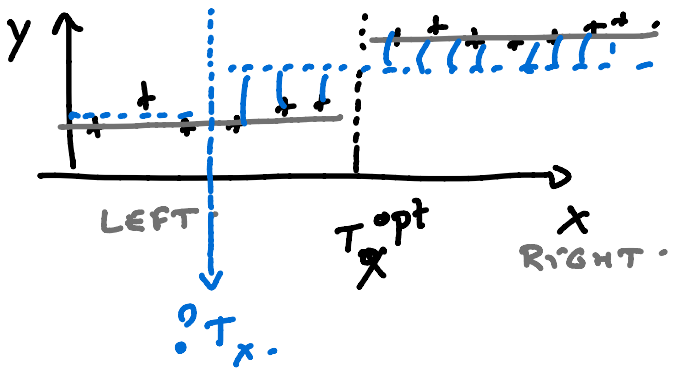
→ X Quantitative, Continuous, Ordinal

$\mathcal{R}_1$ (Left)	$\mathcal{R}_2$ (Right)
$X < S$	$X \geq S$

→ X Qualitative. Example for 4 modalities $X \in \{g_1, g_2, g_3, g_4\}$

$\mathcal{R}_1$ (Left)	$\mathcal{R}_2$ (Right)
g_1	g_2, g_3, g_4
g_2	g_1, g_3, g_4
g_3	g_1, g_2, g_4
g_4	g_1, g_2, g_3
g_1, g_2	g_3, g_4
g_1, g_3	g_2, g_4
g_1, g_4	g_2, g_3

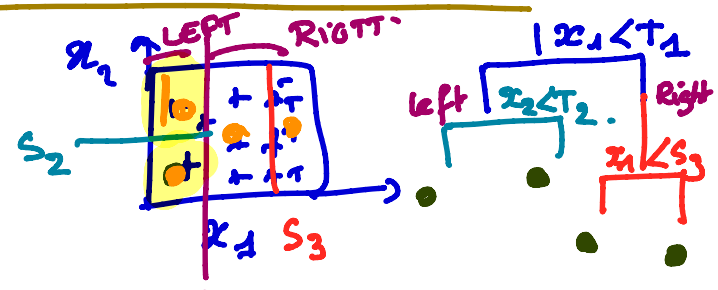
Regression Trees. Construction (1/3)



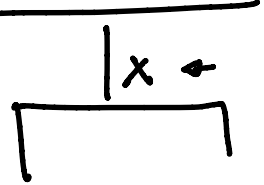
The Target variable Y is a quantitative variable

The X_{j_0} variable is selected if it minimizes the *Deviance* (for Regression) function :

- $(j_0, s_0) = ArgMin_{\{j,s\}} \mathcal{D}(j,s)$
- with
  $\mathcal{D}(j,s) = min_{c1} \sum_{x_i \in R_1(j,s)} (y_i - c_1)^2 + min_{c2} \sum_{x_i \in R_2(j,s)} (y_i - c_2)^2$
- $\hat{c}_1 = mean(y_i / x_i \in R_1(j,s))$ et $\hat{c}_2 = mean(y_i / x_i \in R_2(j,s))$
- $\mathcal{D}(j,s) = \mathcal{D}_{\mathcal{R}_1} + \mathcal{D}_{\mathcal{R}_2}$
  $\mathcal{D}(j,s) = \mathcal{D}_{Left} + \mathcal{D}_{Right}$



$\bar{y}^- = \sum_{x_i \le T} y_i / \text{nbre obs}$



$$\left(X_j^{opt}, T_{x_j}^{opt}\right) = \underset{x_j, T_{x_j}}{\text{Argmin}} \sum_{x_i^j \le T_{x_j}} \left(y_i - \bar{y}^-\right)^2 + \sum_{x_i^j > T_{x_j}} \left(y_i - \bar{y}^+\right)^2$$

LEFT. RIGHT.

Regression Trees. Construction (2/3)

Rule for Stopping the construction of the tree :
A node is a terminal if the observations data (in this node) are "homogeneous".
No more admissible partitions if

- The number of observations (nodes or leaves) is below a given threshold (algorithmic default parameters)
- The deviance ratio (before and after the split) is lower than a given threshold : $\mathcal{D} - (\mathcal{D}_{Left} + \mathcal{D}_{Right}) <$ Threshold (algorithmic default parameter)
- in R for the rpart() function : MinCut, MinSize, MinDev parameters.

3 Hyperparameters for the CART algorithm.

Regression Trees. Prediction (3/3)

- The regression function is given by

$$f(x) = \sum_{m=1}^{M} c_m 1_{x \in \mathcal{R}_m}$$

- The predicted regression model is given by

$$\hat{f}(x) = \sum_{m=1}^{M} \hat{c}_m 1_{x \in \mathcal{R}_m}$$

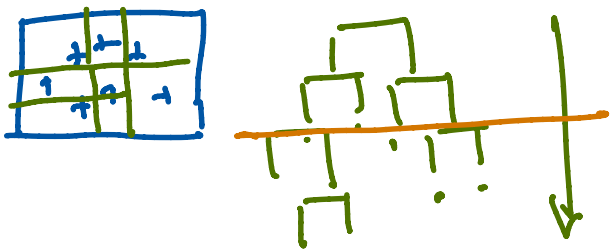
- Notations :
  - $\hat{c}_m$ is the average of the Train observation data in region $\mathcal{R}_m$
  - Prediction for one observation : $x \in \mathcal{R}_m$, $\hat{y} = \hat{c}_m$.

Over fitting is what you want to avoid ! !

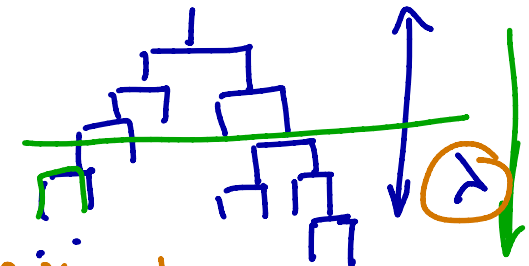
- Question : what is the optimal size of a tree ?
  - Deep enough for a well approximation of the data
  - Not too deep to avoid over fitting
  - The minimization of the Deviance itself is not enough !

- Theory : to able to balance the bias and variance
  - short trees $\rightarrow$ important bias /low variance
  - Deep trees $\rightarrow$ low bias / large variance

- Idea : to be able to prune a original deep tree by cutting some branches using a penalized criteria



$$\text{erreur}(\text{Tree}) + \lambda \cdot |\text{Tree}|$$



Tree drawbacks

- Their instability !
- Very different trees may be computed for different samples (of the same distribution)
- The greedy optimization (very efficient) provides a "local" solution
- For improving the robustness : Aggregation

Outline

Decision trees.

Ensemble methods

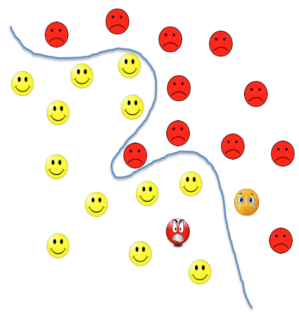
Ensemble methods

- Bagging : Random strategies on the observation data.
  Bagging pour Bootstrap Aggegating (Breiman, 1996)
- Random Forest : Random strategies on both observation data and variables (Breiman, 2001)
- Boosting : strategies on the c_m aggregation parameters
  (ADABOOST : Schapire 1990, Freund & Schapire 1995)

We illustrate these three strategies (Bagging, Random Forest and Boosting) on regression trees.

Decision trees

Bagging



Family of random observation sets. Bagging

- Y target variable, quantitative or qualitative
- $X = (X^1, \ldots, X^p)$ explanatory variables ($\mathbb{R}^p$)
- $\mathcal{S} = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ n sample with a distribution law $\mathcal{F}$.
- $\Phi(x)$ a model function of $x = (X^1, \ldots, X^p)$
- B Bootstrap independant samples $\{\mathcal{S}_b\}_{b=1,B}$
  - $\rightarrow \hat{\Phi}_{\mathcal{S}_b}(.)$
- Aggregation of the different prediction models
  - Y quantitative : $\hat{\Phi}_B(.) = \frac{1}{B}\sum_{b=1}^{B} \hat{\Phi}_{\mathcal{S}_b}(.)$ (average)
  - Y qualitative : $\hat{\Phi}_B(.) = argmax_j card\{b|\hat{\Phi}_{\mathcal{S}_b}\}$ (vote)
- $\Phi(.) = \mathbb{E}_{\mathcal{F}}(\hat{\Phi}_{\mathcal{S}})$ estimator with no bias

Averaging independant prediction in order to decrease the variance
B independant Bootstrap samples, B bootstrap replications.

Bagging. Breiman 1996

Goal : Averaging "independent" predictions in order to reduce the variance using independant classifiers (B bootstrap replications).

$$\text{Var}(\bar{Z}) = \frac{\text{Var}(Z)}{\#\{B\}}$$

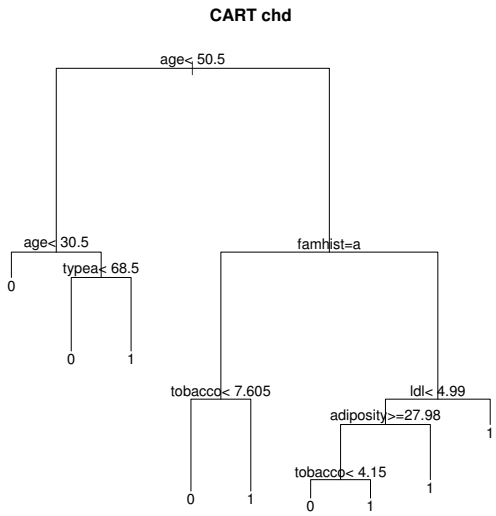
Method :

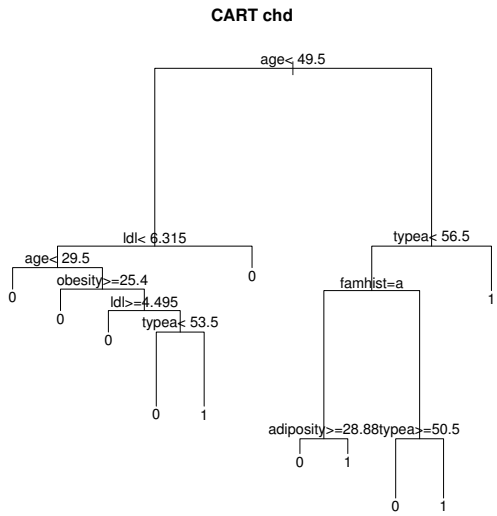
- Y target variable, qualitative or quantitative
- $X = (X^1, \ldots, X^p)$ Multi dimensional co variables ($\mathbb{R}^p$)
- $\Phi(X)$ a given model function of the covariable $X = (X^1, \ldots, X^p)$
- $\mathcal{D}_n = \{(x_1, y_1), \ldots, (x_n, y_n)\}$ n sample of $\mathcal{F}$ distribution law.

Bagging provides a family of random models :

- B independant samples are generated with replacement : $\{\mathcal{S}_b\}_{b=1,B}$
  - Y qualitative : $\hat{\Phi}_B(.) = \arg\max_j \text{card}\{b|\hat{\Phi}_{\mathcal{S}_b}\}$ (vote)
  - Y quantitative : $\hat{\Phi}_B(.) = \frac{1}{B}\sum_{b=1}^{B} \hat{\Phi}_{\mathcal{S}_b}(.)$ average
- $\Phi(.) = \mathbb{E}_{\mathcal{F}}(\hat{\Phi}_{\mathcal{S}})$ estimator with low/ no biais

Bagging. Illustration





Random observations
1^{st} sampling

Random observations
2^{nd} sampling

...
...
...

$\rightarrow$ A tree is built for each Bootstrap sample

Bagging. Benefits and drawbacks

- Complete tree for every bootstrap sample. Faible biais (+)
- Reduced variance for aggregated models. (+)
- Storage of all calibrated models (-)
- Computation time (-)
- Black-box model (-)
- choice of the M value(-)
  -numbers of models (number of trees)

Statistical benefits

- No bias amplification
- With low correlation contributors

$$\mathrm{cov}(g_t(x), g_t'(x)) \simeq 0$$

We observe a variance reduction of the order $1/T$

$$\mathbb{V}(\widetilde{g}_T(x)) \simeq \frac{1}{T}\mathbb{V}(g_1(x))$$

OOB. Out Of Bag Error

$\mathcal{D}_n = \{(x_i, y_i) \;\; y_i \in \{1, .., k..., K\} \; 1 \leq i \leq n\}$ is the original data set.

For each bootstrap sample, (for each b tree) :

- The tree is built using the data of $\mathcal{D}_n^b$, a n Bootstrap sample (n observations drawn with replacement).
- The remaining observations of $\mathcal{D}_n$ which are not in the train data set are used to evaluate the generalization power : $\bar{\mathcal{D}}_n^b = \mathcal{D}_n - \mathcal{D}_n^b$ (observations of $\mathcal{D}_n$ which are not in $\mathcal{D}_n^b$)

For each observation x_i, the OOB performance (or error) is defined

- $\hat{\phi}^{OOB}(x_i)$ computed if $x_i \in \bar{\mathcal{D}}_n^b, b = 1...B$, with $n_B = \sum_{b=1}^{B} 1_{x_i \in \bar{\mathcal{D}}_n^b}$
- $E^{OOB}(x_i) = y_i - \frac{1}{n_B} \sum_{x_i \in \bar{\mathcal{D}}_n^b} \hat{\phi}_{OOB}(x_i)$
- $E^{OOB} = \frac{1}{n} \sum_{i=1}^{n} E^{OOB}(x_i)$

Decision Trees

Random Forest

Random Forest. Breiman 2001.

Similar Goal as Bagging :

Averaging "independent" predictions in order to reduce the variance using independant classifiers (B bootstrap replications). $\text{Var}(\bar{Z}) = \frac{\text{Var}(Z)}{\#\{B\}}$

Method :

- The model is based on a bagging procedure
- At each node, the final variable is selected in a sub-set of variables chosen at random.
- Tuning parameters : R sofware by default : classification : p/3 ; regression $\sqrt{p}$.

Proposition of Breiman

$\rightarrow$ Random choice of the variables to provide more independant classifiers

Feature subsampling

Feature subsampling step : the particularity of random forests is that only a random subset of p features is tried each time when looking for a split. This reduces the correlation between the trees.

Recommendations from the authors (p number of variables) :

- Classification : default value for p_{tried} is $\lfloor \sqrt{p} \rfloor$ and minimum node size is 1.
- Regression : default value for p_{tried} is $\lfloor p/3 \rfloor$ and minimum node size is 5. In practice, best values depend on the problem : tuning parameters.

Some remarks on the RF method

- Usually, trees are not pruned in random forests. Indeed, the gain of pruning does not seem crucial, and hence, this choice allows to save a tuning parameter.
- When the number of variables is large, but the fraction of relevant variables small, random forests do not perform very well for small p, since, at each split, the chance that the relevant variables will be selected is small.

A variant of random forests, ExtraTrees

ExtraTrees : Extremely randomized trees.

Here, trees are built on the initial sample $\mathcal{D}_n$, **no bootstrap**.

1. At each node, a random subset of features is drawn as for random forests.
2. A few number of thresholds is then selected uniformly at random in the feature range.
3. Finally, the best split among these thresholds and features is selected using some impurity criterion (Gini, Entropy).

Remark :

- Due to this random choice, the algorithm is faster.
- Random thresholds lead to more diversified trees, and thus, are some form of regularization.
- Since trees are combined and averaged, not so bad to select the thresholds at random...

→ Python : sklearn.ensemble.ExtraTreesClassifier()

RF Variable importance

Regarding RF interpretability, once again, the resulting estimator is not a tree. Nevertheless, random forests come along with variable importance plots, yielding very useful information.

Several criteria may be found to compute variable importance :

1. At each split in each tree, the improvement in the split-criterion (ex Gini) is attributed to the splitting variable, and then, for each variable, the values are accumulated over all the trees in the forest.
2. A different variable importance measure, based on the OOB samples. When the b-th tree is grown, the prediction accuracy is compared with the prediction accuracy when the values for the j-th variable are randomly permuted in the OOB samples. The decrease in accuracy due to this permuting is averaged over all trees, and is used as a measure of the importance of variable j -th in the random forest.

Variable Importance Measure for Random Forest

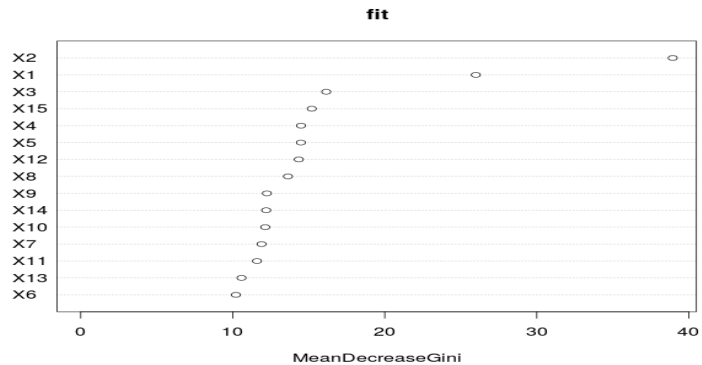
The **V**ariable **I**mportance **M**easure (VIM) quantifies the mean decrease in Accuracy for each covariable thanks to the following protocol.

Considering a RF with B bootstrap sample trees.

- For each b tree, the performance error, $E_{OOB(b)}$ is computed $(1 \leq b \leq B)$
  using the Out Of Bootstrap sample $OOB(b)$.
  1. For each variable X_k, $1 \leq k \leq p$, the observations of the OOB sample are **uniformly shuffled for the b^{th} tree** .
  2. The VIM is then computed for the $X_k$variable and the b tree : $VIM(b,k) = E^k_{OOB(b)} - E_{OOB(b)}$ (several definition/ possible renormalisation)
- The Mean Decrease in Accuracy for each variable X_k is then measured for the RF thanks to all trees :
  $VIM(k) = \frac{1}{B} \sum_{b=1}^{b=B} VIM(k,b)$

Variable Importance Measure (VIM) for Random Forest

- The VIM is computed independently for each variable : two correlated variables have a similar VIM value

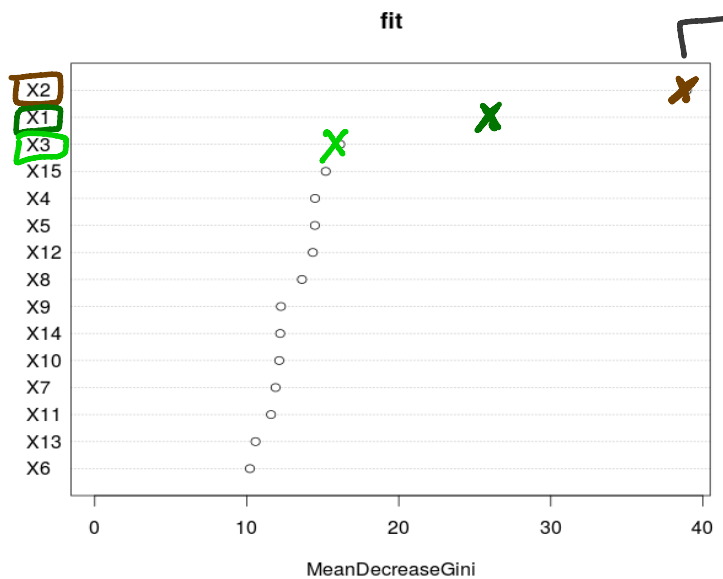


- Several error indexes can be introduced as Gini, entropy... indexes.
- The VIM indicator may be normalized as initially proposed by Leo Breiman :
  $VIM(k) = \frac{1}{B}\sum_{b=1}^{b=B} VIM(k,b)/E_{OOB(b)}$
  $VIM(k) = \frac{1}{B}\sum_{b=1}^{b=B} VIM(k,b)/S_{OOB}$ (S_{OOB} : std of OOB for B trees)

Variable Importance

The variable Importance is computed by the average decrease in impurity provided by each variable calculated by the Gini index. The decrease for each node is cumulative, then an average over all trees is performed.

Target. Covariables.
↓
y $X_1, X_2 \dots X_{15}$.



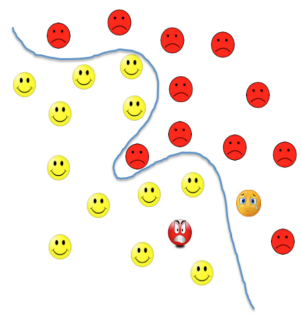
Information of the "importance of the variable" for the predictor in the Ensemble models. (Bagging, RF).

Graph computed with the VarImpPlot() function in R.

Outline

CART-

Classification tree



Classification Trees

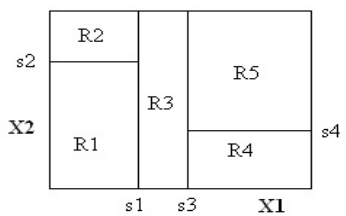
Classification tree is a method which splits the input space in a set of rectangularly domains, in which a **constant model** is adjusted.

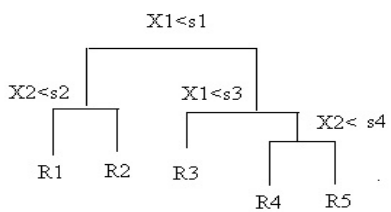
$\rightarrow$ The global classification function is given by

$$f(x) = \sum_{m=1}^{M} c_m 1_{x \in \mathcal{R}_m}$$

c_m is a constant modality for each region $\mathcal{R}_m$

Question : How to compute c_m, $1 \leq m \leq M$, for the M regions ?





Classification Trees

Classification trees are used for a qualitative target variable and are associated in this case with a classification criteria.

- Using the Training set.
  For node m corresponding to region $\mathcal{R}_m$ with N_m observations
  - In node m, the frequency for modality k is estimated :
    for $k \in \{1, ..., K\}$

$$\hat{p}_{mk} = \frac{1}{N_m} \sum_{x_i \in \mathcal{R}_m} I(y_i = k; (x_i, y_i) \in \text{TrainDataSet})$$

  - In region (node) m, an **new** observation is affected to class k_0 if

$$k_0 = \underset{k \in 1..K}{\arg\max} \{\hat{p}_{mk}\}$$

    which represents the most represented class in node m.

Classification Trees

- The classification function is given by

$$f(x) = \sum_{m=1}^{M} c_m 1_{x \in \mathcal{R}_m}$$

- Notations : c_m corresponds to the main modality on the training set for the region $\mathcal{R}_m$
- The estimated classification function is given by

$$\hat{f}(x) = \sum_{m=1}^{M} \hat{c}_m 1_{x \in \mathcal{R}_m}$$

- For an observation $x \in \mathcal{R}_m$, $\hat{y} = \hat{c}_m$. $\hat{c}_m$ estimated on Train DataSet.

Classification Tree. Construction of the Tree

In the classification setting, ther are several ways to measure the quality of a split. **Node Impurity measures (Left ou Right) :**

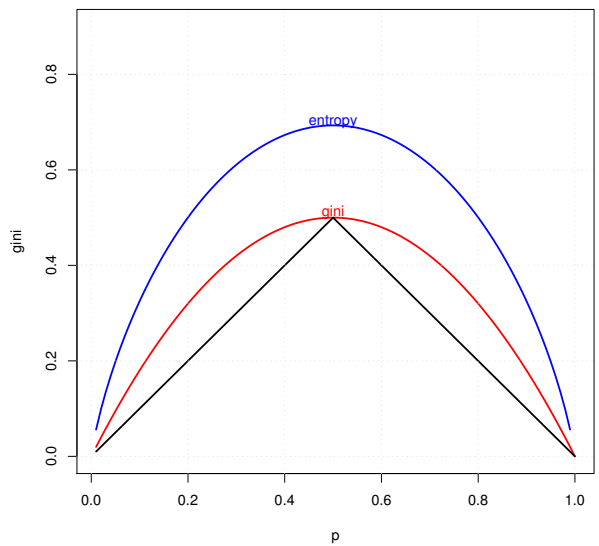
- Missclassification :
  $\mathcal{D}_{\mathcal{R}_m} = \frac{1}{N_m} \sum_{i \in \mathcal{R}_m} I(y \neq k(m)) = 1 - \hat{p}_m$
- Gini index (most used) :
  $\mathcal{D}_{\mathcal{R}_m} = \sum_{k \neq k'} \hat{p}_{mk} \hat{p}_{mk'} = \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk})$
  $= 2p(1-p)$
- Entropy :
  $\mathcal{D}_{\mathcal{R}_m} = -\sum_{k=1}^{K} \hat{p}_{mk} log \hat{p}_{mk}$
  $= -p \log_2 p + (1-p) \log_2 (1-p)$

with $p_m = \frac{1}{N_m} \sum_{i \in \mathcal{R}_m} I(y = k(m))$.

* For 2 classes and for each region

Decision trees

Comparaisons of node impurity



A function of impurity is by default chosen (R : gini)

Classification trees. Node creation

For a impurity measure

- k : node number
- $\mathcal{R}_1$ et $\mathcal{R}_2$ regions of the two leaves
- The algorithm computes the optimal partition for which the value of $\mathcal{D}_{\mathcal{R}_1} + \mathcal{D}_{\mathcal{R}_2}$ is minimal
- i.e. at each step k , the split of "one upper region" in "two lower regions" (corresponding to the recursive construction of the tree) maximizes the difference of node impurity measure (deviance) :

$$\Delta \mathcal{D}_{\mathcal{R} \to \mathcal{R}_1 + \mathcal{R}_2} = \mathcal{D}_{\mathcal{R}} - \left(\frac{N_{\mathcal{R}_1}}{N_{\mathcal{R}}} \mathcal{D}_{\mathcal{R}_1} + \frac{N_{\mathcal{R}_2}}{N_{\mathcal{R}}} \mathcal{D}_{\mathcal{R}_2}\right)$$
$$\{X^j, 1 \leq j \leq p\}$$

Classification tree. Node creation. Illustration

Impurity measure : Gini index

		$Y=0$	$Y=1$	
Left	$X < S$	n_{11}	n_{12}	n_{1+}
Right	$X \geq S$	n_{21}	n_{22}	n_{2+}
Top	global	n_{+1}	n_{+2}	n_{++}

Gini indices :

Top G	$2 * \frac{n_{+1}}{n_{++}}(1 - \frac{n_{+1}}{n_{++}})$
Left G_L	$2 * \frac{n_{11}}{n_{1+}} * (1 - \frac{n_{11}}{n_{1+}})$
Right G_R	$2 * \frac{n_{21}}{n_{2+}} * (1 - \frac{n_{21}}{n_{2+}})$

Classification tree. Node creation. Illustration

Impurity measure. Entropy

		$Y=0$	$Y=1$	
Left	$X < S$	n_{11}	n_{12}	n_{1+}
Right	$X \geq S$	n_{21}	n_{22}	n_{2+}
Top	(global)	n_{+1}	n_{+2}	n_{++}

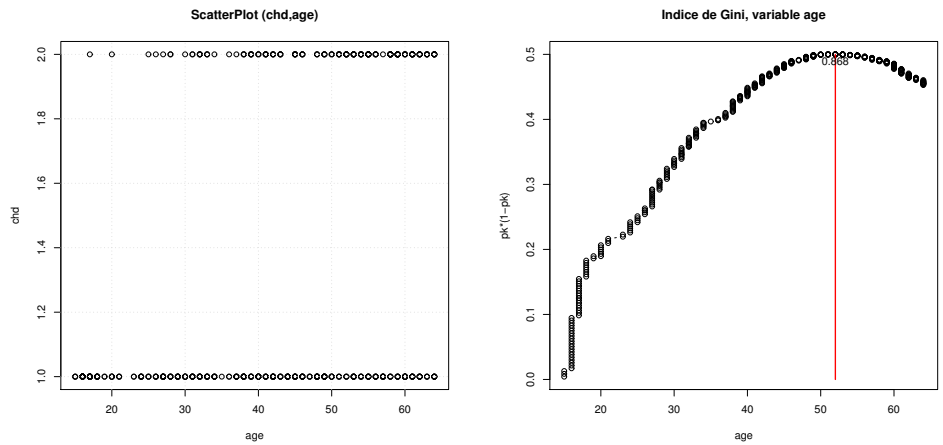
Entropy	
top H	$\frac{n_{+1}}{n_{++}} log \frac{n_{+1}}{n_{++}} + \frac{n_{+2}}{n_{++}} log \frac{n_{+2}}{n_{++}}$

Left H_L $\quad \frac{n_{11}}{n_{1+}} log \frac{n_{11}}{n_{1+}} + \frac{n_{12}}{n_{1+}} log \frac{n_{12}}{n_{1+}}$

Right H_R $\quad \frac{n_{21}}{n_{2+}} log \frac{n_{21}}{n_{2+}} + \frac{n_{22}}{n_{2+}} log \frac{n_{22}}{n_{2+}}$

Decision tree. Cardiac Heart Disease application (chd)

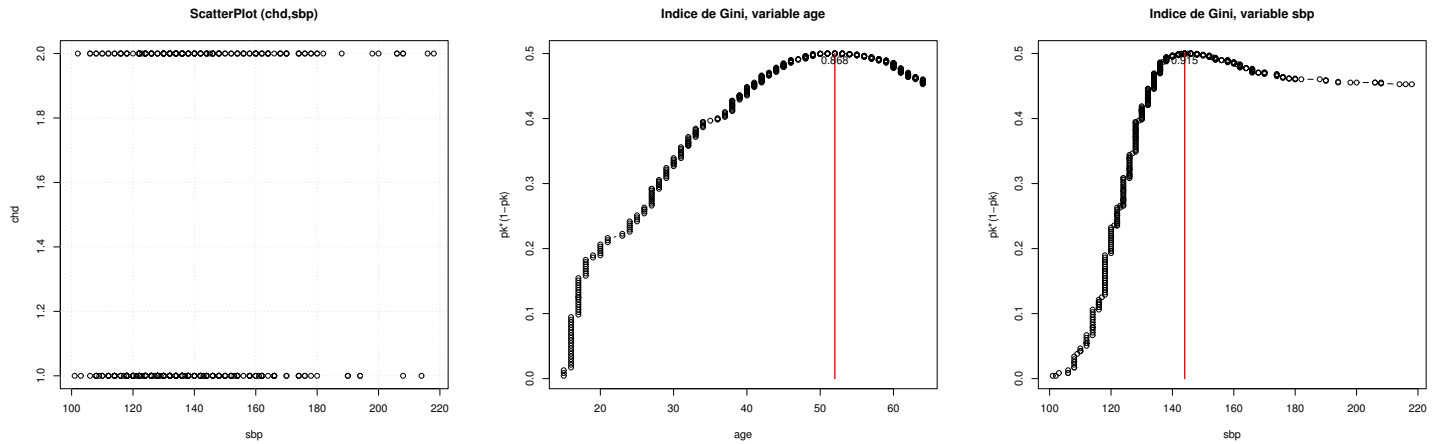
The target variable is chd (binary variable).
$\rightarrow$ **Computation of the decision threshold for the quantitative co-variable age and for the Gini index**



$\mathcal{D}(\text{age})=0.868$

Decision tree. Cardiac Heart Disease application (chd)

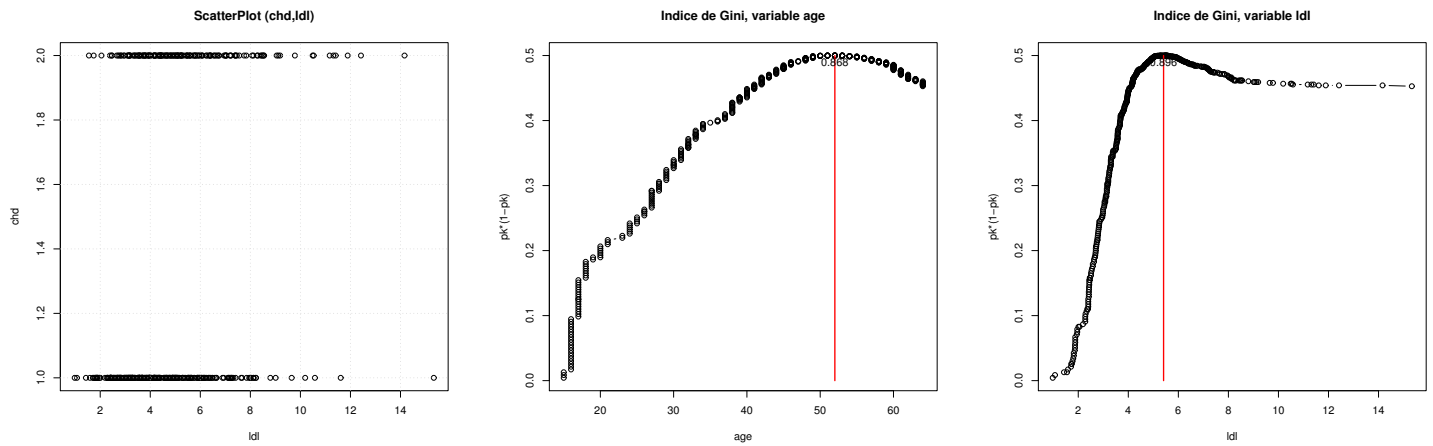
Decision threshold computation and variable selection between two covariables (age, spb) based on the Gini Index



The age variable is selected : $\mathcal{D}(\text{age})=0.868 < \mathcal{D}(\text{spb})=0.915$

Decision Tree, Cardiac Heart Disease application (chd)

Decision threshold computation and variable selection between two covariables (age, ldl) based on the Gini Index



The age variable is selected : $\mathcal{D}(\text{age})=0.868 < \mathcal{D}(\text{ldl})=0.896$

Classification Trees

Stopping the recursive split process

A node is terminal if :

- the region is homogeneous (only one label)
- The is no authorized partitions regarding the algorithmic rule of decreasing the variance criteria ($\Delta\mathcal{D}$).
- The number of observations in the region NCut (or in the sub regions Nsize) is lower than a given threshold then No authorized split. (algorithm parameters).

Software Tuning parameters : (NCut, Nsize, $\Delta\mathcal{D}$)

Classification trees. Estimation. Prediction

From Estimation to Prediction :

- Y quantitative : average of observations of the training data set
- Y qualitative. Each leave is affected to one given class C_k of Y regarding a conditional approach regarding the training data set
  - **The more frequently class represented in the node (training data set)**
  - or
  - the "more probable" class if some apriori exists (training data set)
  - The "cheapest" class if there exists some coast indications.

Outline

Illustration. SPAM classifier

Problem : to be able to automatically classify a regular email from a spam email

SPAM

From : Felix Damians, From .Abidjan Cote D.Ivoire

Hello Dear, Pardon me for not having the pleasure of knowing your mindset before making you this offer and it is utterly confidential and genuine by virtue of its nature. I want someone like you to help me out after i had pray ,then believes that you are a good person and that i can stay with you for the rest of my life , am 24 years old, My late father is a wealthy and successful business man before he died , My mum died when i was a baby, am the only child in my family. Honestly speaking , i am ready to give you 15percent of this total money for your assistance and with extra 5percent for your expenses on phone call, please reply me now if really serious to help me out so that i can tell you more about my intention and forward to you some of the legal papers after knowing you more better. Yours Felix Damians.

Illustration. SPAM classifier

A Text Mining is first performed to compute features

SPAM

From : Felix Damians, From .Abidjan Cote D.Ivoire

Hello Dear, Pardon me for not having the pleasure of knowing your mindset before making you this offer and it is utterly confidential and genuine by virtue of its nature. I want someone like you to **help** me out after i had pray ,then believes that you are a good person and that i can stay with you for the rest of my life , am 24 years old, My late father is a wealthy and successful business man before he died , My mum died when i was a baby, am the only child in my family. And he told me that he used my name to deposit (us dollars 12.5million) in the bank and he seriously advise me to transfer this total **money** to oversea account for my investment, where i will start my new life and finish my education , Because of this reason, i am soliciting your assistance for the claim and transfer to your bank account for the business. Honestly speaking , i am ready to give you 15percent of this total money for your assistance and with extra 5percent for your expenses on phone call, please reply me now if really serious to **help** me out so that i can tell you more about my intention and forward to you some of the legal papers after knowing you more better. All about the money are legal and i have all the legal documents and papers of the money money with me which the bank issued to my late father the day of the deposit, Because of the war in our country now the bank manager here has promised to me that they will use their branch corrospodant bank in Europ or Asia.to transfer the money into any account i provided to them that is why i contacted you to **help** me out in receiveing of the moneymoney into an account over there in your country before i join you over to has rest of mind. Thanks and remain bless with your family as i wait for your

Illustration. SPAM classifier

SPAM data base

- 48 continuous real [0, 100] attributes of type word-freq-WORD = percentage of words in the e-mail that match WORD, i.e. 100 * (number of times the WORD appears in the e-mail) / total number of words in e-mail. A "word" in this case is any string of alphanumeric characters bounded by non-alphanumeric characters or end-of-string.
- 6 continuous real [0, 100] attributes of type char-freq-CHAR = percentage of characters in the e-mail that match CHAR, i.e. 100 * (number of CHAR occurences) / total characters in e-mail
- 1 continuous real [1, ...] attribute of type capital-run-length-average = average length of uninterrupted sequences of capital letters
- 1 continuous integer [1, ...] attribute of type capital-run-length-longest = length of longest uninterrupted sequence of capital letters
- 1 continuous integer [1, ...] attribute of type capital-run-length-total = sum of length of uninterrupted sequences of capital letters = total number of capital letters in the e-mail
- 1 nominal 0,1 class attribute of type spam = denotes whether the e-mail was considered spam (1) or not (0), i.e. unsolicited commercial e-mail.

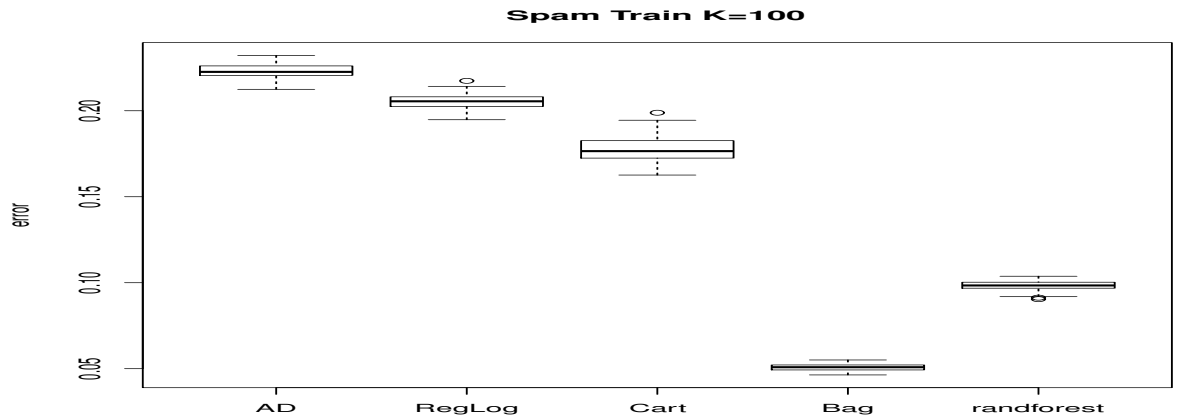
Historical data base

- $p = 57$ features computed from the initial texts ($p = 56$)
- $n = 4601$ Emails with
- $Y \in \{0, 1\}$ a binary indicator
- $n >> p$

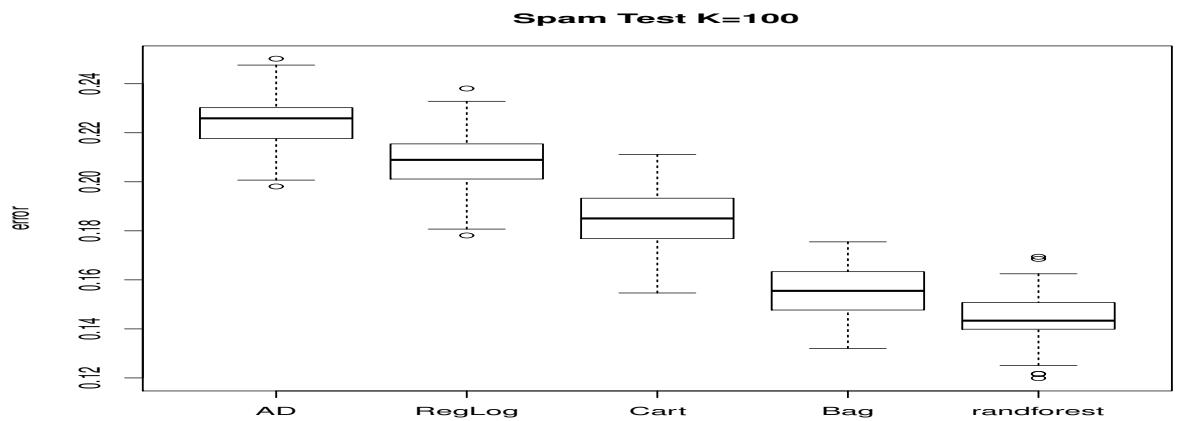
Predictive performance comparison for Several Classifiers

Based on K-fold.

Train data



Test data



Outline

Classification trees. Model selection. Pruning

In order to avoid (minimize) overfitting, the length of the tree is penalized.

One the maximal tree is built (one tree), the pruning algorithm proposes several trees by pruning. A comparison between all these the trees helps to select the tree which minimize the following complexity criteria.
The tree with the lowest error is finally selected.

Complexity criteria :

$$C_\alpha(T) = \sum_{m=1}^{|T|} N_m Q_m(T) + \alpha |T|$$

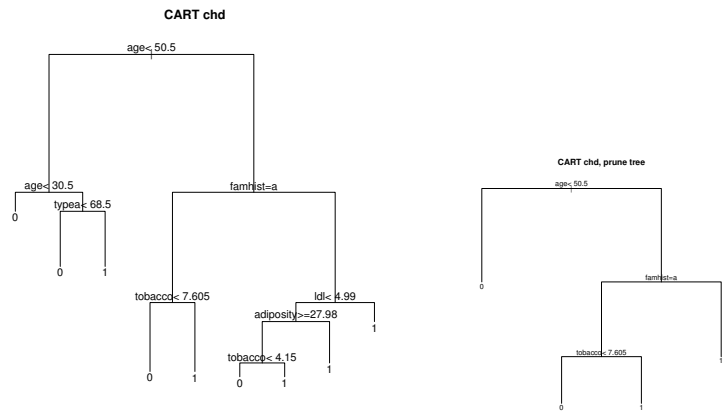
avec

- $|T|$: terminal node number
- $N_m = \sharp\{x_i \in \mathcal{R}_m\}$
- $\hat{c}_m = \frac{1}{N_m} \sum_{x_1 \in \mathcal{R}_m} y_i$
- $\hat{Q}_m(T) = \frac{1}{N_m} \sum_{x_i \in \mathcal{R}_m} 1_{y_i \neq k_m}$
- α is selected by cross-validation

Classification trees & Predictive Power

- A deep decision tree may fit perfectly the training dataset (low biais/ strong variance).

→ Pruning : increasing the Predictive Power for keeping the interpretability with one given decision tree.



Complexity criteria : $C_\alpha(T) = \sum_{m=1}^{|T|} N_m Q_m(T) + \alpha|T|$

α selected by cross-validation