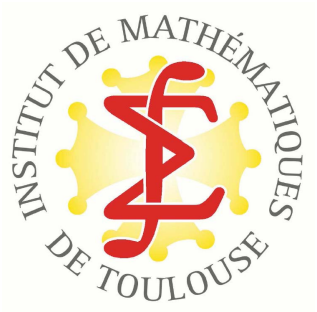


Institut de Mathématiques de Toulouse, INSA Toulouse

Supervised Learning- Part II

Formation en machine Learning
EUR NanoX

Béatrice Laurent - Philippe Besse - Olivier Roustant

Methods studied in this course :

Part I

- Linear models for regression
- Linear models for classification

Part II

- Classification And Regression Trees, Bagging, Random Forests
- Neural networks, Introduction to deep learning

Outline

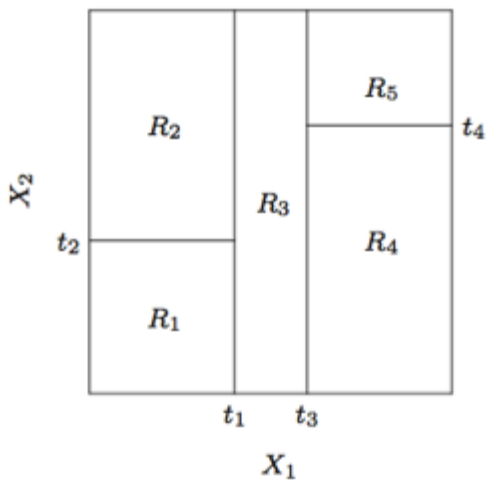
- Classification And Regression Trees (CART)
- Bagging, Random Forests

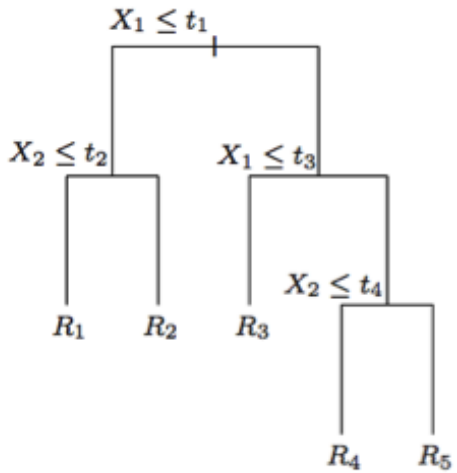
Classification And Regression Trees

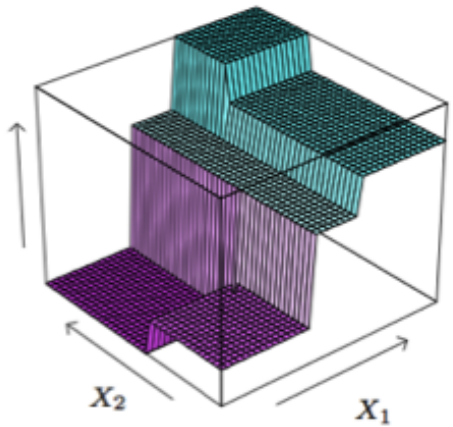
Introduction

- Classification and regression trees (CART) : Breiman et al. (1984)
- X^j explanatory variables (quantitative or qualitative)
- Y qualitative with m levels $\{\mathcal{T}_\ell; \ell = 1 \ldots, m\}$: 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

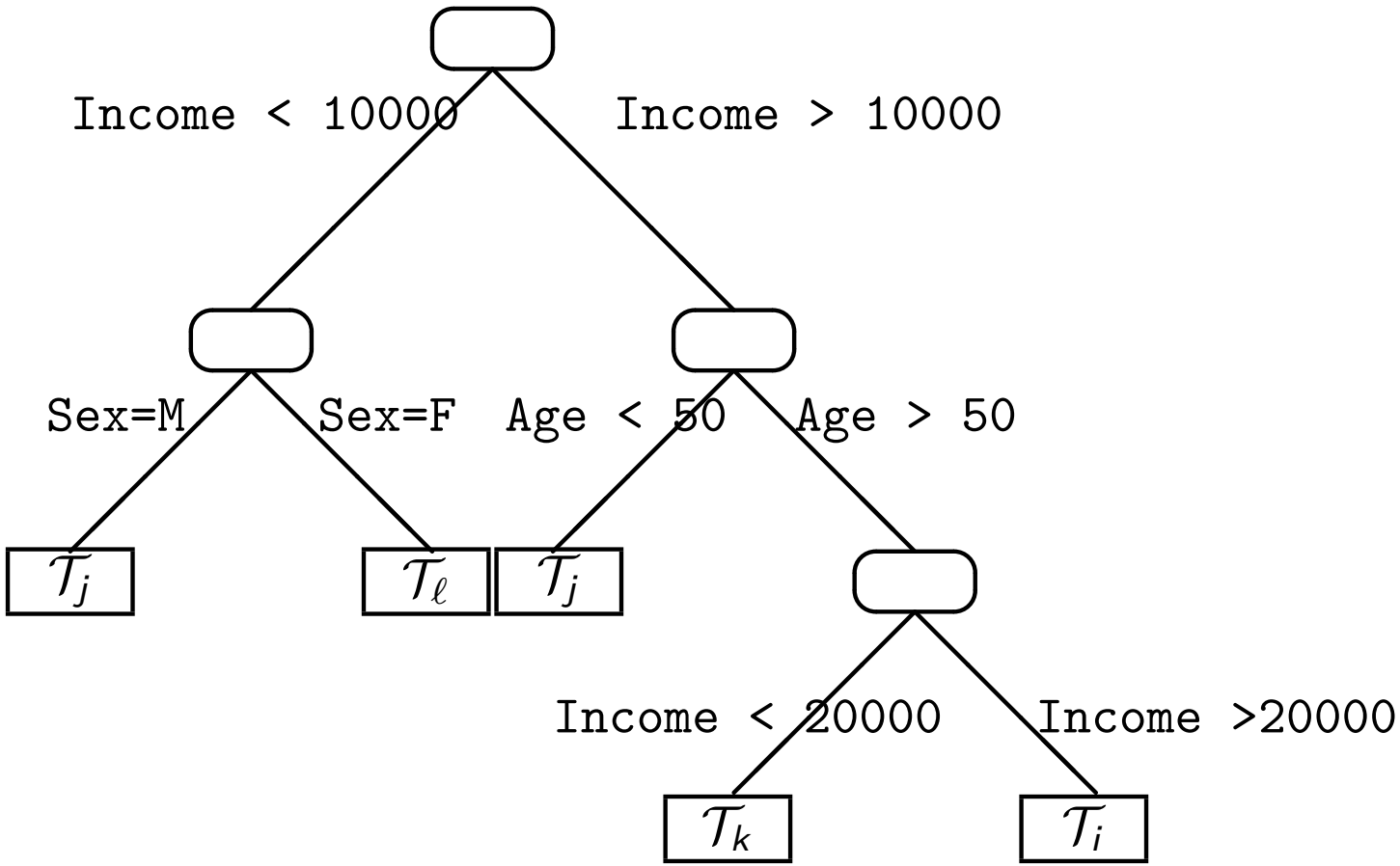






Source : Hastie, Tibshirani, Friedman (2019), "The elements of statistical learning"

Example of binary classification tree



Principles for constructing a tree

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

Constructing regression trees

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

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

Splitting procedure

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

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

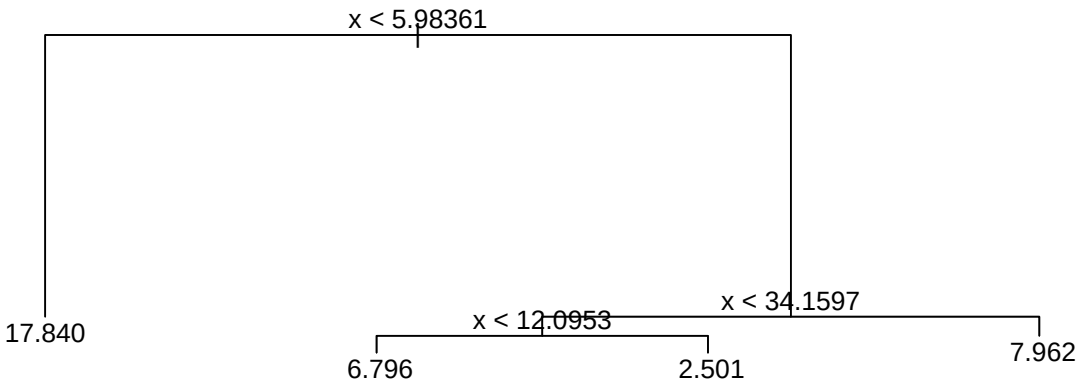
Find (j,t) in order to minimize the intra-class variance

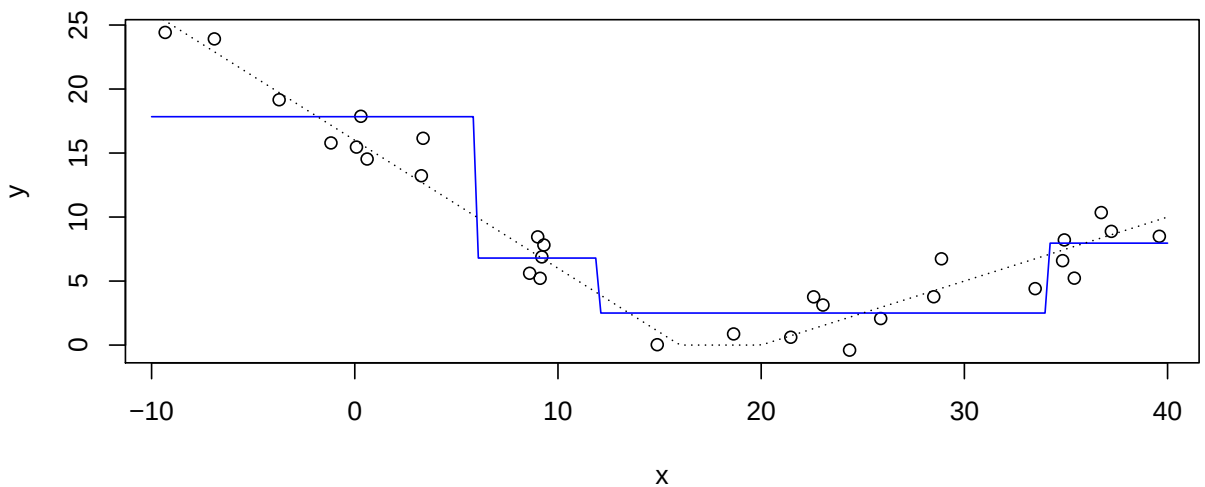
$$J(j,t) = D_{\kappa_L(t,j)} + D_{\kappa_R(t,j)},$$

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_κ^ℓ : proportion of the class $\mathcal{T}_\ell$ of Y in the node κ.

- Shannon Entropy

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

Maximal in $(\frac{1}{m}, \ldots, \frac{1}{m})$, minimal in $(1, 0, \ldots, 0), \ldots, (0, \ldots, 0, 1)$
(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 ($m = 2$)

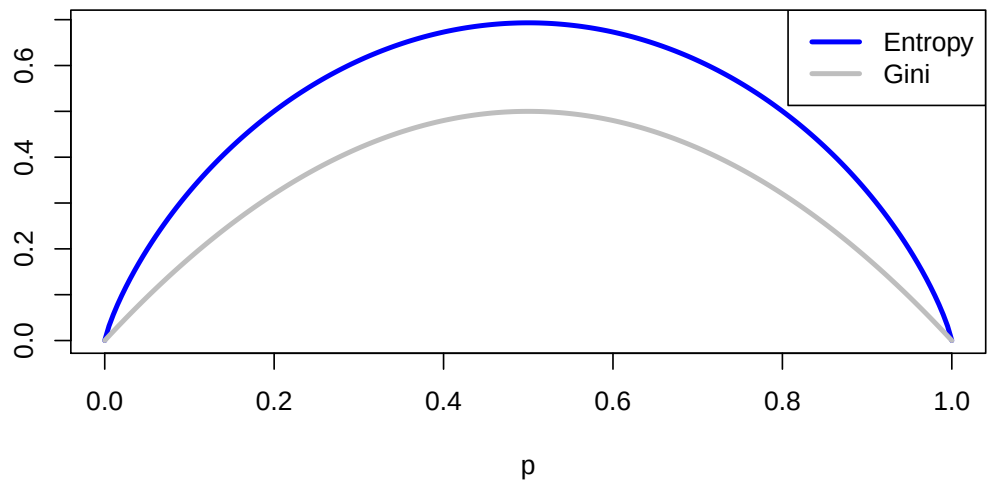
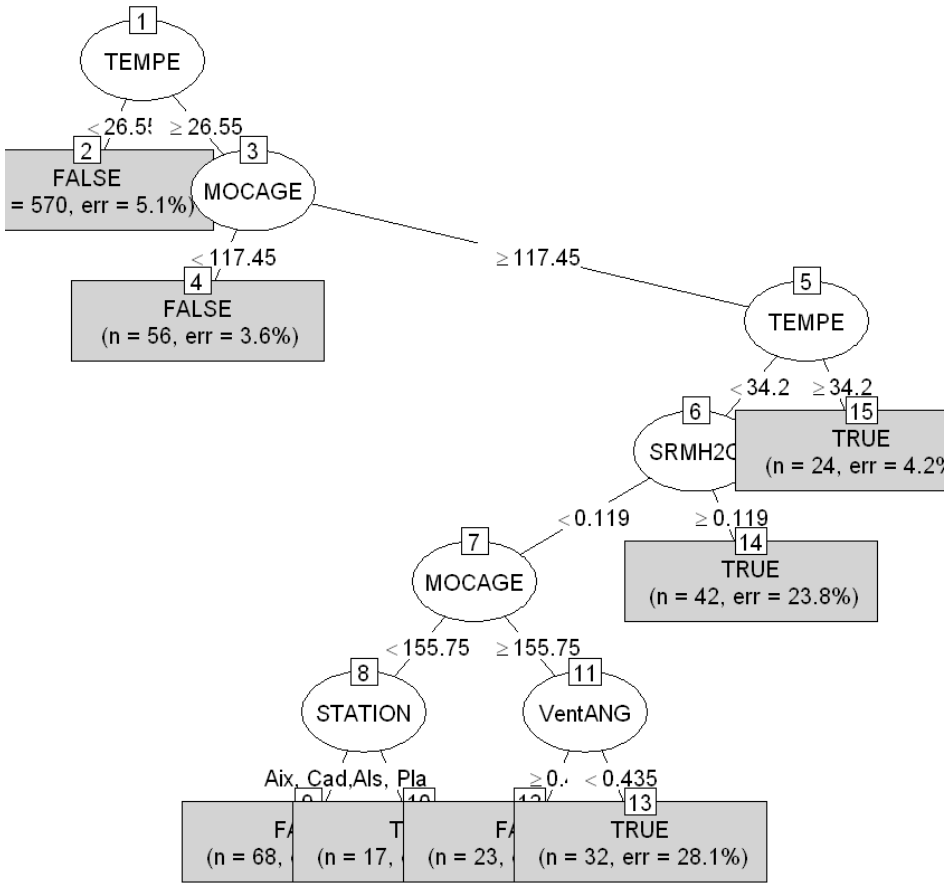


FIGURE – Heterogeneity criterions for classification. Both are minimal for $p = 0$ or $p = 1$, and maximal for $p = 1/2$.

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

Advantages

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

$\Longrightarrow$ 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

$\Longrightarrow$ Aggregation of trees : bagging, random forests

Outline

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

Introduction

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

$^{(\star)}$ *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 - Introductive example

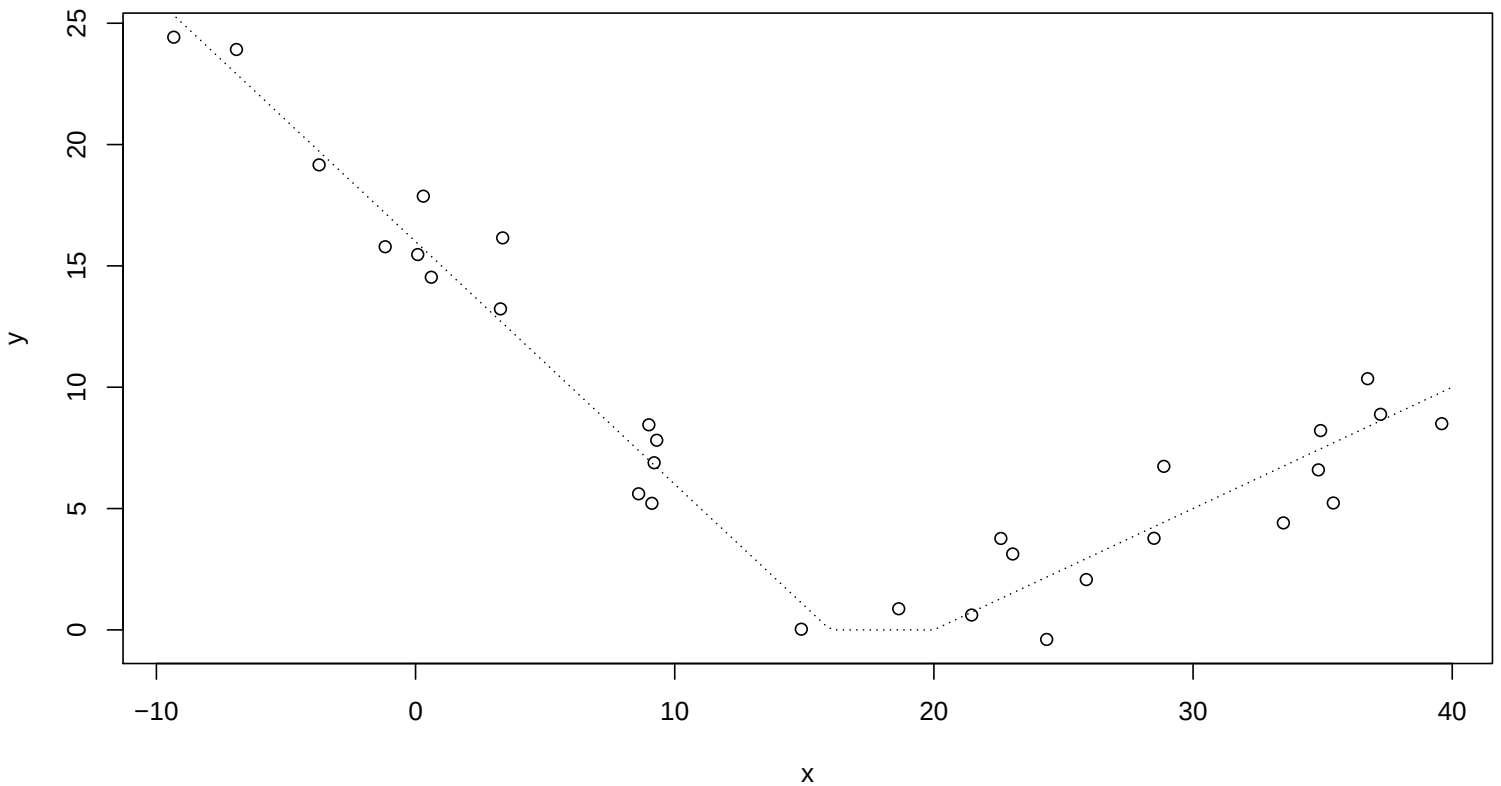


FIGURE – Original data

Bagging - Introductive example

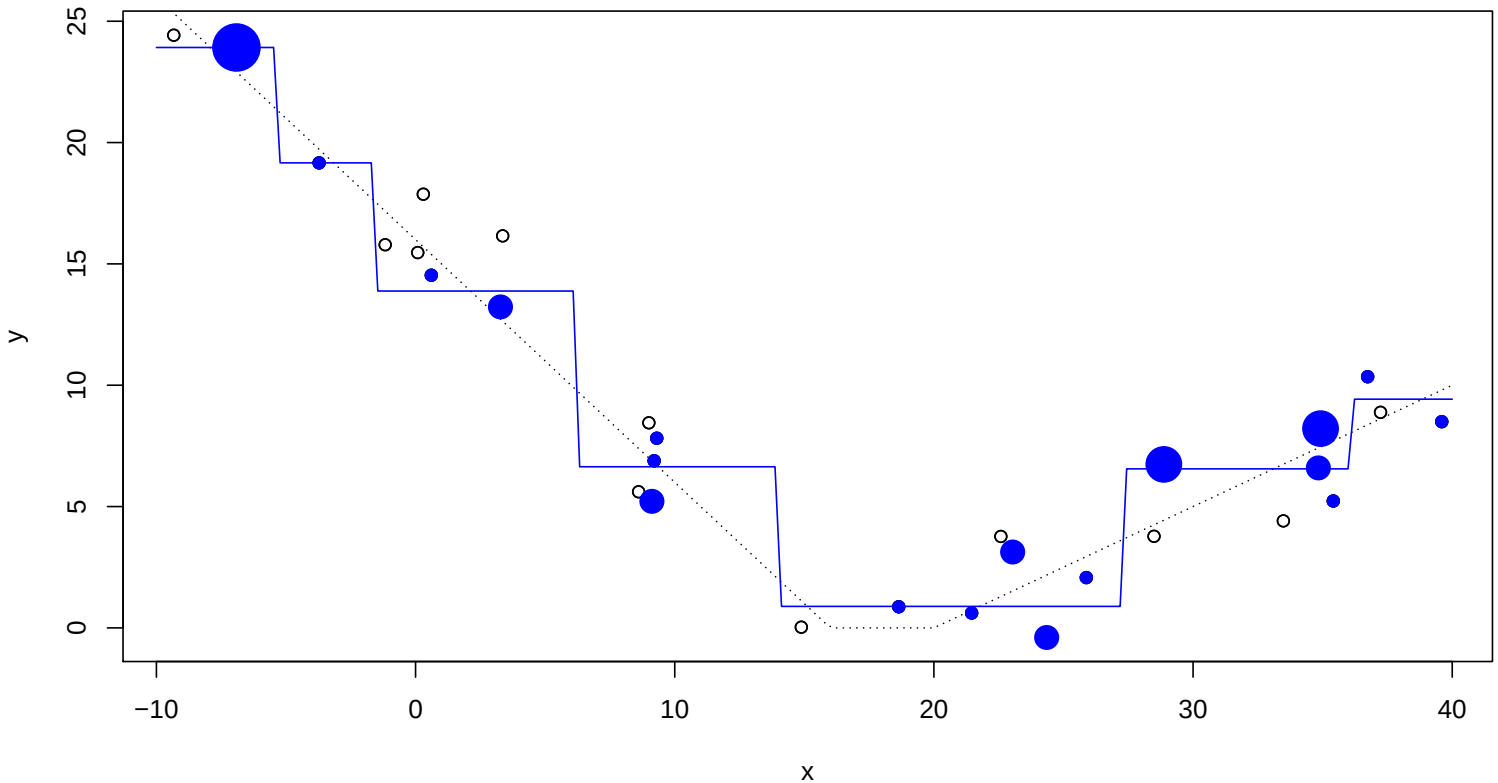


FIGURE – Bootstrap sample $n^o 1$ (in blue), and corresp. prediction with tree. The point size is proportional to the number of replicates.

Bagging - Introductive example

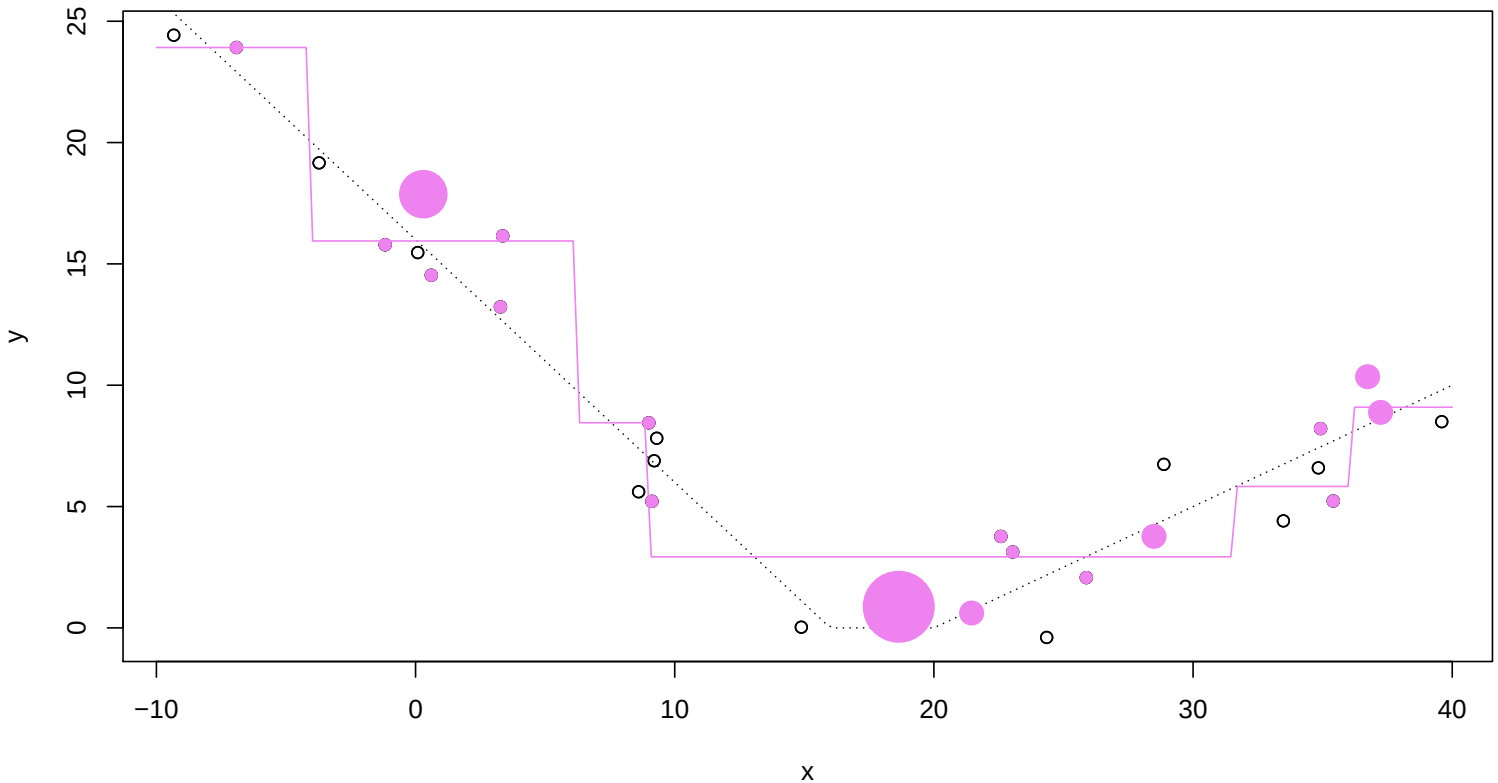


FIGURE – Bootstrap sample $n^o 2$ (in violet), and corresp. prediction with tree. The point size is proportional to the number of replicates.

Bagging - Introductive example

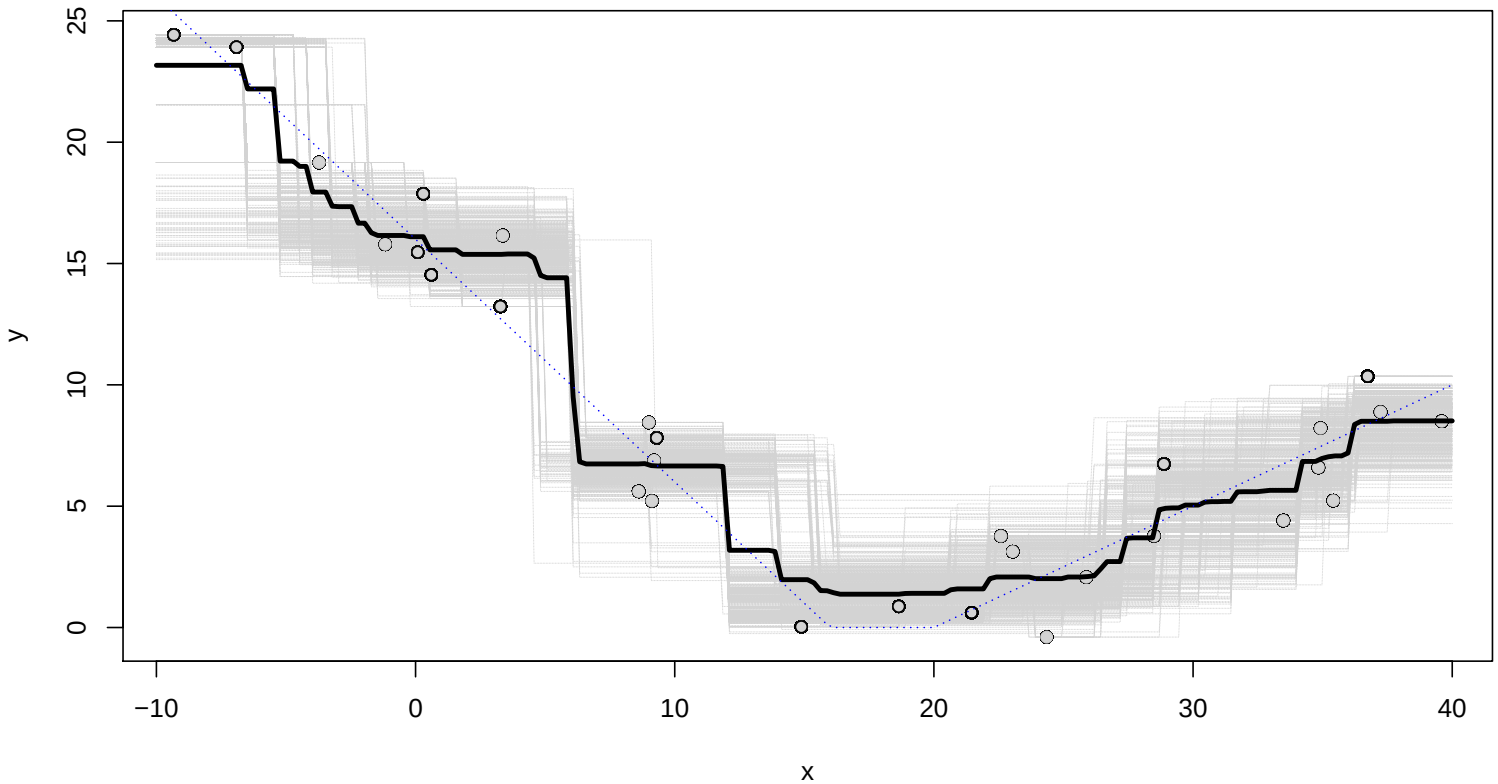


FIGURE – 500 bootstrap samples (grey), corresp. predictions with tree, and their average (bold line).

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 boostrap sample ?

Bagging - Out-Of-Bag data

Out-Of-Bag (OOB) data

For each bootstrap sample :

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

$$\mathbb{P}\left(z_{U_1^\star} \neq z_i, \ldots, z_{U_N^\star} \neq z_i\right) = \left(1 - \frac{1}{N}\right)^N \underset{N \to +\infty}{\longrightarrow} e^{-1} \approx 0.367$$

- 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

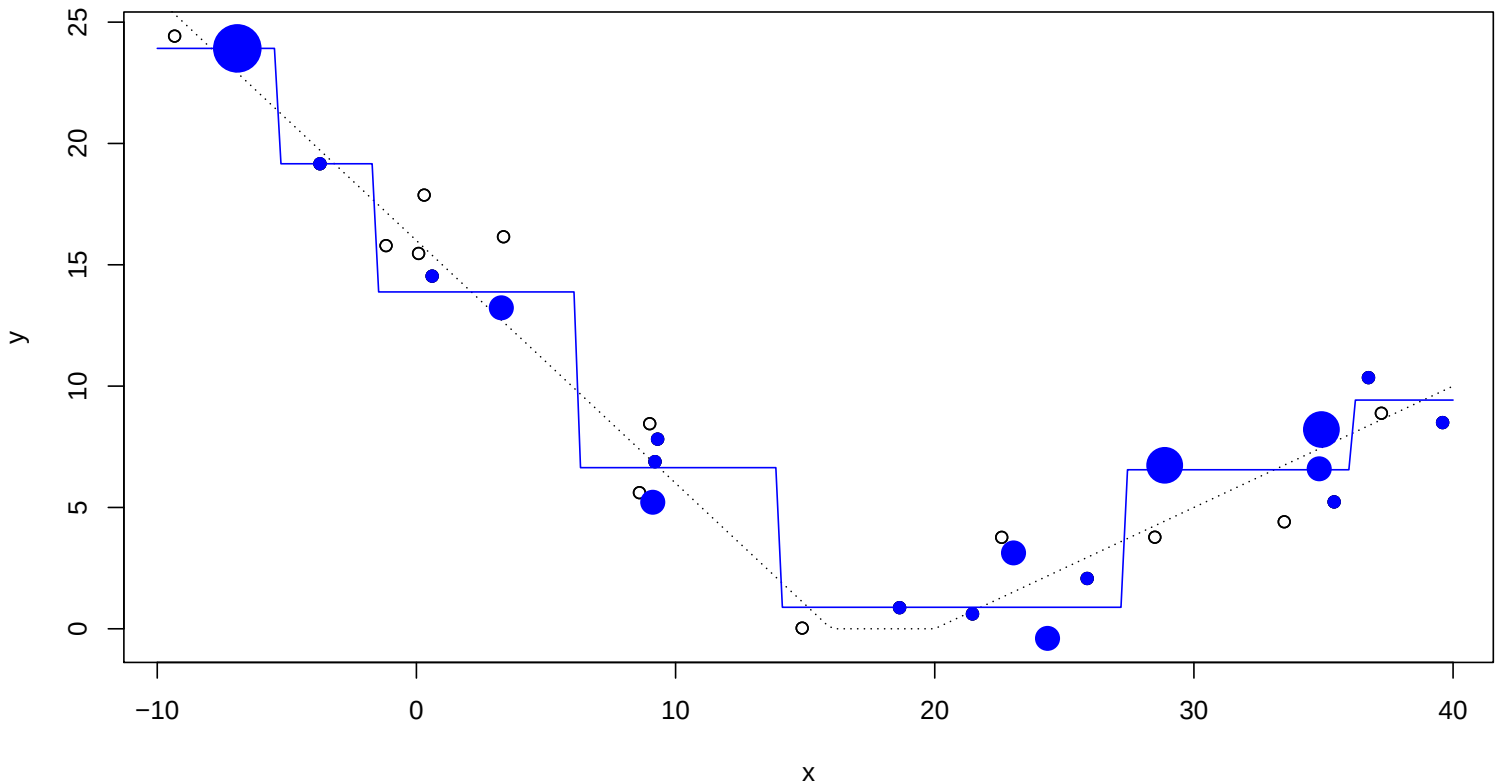


FIGURE – Residuals for the OOB bootstrap sample $n^o 1$ (red bars).

Bagging - Out-Of-Bag data

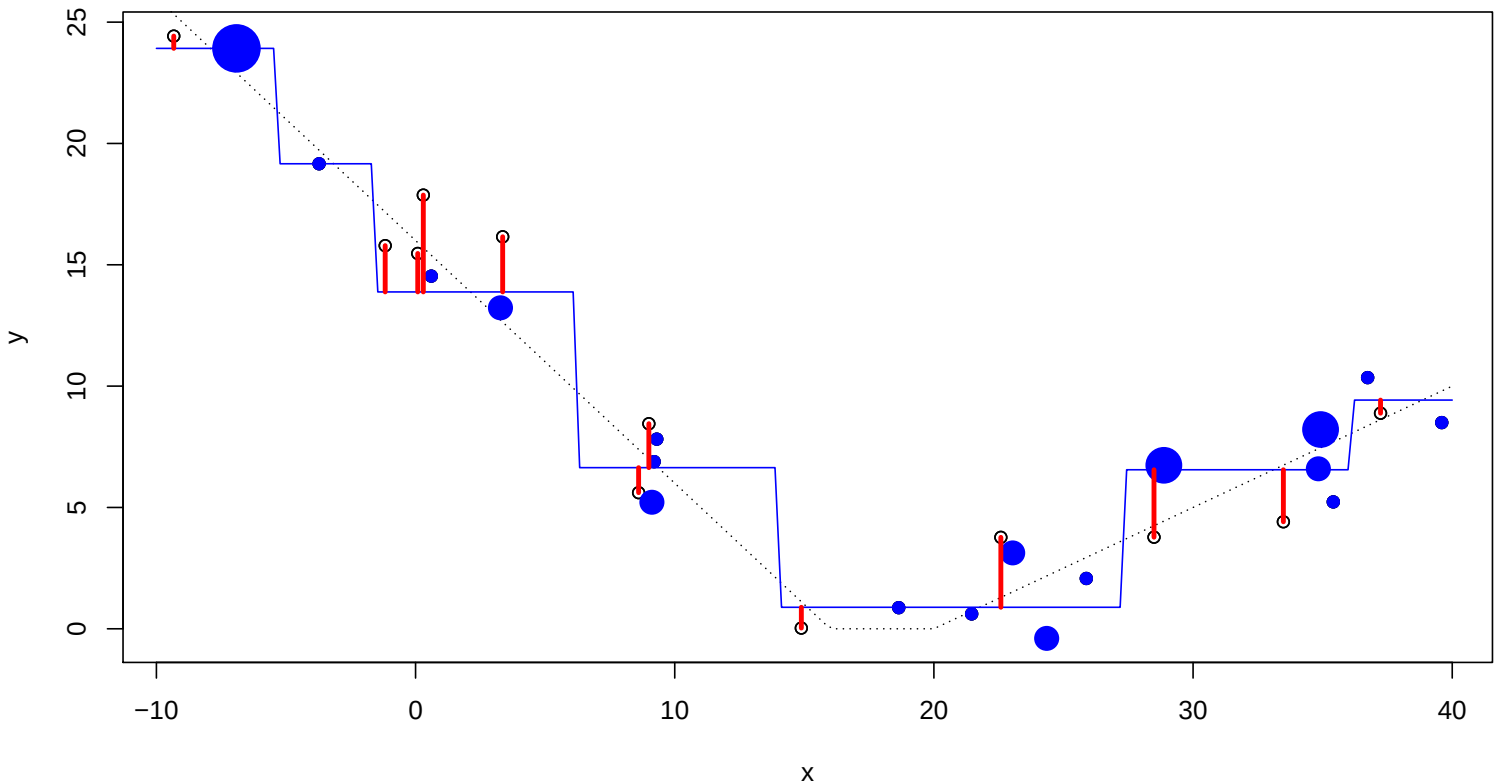


FIGURE – Residuals for the OOB bootstrap sample $n^o 1$ (red bars).

Bagging - Out-Of-Bag data

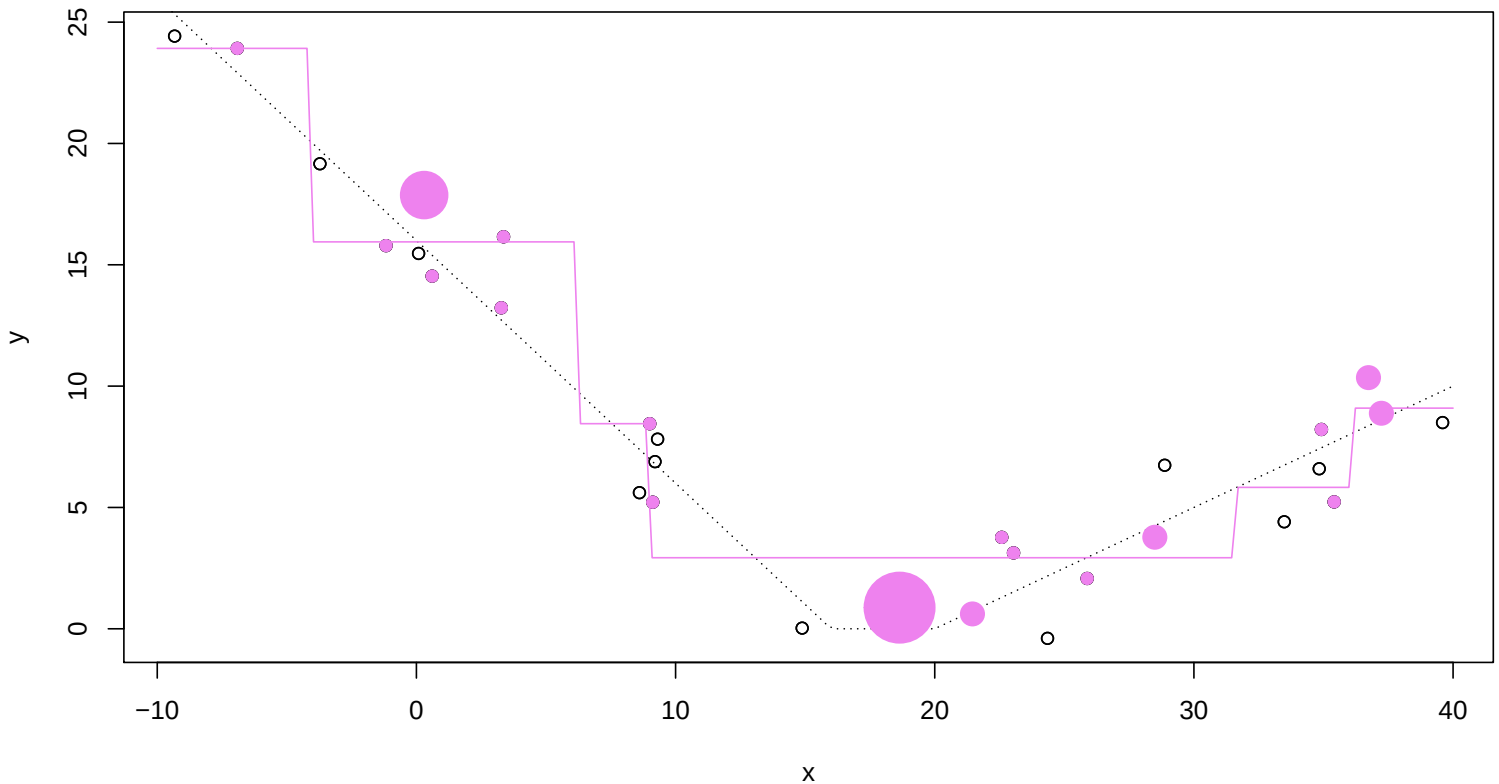


FIGURE – Residuals for the OOB bootstrap sample $n^o 2$ (red bars).

Bagging - Out-Of-Bag data

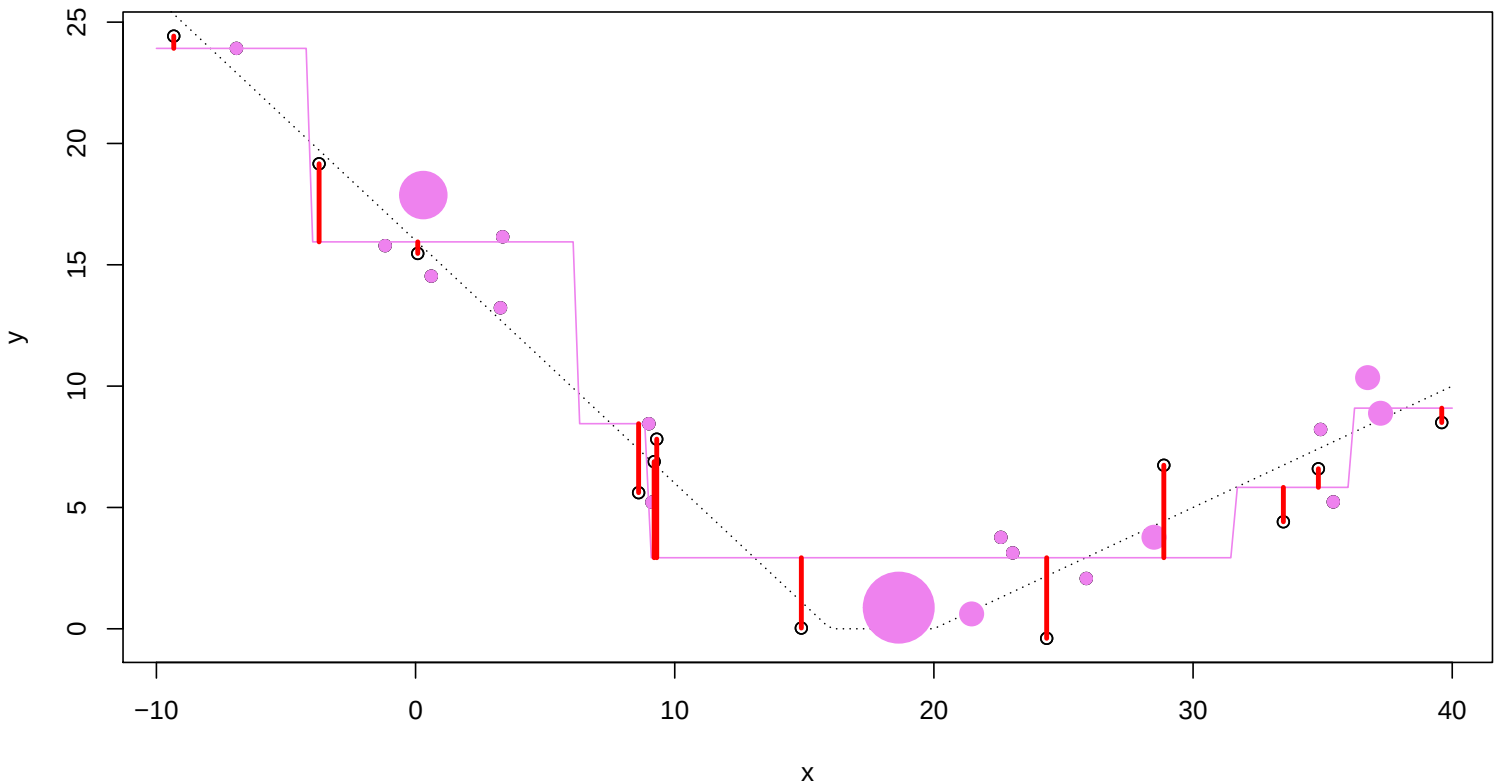


FIGURE – Residuals for the OOB bootstrap sample $n^o 2$ (red bars).

Bagging - Theory

Framework and notations

- Output : Y, a quantitative or qualitative variable to explain
- Inputs : $X^1, \ldots, X^p$, explanatory variables
- Model : $f(\mathbf{x})$, function of $\mathbf{x} = \{x^1, \ldots, x^p\} \in \mathbb{R}^p$
- Learning sample : $\mathbf{z} = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\}$, with distribution F
- A predictor : $\widehat{f}_{\mathbf{z}}$, associated to $\mathbf{z}$, with $f(.) = \mathbb{E}_F(\widehat{f}_{\mathbf{z}})$

- Bootstrap samples : $\{\mathbf{z}_b\}_{b=1,B}$
- Aggregated predictor :
  - Y quantitative : $\widehat{f}_B(.) = \frac{1}{B}\sum_{b=1}^{B} \widehat{f}_{\mathbf{z}_b}(.)$ (mean)
  - Y qualitative : $\widehat{f}_B(.) = \arg\max_j \text{card}\left\{b \mid \widehat{f}_{\mathbf{z}_b}(.) = j\right\}$ (majority vote)

Bagging - Theory

Variance reduction quantification

- The B boostrap samples are built on the same learning sample $\mathbf{z}$ $\Rightarrow$ the estimators $\widehat{f}_{\mathbf{z}_b}(\mathbf{x}_0)$ are not independent

- Regression case : If $\text{Corr}(\widehat{f}_{\mathbf{z}_b}(\mathbf{x}_0), \widehat{f}_{\mathbf{z}_{b'}}(\mathbf{x}_0)) = \rho(x_0)$,

$$\begin{aligned} \text{E}(\widehat{f}_B(\mathbf{x}_0)) &= f(\mathbf{x}_0) \\ \text{Var}(\widehat{f}_B(\mathbf{x}_0)) &= \rho(x_0)\text{Var}(\widehat{f}_b(\mathbf{x}_0)) + \underbrace{\frac{(1-\rho(x_0))}{B}\text{Var}(\widehat{f}_b(\mathbf{x}_0))}_{\longrightarrow 0 \text{ as } B\to\infty} \end{aligned}$$

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

Random forest - Principle

The three ingredients of random forest

- Variance reduction : by aggregating independent predictions
  - Aggregation : average (regression), majority vote (classification)
- Data resampling : get new data from themselves by resampling !
  - Caution : new data remain (slightly) dependent on the initial ones
- Variable resampling : reduces correlation between resampled data
  - The number of resampled variables must be tuned properly

$$\text{Random forest} = \underbrace{\text{data resampling} + \text{aggregation}}_{\text{bagging}} + \text{variable resampling}$$

Random forest

Algorithm

- Let $\mathbf{x}_0$ the point where we want to predict, $\mathbf{z}$ a learning sample
- For $b = 1$ to B, do :
  - Generate a bootstrap sample $\mathbf{z}_b^*$
  - Estimate a tree with randomization of the variables :
    At each node, resample $m < p$ variables to build the subdivision
- Aggregate predictors (average or majority vote)

Random forest

Variance reduction quantification

Consider the regression case. For a large number of boostrap samples,

$$\mathrm{Var}\left(\widehat{f}_B(\mathbf{x}_0)\right) \approx \underbrace{\rho(x_0)}_{\text{small when m small}} \times \underbrace{\mathrm{Var}\left(\widehat{f}_b(\mathbf{x}_0)\right)}_{\text{small when m large}}$$

$\Rightarrow$ Tradeoff required to choose m !

Random forest

Random forest : utilisation

- Pruning : tree with q leaves, or complete tree,
  - Reducing variance by computing the optimal tree is time-consuming
- Random selection of m predictors : default values
  - $m = \frac{p}{3}$ for regression
  - $m = \sqrt{p}$ for classification
- Choice of tuning parameters (including m) by cross-validation

Interpretation - Variable importance

How can we quantifiy the importance of a variable X_i in random forest ?

Decrease in heterogeneity

Average the decrease of heterogeneity when X_i is chosen as a split.

- Mean Decrease Accuracy
- Mean Decrease Gini

Permutation of variables

Compute the OOB error for the subsample of OOB data involving X_i. Compare with the OOB error when permuting at random the inputs (but keeping the output).

Random forest

To go further

- Prediction intervals with `ranger`
- Anomaly detection with `IsolationForest`
- Imputation of missing data with `missForest`
- Survival analysis with `survival forest`
- ...

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 MSE	- bag %Var(y)	Test MSE	set %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
LNO2        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

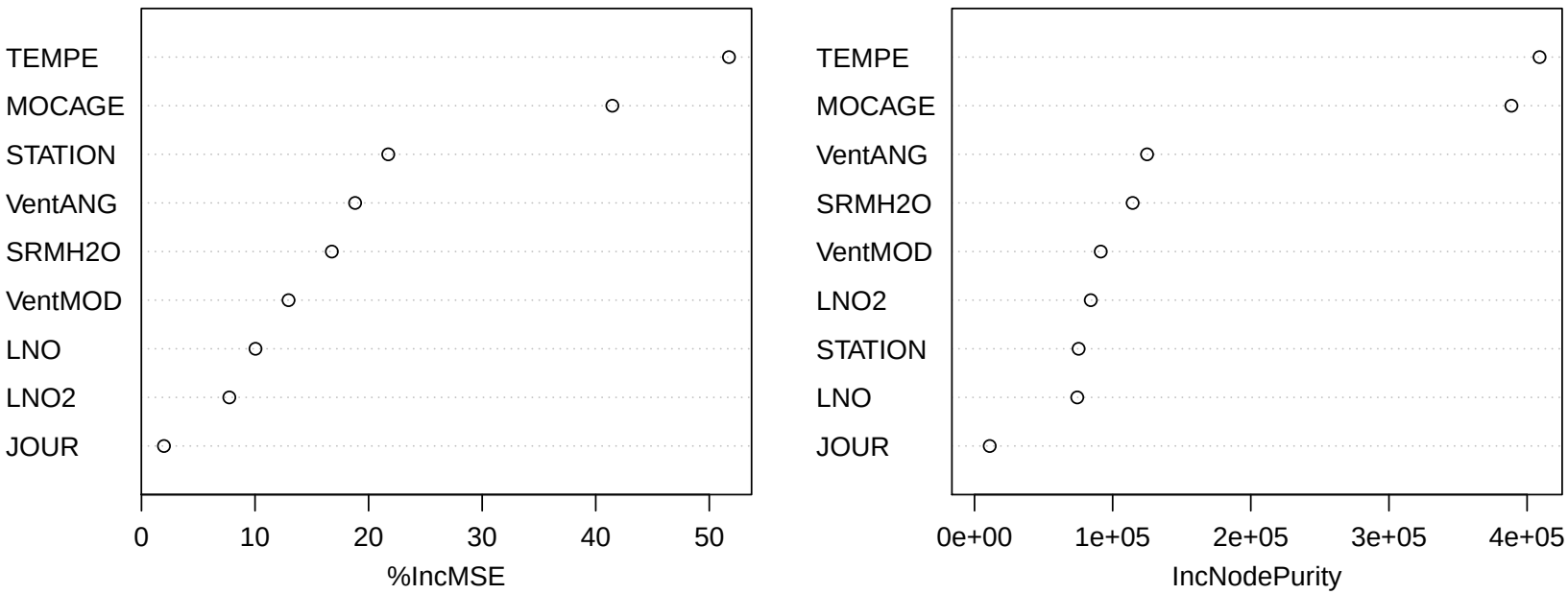


FIGURE – Variable importance plot, returned by the R function `importance`

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- Hastie, T. and Tibshirani, R. and Friedman, J, (2009), *The elements of statistical learning : data mining, inference, and prediction*, Springer.