Institut de Mathématiques de Toulouse, INSA Toulouse

Supervised Learning- Part II

Formation en machine Learning
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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

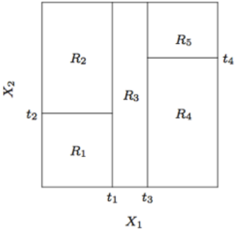
- Classification And Regression Trees (CART)
- Bagging, Random Forests

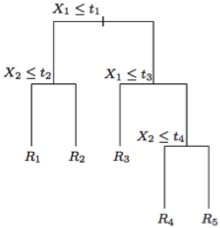
Classification And Regression Trees

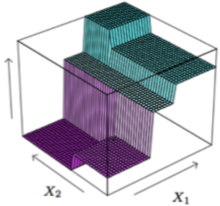
Introduction

- 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

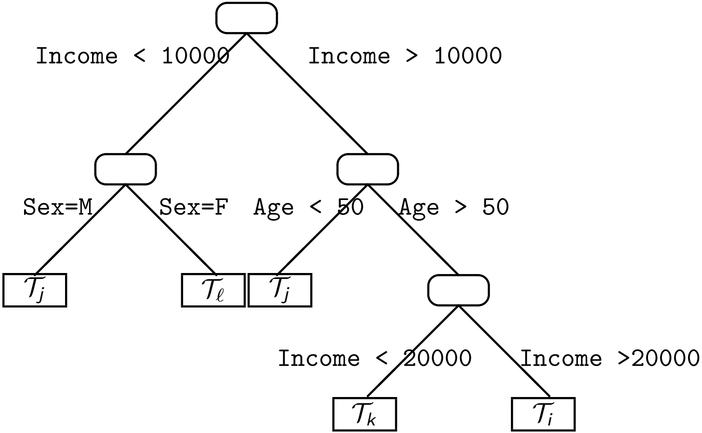






Source : Hastie, Tibshirani, Friedman (2019), "The elements of statistical learning"

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

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

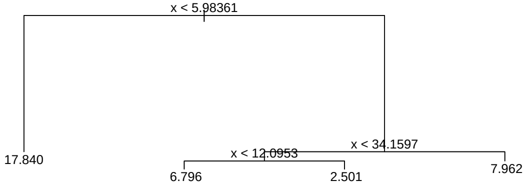
Find (j,t) in order to minimize the intra-class variance

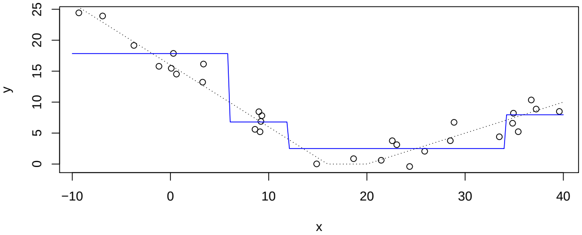
$$J(j,t) = D_{\kappa_L(t,j)} + D_{\kappa_R(t,j)},$$

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 ($m = 2$)

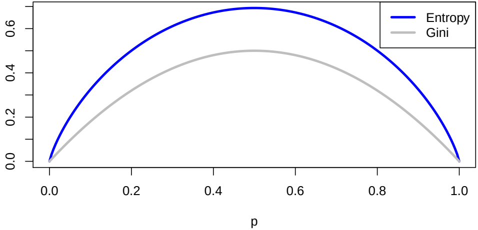
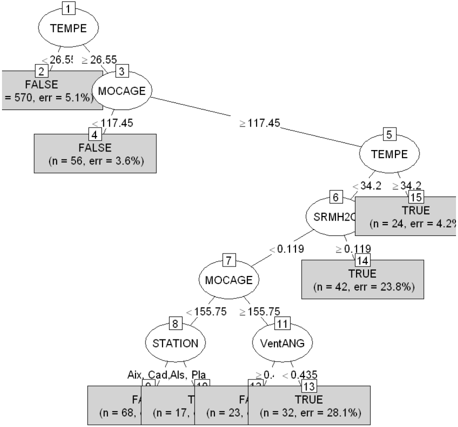


FIGURE – Heterogeneity criterions for classification. Both are minimal for $p = 0$ or $p = 1$, and maximal for $p = 1/2$.

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

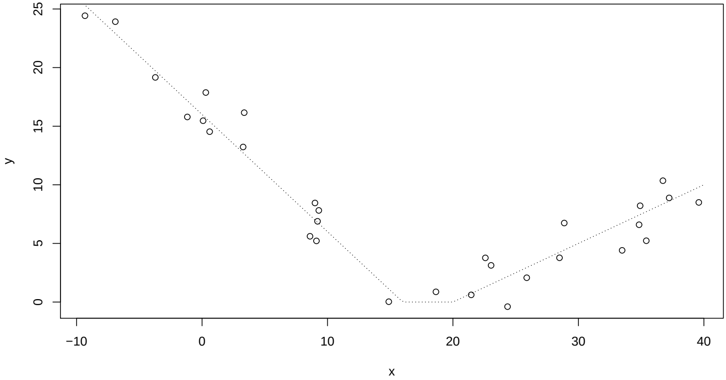


FIGURE – Original data

Bagging - Introductive example

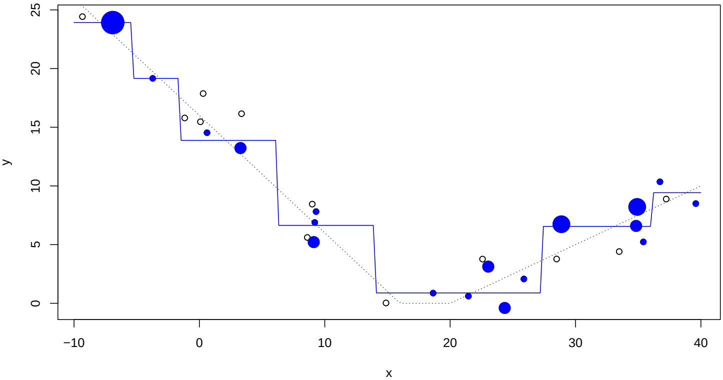


FIGURE – Bootstrap sample n^o1 (in blue), and corresp. prediction with tree. The point size is proportional to the number of replicates.

Bagging - Introductive example

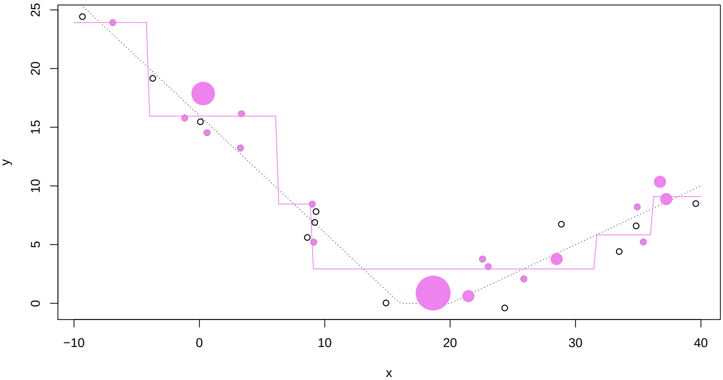


FIGURE – Bootstrap sample $n^o 2$ (in violet), and corresp. prediction with tree. The point size is proportional to the number of replicates.

Bagging - Introductive example

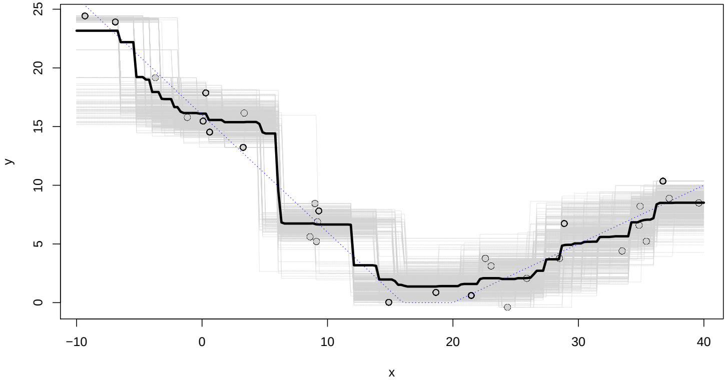


FIGURE – 500 bootstrap samples (grey), corresp. predictions with tree, and their average (bold line).

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

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

- 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

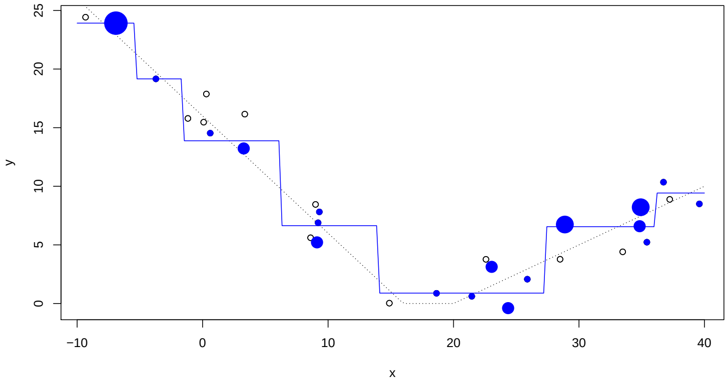


FIGURE – Residuals for the OOB bootstrap sample $n^o 1$ (red bars).

Bagging - Out-Of-Bag data

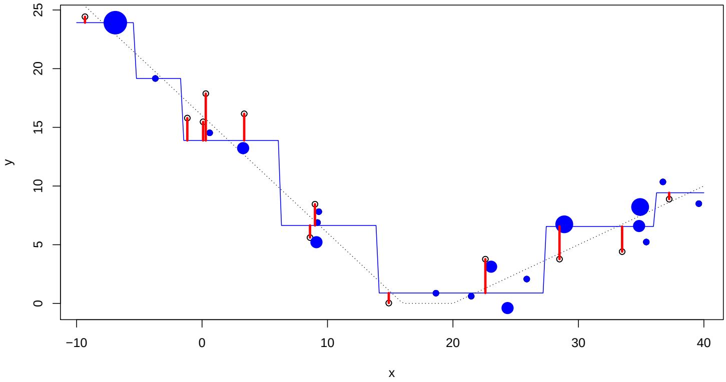


FIGURE – Residuals for the OOB bootstrap sample n^o1 (red bars).

Bagging - Out-Of-Bag data

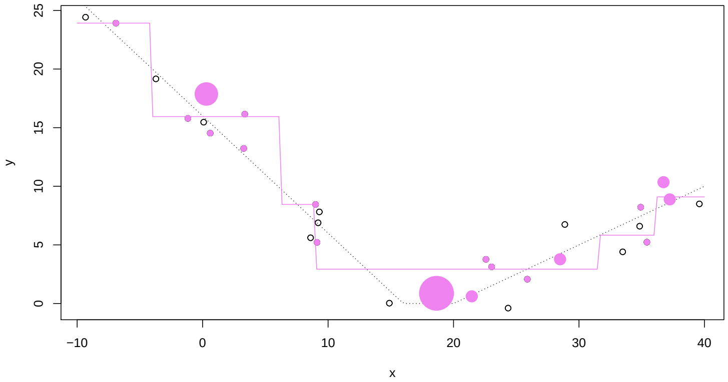


FIGURE – Residuals for the OOB bootstrap sample $n^o 2$ (red bars).

Bagging - Out-Of-Bag data

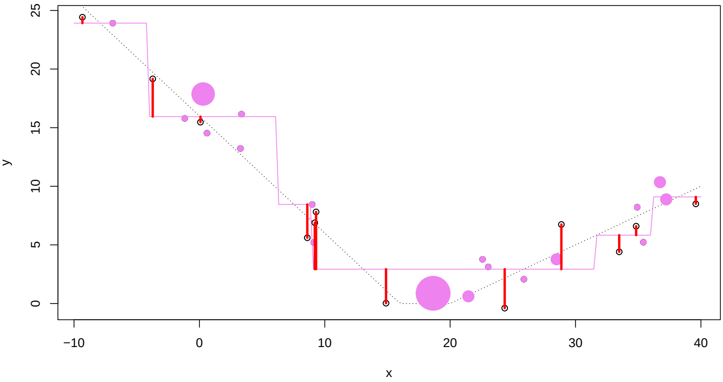


FIGURE – Residuals for the OOB bootstrap sample n^o2 (red bars).

Bagging - Theory

Framework and notations

- Output : Y, a quantitative or qualitative variable to explain
- Inputs : $X^1, \dots, X^p$, explanatory variables
- Model : $f(\mathbf{x})$, function of $\mathbf{x} = \{x^1, \dots, x^p\} \in \mathbb{R}^p$
- Learning sample : $\mathbf{z} = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}$, 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 $\mathrm{Corr}(\widehat{f}_{\mathbf{z}_b}(\mathbf{x}_0), \widehat{f}_{\mathbf{z}_{b'}}(\mathbf{x}_0)) = \rho(x_0)$,

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

- 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`
- ...

References

- L. Breiman, J. Friedman, C. J. Stone, R. A. Olshen (1984). *Classification and regression trees*. Chapman et Hall. CRC Press, Boca Raton.
- Giraud C. (2015) *Introduction to High-Dimensional Statistics* Vol. 139 of Monographs on Statistics and Applied Probability. CRC Press, Boca Raton, FL.
- Hastie, T. and Tibshirani, R. and Friedman, J, (2009), *The elements of statistical learning : data mining, inference, and prediction*, Springer.