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Supervised Learning- Part I

Machine Learning for Data Science
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Introduction

In the framework of **Supervised learning**, we have a **Learning sample** composed with observation data of the type **input/output** :

$$d_1^n = \{(\boldsymbol{x}_1, y_1), \ldots, (\boldsymbol{x}_n, y_n)\}$$

with $\boldsymbol{x}_i \in \mathbb{R}^p$, $y_i \in \mathcal{Y}$ for $i = 1 \ldots n$.

Objectives : From the learning sample, we want to

- **Estimate** the link between the input vector $\boldsymbol{x}$ (explanary variables) and the output y (variable to explain) :

$$y = f(x^1, x^2, \ldots, x^p)$$

- **Predict** the output y associated to a new entry $\boldsymbol{x}$,
- **Select** the important explanatory variables among $x^1, \ldots, x^p$.

quantitative output	qualitative output
$\mathcal{Y} \subset \mathbb{R}^p$	$\mathcal{Y}$ finite
$\downarrow$	$\downarrow$
regression	**classification**
	form recognition

- In this course, we consider supervised learning for real regression ($\mathcal{Y} \subset \mathbb{R}$) and classification ($\mathcal{Y}$ finite).
- The explanatory variables $X^1, \ldots X^p$ can be qualitatives or quantitatives

Choice of the method

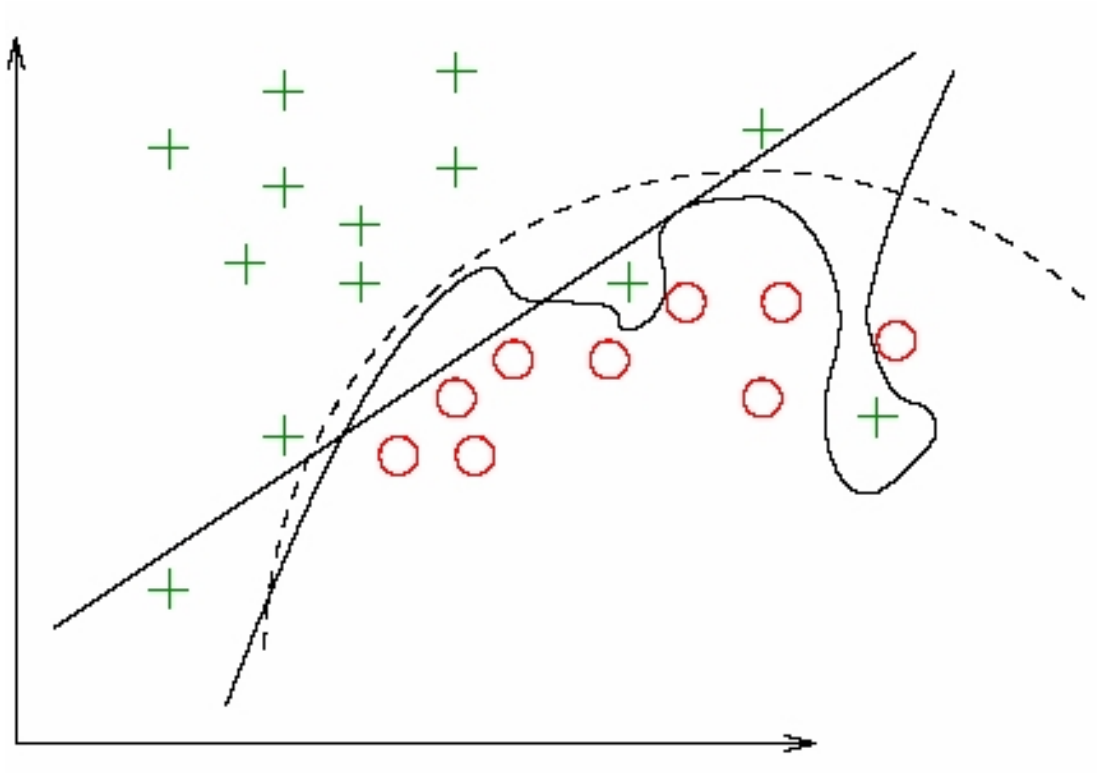
- Huge Bibliography
- No universally best method (several methods can be aggregated)
- Adaptation of the method to the data
- Quality : prediction error

Choice of the model

- Importance of the principle of parcimony : "it is necessary to determine a model that provides an adequate representation of the data, with as few parameters as possible".
- Bias-variance trade-off
- Robustness and prevision

Model selection strategies

- Control of the complexity
- Model choice : selection *vs.* regularisation
  - Variable Selection, selection of the number of parameters
  - Selection and penalisation with $||.||_{l_1}$ penalties
  - Regularisation et penalisation en $||.||_{l_2}$ (*ridge*, *shrinkage*)



Supervised Classification : *Complexity of the models*

First step : *Data munging*

1. Extraction with or without survey
2. Exploration, visualization
3. Cleaning, transformation of the data, choice of a basis (splines, Fourier, wavelets)...
4. New variables (*features*)
5. Management of missing data

Second step : *Learning*

1. Random Partition of the sample : learning, (validation), test
2. **For** each method that we consider :
   - Learning (estimation) depending on θ (complexity)
   - Optimization of θ : validation set or cross-validation with the learning set
3. Comparison of the methods : prediction error on the test sample
4. Eventual Iteration (*Monte Carlo*)
5. Choice of the method (prevision *vs.* interpretability).
6. Estimation of the selected model with all the sample, exploitation

Possibly : Aggregation of several models

Question : Where to bring the effort ?

- *Data munging*
- Selection of the methods to compare
- Optimization of the parameters
- Optimal Combination of the models

Depending on :

- Goal (allotted time)
- Regularity of the underlying problem
- Structure and properties of the data

Methods studied in this course :

Part I

- Linear model, model selection, variable selection, Ridge regression, Lasso.
- Logistic regression
- Support Vector Machine

Part II

- k Nearest Neighbours
- Classification And Regression Trees (CART)
- Bagging, Random Forests, Boosting
- Neural networks, Introduction to deep learning

Part I-1 :

- Linear model, model selection, variable selection, Ridge regression, Lasso.
  - Linear model
  - Least square estimation
  - Confidence intervals and prediction intervals
  - Testing a submodel
  - Determination coefficient, Diagnosis on the residuals
  - Model selection, variable selection : Ridge, Lasso

The Linear model

We have a quantitative variable Y *to explain* which is related with p variables $\boldsymbol{X}^1, \ldots, \boldsymbol{X}^p$ called *explanatory variables*.
The data are obtained from the observation of a n sample of $\mathbb{R}^{(p+1)}$ vectors :

$$(x_i^1, \ldots, x_i^j, \ldots, x_i^p, y_i) \quad i = 1, \ldots, n.$$

We assume in a first time that $n > p + 1$.
In *the linear model*, the regression function $\mathbb{E}(\mathbf{Y}/\mathbf{X})$ is linear in the input variables $\boldsymbol{X}^1, \ldots, \boldsymbol{X}^p$.
If we assume that the regressors are deterministic, this means that $\mathbb{E}(\mathbf{Y})$ is linear in the explanatory variables $\{\mathbf{1}, \boldsymbol{X}^1, \ldots, \boldsymbol{X}^p\}$
where $\mathbf{1}$ denotes the $\mathbb{R}^n$-vector with all components equal to 1.

The Linear model

The linear model is defined by :

$$Y_i = \beta_0 + \beta_1 X_i^1 + \beta_2 X_i^2 + \cdots + \beta_p X_i^p + \varepsilon_i \quad i = 1, 2, \ldots, n$$

with the following assumptions :

1. The random variables ε_i are independent and identically distributed (i.i.d.) ; $\mathbb{E}(\varepsilon_i) = 0$, $Var(\varepsilon_i) = \sigma^2$.
2. The regressors $\boldsymbol{X}^j$ are assumed to be deterministic **or** the errors ε are independent of $(\boldsymbol{X}^1, \ldots, \boldsymbol{X}^p)$. In this case, we have :

   $E(\mathbf{Y}|\boldsymbol{X}^1, \ldots, \boldsymbol{X}^p) = \beta_0 + \beta_1 \boldsymbol{X}^1 + \beta_2 \boldsymbol{X}^2 + \cdots + \beta_p \boldsymbol{X}^p$ and $Var(\mathbf{Y}|\boldsymbol{X}^1, \ldots, \boldsymbol{X}^p) = \sigma^2$.
3. The unknown parameters $\beta_0, \ldots, \beta_p$ are supposed to be constant.
4. It is sometimes assumed that the errors are Gaussian : $\boldsymbol{\varepsilon} = [\varepsilon_1 \cdots \varepsilon_n]' \sim \mathcal{N}_n(0, \sigma^2 \mathbf{I_n})$. The variables ε_i are then i.i.d. $\mathcal{N}(0, \sigma^2)$.

The Linear model

- The explanatory variables are given in the matrix $\mathbf{X}(n \times (p+1))$.
- The regressors $\boldsymbol{X}^j$ can be quantitative variables, nonlinear transformation of quantitative variables (such as log, exp, square ..), interaction between $\boldsymbol{X}^j = \boldsymbol{X}^k.\boldsymbol{X}^l$.
- They can also correspond to qualitative variables : in this case the variables $\boldsymbol{X}^j$ are indicator variables coding the different levels of a factor.
- The response variable is given in the vector $\mathbf{Y}$.
- We set $\boldsymbol{\beta} = [\beta_0 \beta_1 \cdots \beta_p]'$, which leads to the matricial formulation of the linear model :

$$\mathbf{Y} = \mathbf{X}\boldsymbol{\beta} + \boldsymbol{\varepsilon}.$$

Least square estimation

- The unknown parameters of the model are the vector β and σ^2.
- β is estimated by minimizing the residuals sum of square.
- We minimise with respect to the parameter $\beta \in \mathbb{R}^{p+1}$ the criterion :

$$\begin{aligned}\sum_{i=1}^{n}(Y_i - \beta_0 - \beta_1 X_i^1 - \cdots - \beta_p X_i^p)^2 &= \|\mathbf{Y} - \mathbf{X}\beta\|^2 \\ &= (\mathbf{Y} - \mathbf{X}\beta)'(\mathbf{Y} - \mathbf{X}\beta) \\ &= \mathbf{Y}'\mathbf{Y} - 2\beta'\mathbf{X}'\mathbf{Y} + \beta'\mathbf{X}'\mathbf{X}\beta.\end{aligned}$$

Lemma

Let $h : \beta \mapsto \beta' A \beta$ where A is a symmetric matrix.
Then $\bigtriangledown h(\beta) = 2A\beta$.
Let $g : \beta \mapsto \beta' z = z'\beta = \langle z, \beta \rangle$ where $z \in \mathbb{R}^p$.
Then $\bigtriangledown g(\beta) = z$.

Least square estimation

- Derivating the last equation, we obtain the *normal equations* :

$$2(\mathbf{X}'\mathbf{Y} - \mathbf{X}'\mathbf{X}\beta) = 0$$

- The solution is a minimiser of the criterion since the Hessian $2\mathbf{X}'\mathbf{X}$ is positive semi definite (the criterion is convex) .

Least square estimation

We make the additional assumption that the matrix $\mathbf{X}'\mathbf{X}$ is invertible. Under this assumption, the estimation of β is given by :

$$\widehat{\beta} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y}$$

and the predicted values of $\mathbf{Y}$ are :

$$\widehat{\mathbf{Y}} = \mathbf{X}\widehat{\beta} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} = \mathbf{H}\mathbf{Y}$$

where $\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$ is called the "*hat matrix*".

Geometrically, it corresponds to the matrix of orthogonal projection in $\mathbb{R}^n$ onto the subspace Vect($\mathbf{X}$) generated by the columns of $\mathbf{X}$.

Least square estimation

- If $\mathbf{X}'\mathbf{X}$ is not invertible, the application $\beta \mapsto \mathbf{X}\beta$ is not injective, hence the model is not identifiable and β is not uniquely defined.
- In this case, the predicted values $\widehat{\mathbf{Y}}$ are still defined as the projection of $\mathbf{Y}$ onto the space generated by the columns of $\mathbf{X}$.
- In practice, if $\mathbf{X}'\mathbf{X}$ is not invertible (which is necessarily the case in high dimension when $p > n$), we have to remove variables from the model or to consider other approches to reduce the dimension (*Ridge*, Lasso, PLS ...).

Least square estimation

- We define the vector of residuals as :

$$\mathbf{e} = \mathbf{Y} - \widehat{\mathbf{Y}} = \mathbf{Y} - \mathbf{X}\widehat{\beta} = (\mathbf{I} - \mathbf{H})\mathbf{Y}$$

- This is the orthogonal projection of $\mathbf{Y}$ onto the subspace $\text{Vect}(\mathbf{X})^{\perp}$ in $\mathbb{R}^n$.
- The variance σ^2 is estimated by

$$\widehat{\sigma}^2 = \frac{\|\mathbf{e}\|^2}{n-p-1} = \frac{\left\|\mathbf{Y} - \mathbf{X}\hat{\beta}\right\|^2}{n-p-1}.$$

Properties of the least square estimator

Theorem

— *Assuming that*

$$\mathbf{Y} = \mathbf{X}\beta + \varepsilon$$

with $\varepsilon \sim \mathcal{N}_n(0, \sigma^2 \mathbf{I_n})$, *we obtain that* $\widehat{\beta}$ *is a Gaussian vector :*

$$\widehat{\beta} \sim \mathcal{N}_{p+1}(\beta, \sigma^2 (X'X)^{-1}).$$

In particular, the components of $\widehat{\beta}$ *are Gaussian variables :*

$$\widehat{\beta}_j \sim \mathcal{N}(\beta_j, \sigma^2 (X'X)^{-1}_{j,j}).$$

$$\hat{\sigma}^2 \sim \frac{\sigma^2}{n-(p+1)} \chi^2_{(n-(p+1))}$$

and is independent of $\hat{\beta}$.

Properties of the least square estimator

$\widehat{\beta}$ is a linear unbiased estimator of β.
The next theorem, called the *Gauss-Markov* theorem asserts optimality properties.

Theorem

— *Let* $\mathbf{A}$ *and* $\mathbf{B}$ *two matrices.*
We say that $\mathbf{A} \preceq \mathbf{B}$ *if* $\mathbf{B} - \mathbf{A}$ *is positive semi-definite.*
Let $\widetilde{\beta}$ *a linear unbiased estimator of* β*, with variance-covariance matrix* $\widetilde{\mathbf{V}}$.
Then, $\sigma^2(\mathbf{X}'\mathbf{X})^{-1} \preceq \widetilde{\mathbf{V}}$.

In the next section, we will see that it can be preferable to consider biased estimator, if they have a smaller variance than $\widehat{\beta}$, to reduce the quadratic risk.
This will be the case for the Ridge, Lasso, PCR, or PLS regression.

Confidence intervals

One can easily deduce from the Theorem that

$$\frac{\widehat{\beta}_j - \beta_j}{\sqrt{\hat{\sigma}^2 (X'X)^{-1}_{i,i}}} \sim \mathcal{T}_{(n-(p+1))}.$$

This allows to build confidence intervals and tests of significance for the parameters β_j.
The following interval is a 0.95 **confidence interval for** β_j :

$$\left[\widehat{\beta}_j - t_{n-(p+1),0.975}\sqrt{\hat{\sigma}^2 (X'X)^{-1}_{j,j}}, \widehat{\beta}_j + t_{n-(p+1),0.975}\sqrt{\hat{\sigma}^2 (X'X)^{-1}_{j,j}}\right].$$

In order to test $H_0 : \beta_j = 0$ contre $H_1 : \beta_j \neq 0$, we reject the null hypothesis at the level 5% if 0 does not belong to the previous confidence interval.

Prediction

As mentioned above, the vector of predicted values is

$$\widehat{\mathbf{Y}} = \mathbf{X}\widehat{\beta} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\mathbf{Y} = \mathbf{H}\mathbf{Y}.$$

Based on the n previous observations, we may be interested with the prediction of the response of the model for a new point $\mathbf{X_0}' = (1, {X_0}^1, \ldots, {X_0}^p)$:

$$Y_0 = \beta_0 + \beta_1 X_0^1 + \beta_2 X_0^2 + \ldots + \beta_p X_0^p + \varepsilon_0,$$

where $\varepsilon_0 \sim \mathcal{N}(0, \sigma^2)$.
The predicted value is

$$\widehat{Y}_0 = \widehat{\beta}_0 + \widehat{\beta}_1 {X_0}^1 + \ldots \widehat{\beta}_p {X_0}^p = \mathbf{X_0}'\widehat{\beta}.$$

Prediction

- We derive from Theorem 1 that

$$\mathbb{E}(\widehat{Y}_0) = \mathbf{X_0}'\beta = \beta_0 + \beta_1 X_0^1 + \beta_2 X_0^2 + \ldots + \beta_p X_0^p$$

and that $\widehat{Y}_0 \sim \mathcal{N}(\mathbf{X_0}'\beta, \sigma^2 \mathbf{X_0}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X_0})$. Let $t = t_{n-(p+1),0.975}$.

- **Confidence interval for the mean response $\mathbf{X_0}'\beta$** at the new observation point $\mathbf{X_0}$:

$$\left[\mathbf{X_0}'\widehat{\beta} - t\hat{\sigma}\sqrt{\mathbf{X_0}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X_0}}, \mathbf{X_0}'\widehat{\beta} + t\hat{\sigma}\sqrt{\mathbf{X_0}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X_0}}\right].$$

- **Prediction interval for the response Y_0** at the new observation point $\mathbf{X_0}$ is :

$$\left[\mathbf{X_0}'\widehat{\beta} - t\hat{\sigma}\sqrt{1 + \mathbf{X_0}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X_0}}, \mathbf{X_0}'\widehat{\beta} + t\hat{\sigma}\sqrt{1 + \mathbf{X_0}'(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X_0}}\right].$$

Example

We consider the **Ozone data set** .
The data frame has 1041 observations of the following components :

JOUR	type of the day ; public holiday(1) or not (0)
O3obs	Ozone concentration observed the next day at 17h., generally the maximum of the day
MOCAGE	Prediction of this pollution obtained by a deterministic model of fluid mechanics
TEMPE	Temperature forecast by MétéoFrance for the next day 17h
RMH2O	Moisture ratio
NO2	Nitrogen dioxide concentration
NO	Concentration of nitric oxide
STATION	Location of the observation : Aix-en-Provence, Rambouillet, Munchhausen, Cadarache and Plan de Cuques
VentMOD	Wind force
VentANG	Orientation of the wind.

- We denote by Y the variable (**O3obs**) to explain.
- We set $X^1, \ldots X^p$ for the explanatory variables (**MOCAGE** , **TEMPE**, **JOUR** ..). The variables are quantitative (**MOCAGE** , **TEMPE** , ...), or qualitative (**JOUR**, **STATION**).
- We consider the linear model :

$$Y_i = \beta_0 + \beta_1 X_i^1 + \beta_2 X_i^2 + \ldots + \beta_p X_i^p + \varepsilon_i, \ 1 \leq i \leq n,$$

- For the qualitative variables, we consider indicator functions of the different levels of the factor, and introduce some constraints for identifiability. By default, in R, the smallest value of the factor are set in the reference.
  This is an analysis of covariance model (mixing quantitative and qualitative variables).

We consider here a simple linear regression model with the single variable $X =$ **MOCAGE**

$$Y_i = \beta_0 + \beta_1 X_i + \varepsilon_i, \ \ i = 1, \ldots, n.$$

For the least square estimation, we obtain the following results :

Coefficients	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	37.78887	3.42998	11.02	<2e-16 ***
MOCAGE	0.61006	0.02573	23.71	<2e-16 ***

Residual standard error : 33.04 on 1039 degrees of freedom

Multiple R-squared : 0.3511, Adjusted R-squared : 0.3505

F-statistic : 562.1 on 1 and 1039 DF, p-value : $<$ 2.2e-16

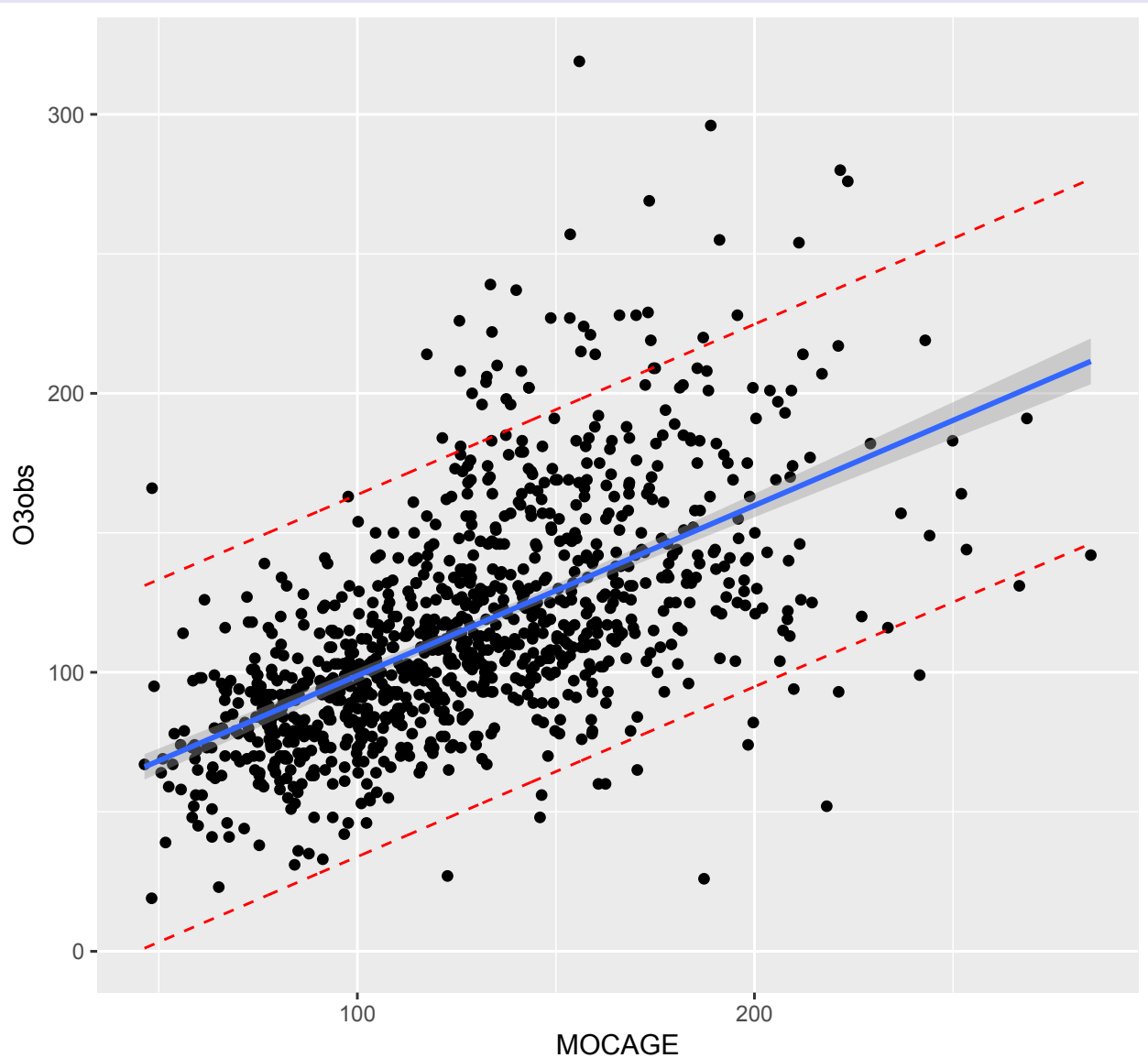


FIGURE: Simple linear regression model : confidence and prediction intervals

We consider here a linear regression model with all the variables :

$$Y_i = \beta_0 + \beta_1 X_i^{(1)} + \ldots + \beta_p X_i^{(p)} + \varepsilon_i, \ i = 1, \ldots, n.$$

For the least square estimation, with the default constraints of R, we obtain the following results :

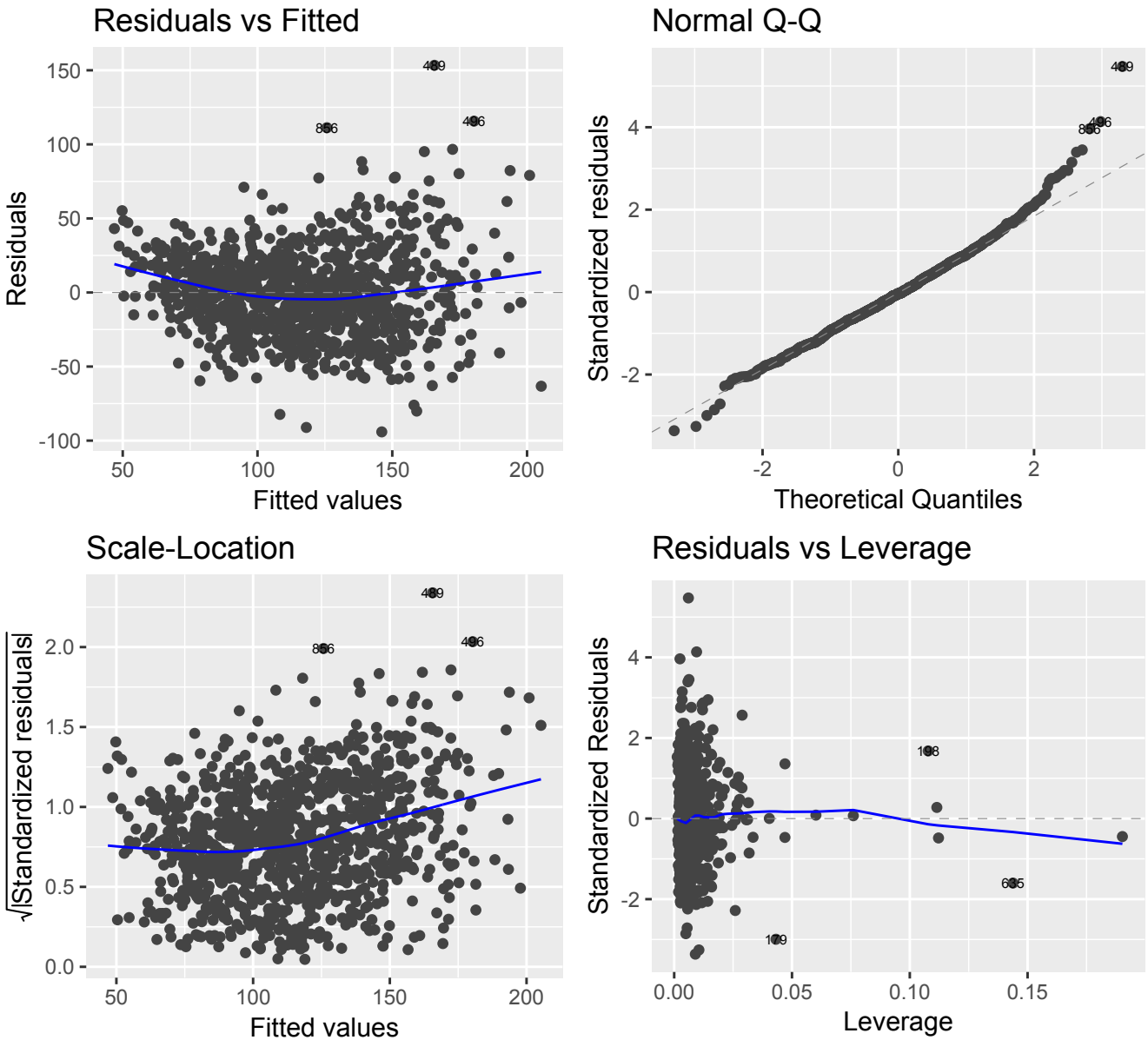
Coefficients	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	-33.43948	6.98313	-4.789	1.93e-06 ****
JOUR1	0.46159	1.88646	0.245	0.806747
MOCAGE	0.37509	0.03694	10.153	$<$ 2e-16 ***
TEMPE	3.96507	0.22135	17.913	$<$ 2e-16 ***
...	...	...	...	...

Residual standard error : 27.83 on 1028 degrees of freedom

Multiple R-squared : 0.5445, Adjusted R-squared : 0.5391

F-statistic : 102.4 on 12 and 1028 DF, p-value : $<$ 2.2e-16

Diagnosis on the residuals



Fisher test of a submodel

Assume that our data obey to the model, called Model (1), where $\beta \in \mathbb{R}^p$

$$\mathbf{Y} = \mathbf{X}\beta + \varepsilon.$$

and consider another model, called Model (0) : $\mathbf{Y} = \widetilde{\mathbf{X}}\theta + \varepsilon$. where $\theta \in \mathbb{R}^l$ with $l < p$.

Definition

We define

$$V = \{\mathbf{X}\beta, \beta \in \mathbb{R}^p\}$$

and

$$W = \left\{\widetilde{\mathbf{X}}\theta, \theta \in \mathbb{R}^l\right\}.$$

We say that Model (0) is a submodel of Model (1) if W is a linear subspace of V.

Fisher test of a submodel

We want to test
H_0 : "the vector $\mathbf{Y}$ of observations obeys to Model (0)" against
H_1 : "the vector $\mathbf{Y}$ of observations obeys to Model (1)".
In the Model (0), the least square estimator of $\boldsymbol{\theta}$ is :

$$\widehat{\boldsymbol{\theta}} = (\widetilde{\mathbf{X}}'\widetilde{\mathbf{X}})^{-1}\widetilde{\mathbf{X}}'\mathbf{Y}.$$

The F-statistics is defined by :

$$F = \frac{\|\mathbf{X}\widehat{\boldsymbol{\beta}} - \widetilde{\mathbf{X}}\widehat{\boldsymbol{\theta}}\|^2/(p-l)}{\|\mathbf{Y} - \mathbf{X}\widehat{\boldsymbol{\beta}}\|^2/(n-p)} = \frac{(\mathrm{SSR}_\mathbf{0} - \mathrm{SSR}_\mathbf{1})/(p-l)}{\mathrm{SSR}_\mathbf{1}/(n-p)},$$

where SSR_0 and SSR_1 respectively denote the residuals sum of square under Model (0) and Model (1).

Fisher test of a submodel

- The numerator of the F-statistics corresponds to $\left\|\widehat{\mathbf{Y}}_{\mathbf{0}} - \widehat{\mathbf{Y}}_{\mathbf{1}}\right\|^2$.
- The null hypothesis is rejected for large values of F, namely, when

$$F > f_{p-l,n-p,1-\alpha},$$

  where $f_{p,q,1-\alpha}$ is the $(1-\alpha)$ quantile of the Fisher distribution with parameters (p, q).
- The statistical softwares provide the $p-$ value of the test :

$$P_{H_0}(F > F_{obs})$$

  where F_{obs} is the observed value for the F-statistics.
- The null hypothesis is rejected at level α if the $p-$ value is smaller than α.

R^2 and adjusted R^2

$$\text{SST} = \sum_{i=1}^{n} (Y_i - \bar{Y})^2 = \left\| \mathbf{Y} - \overline{\mathbf{Y}} \mathbb{1} \right\|^2,$$

$$\text{SSE} = \sum_{i=1}^{n} (\hat{Y}_i - \bar{Y})^2 = \left\| \widehat{\mathbf{Y}} - \overline{\mathbf{Y}} \mathbb{1} \right\|^2,$$

$$\text{SSR} = \sum_{i=1}^{n} (\hat{Y}_i - Y_i)^2 = \left\| \mathbf{Y} - \widehat{\mathbf{Y}} \right\|^2 = \|\mathbf{e}\|^2.$$

$$\left\| \mathbf{Y} - \overline{\mathbf{Y}} \mathbb{1} \right\|^2 = \left\| \mathbf{Y} - \widehat{\mathbf{Y}} \right\|^2 + \left\| \widehat{\mathbf{Y}} - \overline{\mathbf{Y}} \mathbb{1} \right\|^2,$$

hence

$$\text{SST} = \text{SSR} + \text{SSE}.$$

$$R^2 = \frac{\text{SSE}}{\text{SST}} = 1 - \frac{\text{SSR}}{\text{SST}}.$$

Note that $0 \leq R^2 \leq 1$.

Determination coefficient and Model selection

The model is well adjusted to the n training data if the determination coefficient R^2 is close to 1.
Hence, the first hint is that a "good" model is a model for which R^2 is close to 1.
This is in fact not true.
Suppose that we have a training sample $(X_i, Y_i)_{1 \leq i \leq n}$ where $X_i \in [0, 1]$ and $Y_i \in \mathbb{R}$ and we adjust polynomials on these data :

$$Y_i = \beta_0 + \beta_1 X_i + \beta_2 X_i^2 + \ldots + \beta_k X_i^k + \varepsilon_i.$$

When k increases, the model is more and more complex, hence $\left\| \mathbf{Y} - \widehat{\mathbf{Y}} \right\|^2$ decreases, and R^2 increases as shown in Figures 2 and 3.

Determination coefficient and Model selection

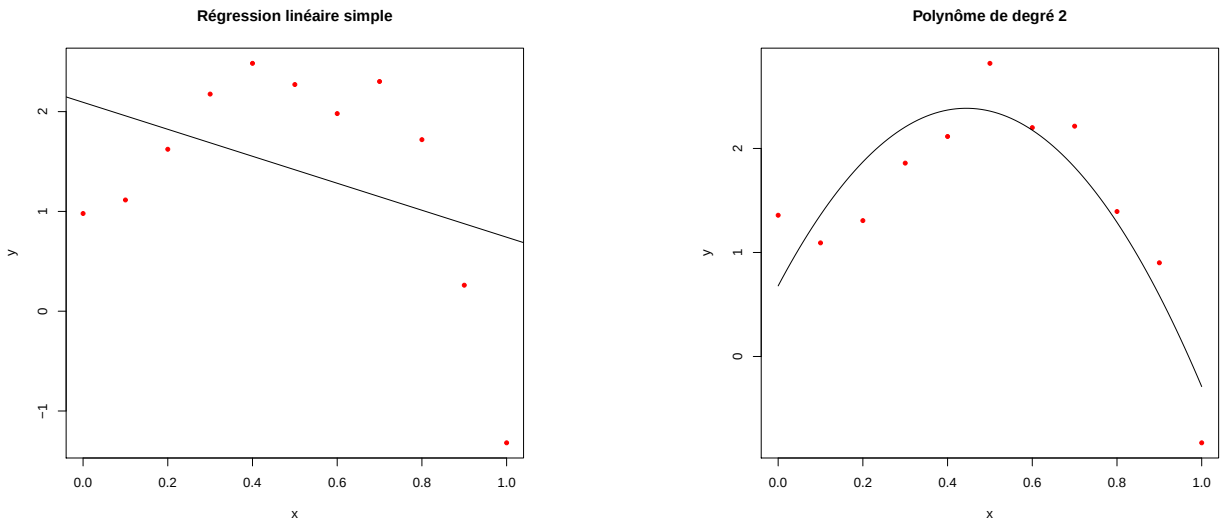


FIGURE: Polynomial regression : adjusted model, on the left : $y = \beta_0 + \beta_1 x + \epsilon$, $R^2 = 0.03$, on the right : $y = \beta_0 + \beta_1 x + \beta_2 x^2 + \epsilon$, $R^2 = 0.73$.

Determination coefficient and Model selection

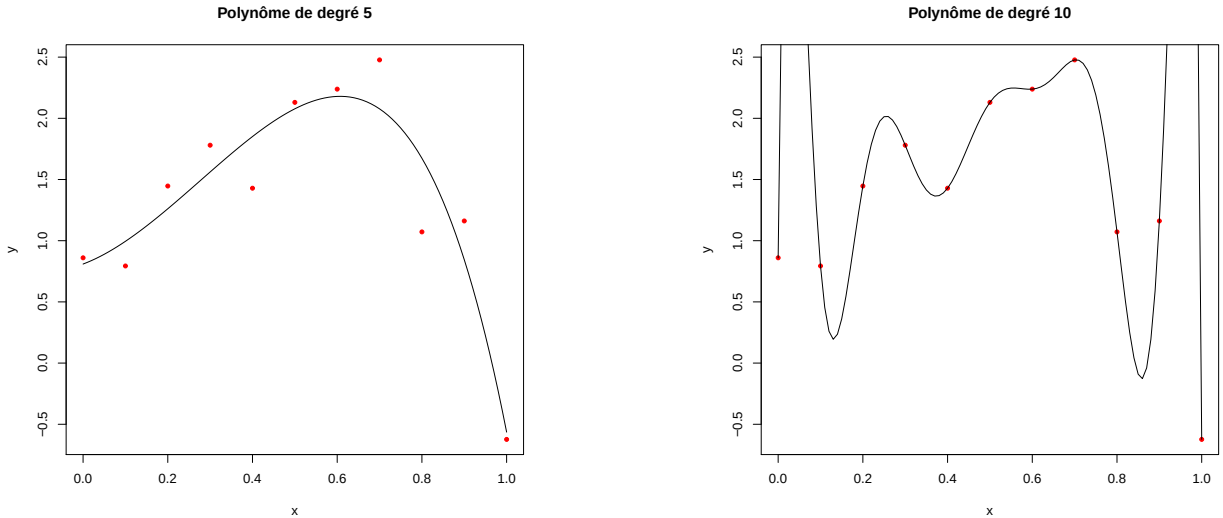


FIGURE: Polynomial regression : adjusted model, on the left : $y = \beta_0 + \beta_1 x + \ldots + \beta_5 x^5 + \epsilon$, $R^2 = 0.874$, on the right : $y = \beta_0 + \beta_1 x + \ldots + \beta_{10} x^{10} + \epsilon$, $R^2 = 1$.

The determination coefficient is equal to 1 for the polynomial of degree $n-1$ (which has n coefficients) and passes through all the training points.

Model selection

- The best model is the one that realizes the best trade-off between the bias term and the variance term.
- Maximizing the determination coefficient is not a good criterion to compare models with various complexity.
- It is more interesting to consider the adjusted determination coefficient defined by :

$$R'^2 = 1 - \frac{\mathrm{SSR}/(n-k-1)}{\mathrm{SST}/(n-1)}.$$

  The definition of R'^2 takes into account the complexity of the model, represented here by its number of coefficients : $k+1$ for a polynomial of degree k, and penalizes more complex models.
- One can choose, between several models, the one which maximizes the adjusted R^2. In the previous example, we would choose a polynomial of degree 3 with this criterion.

Model selection

- We have to define model selection procedures that realize a good compromise between a good adjustment to the data (small bias) and a small variance. We will prefer a biased model if this allows to reduce drastically the variance.
- There are several ways to do that :
  - Reducing the number of explanatory variables and by the same way simplifying the model (variable selection or *Lasso* penalization)
  - Putting some constraints on the parameters of the model by *shrinking* them (*Ridge* or *Lasso* penalization)

Variable selection

- We want to select a subset of variables among all possible subsets taken from the input variables.
- Each subset defines a model, and we want to select the "best model".
- Maximizing the R^2 is not a good criterion since this lead to select the full model.
- It is more interesting to select the model maximizing the adjusted determination coefficient R'^2.
- Many other penalized criterion have been introduce for variable selection such as the Mallow's C_P criterion or the BIC criterion.
- In both cases, it corresponds to the minimization of the least square criterion plus some penalty term, depending on the number k of parameters in the model m that is considered.

$$\text{Crit}(m) = \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2 + \text{pen(k)}.$$

Variable selection

The Mallow's C_P criterion is

$$\text{Crit}_{C_P}(m) = \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2 + 2k\sigma^2,$$

and the BIC criterion penalizes more the dimension of the model with an additional logarithmic term.

$$\text{Crit}_{BIC}(m) = \sum_{i=1}^{n} (Y_i - \hat{Y}_i)^2 + \log(n)k\sigma^2.$$

The aim is to select the model (among all possible subsets) that minimizes one of those criterion. On the example of the polynomial models, we obtain the results summarized in the next Figure.

Variable selection

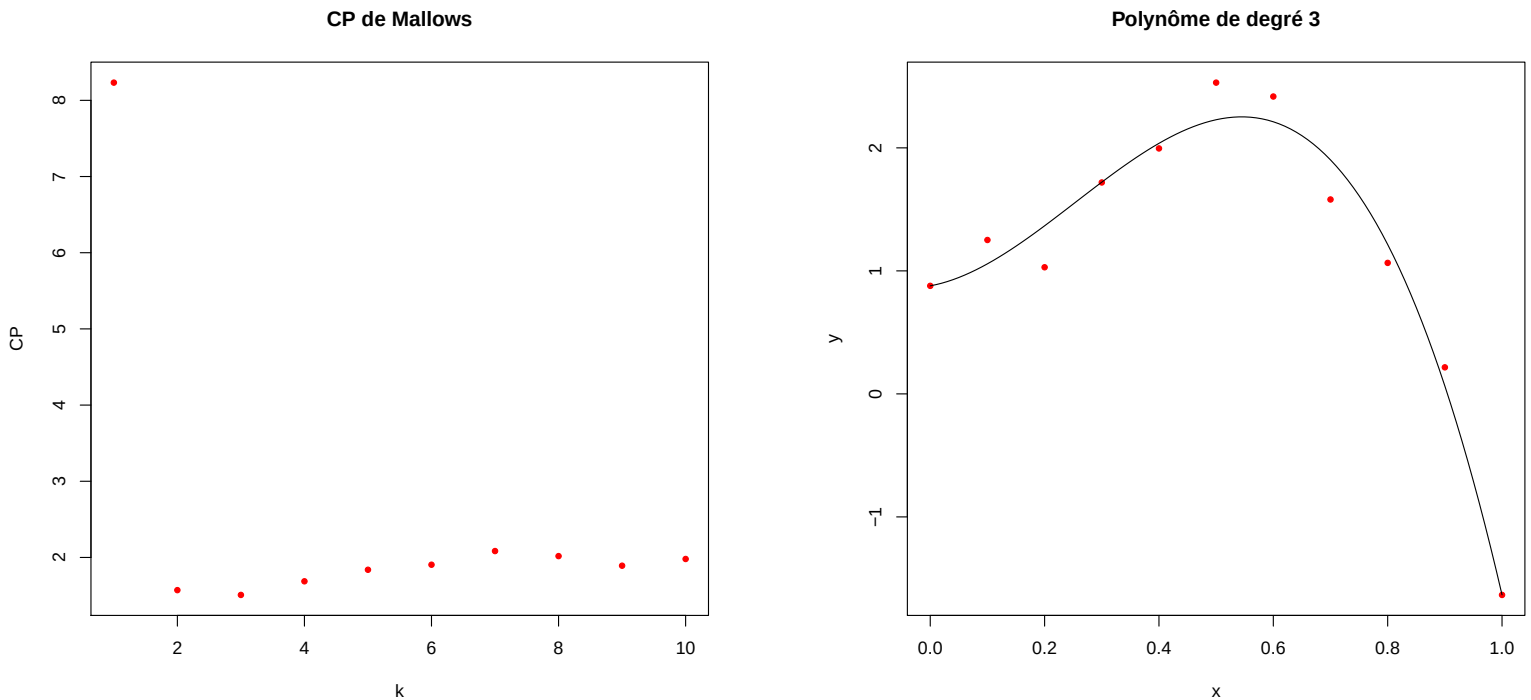


FIGURE: Mallows' C_P in function of the degree of the polynomial. Selected model : polynomial with degree 3.

Variable selection

- The number of subsets of a set of p variables is 2^p, and it is impossible (as soon as $p > 30$) to explore all the models to minimize the criterion.
- Fast algorithms have been developed to find a clever way to explore a subsample of the models.
- This are the *backward, forward* and *stepwise* algorithms :
  - **Forward selection :** We start from the constant model (only the intercept, no explanatory variable), and we add sequentially the variable that allows to reduce the more the criterion.
  - **Backward selection :** This is the same principle, but starting from the full model and removing one variable at each step in order to reduce the criterion.
  - **Stepwise selection :** This is a mixed algorithm, adding or removing one variable at each step in order to reduce the criterion in the best way.

All those algorithms stop when the criterion can no more be reduced.

Variable selection

Applications of the **Stepwise Algorithm** to the `Ozone` data. We apply the `StepAIC` algorithm, with the option **both** of the software R in order to select a subset of variables, and we present here an intermediate result :

```
                    Start:  AIC=6953.05
O3obs ~ MOCAGE + TEMPE + RMH2O + NO2 + NO + VentMOD + VentANG
                 Df  Sum of Sq    RSS     AIC
- VentMOD         1      1484 817158  6952.9
<none>                         815674  6953.0
- RMH2O           1      4562 8202354 6956.9
- VentANG         1     12115 827788  6966.4
- NO2             1     21348 837022  6977.9
- NO              1     21504 837178  6978.1
- MOCAGE          1    225453 1041127 7205.1
- TEMPE           1    268977 1084651 7247.7
                  Step:  AIC= 6952.94
O3obs ~ MOCAGE + TEMPE + RMH2O + NO2 + NO + VentANG
```

Ridge regression

The principle of the Ridge regression is

- to consider all the explanatory variables
- to introduce constraints on the parameters in order to avoid overfitting, and by the same way in order to reduce the variance of the estimators.
- In the case of the Ridge regression, we introduce an l_2 constraint on the parameter β.

Model and estimation

We consider the linear model

$$\mathbf{Y} = \widetilde{\mathbf{X}}\widetilde{\boldsymbol{\beta}} + \boldsymbol{\epsilon},$$

where

$$\widetilde{\mathbf{X}} = \begin{pmatrix} 1 & X_1^1 & X_1^2 & . & X_1^p \\ 1 & X_2^1 & X_2^2 & . & X_2^p \\ . & . & . & . & . \\ 1 & X_n^1 & X_n^2 & . & X_n^p \end{pmatrix},$$

$$\widetilde{\boldsymbol{\beta}} = \begin{pmatrix} \beta_0 \\ \beta_1 \\ . \\ . \\ \beta_p \end{pmatrix}, \quad \boldsymbol{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ . \\ . \\ \beta_p \end{pmatrix}.$$

$\mathbf{X}$ is the matrix $\widetilde{\mathbf{X}}$ where we have removed the first column.

The *ridge* estimator is defined by a least square criterion plus a penalty term, with an l_2 type penalty (note that the parameter β_0 is not penalized).

Definition

The *ridge* estimator of $\widetilde{\beta}$ in the model $\mathbf{Y} = \widetilde{\mathbf{X}}\widetilde{\beta} + \epsilon$, is defined by

$$\widehat{\beta}_{\text{Ridge}} = \text{argmin}_{\beta \in \mathbb{R}^{p+1}} \left(\|\mathbf{Y} - \widetilde{\mathbf{X}}\widetilde{\beta}\|^2 + \lambda \sum_{j=1}^{p} \beta_j^2 \right),$$

where λ is a non negative parameter, that we have to calibrate.

Assume that $\boldsymbol{X}$ and $\boldsymbol{Y}$ are centered. We can find the *ridge* estimator by resolving the normal equations :

$$\mathbf{X}'\mathbf{Y} = (\mathbf{X}'\mathbf{X} + \lambda \mathbf{I}_p)\beta.$$

We get

$$\widehat{\beta}_R = (\mathbf{X}'\mathbf{X} + \lambda \mathbf{I}_p)^{-1}\mathbf{X}'\mathbf{Y}.$$

The solution is therefore explicit and linear with respect to $\mathbf{Y}$.

Remarks :

1. $\mathbf{X}'\mathbf{X}$ is a nonnegative symmetric matrix. Hence, for any $\lambda > 0$, $\mathbf{X}'\mathbf{X} + \lambda \mathbf{I}_p$ is invertible.
2. The constant β_0 is not penalized, otherwise, the estimator would depend on the choice of the origin for $\mathbf{Y}$. We obtain $\widehat{\beta}_0 = \overline{\mathbf{Y}}$, adding a constant to $\mathbf{Y}$ does not modify the values of $\widehat{\beta}_j$ for $j \geq 1$.
3. The *ridge* estimator is not invariant by normalization of the vectors $X^{(j)}$, it is therefore important to normalize the vectors before minimizing the criterion.
4. The *ridge* regression is equivalent to the least square estimation under the constraint that the l_2-norm of the vector β is not too large : $\widehat{\beta}_R = \arg\min_\beta \left\{ \|\mathbf{Y} - \mathbf{X}\beta\|^2 \ ; \ \|\beta\|^2 < c \right\}$. The ridge regression keeps all the parameters, but, introducing constraints on the values of the β_j's avoids too large values for the estimated parameters, which reduces the variance.

Choice of the penalty term

- In the next Figure, we see results obtained by the *ridge* method for several values of the tuning parameter $\lambda = l$ on the polynomial regression example.
- Increasing the penalty leads to more regular solutions, the bias increases, and the variance decreases.
- We have overfitting when the penalty is equal to 0 and under-fitting when the penalty is too large.

Choice of the penalty term

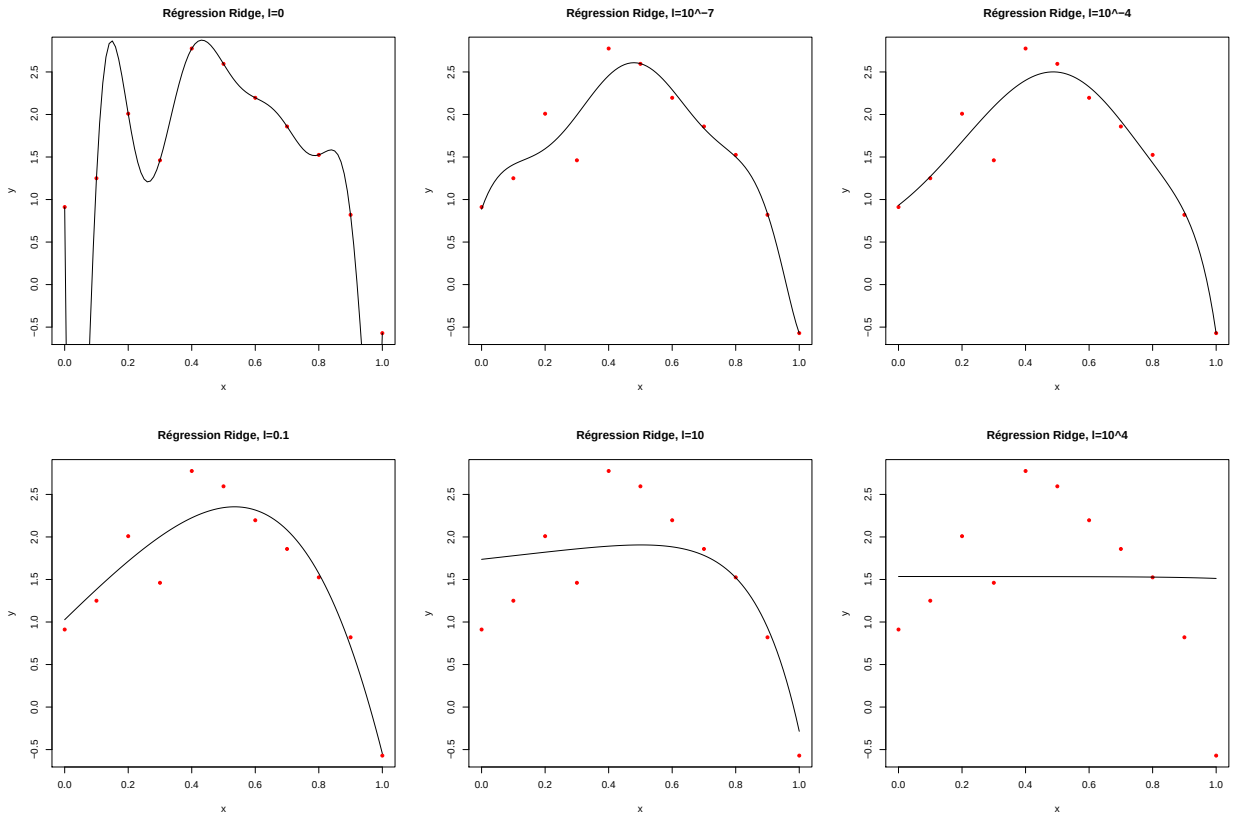
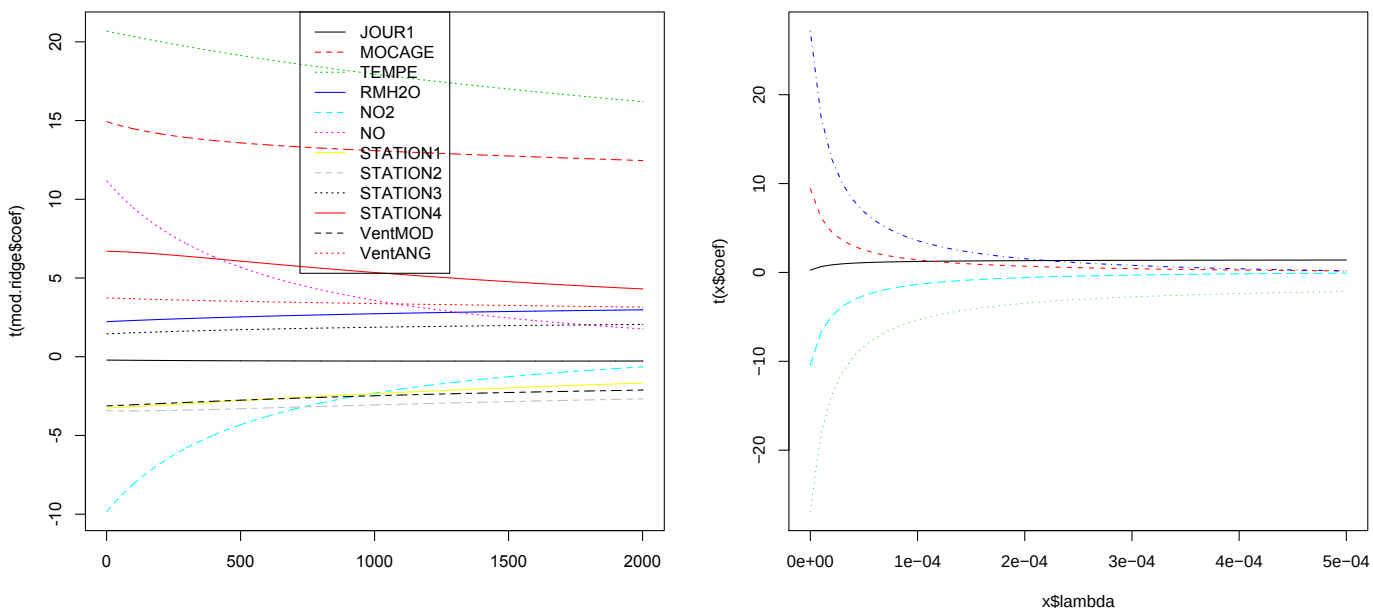


FIGURE: *Ridge* penalisation for the polynomial model

Choice of the penalty term

- For each regularization method, the choice of the parameter λ is determinant for the model selection. We see in next Figure the *Regularisation path*, showing the profiles of the estimated parameters when the tuning parameter λ increases.



Choice of the regularization parameter

Most softwares use the **cross-validation** to select the tuning parameter penalty. The principe is the following :

- We split the data into K sub-samples. For all I from 1 to K :
  - We compute the Ridge estimator associated to a regularization parameter λ from the data of all the subsamples, except the I-th (that will be a "'test"' sample).
  - We denote by $\hat{\beta}_\lambda^{(-I)}$ the obtained estimator.
  - We test the performances of this estimator on the data that have not been used to build it, that is the one of the I-th sub-sample.
- We compute the criterion :

$$CV(\lambda) = \frac{1}{n}\sum_{i=1}^{n}(\boldsymbol{Y}_i - \boldsymbol{X}_i\hat{\beta}_\lambda^{(-\tau(i))})^2.$$

- We choose the value of λ which minimizes $CV(\lambda)$.

Application to the Ozone data : The value of λ selected by cross-validation is 5.4. We show the obtained value in Figure 6.

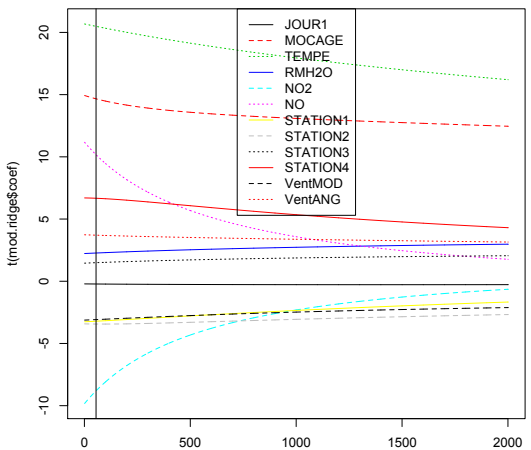


FIGURE: Selection of the regularization parameter by CV

The LASSO regression

- LASSO is the abbreviation of **Least Absolute Shrinkage and Selection Operator.**
- The Lasso estimator is introduced in the paper by Tibshirani, R. (1996) : Regression shrinkage and selection via the lasso. J. Royal. Statist. Soc B., Vol. 58, No. 1, pages 267-288.
- The Lasso corresponds to the minimization of a least square criterion plus an l_1 penalty term.

Definition

The Lasso estimator of β in the model $\mathbf{Y} = \mathbf{X}\beta + \epsilon$, is defined by :

$$\widehat{\beta}_{\text{Lasso}} = \text{argmin}_{\beta \in \mathbb{R}^{p+1}} \left(\sum_{i=1}^{n} (Y_i - \sum_{j=0}^{p} X_i^{(j)} \beta_j)^2 + \lambda \sum_{j=1}^{p} |\beta_j| \right),$$

where λ is a nonnegative tuning parameter.

Model and estimation

We can show that this is equivalent to the minimization problem :

$$\widehat{\beta}_L = \text{argmin}_{\beta \in \mathbb{R}^p, \|\beta\|_1 \leq t}(\|\mathbf{Y} - \mathbf{X}\beta\|^2),$$

where t is suitably chosen, and $\widehat{\beta}_{0\text{Lasso}} = \bar{Y}$.
Like for the Ridge regression, the parameter λ is a regularization parameter :

- If $\lambda = 0$, we recover the least square estimator.
- If λ tends to infinity, all the coefficients $\hat{\beta}_j$ are equal to 0 for $j = 1, \ldots, p$.

The solution to the Lasso is parsimonious (or sparse), since it has many null coefficients.
If the matrix $\mathbf{X}$ is orthogonal : ($\mathbf{X}'\mathbf{X} = Id$), the solution is explicit.

Proposition

— *If* $\mathbf{X}'\mathbf{X} = \mathbf{I}_p$, *the solution* β *of the minimization of the Lasso criterion*

$$\|\mathbf{Y} - \mathbf{X}\beta\|^2 + 2\lambda\|\beta\|_1$$

is defined as follows : for all $j = 1, \ldots, p$,

$$\beta_j = \textit{sign}(\widehat{\beta}_j)(|\widehat{\beta}_j| - \lambda)\mathbb{1}_{|\widehat{\beta}_j| \geq \lambda},$$

where $\widehat{\beta}$ *is the least square estimator :* $\widehat{\beta} = \mathbf{X}'\mathbf{Y}$.

The obtained estimator corresponds to a soft thresholding of the least square estimator.
The coefficients $\widehat{\beta}_j$ are replaced by $\phi_\lambda(\widehat{\beta}_j)$ where

$$\phi_\lambda : x \mapsto \text{sign}(x)(|x| - \lambda)_+.$$

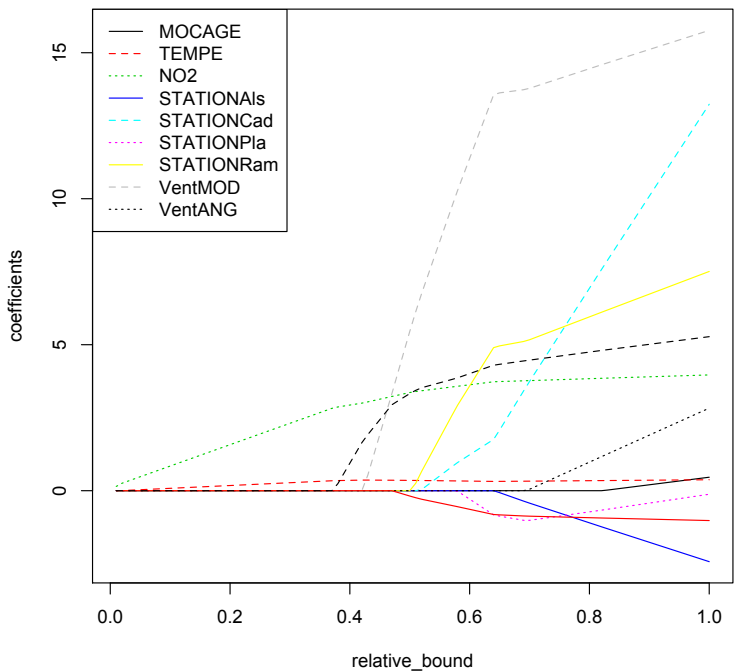
- The LASSO is equivalent to the minimization of the least square criterion under the constraint $\sum_{j=1}^{p} |\beta_j| \leq t$, for some $t > 0$.
- The statistical software R introduces a constraint expressed by a relative bound for $\sum_{j=1}^{p} |\beta_j|$:

$$\sum_{j=1}^{p} |\beta_j| \leq \kappa \sum_{j=1}^{p} |\hat{\beta}_j^{(0)}|,$$

where $\hat{\beta}^{(0)}$ is the least square estimator and $\kappa \in [0, 1]$.
For $\kappa = 1$ we recover the least square estimator and for $\kappa = 0$, all the $\hat{\beta}_j$, $j \geq 1$, vanish.

Applications

We represent in the next Figure the values of the coefficients in function of κ for the Ozone data : this are **the regularization paths of the LASSO**.As for the Ridge regression, the tuning parameter is generally calibrated by cross-validation.



Comparison LASSO/ RIDGE

The next Figure gives a geometric interpretation of the minimization problems for both the Ridge and Lasso estimators. This explains why the Lasso solution is sparse.

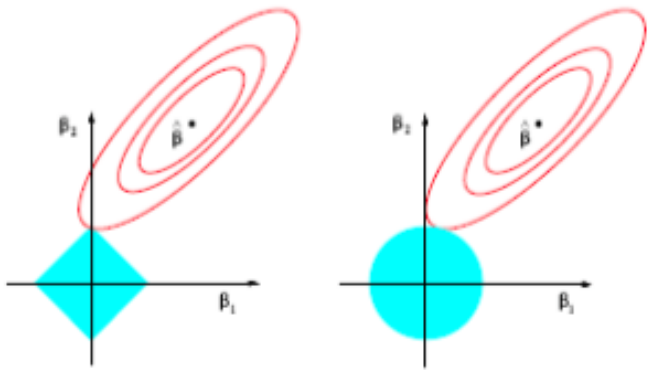


Figure 3.12: *Estimation picture for the lasso (left) and ridge regression (right). Shown are contours of the error and constraint functions. The solid blue areas are the constraint regions* $|\beta_1| + |\beta_2| \leq t$ *and* $\beta_1^2 + \beta_2^2 \leq t^2$*, respectively, while the red ellipses are the contours of the least squares error function.*

Elastic Net

Elastic Net is a method that combines Ridge and Lasso regression, by introducing simultaneously the l_1 and l_2 penalties. The criterion to minimize is

$$\sum_{i=1}^{n}(Y_i - \beta_0 - \beta_1 X_i^{(1)} - \beta_2 X_i^{(2)} - \ldots - \beta_p X_i^{(p)})^2$$
$$+\lambda\left(\alpha\sum_{j=1}^{p}|\beta_j| + (1-\alpha)\sum_{j=1}^{p}\beta_j^2\right)$$

- For $\alpha = 1$, we recover the LASSO.
- For $\alpha = 0$, we recover the Ridge regression.

In this case, we have two tuning parameters to calibrate by cross-validation.

Part I-2 : Classification

- We now consider supervised classification problems. We have a training data set with n observation points (or objects) $\boldsymbol{X}_i$ and their class (or label) Y_i.
- Suppose that $\boldsymbol{d}^n$ corresponds to the observation of a n-sample $\boldsymbol{D}^n = \{(\boldsymbol{X}_1, Y_1), \ldots, (\boldsymbol{X}_n, Y_n)\}$ with joint unknown distribution P on $\mathcal{X} \times \mathcal{Y}$.
- A *classification rule* is a measurable function $f : \mathcal{X} \to \mathcal{Y}$ that associates the output $f(\boldsymbol{x})$ to the input $\boldsymbol{x} \in \mathcal{X}$.
- In order to quantify the quality of the prevision, we introduce a loss function.

Definition

A measurable function $l : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}_+$ is a *loss function* if $l(y, y) = 0$ and $l(y, y') > 0$ for $y \neq y'$.

- **For classification** : $\mathcal{Y}$ is a finite set. We define $l(y, y') = \mathbb{1}_{y \neq y'}$.
- We consider the expectation of this loss, this leads to the definition of the *risk* :

Definition

Given a loss function l, the *risk* - or *generalisation error* - of a prediction rule f is defined by

$$R_P(f) = \mathbb{E}_{(\boldsymbol{X}, Y) \sim P}[l(Y, f(\boldsymbol{X}))].$$

- It is important to note that, in the above definition, $(\boldsymbol{X}, Y)$ is independent of the training sample $\boldsymbol{D}^n$ that was used to build the prediction rule f.

- Let $\mathcal{F}$ denote the set of all possible prediction rules. We say that f^* is an optimal rule if $R_P(f^*) = \inf_{f \in \mathcal{F}} R_P(f)$.
- A natural question arises : is it possible to build optimal rules ?
- We define the Bayes rule, which is an optimal rule for classification.

Definition

We call *Bayes rule* any measurable function f^* in $\mathcal{F}$ such that for all $\boldsymbol{x} \in \mathcal{X}$, $\mathbb{P}(Y = f^*(\boldsymbol{x}) | \boldsymbol{X} = \boldsymbol{x}) = \max_{y \in \mathcal{Y}} \mathbb{P}(Y = y | \boldsymbol{X} = \boldsymbol{x})$.

Theorem

— *If f^* is a Bayes rule, then $R_P(f^*) = \inf_{f \in \mathcal{F}} R_P(f)$.*

- The definition of a Bayes rule depends on the knowledge of the distribution P of $(\boldsymbol{X}, Y)$.
- In practice, we have a training sample $\boldsymbol{D}^n = \{(\boldsymbol{X}_1, Y_1), \ldots, (\boldsymbol{X}_n, Y_n)\}$ with joint unknown distribution P, and we construct a classification rule.
- The aim is to find a "good" classification rule, in the sense that its risk is close to the optimal risk of a Bayes rule.

Part I-2

- Logistic Regression
  - Definitions
  - Estimation of the parameters
  - Application
  - Multiclass classification

Logistic Regression model

- We assume that $\mathcal{X} = \mathbb{R}^p$.
- One of the most popular model for binary classification when $\mathcal{Y} = \{-1, 1\}$ is the **logistic regression model**, for which it is assumed that for all $x \in \mathcal{X}$ and for some $\beta \in \mathbb{R}^p$,

$$\pi(\boldsymbol{x}) = \mathbb{P}(Y = 1/\boldsymbol{X} = \boldsymbol{x}) = \frac{\exp(\langle \beta, \boldsymbol{x} \rangle)}{1 + \exp(\langle \beta, \boldsymbol{x} \rangle)}$$

$$1 - \pi(\boldsymbol{x}) = \mathbb{P}(Y = 0/\boldsymbol{X} = \boldsymbol{x}) = \frac{1}{1 + \exp(\langle \beta, \boldsymbol{x} \rangle)},$$

- The quantity $odds(\boldsymbol{x}) = \frac{\pi(\boldsymbol{x})}{1-\pi(\boldsymbol{x})}$ is called the odds for $\boldsymbol{x}$.
  For example, if $\pi(\boldsymbol{x}) = 0.8$, then $odd(\boldsymbol{x}) = 4$ which means that the chance of success $(Y = 1)$ when $\boldsymbol{X} = \boldsymbol{x}$ is 4 against 1.
- The odds ratio between $\boldsymbol{x}$ and $\tilde{\boldsymbol{x}}$ is $OR(\boldsymbol{x}, \tilde{\boldsymbol{x}}) = odds(\boldsymbol{x})/odds(\tilde{\boldsymbol{x}})$.

- Setting

$$g(\pi) = \mathit{logit}(\pi) = \ln\left(\frac{\pi}{1-\pi}\right),$$

the logistic regression model corresponds to

$$\mathit{logit}(\pi(\boldsymbol{x})) = \ln(\mathit{odds}(\boldsymbol{x})) = \langle \beta, \boldsymbol{x} \rangle.$$

- This is a linear model for the logarithm of the odds.
- g is called the **logit** "link" function.
- Other link functions can be considered such as :
  - The **probit** function $g(\pi) = F^{-1}(\pi)$ where F is the distribution function of the standard normal distribution.
  - The **log-log** function $g(\pi) = \ln(-\ln(1-\pi))$.

Estimation of the parameters

- Given a n-sample $\boldsymbol{D}^n = \{(\boldsymbol{X}_1, Y_1), \ldots, (\boldsymbol{X}_n, Y_n)\}$, we can estimate the parameter β by maximizing the conditional likelihood of $\underline{Y} = (Y_1, \ldots, Y_n)$ given $(\boldsymbol{X}_1, \ldots, \boldsymbol{X}_n)$.
- Since the distribution of Y given $\boldsymbol{X} = \boldsymbol{x}$ is a Bernoulli distribution with parameter $\pi_\beta(\boldsymbol{x})$, the conditional likelihood is

$$L(Y_1, \ldots, Y_n, \beta) = \prod_{i=1}^{n} \pi_\beta(\boldsymbol{X_i})^{Y_i} (1 - \pi_\beta(\boldsymbol{X_i}))^{1-Y_i}$$

$$L(\underline{Y}, \beta) = \prod_{i, Y_i=1} \frac{\exp(\langle \beta, \boldsymbol{X_i} \rangle)}{1 + \exp(\langle \beta, \boldsymbol{X_i} \rangle)} \prod_{i, Y_i=-1} \frac{1}{1 + \exp(\langle \beta, \boldsymbol{X_i} \rangle)}.$$

Estimation of the parameters

- Unlike the linear model, there is no explicit expression for the maximum likelihood estimator $\hat{\beta}$.
- It can be shown that computing $\hat{\beta}$ is a convex optimization problem.
- We compute the gradient of the log-likelihood, also called **the score function** $S(\underline{Y}, \beta)$ and use a **Newton-Raphson algorithm** to approximate $\hat{\beta}$ satisfying $S(\underline{Y}, \hat{\beta}) = 0$.
- Variable selection is also possible by maximizing the penalized likelihood (AIC, BIC, LASSO ..).

- We can then predict the probabilities :

$$\hat{\mathbb{P}}(Y = 1/\boldsymbol{X} = \boldsymbol{x})) = \pi_{\hat{\beta}}(\boldsymbol{x}) = \frac{\exp(\langle \hat{\beta}, \boldsymbol{x} \rangle)}{1 + \exp(\langle \hat{\beta}, \boldsymbol{x} \rangle)}$$

$$\hat{\mathbb{P}}(Y = 0/\boldsymbol{X} = \boldsymbol{x})) = 1 - \pi_{\hat{\beta}}(\boldsymbol{x}) = \frac{1}{1 + \exp(\langle \hat{\beta}, \boldsymbol{x} \rangle)}.$$

- We then compute the logistic regression classifier : we set $\hat{Y}(\boldsymbol{x}) = 1$ if $\hat{\mathbb{P}}(Y = 1/\boldsymbol{X} = \boldsymbol{x})) \geq \hat{\mathbb{P}}(Y = 0/\boldsymbol{X} = \boldsymbol{x})$ which is equivalent to $\langle \hat{\beta}, \boldsymbol{x} \rangle \geq 0$. Hence,

$$\hat{Y}(\boldsymbol{x}) = \mathbb{1}_{\langle \hat{\beta}, \boldsymbol{x} \rangle \geq 0}.$$

Application

- We use the logistic regression model to predict the exceedance of the threshold 150 for the variable O3obs.
- Only with the variable MOCAGE :

```
> logistic=glm(depseuil ~ MOCAGE,
data=ozone,family=binomial(link = "logit"))
> summary(logistic)
```

Coefficients	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	-5.596493	0.389841	-14.36	<2e-16 ***
MOCAGE	0.028659	0.002528	11.34	<2e-16 ***

Application

- We compute the predicted values :

```
> pihat=logistic$fitted.values
> Yhat=(pihat>0.5)
> table(depseuil,Yhat)
```

$\hat{Y} \setminus Y$	0	1
0	830	33
1	152	26

- The misclassification error is 17.7%. There are many false negative .
- The model tends to underestimate the threshold overflow : only 15% of the overflows have been predicted.
- We try to improve the model by considering more variables.

Application

- We consider the variables JOUR, MOCAGE,TEMPE, RMH2O, NO2, NO

```
> logistic2=glm(depseuil ~ MOCAGE+TEMPE+RMH2O+NO2+NO+JOUR,
data=ozone,family=binomial(link = "logit"))
> summary(logistic2)
```

Coefficients	Estimate	Std. Error	t value	Pr(>|t|)
(Intercept)	-14.840457	1.116901	-13.287	< 2e-16 ***
MOCAGE	0.026924	0.004045	6.655	2.82e-11 ***
TEMPE	0.309566	0.029529	10.483	< 2e-16 ***
RMH2O	138.430723	28.548702	4.849	1.24e-06 ***
NO2	-0.210011	0.102607	-2.047	0.0407 *
NO	0.742302	0.552606	1.343	0.1792
JOUR1	0.159047	0.235654	0.675	0.4997

Application

- We compute the predicted values :

```
> pihat=logistic2$fitted.values
> Yhat=(pihat>0.5)
> table(depseuil,Yhat)
```

$\hat{Y}$ \ Y	0	1
0	829	34
1	88	90

- The misclassification error is 11.7%.
- We have improved the results, but there are still many false negative : only 50% of the overflows have been predicted.

Multinomial or polytomic regression

- We consider here the case where the response variable Y has M non ordered modalities $u_1, \ldots, u_M$.
- We set $\pi_m(\boldsymbol{x}) = \mathbb{P}(Y = u_m / \boldsymbol{X} = \boldsymbol{x})$ for $m = 1, \ldots M$.

$$\sum_{m=1}^{M} \pi_m(\boldsymbol{x}) = 1.$$

- We choose a reference in the modalities, we assume that this is the first modality u_1.
- The multinomial regression model is defined by

$$\log\left(\frac{\pi_m(\boldsymbol{x})}{\pi_1(\boldsymbol{x})}\right) = \langle \boldsymbol{\beta^{(m)}}, \boldsymbol{x} \rangle \ \forall m = 2, \ldots M.$$

- This is equivalent to

$$\pi_m(\boldsymbol{x}) = \frac{\exp(\langle \boldsymbol{\beta^{(m)}}, \boldsymbol{x} \rangle)}{1 + \sum_{m'=2}^{M} \exp(\langle \boldsymbol{\beta^{(m')}}, \boldsymbol{x} \rangle)}$$

  which generalizes the logistic regression model (where $u_1 = 0$ and $u_2 = 1$).

- In order to estimate the parameters $\boldsymbol{\beta^{(m)}}$, we maximize the likelihood :

$$L(\underline{Y}, \beta) = \prod_{i=1}^{n} \prod_{m=1}^{M} \pi_m(\boldsymbol{X_i})^{\mathbb{1}_{Y_i = u_m}}.$$

Part I-3 :

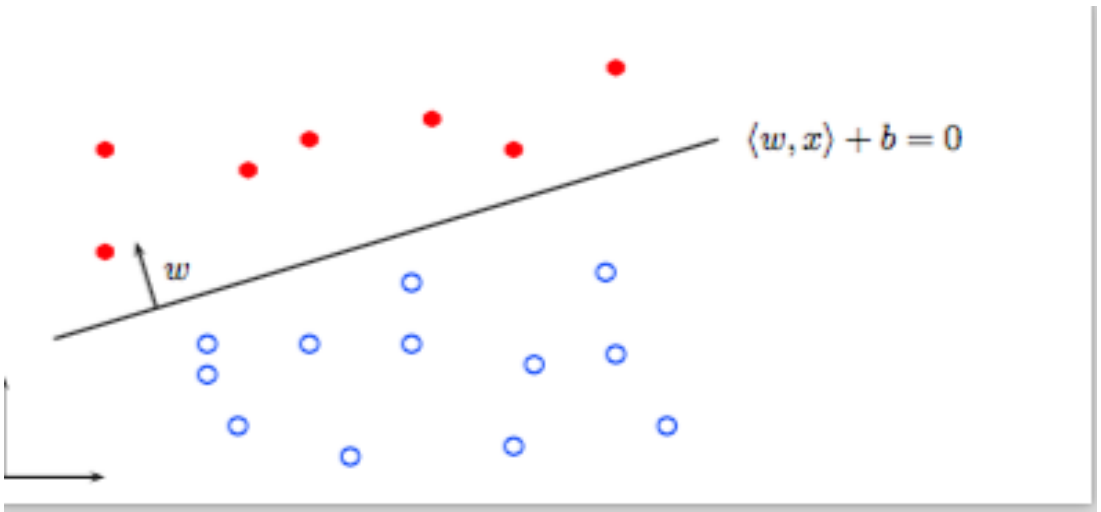
- Support Vector Machines.
  - Linear SVM in the separable case
  - Linear SVM in the non separable case
  - Non linear SVM and kernels
  - Conclusion

Linear Support Vector Machine

Definition

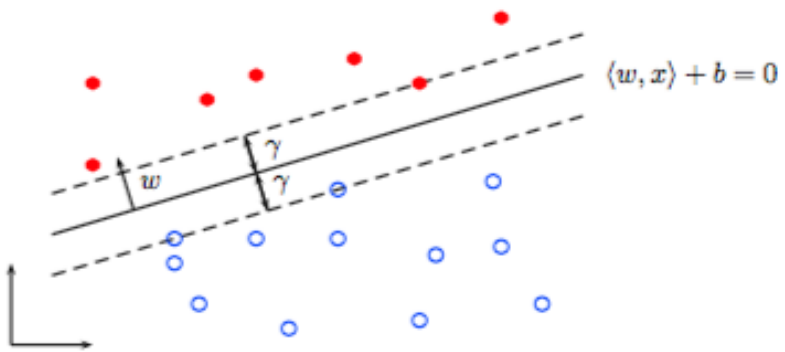
The training set $d_1^n = (x_1, y_1), \ldots, (x_n, y_n)$ is called **linearly separable** if there exists (w, b) such that for all i,
$y_i = 1$ if $\langle w, x_i \rangle + b > 0$, $y_i = -1$ if $\langle w, x_i \rangle + b < 0$,
which means that $\forall i \; y_i \left(\langle w, x_i \rangle + b \right) > 0$.

The equation $\langle w, x \rangle + b = 0$ defines a separating hyperplane with orthogonal vector w.



- The function $f_{w,b}(x) = \mathbb{1}_{\langle w,x\rangle+b\geq 0} - \mathbb{1}_{\langle w,x\rangle+b<0}$ defines a possible linear classification rule.
- The problem is that there exists an infinity of separating hyperplanes, and therefore an infinity of classification rules.
- Which one should we choose ? The response is given by Vapnik (1999).

- The classification rule with the best generalization properties corresponds to the separating hyperplane maximizing the margin γ between the two classes on the training set.



- If we consider two entries of the training set, that are on the border defining the margin, and that we call x_1 and x_{-1} with respective outputs 1 and -1, the separating hyperplane is located at the half-distance between x_1 and x_{-1}.

- The margin is therefore equal to the half of the distance between x_1 and x_{-1} projected onto the normal vector of the separating hyperplane :

$$\gamma = \frac{1}{2} \frac{\langle w, x_1 - x_{-1} \rangle}{\|w\|}.$$

Definition

The hyperplane $\langle w, x \rangle + b = 0$ is **canonical** with respect to the set of vectors $x_1, \ldots, x_k$ if

$$\min_{i=1\ldots k} |\langle w, x_i \rangle + b| = 1.$$

- The separating hyperplane has the canonical form relatively to the vectors $\{x_1, x_{-1}\}$ if it is defined by (w, b) where $\langle w, x_1 \rangle + b = 1$ and $\langle w, x_{-1} \rangle + b = -1$. In this case, we have $\langle w, x_1 - x_{-1} \rangle = 2$, hence

$$\gamma = \frac{1}{\|w\|}.$$

- Finding the separating hyperplane with maximal margin consists in finding (w, b) such that

$$\begin{gathered} \|w\|^2 \text{ or } \tfrac{1}{2}\|w\|^2 \text{ is minimal} \\ \text{under the constraint} \\ y_i \left(\langle w, x_i \rangle + b \right) \geq 1 \text{ for all } i. \end{gathered}$$

This leads to a convex optimization problem with linear constraints, hence there exists a unique global minimizer.

The primal problem to solve is :

$$\text{Minimizing } \tfrac{1}{2}\|w\|^2 \text{ s. t. } y_i\left(\langle w, x_i\rangle + b\right) \geq 1 \ \forall \ i.$$

Lagrangian $L(w, b, \alpha) = \frac{1}{2}\|w\|^2 - \sum_{i=1}^{n} \alpha_i \left(y_i\left(\langle w, x_i\rangle + b\right) - 1\right).$

Dual Function :

$$\frac{\partial L}{\partial w}(w,b,\alpha) = w - \sum_{i=1}^{n} \alpha_i y_i x_i = 0 \Leftrightarrow w = \sum_{i=1}^{n} \alpha_i y_i x_i$$

$$\frac{\partial L}{\partial b}(w,b,\alpha) = -\sum_{i=1}^{n} \alpha_i y_i = 0 \Leftrightarrow \sum_{i=1}^{n} \alpha_i y_i = 0$$

$$\begin{aligned}\theta(\alpha) &= \frac{1}{2}\sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle + \sum_{i=1}^{n} \alpha_i - \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle \\ &= \sum_{i=1}^{n} \alpha_i - \frac{1}{2}\sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle.\end{aligned}$$

The corresponding **dual problem** is :
Maximizing

$$\theta(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle$$

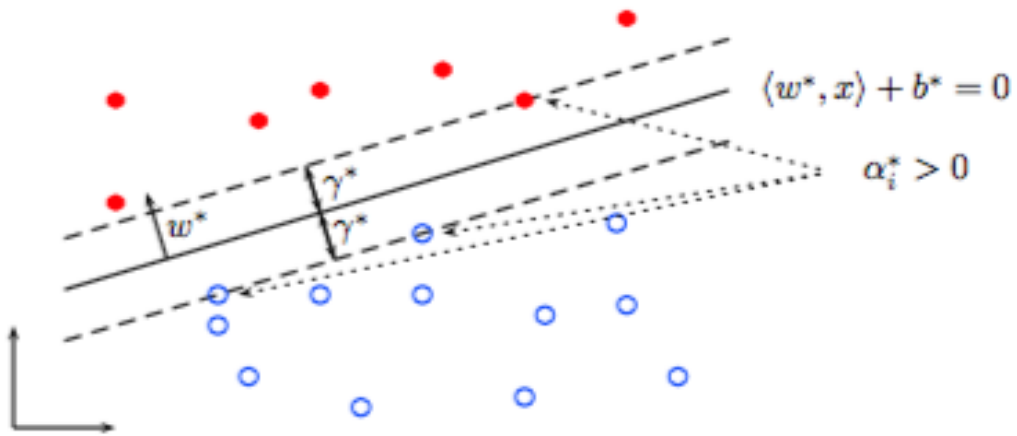
under the constraint $\sum_{i=1}^{n} \alpha_i y_i = 0$ and $\alpha_i \geq 0 \ \forall i$.
The solution α^* of the dual problem can be obtained with classical optimization softwares.
Remark : The solution does not depend on the dimension d, but depends on the sample size n, hence it is interesting to notice that when $\mathcal{X}$ is high dimensional, linear SVM do not suffer from the curse of dimensionality.
For big data sets, n is very large, it is preferable to solve the primal problem.

Supports Vectors

- For our optimization problem, the **Karush-Kuhn-Tucker conditions** are
  - $\alpha_i^* \geq 0 \ \forall i = 1 \dots n.$
  - $y_i \left(\langle w^*, x_i \rangle + b^* \right) \geq 1 \ \forall i = 1 \dots n.$
  - $\alpha_i^* \left(y_i \left(\langle w^*, x_i \rangle + b^* \right) - 1 \right) = 0 \ \forall \ i = 1 \dots n.$ (complementary condition)
- Only the $\alpha_i^* > 0$ are involved in the resolution of the optimization problem.
- If the number of values $\alpha_i^* > 0$ is small, the solution of the dual problem is called **sparse**.

Definition

The x_i such that $\alpha_i^* > 0$ are called the **support vectors**. They are located on the border defining the maximal margin namely $y_i \left(\langle w^*, x_i \rangle + b^* \right) = 1$ (c.f. complementary KKT condition).



We finally obtain the following classification rule :

$$\hat{f}(x) = \mathbb{1}_{\langle w^*, x\rangle + b^* \geq 0} - \mathbb{1}_{\langle w^*, x\rangle + b^* < 0},$$

with

- $w^* = \sum_{i=1}^n \alpha_i^* x_i y_i$,
- $b^* = -\frac{1}{2}\left\{\min_{y_i=1}\langle w^*, x_i\rangle + \min_{y_i=-1}\langle w^*, x_i\rangle\right\}$.

The maximal margin equals $\gamma^* = \frac{1}{\|w^*\|} = \left(\sum_{i=1}^n (\alpha_i^*)^2\right)^{-1/2}$.
The α_i^* that do not correspond to support vectors (sv) are equal to 0, and therefore

$$\hat{f}(x) = \mathbb{1}_{\sum_{x_i \ sv} y_i \alpha_i^* \langle x_i, x\rangle + b^* \geq 0} - \mathbb{1}_{\sum_{x_i \ sv} y_i \alpha_i^* \langle x_i, x\rangle + b^* < 0}.$$

Linear SVM in the non separable case

- The previous method cannot be applied when the training set is not linearly separable. Moreover, the method is very sensitive to outliers.
- In the general case, we allow some points to be in the margin and even on the wrong side of the margin.
- We introduce the slack variable $\xi = (\xi_1, \ldots, \xi_n)$ and the constraint $y_i(\langle w, x_i \rangle + b) \geq 1$ becomes

$$y_i(\langle w, x_i \rangle + b) \geq 1 - \xi_i, \text{ with } \xi_i \geq 0.$$

  - If $\xi_i \in [0, 1]$ the point is well classified but in the region defined by the margin.
  - If $\xi_i > 1$ the point is misclassified.
- The margin is called **flexible margin**.

Optimization problem with relaxed constraints

- In order to avoid too large margins, we penalize large values for the slack variable ξ_i.
- The **primal optimization problem** is formalized as follows :

Minimize with respect to (w, b, ξ) $\quad \frac{1}{2}\|w\|^2 + C\sum_{i=1}^{n}\xi_i$
such that

$$y_i\left(\langle w, x_i\rangle + b\right) \geq 1 - \xi_i \ \forall \ i$$
$$\xi_i \geq 0$$

Remarks :

- $C > 0$ is a tuning parameter of the SVM algorithm. It will determine the tolerance to misclassifications.
- If C increases, the number of misclassified points decreases, and if C decreases, the number of misclassified points increases. C is generally calibrated by cross-validation.
- One can also minimize $\frac{1}{2}\|w\|^2 + C\sum_{i=1}^n \xi_i^k$, $k = 2, 3, \ldots$, we still have a **convex optimization problem**.
  The choice $\sum_{i=1}^n \mathbb{1}_{\xi_i > 1}$ (number of errors) instead of $\sum_{i=1}^n \xi_i^k$ would lead to a non convex optimization problem.

The **Lagrangian** of this problem is :

$$\begin{aligned} L(w, b, \xi, \alpha, \beta) &= \frac{1}{2}\|w\|^2 + \sum_{i=1}^{n} \xi_i (C - \alpha_i - \beta_i) \\ &\quad + \sum_{i=1}^{n} \alpha_i - \sum_{i=1}^{n} \alpha_i y_i \left(\langle w, x_i \rangle + b\right), \end{aligned}$$

with $\alpha_i \geq 0$ and $\beta_i \geq 0$.

The cancellation of the partial derivatives $\frac{\partial L}{\partial w}(w, b, \xi, \alpha, \beta)$, $\frac{\partial L}{\partial b}(w, b, \xi, \alpha, \beta)$ and $\frac{\partial L}{\partial \xi_i}(w, b, \xi, \alpha, \beta)$ leads to the following dual problem.

Dual problem :

Maximizing $\theta(\alpha) = \sum_{i=1}^{n} \alpha_i - \frac{1}{2} \sum_{i,j=1}^{n} \alpha_i \alpha_j y_i y_j \langle x_i, x_j \rangle$

s. t. $\sum_{i=1}^{n} \alpha_i y_i = 0$ and $0 \leq \alpha_i \leq C \ \forall i$.

Karush-Kuhn-Tucker conditions :

- $0 \leq \alpha_i^* \leq C \ \forall i = 1 \dots n.$
- $y_i \left(\langle w^*, x_i \rangle + b^* \right) \geq 1 - \xi_i^* \ \forall i = 1 \dots n.$
- $\alpha_i^* \left(y_i \left(\langle w^*, x_i \rangle + b^* \right) + \xi_i^* - 1 \right) = 0 \ \forall \ i = 1 \dots n.$
- $\xi_i^* (\alpha_i^* - C) = 0.$

Supports vectors

We have the complementary Karush-Kuhn-Tucker conditions :

$$\alpha_i^* \left(y_i \left(\langle w^*, x_i \rangle + b^* \right) + \xi_i^* - 1 \right) = 0 \ \forall \ i = 1 \dots n,$$
$$\xi_i^* (\alpha_i^* - C) = 0$$

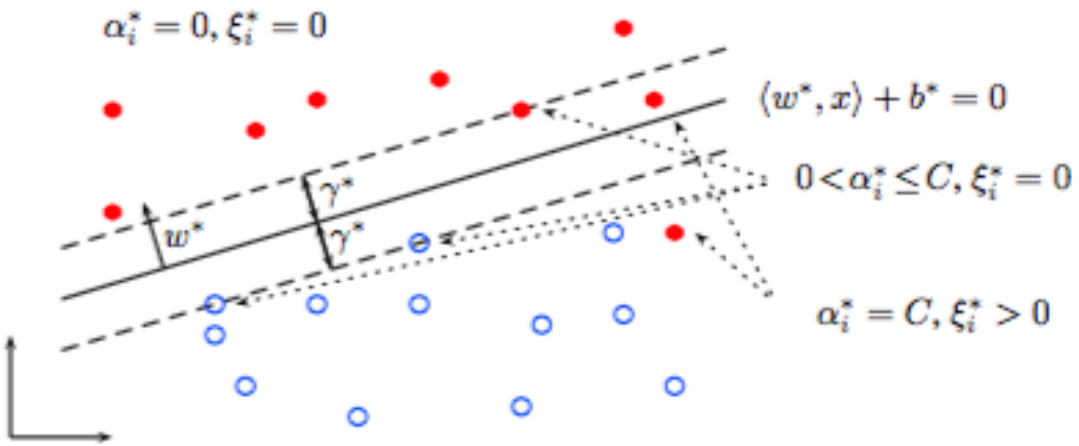
Definition

The points x_i such that $\alpha_i^* > 0$ are the **support vectors**.

We have two types of support vectors :

- The support vectors for which the slack variables are equal to 0. They are located on the border of the region defining the margin.
- The support vectors for which the slack variables are not equal to 0 : $\xi_i^* > 0$ and in this case $\alpha_i^* = C$.

For the vectors that are not support vectors, we have $\alpha_i^* = 0$ and $\xi_i^* = 0$.



The classification rule is defined by

$$\begin{aligned}\hat{f}(x) &= \mathbb{1}_{\langle w^*, x\rangle + b^* \geq 0} - \mathbb{1}_{\langle w^*, x\rangle + b^* < 0}, \\ &= \text{sign}\left(\langle w^*, x\rangle + b^*\right)\end{aligned}$$

with

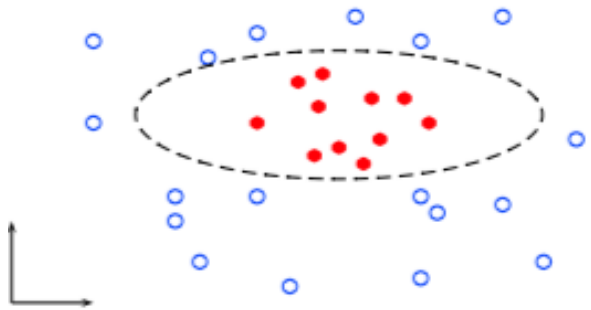
- $w^* = \sum_{i=1}^n \alpha_i^* x_i y_i$,
- b^* such that $y_i \left(\langle w^*, x_i\rangle + b^*\right) = 1 \ \forall x_i, \ 0 < \alpha_i^* < C$.

The maximal margin equals $\gamma^* = \frac{1}{\|w^*\|} = \left(\sum_{i=1}^n (\alpha_i^*)^2\right)^{-1/2}$.
The α_i^* that do not correspond to support vectors are equal to 0, hence

$$\hat{f}(x) = \mathbb{1}_{\sum_{x_i sv} y_i \alpha_i^* \langle x_i, x\rangle + b^* \geq 0} - \mathbb{1}_{\sum_{x_i sc} y_i \alpha_i^* \langle x_i, x\rangle + b^* < 0}.$$

Non linear SVM and kernels

A training set is rarely linearly separable and linear SVM are not appropriate in this case.



- The solution is to enlarge the feature space and send the entries in an Hilbert space $\mathcal{H}$, with high or possibly infinite dimension, via a function ϕ, and to apply a linear SVM procedure on the new training set $\{(\phi(x_i), y_i), i = 1 \dots n\}$. The space $\mathcal{H}$ is called the **feature space**. This idea is due to Boser, Guyon, Vapnik (1992).
- In the previous example, setting $\phi(x) = (x_1^2, x_2^2, x_1, x_2)$, the training set becomes linearly separable in $\mathbb{R}^4$.

The kernel trick

- A natural question arises : how can we choose $\mathcal{H}$ and ϕ ? In fact, we do not choose $\mathcal{H}$ and ϕ but a *kernel* .
- The classification rule is

$$\hat{f}(x) = \mathbb{1}_{\sum y_i \alpha_i^* \langle \phi(x_i), \phi(x) \rangle + b^* \geq 0} - \mathbb{1}_{\sum y_i \alpha_i^* \langle \phi(x_i), \phi(x) \rangle + b^* < 0},$$

  where the α_i^*'s are the solutions of the dual problem in the feature space $\mathcal{H}$:
- Maximizing $\theta(\alpha) = \sum_{i=1}^n \alpha_i - \frac{1}{2} \sum_{i,j=1}^n \alpha_i \alpha_j y_i y_j \langle \phi(x_i), \phi(x_j) \rangle$
  s. t. $\sum_{i=1}^n \alpha_i y_i = 0$ and $0 \leq \alpha_i \leq C \ \forall i$.

- It is important to notice that the final classification rule in the feature space depends on ϕ only through scalar products of the form $\langle \phi(x_i), \phi(x) \rangle$ or $\langle \phi(x_i), \phi(x_j) \rangle$.

- The only knowledge of the function k defined by $k(x, x') = \langle \phi(x), \phi(x') \rangle$ allows to define the SVM in the feature space $\mathcal{H}$ and to derive a classification rule in the space $\mathcal{X}$. The explicite computation of ϕ is not required.

Definition

A function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ such that $k(x, x') = \langle \phi(x), \phi(x') \rangle$ for a given function $\phi : \mathcal{X} \to \mathcal{H}$ is called a **kernel**.

- A kernel is generally more easy to compute than the function ϕ that returns values in a high dimensional space. For example, for $x = (x_1, x_2) \in \mathbb{R}^2$, $\phi(x) = (x_1^2, \sqrt{2}x_1x_2, x_2^2)$, and $k(x, x') = \langle x, x' \rangle^2$.
- Let us now give a property to ensure that a function $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ defines a kernel.

Proposition

—**Mercer condition** *If the function* $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ *is continuous, symmetric, and if for all finite subset* $\{x_1, \ldots, x_k\}$ *in* $\mathcal{X}$*, the matrix* $(k(x_i, x_j))_{1 \leq i,j \leq k}$ *is positive definite :*

$$\forall c_1, \ldots, c_n \in \mathbb{R}, \sum_{i,j=1}^{k} c_i c_j k(x_i, x_j) \geq 0,$$

then, there exists an Hilbert space $\mathcal{H}$ *and a function* $\phi : \mathcal{X} \to \mathcal{H}$ *such that* $k(x, x') = \langle \phi(x), \phi(x') \rangle_{\mathcal{H}}$*. The space* $\mathcal{H}$ *is called the* **Reproducing kernel Hilbert Space (RKHS)** *associated to* k*.*
We have :

1. *For all* $x \in \mathcal{X}$*,* $k(x, .) \in \mathcal{H}$ *where* $k(x, .) : y \mapsto k(x, y)$*.*
2. **Reproducing property** *:*

$$h(x) = \langle h, k(x, .) \rangle_{\mathcal{H}} \text{ for all } x \in \mathcal{X} \text{ and } h \in \mathcal{H}.$$

- Let us give some examples. The Mercer condition is often hard to verify but we know some classical examples of kernels that can be used.
- We assume that $\mathcal{X} = \mathbb{R}^d$.
  - p **degree polynomial kernel** : $k(x, x') = (1 + \langle x, x' \rangle)^p$
  - **Gaussian kernel (RBF)** : $k(x, x') = e^{-\frac{\|x - x'\|^2}{2\sigma^2}}$
    ϕ returns values in a infinite dimensional space.
  - **Laplacian kernel** : $k(x, x') = e^{-\frac{\|x - x'\|}{\sigma}}$.
  - **Sigmoid kernel** : $k(x, x') = \tanh(\kappa \langle x, x' \rangle + \theta)$ (this kernel is not positive definite).

- We have seen some examples of kernels. One can construct new kernels by aggregating several kernels.
- For example let k_1 and k_2 be two kernels and f a function $\mathbb{R}^d \to \mathbb{R}$, $\phi : \mathbb{R}^d \to \mathbb{R}^{d'}$, B a positive definite matrix, P a polynomial with positive coefficients and $\lambda > 0$.
  The functions defined by $k(x, x') = k_1(x, x') + k_2(x, x')$, $\lambda k_1(x, x')$, $k_1(x, x')k_2(x, x')$, $f(x)f(x')$, $k_1(\phi(x), \phi(x'))$, $x^T Bx'$, $P(k_1(x, x'))$, or $e^{k_1(x,x')}$ are still kernels.
- We have presented examples of kernels for the case where $\mathcal{X} = \mathbb{R}^d$ but a very interesting property is that kernels can be defined for very general input spaces, such as **sets, trees, graphs, texts, DNA sequences ...**

Conclusion

- Using kernels allows to delinearize classification algorithms by mapping $\mathcal{X}$ in the RKHS $\mathcal{H}$ with the map $x \mapsto k(x, .)$. It provides nonlinear algorithms with almost the same computational properties as linear ones.
- SVM have nice theoretical properties, cf. Vapnik's theory for empirical risk minimization.
- The use of RKHS allows to apply to any set $\mathcal{X}$ (such as set of graphs, texts, DNA sequences ..) algorithms that are defined for vectors as soon as we can define a kernel $k(x, y)$ corresponding to some measure of similarity between two objects of $\mathcal{X}$.

Conclusion

- Important issues concern the choice of the kernel, and of the tuning parameters to define the SVM procedure.
- Note that SVM can also be used for multi-class classification problems for example, one can built a SVM classifier for each pair of classes and predict the class for a new point by a majority vote.
- Kernels are also used for regression as mentioned above or for non supervised classification (kernel PCA).

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