Regularization Methods for Linear Regression

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ENSIIE

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Agenda

Lessons

- 3 plenatory lessons (MRR)
- 3 Practical work sessions using R (mrr)
- 10 Project sessions (ipR)

Before next session, install on your computer

1. R software, `https://www.r-project.org/`
2. Rstudio, `https://www.rstudio.com/`

Documents are availabale (at this stage)

- `https://sites.google.com/site/MougeotMathilde/teaching`

A word on data and predictive models

Data are everywhere

- Industry (Temperature, IR sensors...)
- Finance : transactions
- Marketing : consumer data.
- on your phone (GPS, mail, musique ...)

$\rightarrow$ Data base are available everywhere : from small data set to Big Data

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Nowadays, predictive models are crutial for monitoring, for diagnosis

- Industry : Health monitoring, Energy...
- Finance : forecast of the evolution of the market
- Marketing : scoring
- Health

→ Machine learning models are used to mine, to operate the data.

Regularization Methods for Linear Regression

-Linear regression and Regularized Linear Regression belongs to the Predictive model family.
-Linear regression is an old model but still very useful !
Gauss, 1785 ; Legendre 1805

Outline of the lesson

- Motivations
- Ordinary Least Square -OLS- (geometrical approach)
- The linear Model (probabilistic approach)
- Using R software for modeling

Evolution of the average age of the French population

Évolution de l'âge moyen et de l'âge médian jusqu'en 2012

Source : Insee, estimations de population.

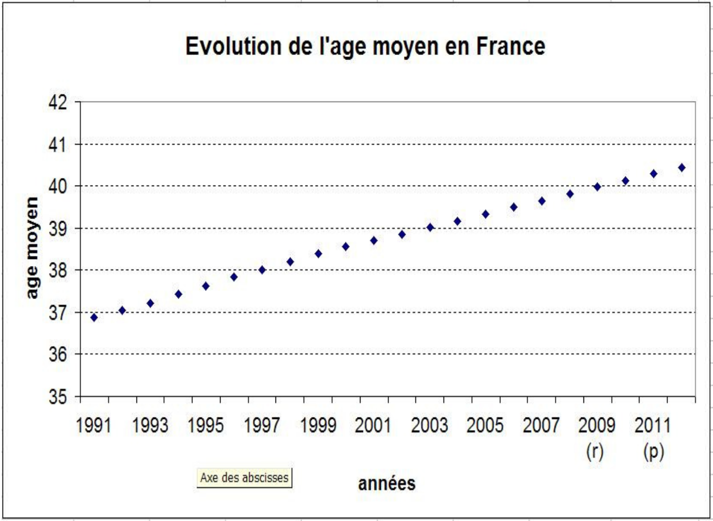
	Âge moyen			Âge médian		
	Ensemble	**Hommes**	**Femmes**	**Ensemble**	**Hommes**	**Femmes**
1991	**36,9**	35,3	38,4	**33,7**	32,4	35,0
1992	**37,0**	35,5	38,5	**34,0**	32,7	35,3
1993	**37,2**	35,7	38,7	**34,3**	32,9	35,6
1994	**37,4**	35,9	38,9	**34,6**	33,2	35,9
1995	**37,6**	36,1	39,1	**34,9**	33,6	36,2
1996	**37,8**	36,3	39,3	**35,2**	33,9	36,5
1997	**38,0**	36,5	39,5	**35,5**	34,1	36,8
1998	**38,2**	36,7	39,7	**35,8**	34,4	37,1
1999	**38,4**	36,9	39,8	**36,1**	34,7	37,4
2000	**38,6**	37,0	40,0	**36,3**	35,0	37,7
2001	**38,7**	37,2	40,1	**36,6**	35,3	38,0
2002	**38,9**	37,3	40,3	**36,9**	35,5	38,2
2003	**39,0**	37,5	40,4	**37,1**	35,8	38,5
2004	**39,2**	37,6	40,6	**37,4**	36,0	38,8
2005	**39,3**	37,8	40,8	**37,7**	36,2	39,1
2006	**39,5**	38,0	40,9	**37,9**	36,4	39,3
2007	**39,7**	38,1	41,1	**38,1**	36,7	39,6
2008 (r)	**39,8**	38,3	41,3	**38,3**	36,9	39,8
2009 (r)	**40,0**	38,5	41,4	**38,6**	37,1	40,0
2010 (p)	**40,1**	38,6	41,6	**38,8**	37,4	40,3
2011 (p)	**40,3**	38,8	41,7	**39,0**	37,6	40,5
2012 (p)	**40,4**	38,9	41,9	**39,3**	37,9	40,7

p : données provisoires, résultats arrêtés à fin 2011.

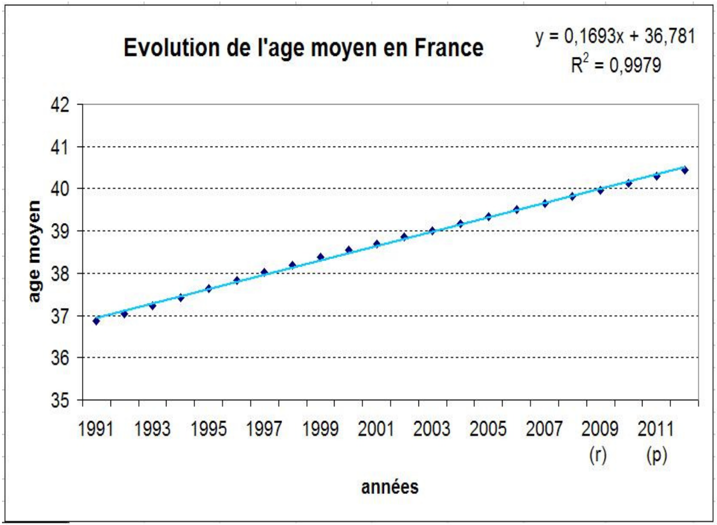
r : données révisées.

Champ : France.

Evolution of the average age of the French population



Modeling the average age of the French population

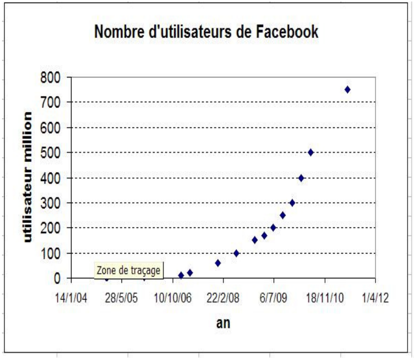


Application : Social Networks

Facebook users :

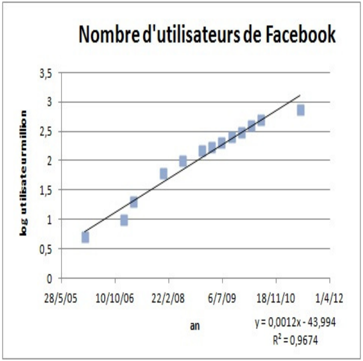
an	user(million)
31/12/04	0
31/12/05	5
31/12/06	10
31/3/07	20
30/12/07	60
30/6/08	100
30/12/08	150
30/3/09	170
30/6/09	200
30/9/09	250
30/12/09	300
30/3/10	400
30/6/10	500
30/6/11	750

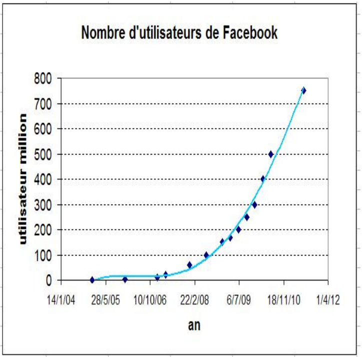
Evolution of the number of Facebook users



Motivations : investment, forecast

Modeling the evolution of the number of Facebook users





Introduction : Regression model

- (Y,X) : couple of variables
  Y : Target quantitative variable
  $X = (X_1, X_2, \ldots, X_p)$: Co-variates, quantitative variables

- The goal is to propose a Regression model to explain Y given X.
  The parameters of the model are computed using a set of data

$$Y = \mathcal{F}_{data}(X) = \mathcal{F}_{data}(X_1, \ldots, X_p)$$

  here, $\mathcal{F}$ is a linear function.

- Questions :
  - What are the performances of this model ?
  - What are the main explicative variables ?
  - Is-it possible to use the model to predict new values ? to forecast ?
  - Can we improve the model ?

Boston Housing Data

The original data are $n = 506$ observations on $p = 14$ variables,

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

Boston Housing Data

The data :

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

Boston Housing Data

- Model $Y = \mathcal{F}_{data}(X)$
- Evaluate the performances of the model
- What are the most important variables ? (variable selection)
  $\rightarrow$ sparse models, less complex, best performances
- Inference and simulation
  $\rightarrow$ Ponctual estimation for new values of the co-variables
  $\rightarrow$ Confidence interval computation.

Outline

- Applications
- Ordinary Least Square (OLS) / Moindre Carrés Ordinaires (MCO)
- Linear Model
- Regularization methods : ridge, lasso

Ordinary Least Square (OLS)

Ordinary Least Square (OLS)

- Values/Variables :
  - Y, $Y \in \mathbb{R}$ **value/ Target variable**
  - $X = (X^1, ..., X^p)$, $X \in \mathbb{R}^p$ **values/ covariates**

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- Data : $S = \{(x_i, y_i)\ i = 1, ..., n,\ y_i \in \mathbb{R},\ x_i \in \mathbb{R}^p\}$

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- Data : $S = \{(x_i, y_i) \; i = 1, ..., n, \; y_i \in \mathbb{R}, \; x_i \in \mathbb{R}^p\}$

- Goal : Modeling Y linearly with X, with a "small" ϵ term

$$Y = \beta_1 + \beta_2 X_2 + \cdots + \beta_p X_p + \boxed{\epsilon}$$

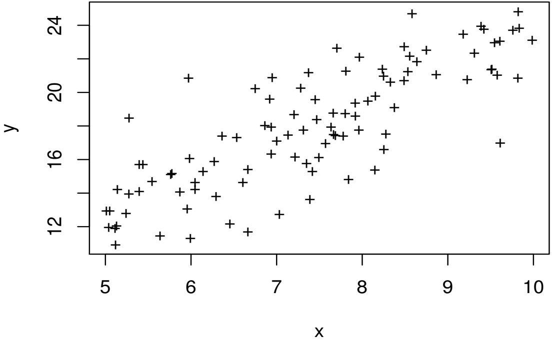
$$Y = \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_p X_p + \boxed{\epsilon}$$

$$Y = \sum_j^p \beta_j X_j + \boxed{\epsilon}$$

Ordinary Least Square (OLS)
Simple Linear Regression model

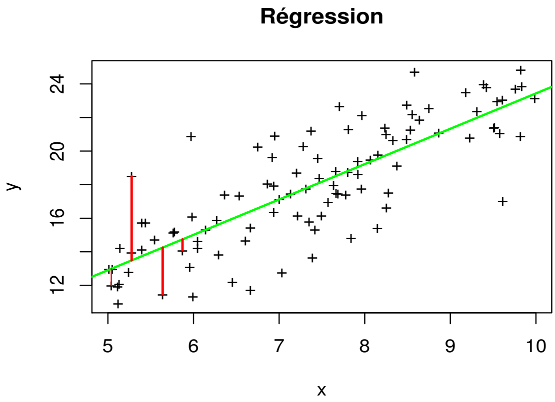
Simple Linear Regression : example

We only have one co-variable (X) to explain the target variable (Y).
The scatter plot is represented by :



Simple Linear Regression : example

For all observation couples i, $1 \leq i \leq n$ (Y_i, X_i),
the goal is here to minimize $(Y_i - (\beta_1 + \beta_2 X_i))^2$



Ordinary Least Square : simple linear model

Formalism :

- Distance to a single point : $(y_i - x_i\beta_2 - \beta_1)^2$
- Distance to the whole sample : $\sum_{i=1}^n (y_i - x_i\beta_2 - \beta_1)^2$
  $\rightarrow$ Best line : intercept $\hat{\beta}_1$ and slope $\hat{\beta}_2$ such that $\sum_{i=1}^n (y_i - x_i\beta_2 - \beta_1)^2$ is minimum, among all possible values of β_1 and β_2.

OLS estimator :

The values estimated by OLS (the estimates) for β_1 and β_2 verify :

$$(\hat{\beta}_1^{ols}, \hat{\beta}_2^{ols}) = \arg\min_{\beta_1, \beta_2 \in \mathbb{R}^2} \{\sum_{i=1}^n (y_i - x_i\beta_2 - \beta_1)^2\}$$

Ordinary Least Square : simple linear model

OLS estimator (observations) :

The values estimated by OLS (the estimates) for β_1 and β_2 verify :

$$(\hat{\beta}_1^{ols}, \hat{\beta}_2^{ols}) = \underset{\beta_1, \beta_2 \in \mathbb{R}^2}{\arg\min} \{ \sum_{i=1}^{n} (y_i - x_i \beta_2 - \beta_1)^2 \}$$

OLS estimator (vector notations) : y, x, 1_n

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$$(\hat{\beta}_1^{ols}, \hat{\beta}_2^{ols}) = \underset{\beta_1, \beta_2 \in \mathbb{R}^2}{\arg\min} \| y - x\beta_2 - 1_n \beta_1 \|_2^2$$

OLS estimator (matrix notations Y (n,1) ; X (n,2)) :

The values estimated by OLS (the estimates) for β_1 and β_2 verify :

$$(\hat{\beta}_1^{ols}, \hat{\beta}_2^{ols}) = \underset{\beta_1, \beta_2 \in \mathbb{R}^2}{\arg\min} \| Y - X\beta \|_2^2$$

Ordinary Least Square : simple linear model

Theorem :
The OLS estimators have the following expressions :

$$\hat{\beta}_1 = \bar{y} - \hat{\beta}_2 \bar{x}$$

$$\hat{\beta}_2 = \frac{\sum_{i=1}^{n}(x_i - \hat{x})(y_i - \hat{y})}{\sum_{i=1}^{2}(x_i - \bar{x})^2} = \frac{Cov(x,y)}{Var(x)}$$

Proof :
by zeroing the derivative of the objective function, which is convex.

Ordinary Least Square : simple linear model

For the simple linear model, the correlation coefficient may be very useful :

- $r(x, y)$: correlation coefficient/ coefficient de corrélation linéaire

$$r(x, y) = \frac{cov(X, Y)}{\sqrt{var(x)}\sqrt{var(y)}}$$

- $r(x, y) = 1$ if and only if $Y = aX + b$, linear relation between Y et X

Ordinary Least Square : simple linear model

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R-square used in multiple regression

- $R^2 = \frac{Var\,\hat{Y}}{Var(Y)}$
- $R^2 \in [0, 1]$
- **Simple regression $R^2 = r^2$:**

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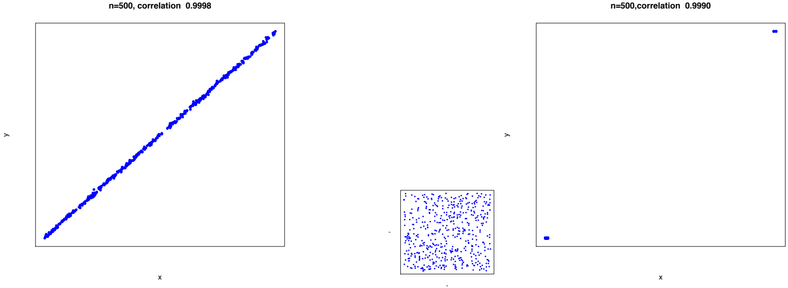
Best Practices

The correlation coefficient equals 1 for these two cases :



Always looking at the data ! !

Ordinary Least Square (OLS)
Multiple Linear Regression model

Ordinary Least Square : multiple linear model

- **We suppose** $Y = \sum_j^p \beta_j X^j + \epsilon$ and $S = \{(x_i, y_i)\ i = 1...n,\ y_i \in \mathbb{R}\ x_i \in \mathbb{R}^p\}$
- The Quadratic error is defined by :

$$E(\beta) = \sum_i^n \epsilon_i^2 = \sum_i^n (y_i - \sum_j x_i^j \beta_j)^2$$

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with matrix notation :

$$E(\beta) = (Y - X\beta)^T (Y - X\beta)$$

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  with matrix notation :

  $$E(\beta) = (Y - X\beta)^T (Y - X\beta)$$

- **Goal :** To minimize the error $E(\beta)$ on the data set S.
  To compute $\hat{\beta} \in \mathbb{R}^p$:

  $$\hat{\beta} = \arg\min_{\beta \in \mathbb{R}^p} E(\beta)$$

Ordinary Least Square. multiple regression model

- We aim to compute β which minimize :

$$\begin{aligned} E(\beta) &= ||Y - X\beta||_2^2 \\ &= (Y - X\beta)^T (Y - X\beta) \end{aligned}$$

- Assumption : $X^T X$ **inversible**. $(n \geq p)$

Theorem :

$$\hat{\beta}_{MCO} = (X^T X)^{-1} X^T Y$$

MCO

- Estimation

$$\hat{\beta} = (X^T X)^{-1} X^T Y$$

MCO

- Estimation

$$\hat{\beta} = (X^T X)^{-1} X^T Y$$

- Prediction Knowing $\hat{\beta}$ and given $X_1, \dots, X_p$,
  the prediction of the target can be computed : $\hat{Y} = \sum_j \hat{\beta}_j X_j$

$$\begin{aligned} \hat{Y} &= X\hat{\beta} \\ &= X(X^T X)^{-1} X^T Y \end{aligned}$$

MCO

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- P Projection matrix on the Hyperplan (hat matrix)

$$\begin{aligned} P &= X(X^T X)^{-1} X^T \\ P^2 &= P \end{aligned}$$

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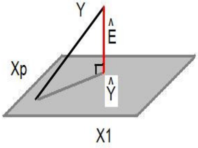
- Residuals
  - $\hat{\epsilon} = Y - \hat{Y}$
  - **Remarque : no assumption on the law or distribution of ϵ**

Ordinary Least Square. Geometrical interpretation



$$\begin{array}{lcccl} Y & = & \sum_j^p X^j \beta_j & + & \epsilon \\ \in \mathcal{R}^n & & \in \mathcal{R}^p & & \in \mathcal{R}^{(n-p)} \end{array}$$

Ordinary Least Square. Properties

- Orthogonality :
  - $\hat{Y} \perp \hat{\epsilon}$
  - $X_j \perp \hat{\epsilon} \qquad \forall j \in [1 \ldots p] < X^j, \hat{\epsilon} >= 0$

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- Residual average :
  - $\sum_i \hat{\epsilon}_i = 0$ if there is an intercept in the model $X^1 = (1, 1, \dots, 1)$

  $\rightarrow$ the average point belongs to the hyperplan
  - $\bar{\hat{Y}} = \bar{Y}$

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- Analysis of Variance -ANAVAR- (Pythagore)
  - $var(Y) = var(\hat{Y}) + var(\hat{E})$

Multiple Linear model : example with R

```
head(mydata,3);
y x1 x2 x3
1 -2.20 0.38 0.98 0.46
2 -1.75 0.11 0.62 0.37
3 -0.24 0.80 0.59 0.87
...
> modlm=lm(y ~ x1+x2+x3,data=mydata);
Call :
lm(formula = y ~ x1+x2+x3, data = mydata)
Coefficients :
(Intercept) x1 x2 x3
0.02754 1.98163 -3.03612 0.01903
```

Multiple Linear model : example with R

```
> modlm=lm(y ~ x1+x2+x3,data=mydata);
> summary(modlm)
lm(formula = y ~ x1+x2+x3, data = mydata)
Residuals :
Min 1Q Median 3Q Max
-0.29 -0.075 -0.0035 0.073 0.281
Coefficients :
Estimate Std. Error t value Pr(>|t|)
(Intercept) 0.02754 0.01503 1.833 0.0674 .
x1      1.98163 0.01577 125.652 <2e-16 ***
x2      -3.03612 0.01621 -187.286 <2e-16 ***
x3      0.01903 0.01576 1.208 0.2277
— Signif. codes : 0 /*** 0.001 /** 0.01 / * 0.05 / . 0.1/ 1
Residual standard error : 0.1009 on 496 degrees of freedom
Multiple R-squared : 0.9904, Adjusted R-squared : 0.9904
F-statistic : 1.707e+04 on 3 and 496 DF, p-value : < 2.2e-16
```

Ordinary Least Square, quality of the adjustment

- R^2, R-square (French : coefficient de détermination)
  - $R^2 = \frac{var(\hat{Y})}{var(Y)}$, remark : no unit

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  - $cos^2 w = R^2 = \frac{||\hat{Y} - \bar{\hat{Y}}_{1,n}||^2}{||Y - \bar{Y}_{1,n}||^2}$
    w : angle between the centered vector $(Y - \bar{Y}_{1,n})$ and its centered prediction $(\hat{Y} - \bar{\hat{Y}}_{1,n})$

Ordinary Least Square, quality of the adjustment

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    w : angle between the centered vector $(Y - \bar{Y}_{1,n})$ and its centered prediction $(\hat{Y} - \bar{\hat{Y}}_{1,n})$
- $var(\hat{E}) = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$
  $= (1 - R^2)var(Y)$, unit of Y^2

Ordinary Least Square : Quality of the Ajustement

- R-square (for few variables)
  - $R^2 = \cos^2 \omega = \frac{Var \hat{Y}}{Var(Y)}$
  - $R^2 \in [0, 1]$
  - $R^2 =$ increases mechanically with the number of variables

Ordinary Least Square : Quality of the Ajustement

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- Adjusted R-squared is sometimes preferred (penalization with the number of variables)
  - $R^2_{adj} = 1 - (1 - R^2)\frac{n-1}{n-p}$
  - R^2_{adj} may be negtive

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  - R^2_{adj} may be negtive

- Residual study :
  - $\hat{\epsilon}_i = y_i - \hat{y}_i \qquad \forall i \in 1..n$
  - Vizualization of
    - $(\hat{\epsilon}_i, i)\ \forall i \in 1..n$
    - $(\hat{\epsilon}_i, y_i)$ homoscedastic vs heteroscedasticbissectrice model

Ordinary Least Square : Quality of the Ajustement

- R-square (for few variables)
  - $R^2 = \cos^2 \omega = \frac{Var \hat{Y}}{Var(Y)}$
  - $R^2 \in [0, 1]$
  - $R^2 =$ increases mechanically with the number of variables

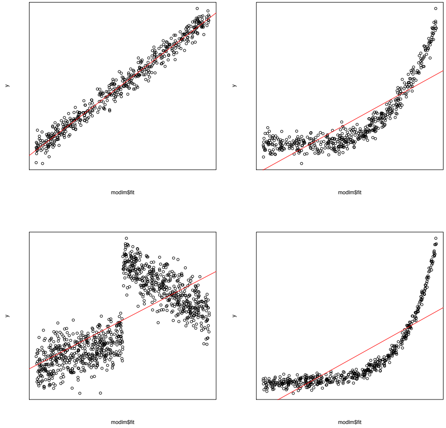
- Adjusted R-squared is sometimes preferred (penalization with the number of variables)
  - $R^2_{adj} = 1 - (1 - R^2)\frac{n-1}{n-p}$
  - R^2_{adj} may be negtive

- Residual study :
  - $\hat{\epsilon}_i = y_i - \hat{y}_i \qquad \forall i \in 1..n$
  - Vizualization of
    - $(\hat{\epsilon}_i, i)$ $\forall i \in 1..n$
    - $(\hat{\epsilon}_i, y_i)$ homoscedastic vs heteroscedasticbissectrice model

- Prediction : Vizualization of
  - $(\hat{y}_i, y_i) \qquad \forall i \in 1..n$
  - comparison with the first bisector.

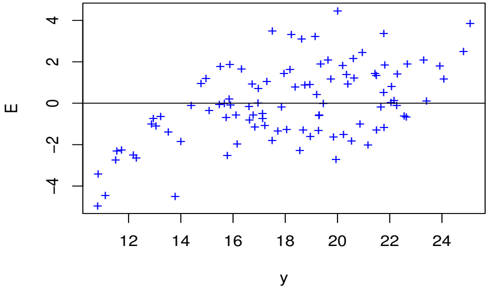
Ordinary Least Square : Quality of the Adjustement

Graphics $(y_i, \hat{y}_i)$ $1 \leq i \leq j$ VERY USEFUL



Ordinary Least Square : Student Residual graph

$\frac{\hat{\epsilon}_i}{S_E} = \frac{y_i - \hat{y}_i}{S_E}$ (no unit term)

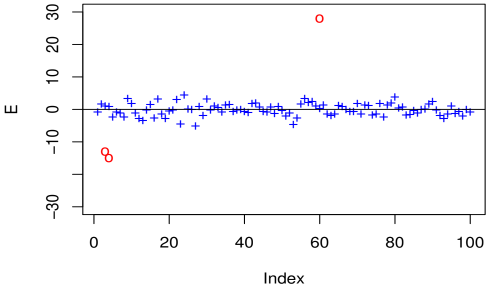


Residual graph

→ Random distribution. There is no information to be capture

Ordinary Least Square : Student Residual graph

$\frac{\hat{\epsilon}_i}{S_E} = \frac{y_i - \hat{y}_i}{S_E}$ (with non unit)

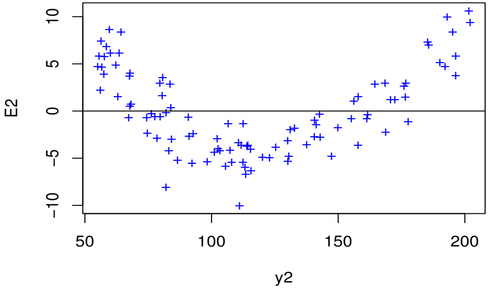


Residual graph function of Y

$\rightarrow$ Large values for some points ? Outliers detection ?

Ordinary Least Square : Student Residual graph

$\frac{\hat{\epsilon}_i}{S_E} = \frac{y_i - \hat{y}_i}{S_E}$ (with non unit)



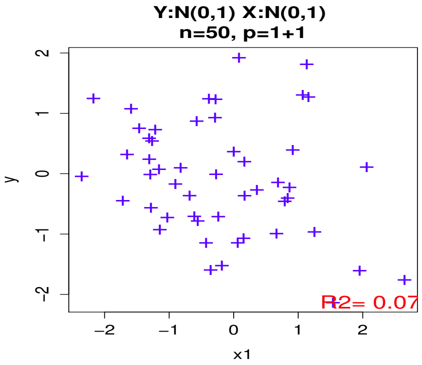
Graphe des résidus en fonction de Y

$\rightarrow$ there is still some information in the residuals.

$\rightarrow$ The model needs to be changed.

Ordinary Least Square : curse of dimension

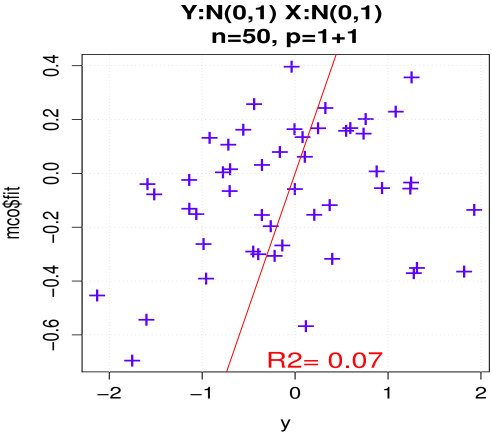
Data set : $\{(y_i, x_i) 1 \leq i \leq n\}$. One target variable, one covariable



$\rightarrow R^2 =, \; R^2_{adj} = -0.02$

Ordinary Least Square : illustration of the impact of the number of covariables on the model

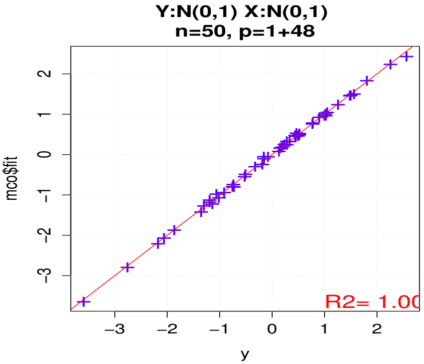
initial data and OLS line



$\rightarrow R^2 =, \; R^2_{adj} = -0.02$

Ordinary Least Square : illustration of the impact of the number of covariables on the model

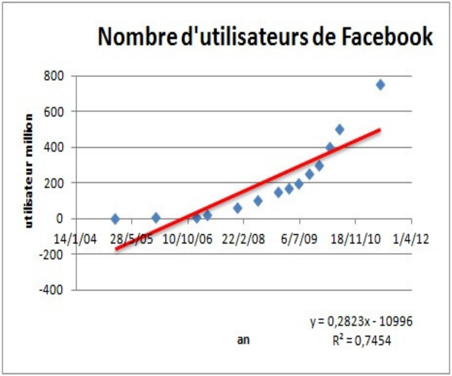
initial data and 48 more covariables $\mathcal{N}(0,1)$ are added to the initial data set.



$\rightarrow R^2 = 0.99,\ R^2_{adj} = 0.93$

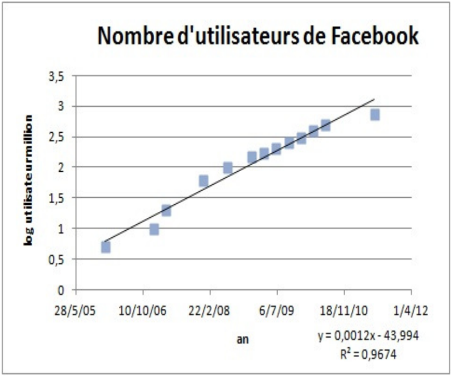
Ordinary Least Square : need to change the model (1/2)

initial data set :



Ordinary Least Square : need to change the model (1/2)

logarithmic transformation



MCO Regression. Some limits :

If $X^T X$ is non inversible

- $n >> p$, collinearity between some X_j.
  - Pseudo-inverse, the solution is not unique
  - Variable selection

- $p >> n$, when the number of variables is larger than the number of observations
  - Regularization method
  - Ridge -$L2$-, Lasso -$L1$-.
  - Variable selection

  OLS model
  Ponctual estimation.

OLS, X^TX non inversible $\rightarrow$

Pseudo inverse computation

Solution ($n > p$), X^TX is non invertible with the rank k, $k < p$:

$$\begin{aligned} X^TX &= U\Sigma^2U^T \\ &= U \begin{pmatrix} \sigma_1^2 & 0 & 0 & 0 \\ 0 & \vdots & 0 & 0 \\ 0 & 0 & \sigma_k^2 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix} U^T \\ &= U_k\Sigma_k^2U_k^T \end{aligned}$$

$$(X^TX)^{*-1} = U_k{\Sigma_k^2}^{-1}U_k^T \text{ avec } \Sigma_k^2 = \begin{pmatrix} \sigma_1^2 & 0 & 0 \\ 0 & \vdots & 0 \\ 0 & 0 & \sigma_k^2 \end{pmatrix}$$

$\hat{\beta} = (X^TX)^{*-1}X^TY$

The solution non unique

Outline

- Motivations
- Ordinary Least Square
- Linear Model
- Penalized regression, ridge, lasso

Linear Model

Probabilistic assumption on the residuals

LInear model

- We write : $Y = X\beta + \epsilon$ avec $\epsilon \sim \mathcal{N}(0, \sigma^2)$
- We have
  - $\epsilon_i = Y_i - \sum X_i^j \beta_j$ avec $f(\epsilon) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{\epsilon^2}{2\sigma^2}}$ i.i.d.

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- Residual density & Maximum Likelihood Estimation
  $f(\epsilon_1, \ldots, \epsilon_n) = \prod_i f(\epsilon_i)$

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- Residual density & Maximum Likelihood Estimation

$$
\begin{aligned}
f(\epsilon_1, \ldots, \epsilon_n) &= \prod_i f(\epsilon_i) \\
&= \frac{1}{(2\pi)^{n/2}\sigma^n} e^{-\frac{\sum \epsilon_i^2}{2\sigma^2}} \\
&= \frac{1}{(2\pi)^{n/2}\sigma^{2n/2}} e^{-\frac{||Y - X\beta||^2}{2\sigma^2}}
\end{aligned}
$$

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&= \frac{1}{(2\pi)^{n/2}\sigma^{2n/2}} e^{-\frac{||Y - X\beta||^2}{2\sigma^2}}
\end{aligned}
$$

- the goal is to compute $\hat{\beta}$, σ^2 solutions of the maximum likelihood Estimation (MLE)
  Same solution for the MLE and the OLS :
  - $\hat{\beta} = (X^T X)^{-1} X^T Y$
  - $\hat{\sigma}^2 = \frac{1}{n} \sum_{i=1}^{i=n} \hat{\epsilon}_i^2$

Linear model : What are the laws of the estimators ?

$Y = X\beta + \epsilon$ avec $\epsilon \sim \mathcal{N}(0, \sigma^2)$

Law of the estimators :

- Law of $\hat{\beta}$?
- Law of $\hat{Y}$?
- Law of $\hat{\sigma}^2$?

Benefits
$\rightarrow$ let to compute confidence intervals for β and Y.
$\rightarrow$ let to test the parameters.

Law of $\hat{\beta}$:

$$\boxed{\hat{\beta} \sim \mathcal{N}(\beta, \sigma^2 (X^T X)^{-1})}$$

Law of $\hat{\beta}$:

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Expectation and Variance of $\hat{\beta}$? :

$\hat{\beta} = (X^T X)^{-1} X^T Y \qquad et\ Y = X\beta + \epsilon$

Law of $\hat{\beta}$:

$$\boxed{\hat{\beta} \sim \mathcal{N}(\beta, \sigma^2 (X^T X)^{-1})}$$

Expectation and Variance of $\hat{\beta}$? :

$\hat{\beta} = (X^T X)^{-1} X^T Y \qquad et\ Y = X\beta + \epsilon$

- $\mathbb{E}(\hat{\beta}) = \beta$ Non biased estimator $\mathbb{E}(\hat{\beta}) - \beta = 0$

Law of $\hat{\beta}$:

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Expectation and Variance of $\hat{\beta}$? :

$\hat{\beta} = (X^T X)^{-1} X^T Y \qquad et \; Y = X\beta + \epsilon$

- $\mathbb{E}(\hat{\beta}) = \beta$ Non biased estimator $\mathbb{E}(\hat{\beta}) - \beta = 0$
- $Var(\hat{\beta}) = \sigma^2 (X^T X)^{-1}$

$$\begin{aligned} Var(\hat{\beta}) \quad &= (X^T X)^{-1} X^T ([var(Y)] X (X^T X)^{-1} \\ &= (X^T X)^{-1} X^T ([var(\epsilon)] X (X^T X)^{-1} \\ &= \sigma^2 (X^T X)^{-1} \end{aligned}$$

- $\mathbb{E}[(\hat{\beta} - \beta)^2] = Var(\hat{\beta}) + 0$

Recall $Var(aY) = aVar(Y)a^T$

Law of $\hat{Y}$

$$\boxed{\hat{Y} \sim \mathcal{N}(X\beta, \sigma^2 X(X^T X)^{-1} X^T)}$$

Expectation and Variance of $\hat{Y}$?, $\hat{Y} = X\hat{\beta}$

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$$\boxed{\hat{Y} \sim \mathcal{N}(X\beta, \sigma^2 X(X^T X)^{-1} X^T)}$$

Expectation and Variance of $\hat{Y}$?, $\hat{Y} = X\hat{\beta}$

- $\mathbb{E}(\hat{Y}) = X\beta$
  $\mathbb{E}(\hat{Y}) = \mathbb{E}(X\hat{\beta}) = X\mathbb{E}(\hat{\beta}) = X\beta = \mathbb{E}(Y)$

Law of $\hat{Y}$

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Expectation and Variance of $\hat{Y}$?, $\hat{Y} = X\hat{\beta}$

- $\mathbb{E}(\hat{Y}) = X\beta$
  $\mathbb{E}(\hat{Y}) = \mathbb{E}(X\hat{\beta}) = X\mathbb{E}(\hat{\beta}) = X\beta = \mathbb{E}(Y)$
- $Var(\hat{Y}) = \sigma^2\ X(X^T X)^{-1}\ X^T$

$$\begin{aligned} Var(\hat{Y}) \quad &= Var(X\hat{\beta}) \\ &= X\ Var(\hat{\beta})\ X^T \\ &= \sigma^2\ X(X^T X)^{-1}\ X^T \end{aligned}$$

Law of $\hat{\epsilon}$

$$\boxed{\hat{\epsilon} \sim \mathcal{N}(0, \sigma^2(I_n - X(X^T X)^{-1} X^T)}$$

Expectation and Variance of $\hat{\epsilon} = Y - \hat{Y}$? :

Law of $\hat{\epsilon}$

$$\boxed{\hat{\epsilon} \sim \mathcal{N}(0, \sigma^2(I_n - X(X^TX)^{-1}X^T)}$$

Expectation and Variance of $\hat{\epsilon} = Y - \hat{Y}$? :

- $\mathbb{E}(\hat{\epsilon}) = 0$

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Expectation and Variance of $\hat{\epsilon} = Y - \hat{Y}$? :

- $\mathbb{E}(\hat{\epsilon}) = 0$
- $Var(\hat{\epsilon}) = \sigma^2(I_n - X(X^TX)^{-1}X^T)$

$$\begin{aligned} Var(\hat{\epsilon}) &= Var(Y - \hat{Y}) \\ &= Var(Y - X\hat{\beta}) \\ &= \sigma^2(I_n) - XVar(\hat{\beta})X^T \\ &= \sigma^2(I_n - X(X^TX)^{-1}X^T) \end{aligned}$$

Recal : $Var(aY) = aVar(Y)a^T$

Linear model : law of the estimators

Under the assumption that ϵ_i are i.i.d. with $\epsilon_i \sim \mathcal{N}(0, \sigma^2)$

Theorem

if $p \leq n$ and $X^T X$ inversible,

The vector $\begin{pmatrix} \hat{\beta} \\ \hat{\epsilon} \end{pmatrix}$ of dimension $(p+n)$ is a gaussian vector

with mean $\begin{pmatrix} \beta \\ 0 \end{pmatrix}$, and

and variance $\sigma^2 \begin{pmatrix} (X^T X)^{-1} & 0 \\ 0 & I_n - X(X^T X)^{-1} X^T \end{pmatrix}$

Loi $\hat{\sigma}^2$

$$\frac{n-p}{\sigma^2}\hat{\sigma}^2 \sim \chi^2_{n-p}$$

We note : $\hat{\sigma}^2 = \frac{||\hat{\epsilon}||^2}{n-p}$

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$||\hat{\epsilon}||^2 = \sum_i^n \hat{\epsilon}_i^2$ $\qquad$ $||\hat{\epsilon}||^2$ suit une loi $\sigma^2\chi^2(n-p)$ (Cochran theorem)

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$||\hat{\epsilon}||^2 = \sum_i^n \hat{\epsilon}_i^2$ $\qquad$ $||\hat{\epsilon}||^2$ suit une loi $\sigma^2\chi^2(n-p)$ (Cochran theorem)

Then, the expectation of $\hat{\sigma}^2 = \frac{||\hat{\epsilon}||^2}{n-p}$ is σ^2,
$(\mathbb{E}(\chi^2(n-p)) = n-p)$

We deduce the law of $\hat{\sigma}^2$:
$\hat{\sigma}^2 \sim \frac{\sigma^2}{n-p}\chi^2(n-p)$

Recall : Student theorem.
$U \sim \mathcal{N}(0,1)$ and $V \sim \chi^2(d)$, U and V are independant, the, we have
$Z = \frac{U}{\sqrt{V/d}}$ follows a Student law of parameter d.

Significativity test of $\hat{\beta}_j$, σ^2 **inconnu**

- Student Statistics : T

Significativity test of $\hat{\beta}_j$, σ^2 **inconnu**

- Student Statistics : T
- Significativity test (bilateral)
  - $H_0 : \beta_j = 0$
  - $H_1 : \beta_j \neq 0$

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- Decision with a risk α, **Reject of H_0 if**
  - $\frac{\hat{\beta}_j}{\sqrt{\hat{\sigma}^2 S_{j,j}}} > t_{n-p}(1-\alpha/2)$ with $S_{j,j}$ jème term of the diagonal of $(X^T X)^{-1}$
  - pvalue $< \alpha$

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- Conclusion :
  - β_j is significatively different of zero
  - X_j a une influence dans le modèle

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  - pvalue $< \alpha$
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  - X_j a une influence dans le modèle

Not true if there exists colinearity between the variables

Global significativity of the model

Test of the model with a risk α

$$
\begin{array}{rl}
H_0: & \beta_2 = \beta_3 = \ldots = \beta_p = 0 \\
H_1: & \exists j = 2, \ldots, p, \beta_j \neq 0
\end{array}
$$

Global significativity of the model

Test of the model with a risk α

$$\begin{array}{c} H_0 : \quad \beta_2 = \beta_3 = \ldots = \beta_p = 0 \\ H_1 : \quad \exists j = 2, \ldots, p, \beta_j \neq 0 \end{array}$$

Statistics

$$F = \frac{n-p}{p-1} \frac{||\hat{Y} - \bar{\hat{Y}}||^2}{||Y - \hat{Y}||^2} \sim Fisher(p-1, n-p)$$

Global significativity of the model

Test of the model with a risk α

$$H_0 : \quad \beta_2 = \beta_3 = \ldots = \beta_p = 0$$
$$H_1 : \quad \exists j = 2, \ldots, p, \beta_j \neq 0$$

Statistics

$$F = \frac{n-p}{p-1} \frac{||\hat{Y} - \bar{\hat{Y}}||^2}{||Y - \hat{Y}||^2} \sim Fisher(p-1, n-p)$$

Remarque : $\frac{n-p}{p-1} \frac{||\hat{Y} - \bar{\hat{Y}}||^2}{||Y - \hat{Y}||^2} = \frac{SSE/(p-1)}{SSR/(n-p)}$ (E :Estimated ; R : Residuals)

Decision rule

- si $F_{obs} > q_\alpha^F$, H_0 is rejected, and there exist a coefficient which is not zero. **The regression is "useful"**
- si $F_{obs} \leq q_\alpha^F$, H_0 is acceted, all the coefficients are supposed to be null **The regression is not "useful"**

Global significativity of the model

- Fisher Statistic

Global significativity of the model

- Fisher Statistic
- Significativity test (bilateral)
  - $H_0 : \beta_2 = \ldots = \beta_p = 0$
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Global significativity of the model

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- Decision with a rish α, **Reject H_0 if**
  - si $\frac{n-p}{p-1} \frac{R^2}{1-R^2} > f_{p-1,n-p}(1-\alpha)$
  - si pvalue $< \alpha$

$\rightarrow$ The linear model has an added value

Global significativity of the model

Remarque1 : sur la statistique de Fisher :

$F = \frac{n-p}{p-1}\frac{R^2}{1-R^2}$

The R^2 coefficient increase mechanically with the number of variables

Global significativity of the model

Remarque1 : sur la statistique de Fisher :
$F = \frac{n-p}{p-1}\frac{R^2}{1-R^2}$
The R^2 coefficient increase mechanically with the number of variables

Remarque : the adjusted R^2 may be used

$R^2_{adj} = 1 - \frac{(1-R^2)(n-1)}{n-p}$

The R^2_{adj} does not increase ith the number of variables.

Boston Housing Data

The original data are $n = 506$ observations on $p = 14$ variables,

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

Boston Housing Data

Les données :

nř	crim	zn	indus	chas	nox	rm	age	dis	rad	tax	ptratio	b	lstat	medv
1	0.00632	18	2.31	0	0.538	6.575	65.2	4.0900	1	296	15.3	396.90	4.98	24.0
2	0.02731	0	7.07	0	0.469	6.421	78.9	4.9671	2	242	17.8	396.90	9.14	21.6
3	0.02729	0	7.07	0	0.469	7.185	61.1	4.9671	2	242	17.8	392.83	4.03	34.7
4	0.03237	0	2.18	0	0.458	6.998	45.8	6.0622	3	222	18.7	394.63	2.94	33.4
5	0.06905	0	2.18	0	0.458	7.147	54.2	6.0622	3	222	18.7	396.90	5.33	36.2
...	...	...	...	...	...	...	...	...	...	...	...	...	...	...

Boston Housing Data

MCO sous R

```
library(mlbench)
#Data data(BostonHousing) tab=BostonHousing;names(tab)
target="medv"; Y=tab[,target]; X=tab[,names(tab)!=target]; names(X)
#MCO resfit=lsfit(x=X,y=Y,intercept=T);
resfit$coef hist(resfit$res)
```

Cst	crim	zn	indus	chas	nox	rm	age	dis	rad	tax	ptratio	b	lstat	medv
36.45	-0.10	0.046	0.020	2.68	-17.76	3.80	0.00	-1.47	0.30	-0.01	-0.95			

Boston Housing Data

Modèle Linéaire sous R
code R

`reslm=lm(medv ~ .,data=tab); summary(reslm)` **Résultats :**

$n = 506$, $p = 14$

Residuals:

Min	1Q	Median	3Q	Max
-15.595	-2.730	-0.518	1.777	26.199

Coefficients:

	Estimate	Std. Error	t value	Pr(>|t|)	
(Intercept)	3.646e+01	5.103e+00	7.144	3.28e-12	***
crim	-1.080e-01	3.286e-02	-3.287	0.001087	**
zn	4.642e-02	1.373e-02	3.382	0.000778	***
indus	2.056e-02	6.150e-02	0.334	0.738288	
chas1	2.687e+00	8.616e-01	3.118	0.001925	**
nox	-1.777e+01	3.820e+00	-4.651	4.25e-06	***
rm	3.810e+00	4.179e-01	9.116	< 2e-16	***
age	6.922e-04	1.321e-02	0.052	0.958229	
dis	-1.476e+00	1.995e-01	-7.398	6.01e-13	***
rad	3.060e-01	6.635e-02	4.613	5.07e-06	***
tax	-1.233e-02	3.760e-03	-3.280	0.001112	**
ptratio	-9.527e-01	1.308e-01	-7.283	1.31e-12	***
b	9.312e-03	2.686e-03	3.467	0.000573	***
lstat	-5.248e-01	5.072e-02	-10.347	< 2e-16	***

```
Signif. codes: 0 *** 0.001/ ** 0.01 /* 0.05 /. 0.1 / 1
Residual standard error: 4.745 on 492 degrees of freedom
Multiple R-squared: 0.7406, Adjusted R-squared: 0.7338
F-statistic: 108.1 on 13 and 492 DF, p-value: < 2.2e-16
```

Précautions

- Multicolinéarité
  la solution des MCO nécessite de calculer $(X^T X)^{-1}$.
  Lorsque le déterminant de cette matrice est très proche de zéro, le problème est mal conditionné.

- Choix des variables
  Le coefficient de détermination R^2 augmente en fonction du nombre de variables.
  si $p = n$ $R^2 = 1$, ce qui n'est pas forcément pertinent.

Démonstration sous R