SD TSIA 204
Linear Models
Intro to linear models

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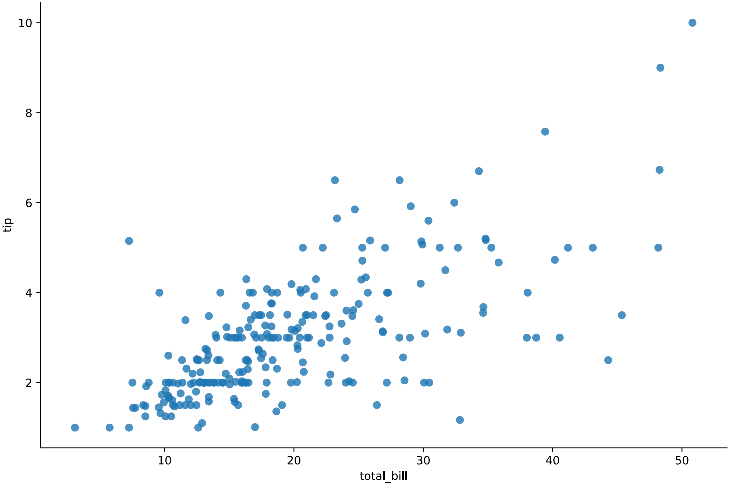
A 2D starting example



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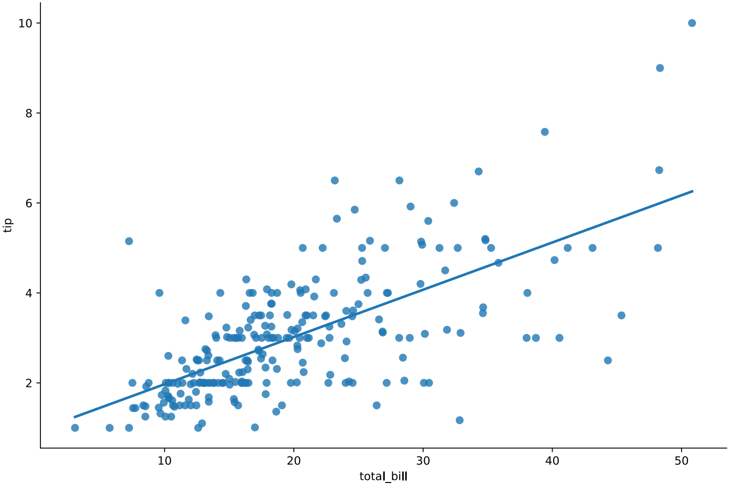

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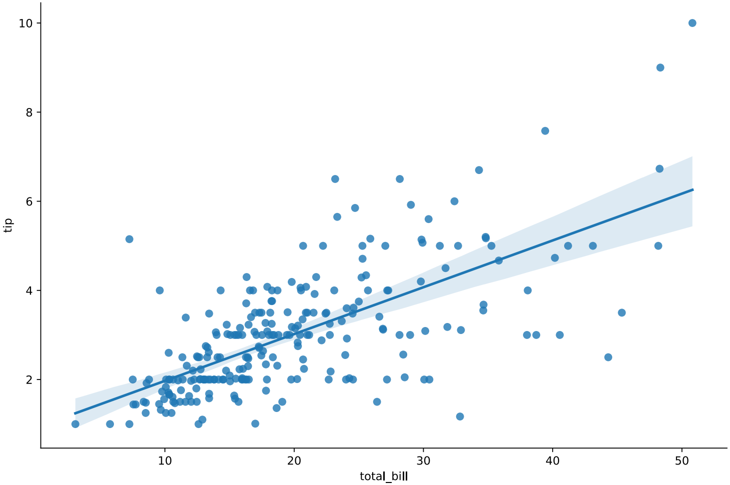


Notation interpretation

- $n = 244$
- $p = 1$
- y_i : tip let by the i-th customer
- x_i : total bill payed by the i-th customer
- y : the observation is the tips, dependent variable
- x : the feature/covariate, price of the bill, independent variable

Linear model / Linear regression hypothesis : assume that the price of the bill and the tip let are linearly correlated

Exo : use `describe()` from `Pandas` to get a rough data summary

Three questions to be covered : modeling, learning and predicting

```python
import numpy as np
import matplotlib.pyplot as plt
from sklearn.linear_model import LinearRegression
# Generate example data
np.random.seed(42)
X = np.random.rand(20, 1)*10 # Independent variable
y = 2 * X + 3 + np.random.randn(20, 1) # Dependent variable
# Fit linear regression model
model = LinearRegression()
model.fit(X, y)
# Predict y values using the model
X_new = np.linspace(0, 10, 100).reshape(-1, 1)
y_pred = model.predict(X_new)
# Create a scatter plot of the data points
plt.scatter(X, y, label='Data Points')
# Plot the linear regression line
plt.plot(X_new, y_pred, color='red', label='Linear Regression Line')
plt.xlabel('X')
plt.ylabel('y')
```

Modeling I, the 1D case

$$\text{Given a sample : } \quad (y_i, x_i), \text{ for } i = 1, \dots, n$$

Linear model or linear regression hypothesis assume :

$$\boxed{y_i \approx \theta_0^\star + \theta_1^\star x_i}$$

Model coefficients

- $\theta_0^\star$: intercept (unknown)
- $\theta_1^\star$: slope (unknown)

<u>Rem</u>: both parameters are unknown from the statistician

Data

- y is an **observation** or a variable to explain
- x is a **feature** or a covariate

Modeling II

Probabilistic model. Let us give a precise meaning to the sign $\approx$:

$$
\begin{aligned}
& y_i = \theta_0^\star + \theta_1^\star x_i + \varepsilon_i, \\
& \varepsilon_i \overset{i.i.d}{\sim} \varepsilon, \text{ for } i = 1, \ldots, n \\
& \mathbb{E}(\varepsilon) = 0
\end{aligned}
$$

where i.i.d. means "independent and identically distributed"

Interpretation : $\varepsilon_i = y_i - \theta_0^\star - \theta_1^\star x_i$: represent the error between the theoretical model and the observations, represented by random variables ε_i centered (often referred to as **white noise**).

<u>Rem</u>: motivation for the random nature of the noise – measurement noise, transmission noise, in-population variability, etc.

Modeling III

$$y_i = \theta_0^\star + \theta_1^\star x_i + \varepsilon_i$$

We call

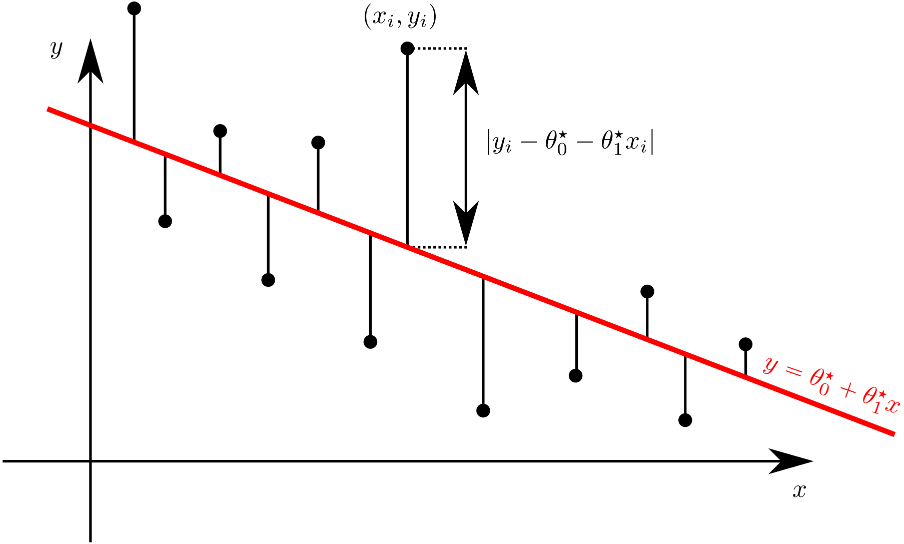
- **intercept** the scalar $\theta_0^\star$ (: *ordonnée à l'origine*)
- **slope** the scalar $\theta_1^\star$ (: *pente*)

Our **goal in the learning stage** is to estimate $\theta_0^\star$ and $\theta_1^\star$ (unknown) by $\widehat{\theta}_0$ and $\widehat{\theta}_1$ relying on observations (y_i, x_i) for $i = 1, \dots, n$

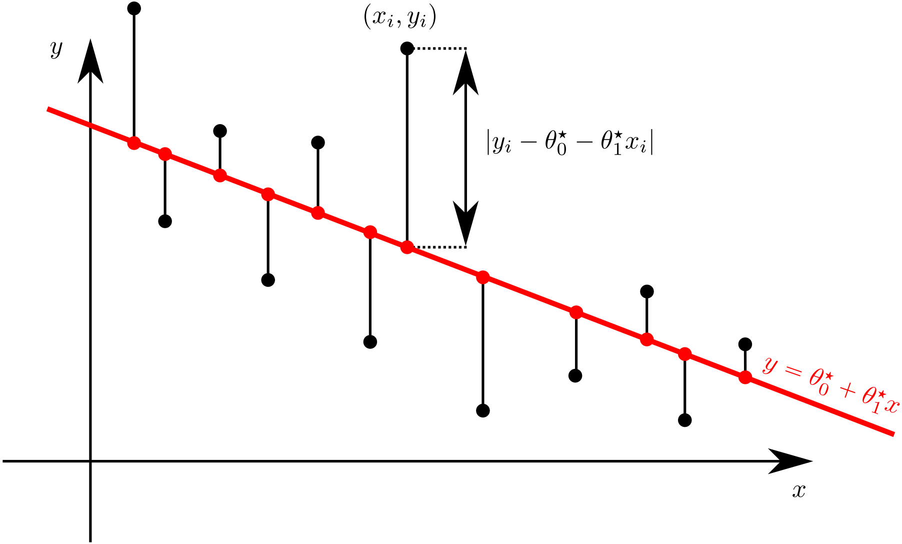
<u>Rem</u>: The "hat" notation is classical in statistics for referring to estimators

In **prediction time** $\widehat{y}_i = \widehat{\theta}_0 + \widehat{\theta}_1 x_i$

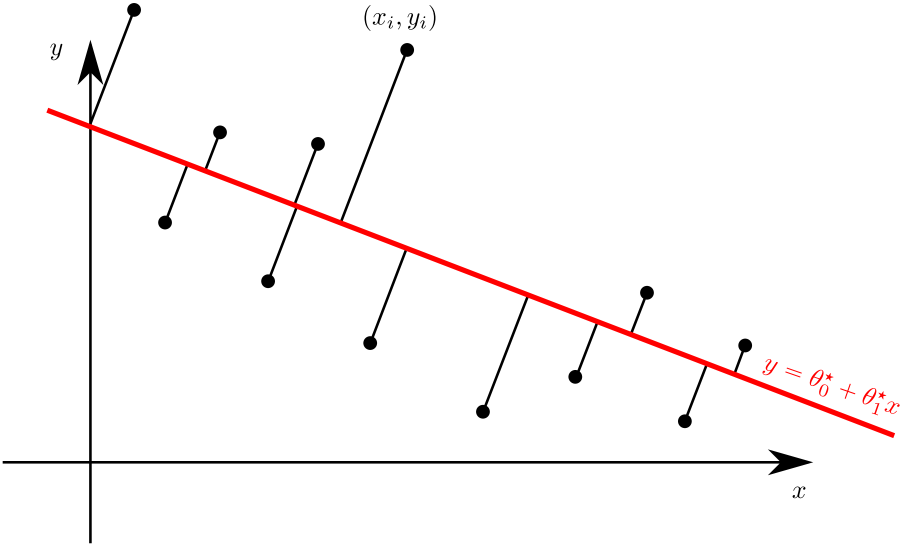
Least squares : visualization



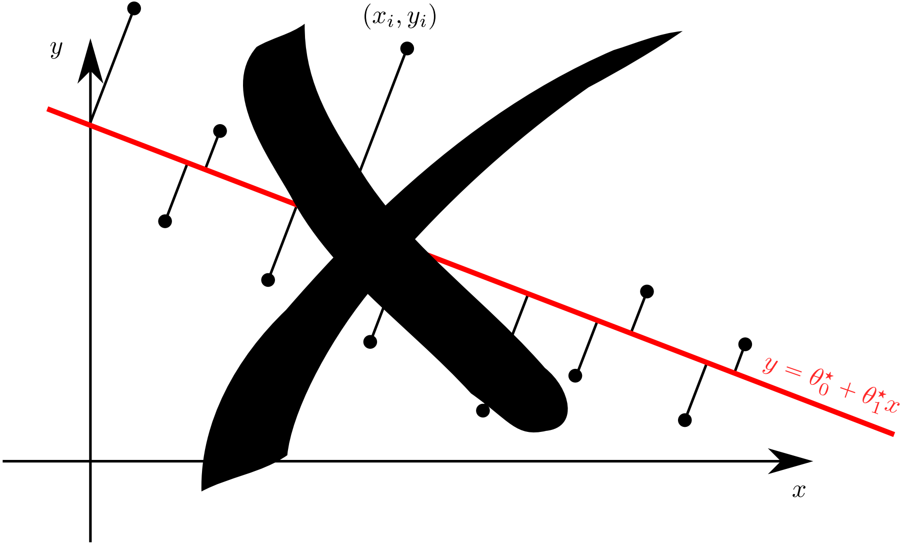
Least squares : visualization



(Total) Least squares : visualization



(Total) Least squares : visualization



Learning : mathematical formulation of Least squares

The **least squares** estimator is defined as :

$$(\widehat{\theta}_0, \widehat{\theta}_1) \in \operatorname{argmin}_{(\theta_0,\theta_1)\in\mathbb{R}^2} \sum_{i=1}^{n} \left(y_i - \theta_0 - \theta_1 x_i\right)^2$$

- Differentiate between θ^*, θ and $\widehat{\theta}$!!!!!
- it is also referred to as “ordinary least squares” (OLS)
- an original motivation for the squares is computational : first order conditions only require solving a linear system
- a solution always exists : minimizing a **coercive** continuous function (coercive : $\lim_{\|x\|\to+\infty} f(x) = +\infty$)

<u>Rem</u>: write « $\in$ argmin » as long as you do not know if the solution is unique

Least square authorship (controversial)

FIGURE – Adrien-Marie Legendre and Carl Friedrich Gauss

Historical / robust detour

The **least absolute deviation** (LAD) estimator reads :

$$(\widehat{\theta}_0, \widehat{\theta}_1) \in \operatorname{argmin}_{(\theta_0,\theta_1)\in\mathbb{R}^2} \sum_{i=1}^{n} |y_i - \theta_0 - \theta_1 x_i|$$

Rem: hard to compute without computer ; requires an optimization solver for non-smooth function (or a Linear Programming solver)

Rem: more robust to outliers (: *données aberrantes*)

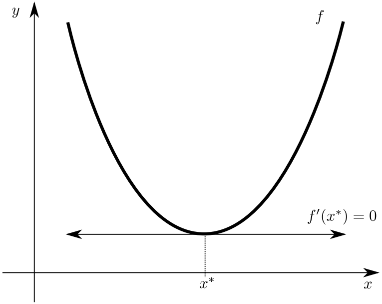
Least absolute deviation authorship

FIGURE – Ruđer Josip Bošković and Pierre-Simon de Laplace

Existence and uniqueness of the solution

Existence of a Local minimum : first order condition

Fermat's rule Theorem If f is differentiable, then at a local minimum x^* the gradient of f vanishes at x^*, *i.e.* $\nabla f(x^*) = 0$.



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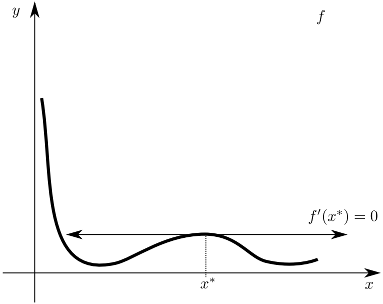

Rem: sufficient condition when f is strongly convex!

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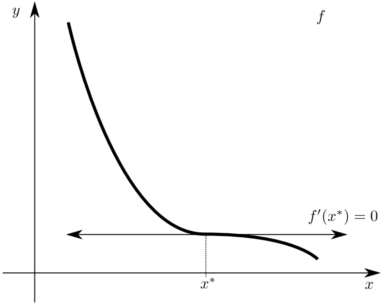


Rem: sufficient condition when f is strongly convex !

The Hessian Matrix and Gradients

The **gradient** ∇f is a vector of first-order partial derivatives :

$$\nabla f = \begin{bmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{bmatrix}$$

The **Hessian Matrix H** of f is a square matrix of second-order partial derivatives :

$$\mathbf{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial x_1^2} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2^2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n^2} \end{bmatrix}$$

The minimizer is unique $\Leftrightarrow$ f its strictly convex

f is quadratic $\implies$ f is convex.

$f(\widehat{\boldsymbol{\theta}})$ strictly convex $\Leftrightarrow \nabla^2 f(\widehat{\boldsymbol{\theta}})$ positive definite $\Leftrightarrow det(\nabla^2 f(\widehat{\boldsymbol{\theta}})) > 0$

Back to least squares

$$\widehat{\boldsymbol{\theta}} = (\widehat{\theta}_0, \widehat{\theta}_1) \in \operatorname{argmin}_{(\theta_0,\theta_1)\in\mathbb{R}^2} \frac{1}{2}\sum_{i=1}^{n}(y_i - \theta_0 - \theta_1 x_i)^2$$

For least squares, minimize the function of two variables :

$$f(\theta_0, \theta_1) = f(\boldsymbol{\theta}) = \frac{1}{2}\sum_{i=1}^{n}(y_i - \theta_0 - \theta_1 x_i)^2$$

First order condition / Fermat's rule :

$$\begin{cases} \frac{\partial f}{\partial \theta_0}(\widehat{\boldsymbol{\theta}}) = \sum_{i=1}^{n}(y_i - \widehat{\theta}_0 - \widehat{\theta}_1 x_i) = 0 \\ \frac{\partial f}{\partial \theta_1}(\widehat{\boldsymbol{\theta}}) = \sum_{i=1}^{n}(y_i - \widehat{\theta}_0 - \widehat{\theta}_1 x_i) x_i = 0 \end{cases}$$

Calculus continued

$$\text{Usual mean notation : } \overline{x}_n = \frac{1}{n}\sum_{i=1}^{n} x_i \text{ and } \overline{y}_n = \frac{1}{n}\sum_{i=1}^{n} y_i$$

With that, Fermat's rule states (dividing by n) :

$$\begin{cases} \frac{\partial f}{\partial \theta_0}(\widehat{\boldsymbol{\theta}}) = \sum_{i=1}^{n}(y_i - \widehat{\theta}_0 - \widehat{\theta}_1 x_i) = 0 \\ \frac{\partial f}{\partial \theta_1}(\widehat{\boldsymbol{\theta}}) = \sum_{i=1}^{n}(y_i - \widehat{\theta}_0 - \widehat{\theta}_1 x_i)x_i = 0 \end{cases}$$

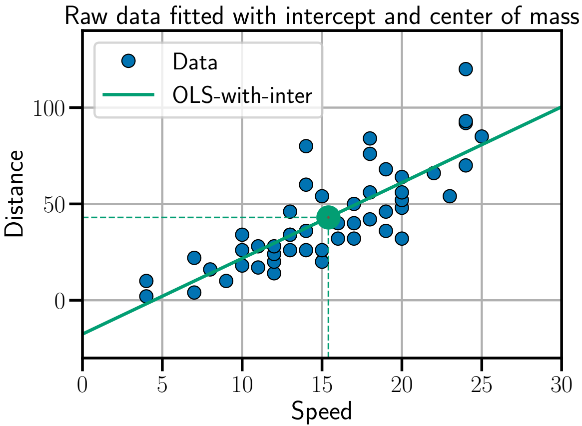
$$\Leftrightarrow$$

$$\begin{cases} \widehat{\theta}_0 = \overline{y}_n - \widehat{\theta}_1 \overline{x}_n & \text{(CNO1)} \\ \widehat{\theta}_1 = \dfrac{\sum_{i=1}^{n}(x_i - \overline{x}_n)(y_i - \overline{y}_n)}{\sum_{i=1}^{n}(x_i - \overline{x}_n)^2} & \text{(CNO2)} \end{cases}$$

Exo : Show that the solution to the OLS is unique iff $Var(x) \neq 0$

Center of gravity and interpretation

$$(\text{CNO1}) \Leftrightarrow (\overline{x}_n, \overline{y}_n) \in \{(x,y) \in \mathbb{R}^2 : y = \widehat{\theta}_0 + \widehat{\theta}_1 x\}$$



- $\overline{speed} = 15.4$
- $\overline{dist} = 42.98$
- $\widehat{\theta}_0 = -17.579095$ intercept (negative !)
- $\widehat{\theta}_1 = 3.932409$ slope

Physical interpretation : the cloud of points' center of gravity belongs to the (estimated) regression line

Vector formulation

<u>Notation</u> : $\mathbf{x} = (x_1, \ldots, x_n)^\top$ and $\mathbf{y} = (y_1, \ldots, y_n)^\top$

$$\text{(CNO2)} \Leftrightarrow \widehat{\theta}_1 = \frac{\sum_{i=1}^n (x_i - \overline{x}_n)(y_i - \overline{y}_n)}{\sum_{i=1}^n (x_i - \overline{x}_n)^2}$$

$$\text{(CNO2)} \Leftrightarrow \widehat{\theta}_1 = \mathrm{corr}_n(\mathbf{x}, \mathbf{y}) \cdot \frac{\sqrt{\mathrm{var}_n(\mathbf{y})}}{\sqrt{\mathrm{var}_n(\mathbf{x})}}$$

where $$\mathrm{corr}_n(\mathbf{x}, \mathbf{y}) = \frac{\frac{1}{n}\sum_{i=1}^n (x_i - \overline{x}_n)(y_i - \overline{y}_n)}{\sqrt{\mathrm{var}_n(\mathbf{x})}\sqrt{\mathrm{var}_n(\mathbf{y})}}$$

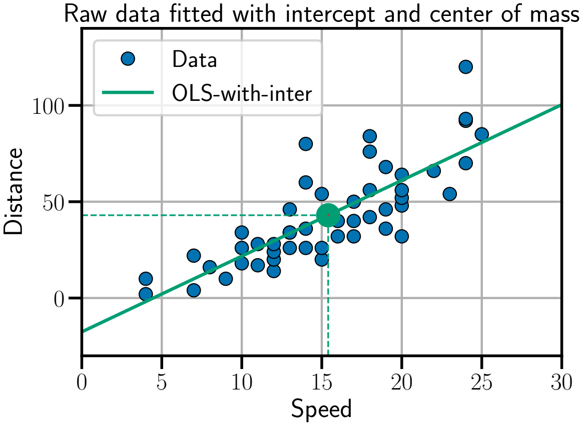
and $$\mathrm{var}_n(\mathbf{z}) = \frac{1}{n}\sum_{i=1}^n (z_i - \overline{z}_n)^2 \text{ (for any } \mathbf{z} = (z_1, \ldots, z_n)^\top\text{)}$$

respectively **empirical correlation**, **empirical variances**

cars example

Braking distance for cars as a sunction of the speed

Line slope : $\mathrm{corr}_n(\mathbf{x},\mathbf{y}) \cdot \frac{\sqrt{\mathrm{var}_n(\mathbf{y})}}{\sqrt{\mathrm{var}_n(\mathbf{x})}} = 3.932409.$



Centering

Centered model :

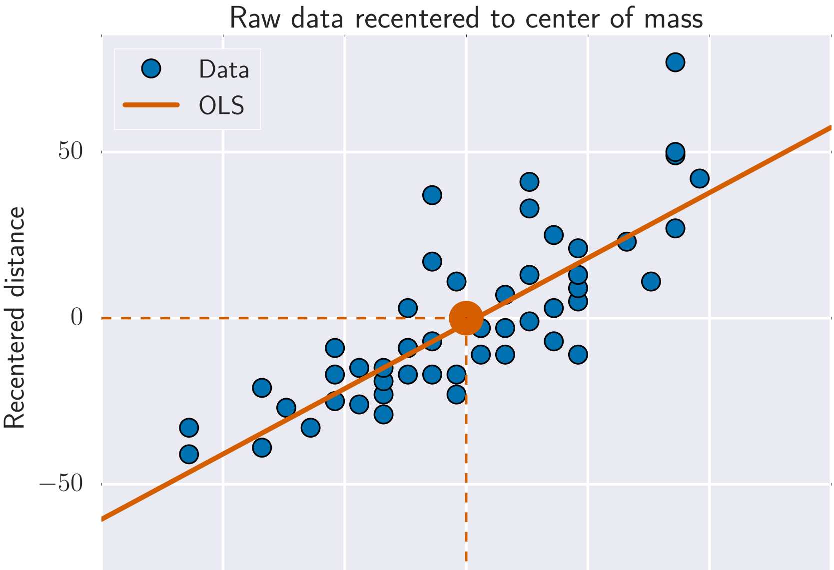
$$\text{Write for any } i = 1, \dots, n : \begin{cases} x'_i = x_i - \overline{x}_n \\ y'_i = y_i - \overline{y}_n \end{cases} \quad \Leftrightarrow \begin{cases} \mathbf{x}' = \mathbf{x} - \overline{x}_n \mathbf{1}_n \\ \mathbf{y}' = \mathbf{y} - \overline{y}_n \mathbf{1}_n \end{cases}$$

and $\mathbf{1}_n = (1, \dots, 1)^\top \in \mathbb{R}^n$, then solving the OLS with $(\mathbf{x}', \mathbf{y}')$ leads to

$$\begin{cases} \widehat{\theta}'_0 = 0 \\ \widehat{\theta}'_1 = \dfrac{\dfrac{1}{n}\displaystyle\sum_{i=1}^n x'_i y'_i}{\dfrac{1}{n}\displaystyle\sum_{i=1}^n x'^2_i} \end{cases}$$

<u>Rem</u>: equivalent to choosing the cloud of points' center of mass as origin, *i.e.* $(\overline{x}'_n, \overline{y}'_n) = (0, 0)$

Centering (II)



Centering and interpretation

Consider the coefficient $\widehat{\theta}'_1$ ($\widehat{\theta}'_0 = 0$) for centered points $\mathbf{y}', \mathbf{x}'$, then :

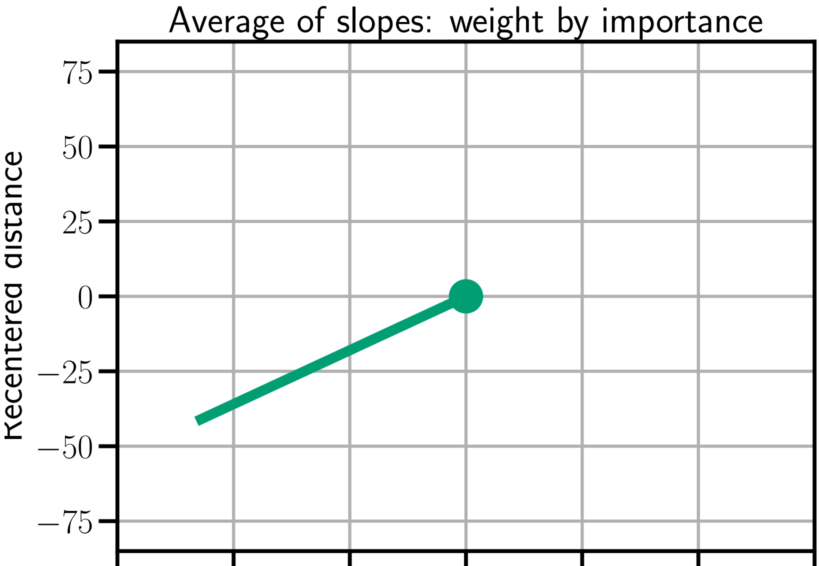
$$\widehat{\theta}'_1 \in \text{argmin}_{\theta_1} \sum_{i=1}^{n} (y'_i - \theta_1 x'_i)^2 = \text{argmin}_{\theta_1} \sum_{i=1}^{n} x'^2_i \left(\frac{y'_i}{x'_i} - \theta_1 \right)^2$$

<u>Interpretation</u> : $\widehat{\theta}'_1$ is a weighted average of the slopes $\frac{y'_i}{x'_i}$

$$\widehat{\theta}'_1 = \frac{\displaystyle\sum_{i=1}^{n} x'^2_i \frac{y'_i}{x'_i}}{\displaystyle\sum_{j=1}^{n} x'^2_j}$$

<u>Influence of extreme points</u> : weights proportional to x'^2_i ; connected to the **leverage** (🇫🇷 : *levier*) effect

Extreme points – leverage effect



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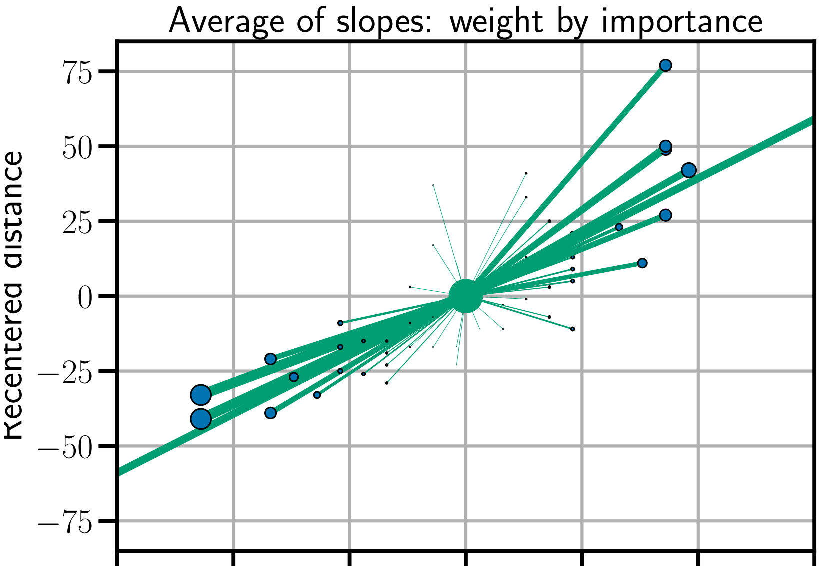
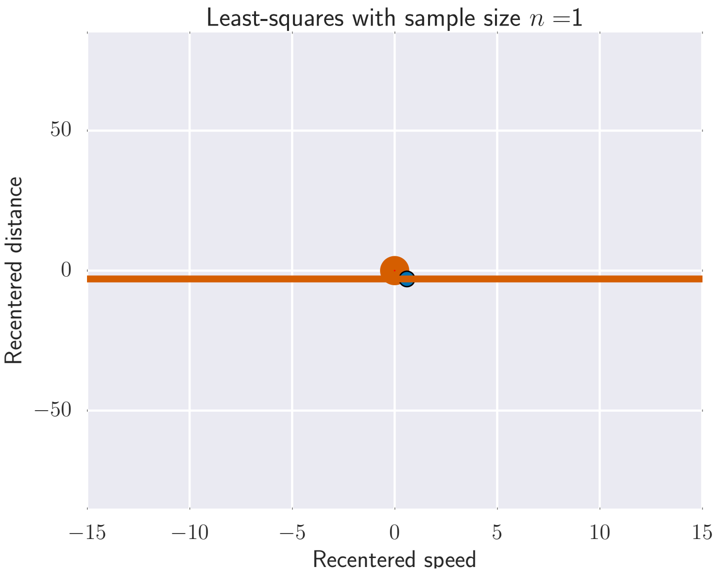


Extreme points – leverage effect (II)



Centering + scaling (standardization)

Centered-scaled model :

$$\forall i = 1, \dots, n : \begin{cases} x_i'' = (x_i - \overline{x}_n)/\sqrt{\mathrm{var}_n(\mathbf{x})} \\ y_i'' = (y_i - \overline{y}_n)/\sqrt{\mathrm{var}_n(\mathbf{y})} \end{cases} \quad \Leftrightarrow \begin{cases} \mathbf{x}'' = \dfrac{\mathbf{x} - \overline{x}_n \mathbf{1}_n}{\sqrt{\mathrm{var}_n(\mathbf{x})}} \\ \mathbf{y}'' = \dfrac{\mathbf{y} - \overline{y}_n \mathbf{1}_n}{\sqrt{\mathrm{var}_n(\mathbf{y})}} \end{cases}$$

Solving OLS with $(\mathbf{x}'', \mathbf{y}'')$ then

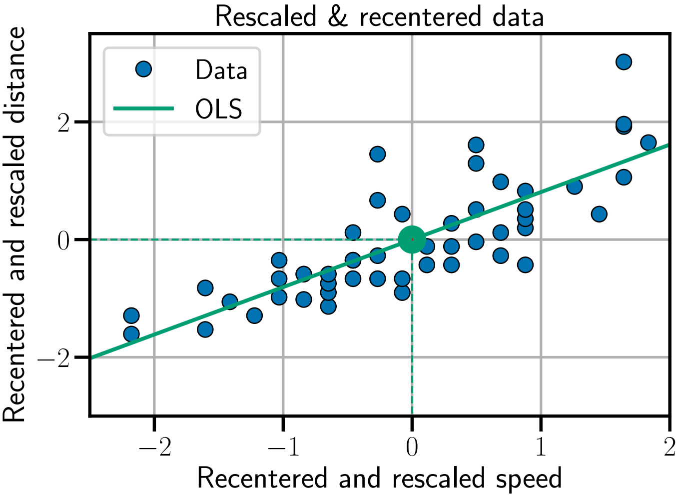
$$\begin{cases} \widehat{\theta}_0'' = 0 \\ \widehat{\theta}_1'' = \dfrac{1}{n} \displaystyle\sum_{i=1}^{n} x_i'' y_i'' \end{cases}$$

Rem: equivalent to choosing the points cloud center of mass as origin and normalize $\mathbf{x}$ and $\mathbf{y}$ to have unit **empirical norm** $\|\cdot\|_n$:

$$\|\mathbf{x}''\|_n^2 = \frac{1}{n} \sum_{i=1}^{n} (x_i'')^2 = 1$$

$$\|\mathbf{y}''\|_n^2 = \frac{1}{n} \sum_{i=1}^{n} (y_i'')^2 = 1$$

Centering + scaling



When/why preprocessing ?

Centering **y** or using an intercept (or adding a constant feature) is equivalent

Rem: for sparse (🇫🇷 : *creux*) cases centering **y** adding a constant feature could be preferred

Scaling features is important :

- if you want to interpret the coefficients' amplitude in regression (better solution : t-tests)
- if you want to penalize or regularize coefficients (*c.f.* Lasso, Ridge, etc.) a single scale is needed
- for computing reasons (*e.g.* store scaling to improve efficiency, etc.)

Rem: in practice centering/scaling is useful for **estimation** not so much for **prediction** (see next courses)

What happens with the logarithm scaling ?

Centering with `Python`

Use centering classes from `sklearn`, see `preprocessing` :

http://scikit-learn.org/stable/modules/preprocessing.html

```
from sklearn import preprocessing

scaler = preprocessing.StandardScaler().fit(X)

print(np.isclose(scaler.mean_, np.mean(X)))

print(np.array_equal(scaler.std_, np.std(X)))

print(np.array_equal(scaler.transform(X),
                     (X - np.mean(X)) / np.std(X)))

print(np.array_equal(scaler.transform([26]),
                     (26 - np.mean(X)) / np.std(X)))
```

Rem:most valuable with `pipeline`

http://scikit-learn.org/stable/modules/pipeline.html

Prediction

We call **prediction** function the function that associates an estimation of the variable of interest to a new sample. For least squares the prediction is given by :

$$\mathrm{pred}(x_{n+1}) = \widehat{\theta}_0 + \widehat{\theta}_1 x_{n+1}$$

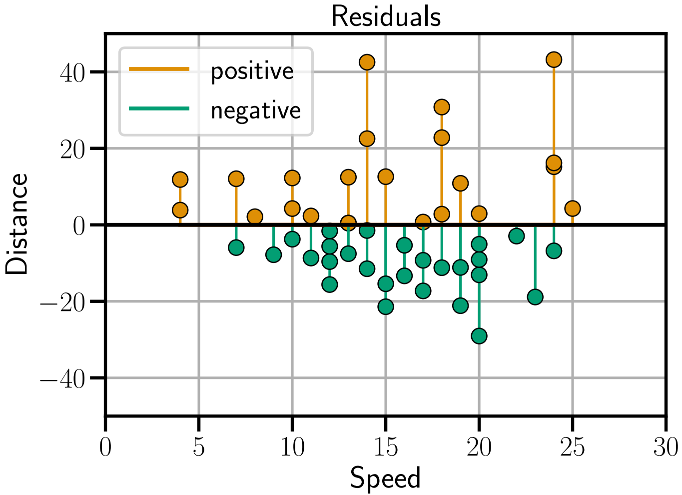
<u>Rem</u>: often written $\widehat{y}_{n+1}$ (implicit dependence on x_{n+1})

The **residual** : difference between observations and predicted values

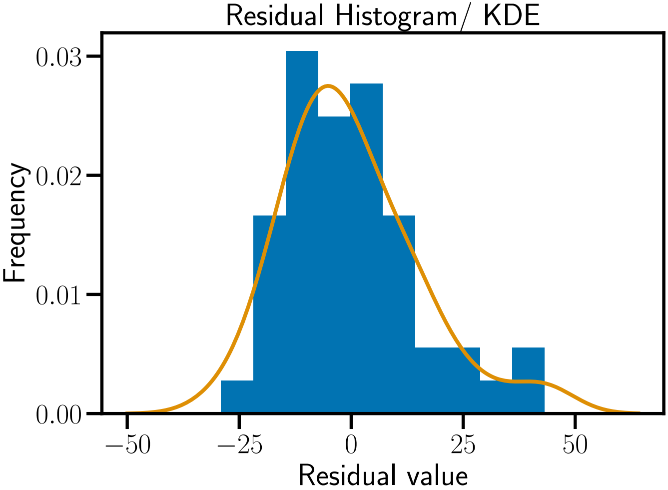
$$\epsilon_i = y_i - \mathrm{pred}(x_i) = y_i - \widehat{y}_i = y_i - (\widehat{\theta}_0 + \widehat{\theta}_1 x_i)$$

<u>Rem</u>: observable estimate of the unobservable statistical error

Residuals (on cars)



Residual histograms



Least squares motivation

- Computing advantage : computationally heavy methods avoided before computers (*e.g.* iterative methods)
- Theoretical advantage : least square analysis easy under simple hypothesis
- Interpretability : how much does the regressor increase with the features

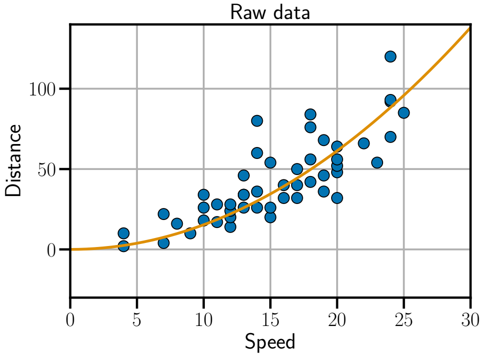
Example : under additive white Gaussian noise assumption *i.e.*, $\varepsilon \sim \mathcal{N}(0, \sigma^2)$ the maximum likelihood is equivalent to solving least squares to estimate $(\theta_0^\star, \theta_1^\star)$

Rem: for another noise model and/or to limit outliers influence one can solve (see *e.g.* `QuantReg` in `statsmodels`)

$$\boxed{\widehat{\boldsymbol{\theta}} = (\widehat{\theta}_0, \widehat{\theta}_1) \in \mathrm{argmin}_{(\theta_0,\theta_1)\in\mathbb{R}^2} \sum_{i=1}^{n} |y_i - \theta_0 - \theta_1 x_i|}$$

Discussion : toward multivariate cases

Physical laws (or your driving school memories) would lead to rather pick a **quadratic** model instead of a **linear** one : the OLS can be applied by choosing x_i^2 as features instead of x_i :

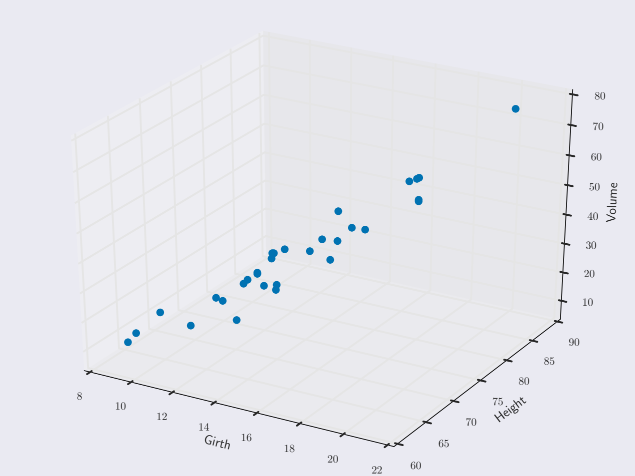


Web sites and books to go further

- Datascience in general : Blog + videos by Jake Vanderplas `http://jakevdp.github.io/`
  Homework for next lesson : watch the following videos `http://jakevdp.github.io/blog/2017/03/03/reproducible-data-analysis-in-jupyter/`
- A few notebooks of OLS with `statsmodels`
- McKinney (2012) about `Python` for statistics
- Lejeune (2010) about linear models (in French)
- Regression course by B. Delyon (in French, more technical)

Toward multivariate models

Tree volume as a function of height / girth (🇫🇷 : *circonférence*)



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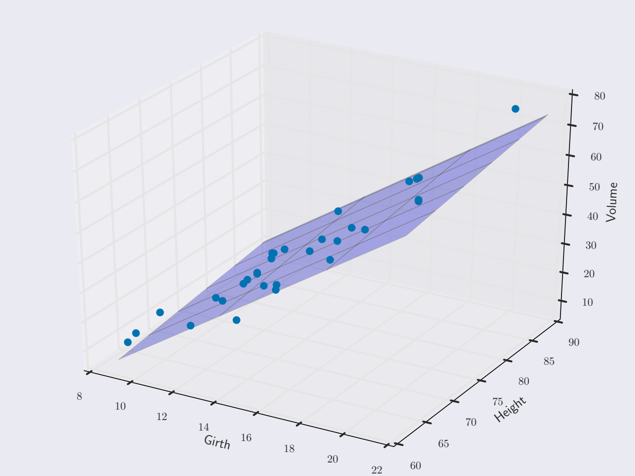


Python commands

```python
import numpy as np
import matplotlib.pyplot as plt
from sklearn.linear_model import LinearRegression

# Generate example data
...

# Fit linear regression model
model = LinearRegression()
model.fit(X, y)
```

Model

One observes p features $(\mathbf{x}_1, \ldots, \mathbf{x}_p)$. Model in dimension p

$$\begin{aligned}
y_i &= \theta_0^\star + \sum_{j=1}^{p} \theta_j^\star x_{i,j} + \varepsilon_i \\
\varepsilon_i &\overset{i.i.d}{\sim} \varepsilon, \text{ pour } i = 1, \ldots, n \\
\mathbb{E}[\varepsilon] &= 0
\end{aligned}$$

Rem: we assume (frequentist point of view) there exists a “true” parameter $\boldsymbol{\theta}^\star = (\theta_0^\star, \ldots, \theta_p^\star)^\top \in \mathbb{R}^{p+1}$

Dimension p

Matrix model

$$\underbrace{\begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}}_{\mathbf{y}} = \underbrace{\begin{pmatrix} 1 & x_{1,1} & \dots & x_{1,p} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & x_{n,1} & \dots & x_{n,p} \end{pmatrix}}_{X} \underbrace{\begin{pmatrix} \theta_0^\star \\ \vdots \\ \theta_p^\star \end{pmatrix}}_{\boldsymbol{\theta}^\star} + \underbrace{\begin{pmatrix} \varepsilon_1 \\ \vdots \\ \varepsilon_n \end{pmatrix}}_{\boldsymbol{\epsilon}}$$

$$\text{Equivalently :} \quad \boxed{\mathbf{y} = X\boldsymbol{\theta}^\star + \boldsymbol{\epsilon}} \tag{1}$$

Column notation : $X = (\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_p)$ with $\mathbf{x}_0 = \mathbf{1}_n = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix}$.

Line notation : $X = \begin{pmatrix} x_1^\top \\ \vdots \\ x_n^\top \end{pmatrix} = (x_1, \dots, x_n)^\top$

Matrix Notation and L_2 Norm

Matrix notation is a powerful way to represent mathematical operations involving vectors and matrices.

The **Inner Product** (dot product) of two vectors $\mathbf{u}$ and $\mathbf{v}$ is defined as :

$$\langle \mathbf{u}, \mathbf{v} \rangle = \sum_{i=1}^{n} u_i v_i = \mathbf{u} \cdot \mathbf{v}^T$$

Let $\mathbf{A}$ be an $m \times n$ matrix and $\mathbf{B}$ be an $n \times p$ matrix. The **matrix product** $\mathbf{C} = \mathbf{AB}$ is an $m \times p$ matrix with elements :

$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj}$$

The L_2 **Norm** (Euclidean norm) of a vector $\mathbf{v}$ is defined as :

$$\|\mathbf{v}\|_2 = \sqrt{\sum_{i=1}^{n} v_i^2}$$

Matrix notation simplifies operations and equations involving vectors and matrices.

Vocabulary

$$\boxed{\mathbf{y} = X\boldsymbol{\theta}^\star + \boldsymbol{\epsilon}}$$

- $\mathbf{y} \in \mathbb{R}^n$: observations vector
- $X \in \mathbb{R}^{n\times(p+1)}$: **design** matrix (with features as columns and a first column of 1s)
- $\tilde{X} \in \mathbb{R}^{n\times(p)}$: **reduced design** matrix (with features as columns and NO column of ones)
- $\boldsymbol{\theta}^\star \in \mathbb{R}^{p+1}$: (unknown) **true** parameter to be estimated
- $\boldsymbol{\epsilon} \in \mathbb{R}^n$: noise vector

(Ordinary) Least squares

A least square estimator is **any** solution of the following problem :

$$\widehat{\boldsymbol{\theta}} \in \operatorname{argmin}_{\boldsymbol{\theta} \in \mathbb{R}^{p+1}} \left(\|\mathbf{y} - X\boldsymbol{\theta}\|_2^2 \right)$$

$$\widehat{\boldsymbol{\theta}} \in \operatorname{argmin}_{\boldsymbol{\theta} \in \mathbb{R}^{p+1}} \sum_{i=1}^{n} \left[y_i - \left(\theta_0 + \sum_{j=1}^{p} \theta_j x_{i,j} \right) \right]^2$$

$$\widehat{\boldsymbol{\theta}} \in \operatorname{argmin}_{\boldsymbol{\theta} \in \mathbb{R}^{p+1}} \sum_{i=1}^{n} \left[y_i - \langle x_i, \boldsymbol{\theta} \rangle \right]^2$$

- Does the solution exist ? A solution always exists, as we are minimizing a coercive continuous function (**coercive** : $\lim_{\|x\| \to +\infty} f(x) = +\infty$)
- Is the solution unique ? not guaranteed

Exo how do we make the prediction ?

Row / column interpretation

Row interpretation

Let $\tilde{x}_1^\top, \ldots, \tilde{x}_{p+1}^\top$ be the rows of X. The residuals are $r_i = \tilde{x}_i \boldsymbol{\theta} - y_i$ and the OLS is equivalent to minimizing the sum of squares residuals

Column interpretation

Let $x_1, \ldots, x_{p+1}$ be the columns of X. Then $\|\mathbf{y} - X\boldsymbol{\theta}\|_2^2 = \|(\theta_0 x_0, \ldots, \theta_p x_p) - \mathbf{y}\|_2^2$, so OLS is to find a linear combination of columns of X that is closest to $\mathbf{y}$.

Vocabulary (and abuse of terms)

We call **Gram matrix** the matrix

$$X^\top X$$

whose general term is $[X^\top X]_{i,j} = \langle \mathbf{x}_i, \mathbf{x}_j \rangle$

If the design matrix X is centered and scaled, the Gram matrix is proportional to the correlation between columns. $X^\top X$ is often referred to as the feature correlation matrix

<u>Rem</u>: when columns are scaled such that $\forall j \in [\![0, p]\!], \|\mathbf{x}_j\|^2 = n$, the Gramian diagonal is $(n, \dots, n)$

The vector $X^\top \mathbf{y} = \begin{pmatrix} \langle \mathbf{x}_0, \mathbf{y} \rangle \\ \vdots \\ \langle \mathbf{x}_p, \mathbf{y} \rangle \end{pmatrix}$ represents the correlation between the observations and the features

Hilbert projection theorem (HPT)

Let $C \subset \mathbb{R}^d, Y \in \mathbb{R}^d$. Let $\widehat{z} = \arg\min_{z \in C} \|Y - z\|_2^2$. Then $\widehat{z}$ always exists and is given by

$$\boxed{< Y - \widehat{z}, z >= 0 \qquad \forall z \in C}$$

Hilbert projection theorem (HPT) and application to OLS

$$\widehat{\boldsymbol{\theta}} \in \text{argmin}_{\theta\in\mathbb{R}^{p+1}} \|\mathbf{y} - X\boldsymbol{\theta}\|_2^2$$

Note $col(X) = span([x_0, ..., x_p]) = \sum_{j=0}^{p} x_j\theta_j = X\boldsymbol{\theta}$ OLS :
$\widehat{W} \in \text{argmin}_{W\in col(X)} \left(\|\mathbf{y} - W\|_2^2\right)$

$$\begin{aligned}
< \mathbf{y} - \widehat{W}, W > &= 0 \\
(\mathbf{y} - \widehat{W})^\top W &= 0 \\
(\mathbf{y} - \widehat{W})^\top X\boldsymbol{\theta} &= 0 \\
(\mathbf{y} - \widehat{W})^\top X &= 0 \\
(\mathbf{y} - X\widehat{\boldsymbol{\theta}})^\top X &= 0 \\
X^\top(\mathbf{y} - X\widehat{\boldsymbol{\theta}}) &= 0 \\
X^\top X\widehat{\boldsymbol{\theta}} &= X^\top\mathbf{y}
\end{aligned} \tag{2}$$

OLS normal equations

The solution to the OLS problem is given by the solution to the normal equation

$$\textbf{Normal equation :} \boxed{X^\top X \widehat{\boldsymbol{\theta}} = X^\top \mathbf{y}}$$

As a consequence,

- a solution always exists.
- its unique if the solution to the normal equations is unique

Hilbert projection theorem

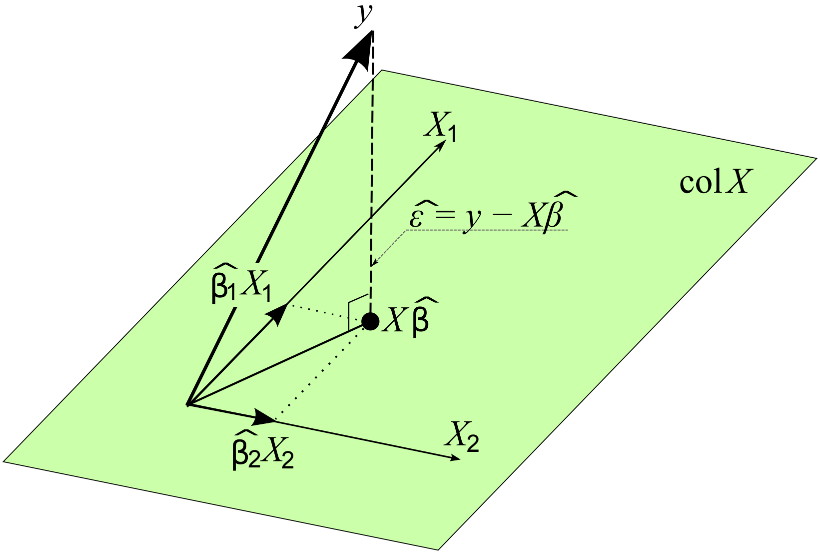


FIGURE – Souce : Wikipedia

Least squares and uniqueness

Let $\widehat{\boldsymbol{\theta}}$ be a solution of $\boxed{X^\top X\widehat{\boldsymbol{\theta}} = X^\top \mathbf{y}}$

Non uniqueness : happens for non trivial kernel,*i.e.* when $\ker(X) = \{\boldsymbol{\theta} \in \mathbb{R}^{p+1} : X\boldsymbol{\theta} = 0\} \neq \{0\}$

Assume $\boldsymbol{\theta}_K \in \ker(X)$ with $\boldsymbol{\theta}_K \neq 0$, then

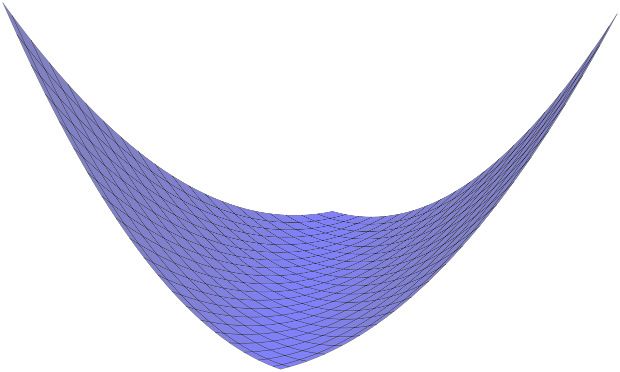
$$\begin{aligned} X(\widehat{\boldsymbol{\theta}} + \boldsymbol{\theta}_K) &= X\widehat{\boldsymbol{\theta}} \\ \text{and then} \quad (X^\top X)(\widehat{\boldsymbol{\theta}} + \boldsymbol{\theta}_K) &= X^\top \mathbf{y} \end{aligned}$$

<u>Conclusion</u> : the set of least squares solutions is an affine sub-space

$$\boxed{\widehat{\boldsymbol{\theta}} + \ker(X)}$$

Optimization in $\mathbb{R}^d$

Convex case, $f(\boldsymbol{\theta}) = \|\mathbf{y} - X\boldsymbol{\theta}\|_2^2$, where the set of minimizers is non-unique :



Optimization in $\mathbb{R}^d$

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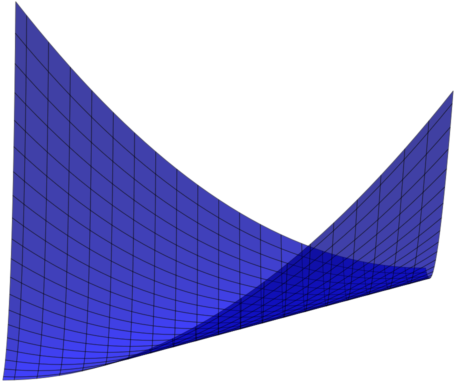

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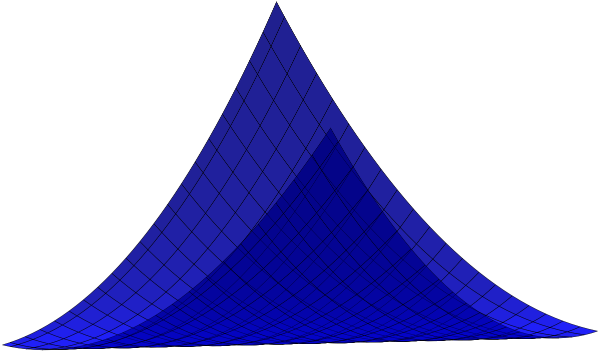

Optimization in $\mathbb{R}^d$

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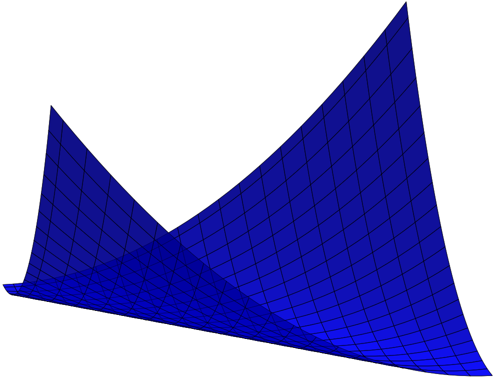
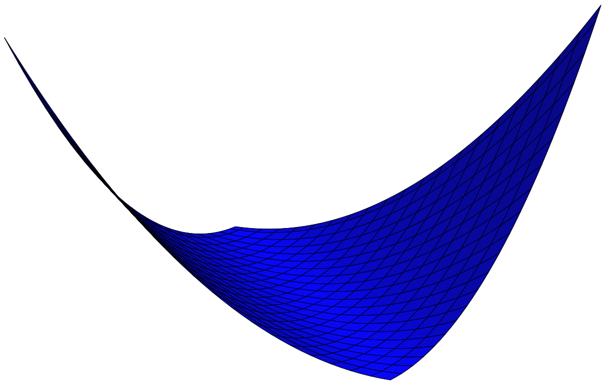


Optimization in $\mathbb{R}^d$

Convex case, $f(\boldsymbol{\theta}) = \|\mathbf{y} - X\boldsymbol{\theta}\|_2^2$, where the set of minimizers is non-unique :



Non uniqueness : single feature case

Reminder : $$X = \begin{pmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix}$$

If $\ker(X) = \{\boldsymbol{\theta} \in \mathbb{R}^2 : X\boldsymbol{\theta} = 0\} \neq \{0\}$ there exists $(\theta_0, \theta_1) \neq (0, 0)$:

$$\begin{cases} \theta_0 + \theta_1 x_1 & = 0 \\ \vdots \qquad \vdots & = \vdots \\ \theta_0 + \theta_1 x_n & = 0 \end{cases} \qquad (\star)$$

1. If $\theta_1 = 0$: $(\star) \Rightarrow \theta_0 = 0$, so $(\theta_0, \theta_1) = (0, 0)$, **contradiction**
2. If $\theta_1 \neq 0$:
   2.1 If $\forall i, x_i = 0$ then $X = (\mathbf{1}_n, 0)$ and $\theta_0 = 0$
   2.2 Otherwise there exists $x_{i_0} \neq 0$ and $\forall i, x_i = -\theta_0/\theta_1 = x_{i_0}$, *i.e.* $X = [\mathbf{1}_n \quad x_{i_0} \cdot \mathbf{1}_n]$

Interpretation : $\mathbf{x}_1 \propto \mathbf{1}_n$, *i.e.* $\mathbf{x}_1$ is constant

Interpretation for multivariate cases

Reminder : we write $X = (\mathbf{1}_n, \mathbf{x}_1, \ldots, \mathbf{x}_p)$, the features being column-wise (each are of length n)

The property $\ker(X) = \{\boldsymbol{\theta} \in \mathbb{R}^{p+1} : X\boldsymbol{\theta} = 0\} \neq \{0\}$ means that there exists a linear dependence between the features $\mathbf{1}_n, \mathbf{x}_1, \ldots, \mathbf{x}_p$,

Reformulation : $\exists \boldsymbol{\theta} = (\theta_0, \ldots, \theta_p)^\top \in \mathbb{R}^{p+1} \setminus \{0\}$ s.t.

$$\theta_0 \mathbf{1}_n + \sum_{j=1}^{p} \theta_j \mathbf{x}_j = 0$$

Algebra reminder

Rank of a matrix : $\quad \mathrm{rank}(X) = \dim(\mathrm{span}(\mathbf{1}_n, \mathbf{x}_1, \ldots, \mathbf{x}_p))$; $\mathrm{span}(\cdot)$: the space generated by $\cdot$

Property : $\mathrm{rank}(X) = \mathrm{rank}(X^\top)$

Rank–nullity theorem :

- $\mathrm{rank}(X) + \dim(\ker(X)) = p + 1$
- $\mathrm{rank}(X^\top) + \dim(\ker(X^\top)) = n$

Property : $\boxed{\mathrm{rank}(X) \leq \min(n, p+1)}$

See Golub and Van Loan (1996) for details

Algebra reminder (continued)

Matrix inversion : A square matrix $A \in \mathbb{R}^{m \times m}$ is invertible

- if and only if its kernel is trivial : $\ker(A) = \{0\}$
- if and only if it is full rank $\text{rank}(A) = m$

OLS is unique iff $X^\top X$ is invertible

$\Leftrightarrow \ker(X^\top X) = \{0\}$

$\Leftrightarrow \ker(X) = \{0\}$

$\Leftrightarrow X$ has full rank

Exo: $\ker(X) = \ker(X^\top X)$

Prediction

$$\textbf{Prediction vector :} \qquad \widehat{\mathbf{y}} = X\widehat{\boldsymbol{\theta}}$$

Rem: $\widehat{\mathbf{y}}$ depends linearly on the observation vector $\mathbf{y}$

Rem: an **orthogonal projector** is a matrix H such that

1. H is symmetric : $H^\top = H$
2. H is idempotent : $H^2 = H$

Proposition Writing H_X the orthogonal projector onto the space span by the columns of X, one gets $\widehat{\mathbf{y}} = H_X\mathbf{y}$

If X is full (column) rank, then $H_X = X(X^\top X)^{-1}X^\top$ is called the **hat matrix**

Exo: Show that H_X is an orthogonal projector

Prediction (continued)

If a new observation $x_{n+1} = (x_{n+1,1}, \ldots, x_{n+1,p})$ is provided, the associated prediction is :

$$\widehat{y}_{n+1} = \langle \widehat{\boldsymbol{\theta}}, (1, x_{n+1,1}, \ldots, x_{n+1,p})^\top \rangle$$
$$\widehat{y}_{n+1} = \widehat{\theta}_0 + \sum_{j=1}^{p} \widehat{\theta}_j x_{n+1,j}$$

<u>Rem</u>: the normal equation ensures **equi-correlation** between observations and features :

$$\begin{aligned}(X^\top X)\widehat{\boldsymbol{\theta}} = X^\top \mathbf{y} \Leftrightarrow X^\top \widehat{\mathbf{y}} &= X^\top \mathbf{y} \\ \Leftrightarrow \begin{pmatrix} \langle \mathbf{x}_0, \widehat{\mathbf{y}} \rangle \\ \vdots \\ \langle \mathbf{x}_p, \widehat{\mathbf{y}} \rangle \end{pmatrix} &= \begin{pmatrix} \langle \mathbf{x}_0, \mathbf{y} \rangle \\ \vdots \\ \langle \mathbf{x}_p, \mathbf{y} \rangle \end{pmatrix}\end{aligned}$$

Residuals and normal equation

$$\textbf{Residual(s)}: \quad \widehat{\boldsymbol{\varepsilon}} = \mathbf{y} - \widehat{\mathbf{y}} = \mathbf{y} - X\widehat{\boldsymbol{\theta}} = (\mathrm{Id}_n - H_X)\mathbf{y}$$

Proposition

$$\begin{aligned} < \widehat{\boldsymbol{\varepsilon}}, X >&= 0_n \\ < \widehat{\boldsymbol{\varepsilon}}, \widehat{\mathbf{y}} >&= 0 \\ < \widehat{\boldsymbol{\varepsilon}}, \bar{\mathbf{y}}\mathbf{1}_n >&= 0 \end{aligned} \tag{3}$$

<u>Rem</u>: The Normal equation is $(X^\top X)\widehat{\boldsymbol{\theta}} = X^\top \mathbf{y}$. It follows that $X^\top(X\widehat{\boldsymbol{\theta}} - \mathbf{y}) = 0 \Leftrightarrow X^\top \widehat{\boldsymbol{\varepsilon}} = 0 \Leftrightarrow \widehat{\boldsymbol{\varepsilon}}^\top X = 0$

With $X = (\mathbf{1}_n, \mathbf{x}_1, \ldots, \mathbf{x}_p)$, this can be rewritten

$$\forall j = 1, \ldots, p : \langle \widehat{\boldsymbol{\varepsilon}}, \mathbf{x}_j \rangle = 0 \text{ and } \overline{r}_n = 0$$

<u>Interpretation</u> : (1,2) residuals are $\perp$ to features and (3) $\widehat{\boldsymbol{\varepsilon}}$ is centered ($\sum \widehat{\epsilon}_i = 0$)

How good is our model ? RSS and the determination coefficient R^2

The ratio of the variation explained by the model and the total variation of the data $R^2 = \frac{\|\widehat{\mathbf{y}}-\bar{\mathbf{y}}\mathbf{1}_n\|^2}{\|\mathbf{y}-\bar{\mathbf{y}}\mathbf{1}_n\|^2}$ We can write also, by orthogonality :

$$\|\mathbf{y} - \bar{\mathbf{y}}\mathbf{1}_n\|^2 = \|\mathbf{y} - \widehat{\mathbf{y}}\|^2 + \|\widehat{\mathbf{y}} - \bar{\mathbf{y}}\mathbf{1}_n\|^2 \quad (4)$$

Reordering

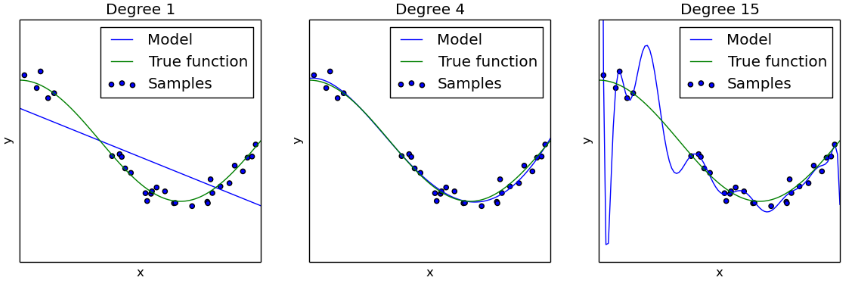
$$\|\widehat{\mathbf{y}} - \bar{\mathbf{y}}\mathbf{1}_n\|^2 = \|\mathbf{y} - \bar{\mathbf{y}}\mathbf{1}_n\|^2 - \|\mathbf{y} - \widehat{\mathbf{y}}\|^2 \quad (5)$$

So

$$R^2 = 1 - \frac{\|\mathbf{y} - \widehat{\mathbf{y}}\|^2}{\|\mathbf{y} - \bar{\mathbf{y}}\mathbf{1}_n\|^2} \quad (6)$$

Exo: Show that $0 \leq R^2 \leq 1$

Polynomial regression and overfitting



Source : sklearn

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