SD-TSIA204
Statistics : linear models

Joseph Salmon
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Teachers

- **Joseph Salmon** (Assistant Professor) :
  - Positions : Paris Diderot-Paris 7, Duke University, Télécom ParisTech
  - Research themes : high dimensional statistics, aggregation, image processing, optimization
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  - Office : E410
- **Francois Portier** (Assistant Professor) :
  - Positions : Université catholique de Louvain, Université de Rennes 1, Télécom ParisTech
  - Research themes : sparse regression, bootstrap, semi-parametric statistic, kernel smoothing
  - Email : *fportier@enst.fr*
  - Office : E 302

Teaching assistants

- **Gower Robert** (Assistant Professor) : Optimization for machine learning, randomized numerical linear algebra, variable metric and quasi-Newton methods
- **Giovanna Varni** (Assistant Professor) : Social Signal Processing (SSP), human-human/human-computer/human-robot interaction, expressive gesture, and interpersonal synchrony
  - **Garcia Alexandre** (PhD Student) : semi-supervised prediction for structured variables, sentiment analysis
  - **Korba Anna** (PhD Student) : ranking, preference learning, voting rules, recommender systems
  - **Ndiaye Eugene** (PhD Student) : sparse estimators, optimization with coordinates descent methods, safe screening rules

Grades : SD-TSIA204

- Practical 1 : **20% final grade**
  - Problem statement available on Wednesday 06/12/2017 at 1 : 30 PM, deadline 23 : 59 the same day.
  - Single accepted file : **IPython Notebook**

- Practical 2 : **20% final grade**
  - Problem statement available on Wednesday 10/01/2018 at 3 : 15 PM, deadline 23 : 59 the same day.
  - Single accepted file : **IPython Notebook**

- Final exam : **60% note finale**
  - Date : 24/01/2018
  - Format : Quiz + exercises

  Rem: Quiz questions samples are available on the course website (cf. Liste de questions section)

BEWARE : your practical should be personal not copy pasted from your neighbor ! ! !

Practical notation

Practicals are graded on a scale from 0 to **20**, as follows

- scientific quality of answer **15** pts
- language/writing quality of answer (spelling, etc.) **2** pts
- indentation, PEP8 Style, useful comments in code, no/few warnings **2** pts
- no bug **1** pt (at least https://github.com/agramfort/check_notebook)
- one single **.ipynb** file expected, submitted on the "Site pédagogique" of the course ; emailed work will receive a zero score and will not be graded

Late : **no Late work** work will be accepted, unless official reason accepted by Télécom ParisTech's administration ; late work will receive a zero score and will not be graded

Bonus

1 pt out of the **final grade** could be rewarded for any useful contribution to improve this course (slides, codes, etc.)

Constraints :

- only the first contribution received on one aspect will be rewarded
- upload a **.txt** file for each proposition the "Propositions d'amélioration" section of the Site pédagogique
- detail precisely (code lines, slide page, etc.) the contribution proposed, and what it is improving/solving
- For typos : a minimum number of 5 typos is required to get the 1pt bonus

Outline of the course

Course 1 Joseph Salmon (08/11) : Introduction

Course 2 Francois Portier (29/11) : Least squares properties

Course 3 A. K./R. G./A. G./E. N./F. P./J. S. (06/12) :
Practical 1 Regression / Regularization

Course 4 Francois Portier (13/12) : CI / Bootstrap

Course 5 Francois Portier (20/12) : Ridge/Greedy/Lasso

Course 6 Joseph Salmon (10/01) : PCA/SVD

Course 7 G. V./A. K./A. G./E. N./F. P. /J. S. (10/01) :
Practical 2 (PCA/SVD)

Course 8 Joseph Salmon (17/01) : GLM/Logistic regression

Course 9 (24/01) : **Final Exam**

Prerequisites

- **Probability** basis : probability, expectation, law of large number, Gaussian distribution, central limit theorem.
  Books : Foata et Fuchs (1996) (in French) or Murphy (2012, ch.1 and 2)
- **Optimisation** basis : (differential) calculus, convexity, first order conditions, gradient descent, Newton method
  Lecture : Boyd et Vandenberghe (2004), Bertsekas (1999)

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Algorithmic aspects : some advice

`Python` installation : use **Conda / Anaconda**

Rem: you are on your own for this (or use the school machines)

Recommended tools : **Jupyter / IPython Notebook** (mandatory for your practical) **IPython** with a text editor *e.g.*, **Atom**, **Sublime Text**, **Visual Studio Code**, etc., for larger projects

- **Python**, **Scipy**, **Numpy** :
  http://perso.telecom-paristech.fr/~gramfort/liesse_python/
- **Pandas** : http://pandas.pydata.org/
- **scikit-learn** : http://scikit-learn.org/stable/

Rem: for practicals, bring your own machine if you prefer but install your `Python` environment upfront

General advice

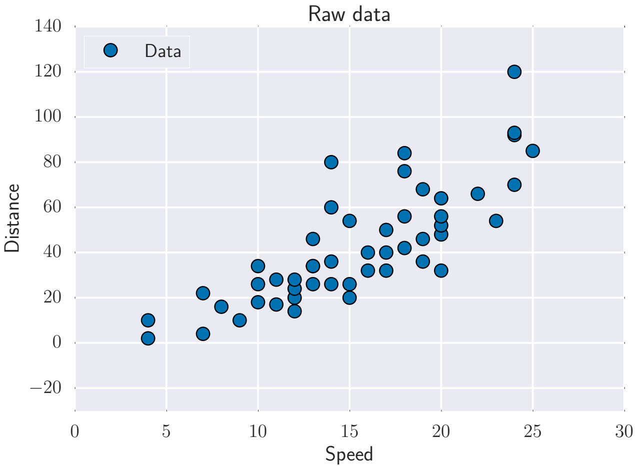
- Use version control system for your work : **Git** (*e.g.*, **Bitbucket**, **Github**, etc.)
- Use clean way of writing code/ presenting your code
  Example : **PEP8** for Python (use for instance **AutoPEP8**, `https://github.com/kenkoooo/jupyter-autopep8`)
- Learn from good examples :
  `https://github.com/scikit-learn/`,
  `http://jakevdp.github.io/`, etc.

Outline

Outline

A 2D starting example

Example : breaking distance for cars as a function of speed ($n = 50$ measurements)



Dataset *cars* : https://stat.ethz.ch/R-manual/R-devel/library/datasets/html/cars.html

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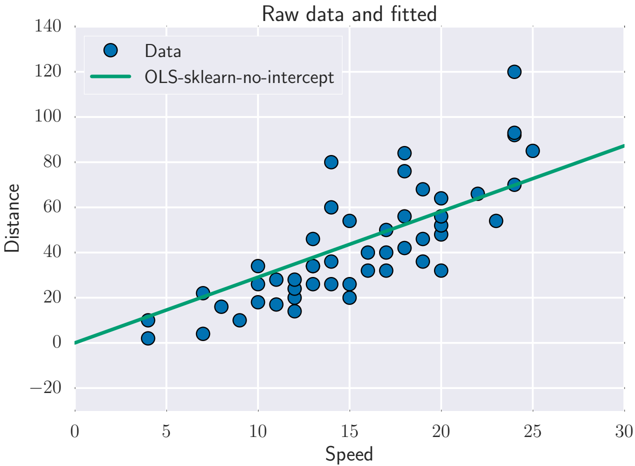

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Python command

```python
import pandas as pd
import matplotlib.pyplot as plt
import sklearn.linear_model as lm
# Load data
url = 'cars.csv'
dat = pd.read_csv(url)
y = dat['dist']
X = dat[['speed']] # sklearn needs X to have 2 dim.

skl_linmod = lm.LinearRegression(fit_intercept=False)
skl_linmod.fit(X, y) # Fit regression model

fig = plt.figure(figsize=(8, 6))
plt.plot(X, y, 'o', label="Data")
plt.plot(X, skl_linmod.predict(X),
        label="OLS-sklearn-no-intercept")
plt.legend(loc='upper left')
plt.show()
```

A 2D starting example : with an intercept

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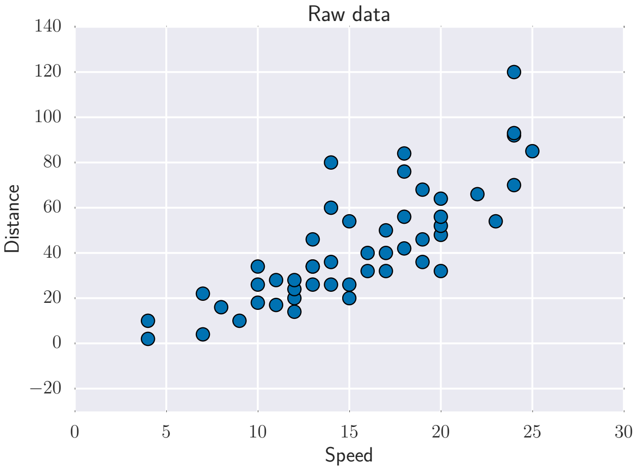

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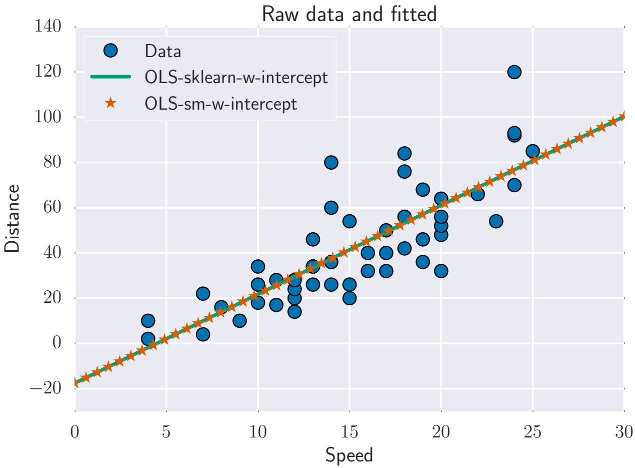


Dataset *cars* : https://stat.ethz.ch/R-manual/R-devel/library/datasets/html/cars.html

Python commands : with intercept

```python
import statsmodels.api as sm

# data, fitted, etc
y = dat['dist']
X = dat[['speed']]
X = sm.add_constant(X)
results = sm.OLS(y,X).fit()

# plot
fig, ax = plt.subplots(figsize=(8,6))
ax.plot(X['speed'], y, 'o', label="data")
ax.plot(X['speed'], results.fittedvalues,
        linewidth=3, label="OLS-sklearn-no-intercept")
ax.legend(loc='best')
```

Alternative : use `lm.LinearRegression(fit_intercept=True)`

Outline

Modeling I

$$\text{Observations :} \quad (y_i, x_i), \text{ for } i = 1, \ldots, n$$

Linear model or linear regression hypothesis assume :

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

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

Rem: both parameters are unknown from the statistician

Definition

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

Notation interpretation

Example : dataset *cars*

- $n = 50$
- y_i : breaking time for i-th car
- x_i : speed of i-th car
- y : the observation is the car's breaking time
- x : the feature/covariate is the car's speed

Linear model / Linear regression hypothesis : assume that breaking time is proportional to speed

---

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

Modeling II

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

Probabilist model

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

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**).

Rem: motivation for the randomness nature of the noise – measurement noise, transmission noise, in-population variability, etc.

Modeling III

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

Definition

We call

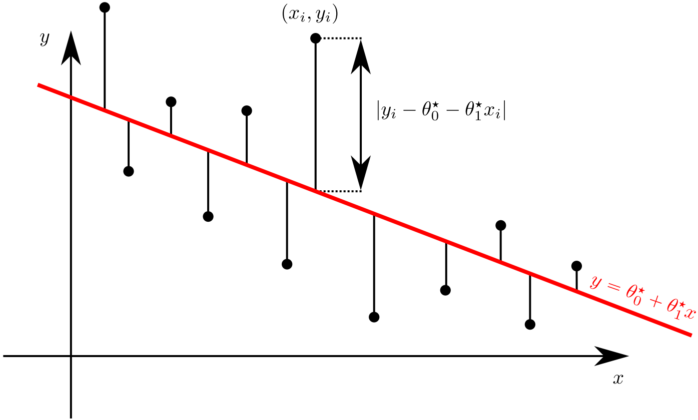
- **intercept** the scalar $\theta_0^\star$ (: *ordonnée à l'origine*)
- **slope** the scalar $\theta_1^\star$ (: *pente*)

Goal

Estimate $\theta_0^\star$ and $\theta_1^\star$ (unknown) by $\hat{\theta}_0$ and $\hat{\theta}_1$ relying on observations (y_i, x_i) for $i = 1, \ldots, n$

Rem: The "hat" notation is classical in statistics for referring to estimators

Least squares : visualization



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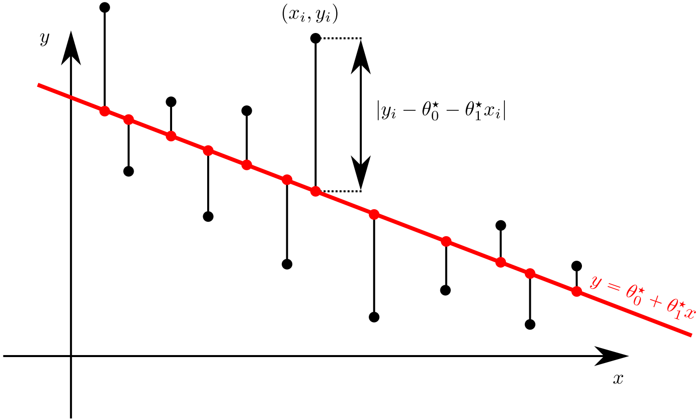
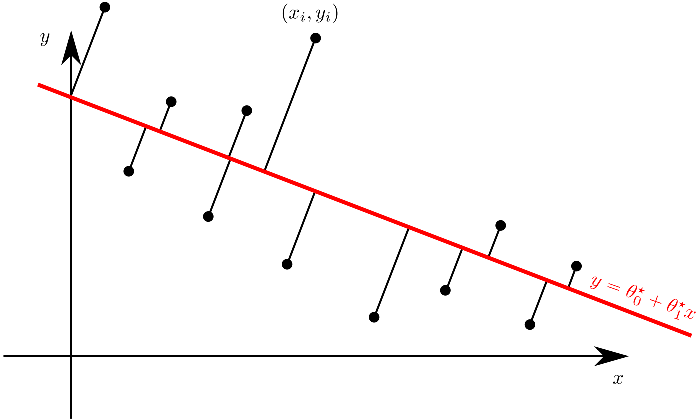


(Total) Least squares : visualization



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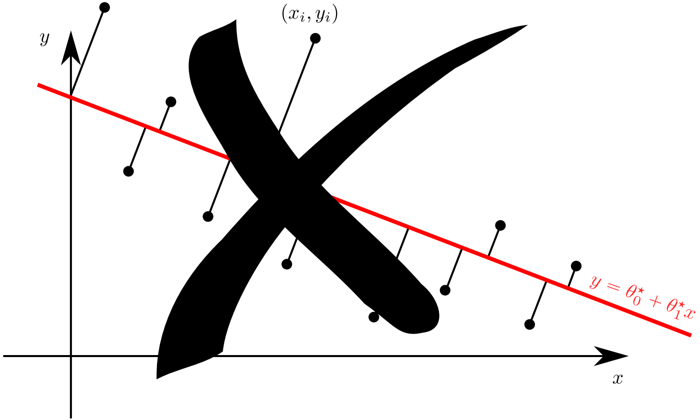


Least squares : mathematical formulation

Definition

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

$$(\hat{\theta}_0, \hat{\theta}_1) \in \underset{(\theta_0,\theta_1)\in\mathbb{R}^2}{\arg\min} \sum_{i=1}^{n} \left(y_i - \theta_0 - \theta_1 x_i\right)^2$$

- it is also referred to as "ordinary least squares" (OLS)
- an original motivation for the squares is computational : first oder conditions only require solving a linear system
- a solution always exists : minimizing a **coercive** continuous function (coercive : $\lim_{\|x\|\to+\infty} f(x) = +\infty$)

Rem: write « $\in \arg\min$ » as long as you do not know if the solution is unique

Least square authorship (controversial)

(a) **Adrien-Marie Legendre** :“Nouvelles méthodes pour la détermination des orbites des comètes”, 1805

(b) **Carl Friedrich Gauss** : “Theoria Motus Corporum Coelestium in sectionibus conicis solem ambientium” 1809

Historical / robust detour

Definition

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

$$(\hat{\theta}_0, \hat{\theta}_1) \in \underset{(\theta_0,\theta_1)\in\mathbb{R}^2}{\arg\min} \sum_{i=1}^{n} |y_i - \theta_0 - \theta_1 x_i|$$

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

(c) **Ruđer Josip Bošković** :"???", 1757

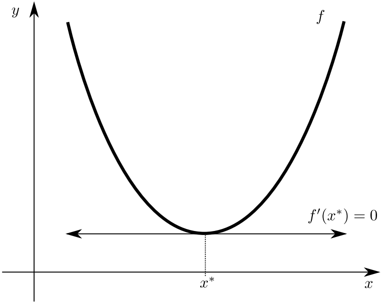
(d) **Pierre-Simon de Laplace** : "Traité de mécanique céleste", 1799

Outline

Local minimum : first order condition

Theorem : Fermat's rule

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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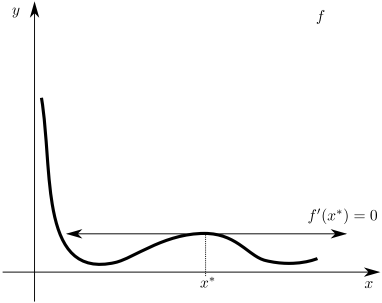

Rem: sufficient condition when f is convex !

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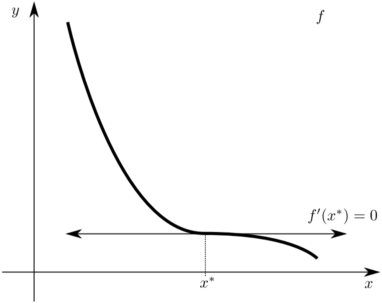


Rem: sufficient condition when f is convex !

Back to least squares

$$\boxed{\hat{\boldsymbol{\theta}} = (\hat{\theta}_0, \hat{\theta}_1) \in \mathop{\arg\min}_{(\theta_0,\theta_1)\in\mathbb{R}^2} \frac{1}{2}\sum_{i=1}^{n}(y_i - \theta_0 - \theta_1 x_i)^2}$$

For least squares, minimize the function of two variables :

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

Firs order condition / Fermat's rule :

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

Exo: Is f convex ? help : a sum of convex function is convex

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) :

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

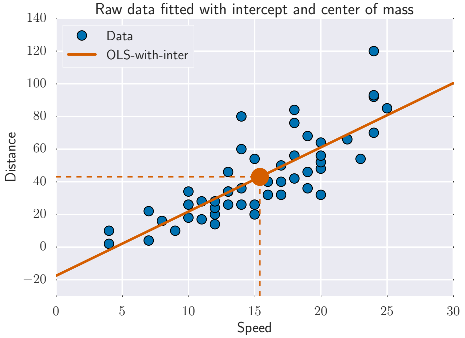
$$\Leftrightarrow$$

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

Exo: Prove that (CNO2) holds if and only if $\mathbf{x} = (x_1, \dots, x_n)^\top$ is non constant, *i.e.*, $\mathbf{x}$ is not proportional to $\mathbf{1}_n = (1, \dots, 1)^\top \in \mathbb{R}^n$

Center of gravity and interpretation

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



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

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

Vector formulation

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

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

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

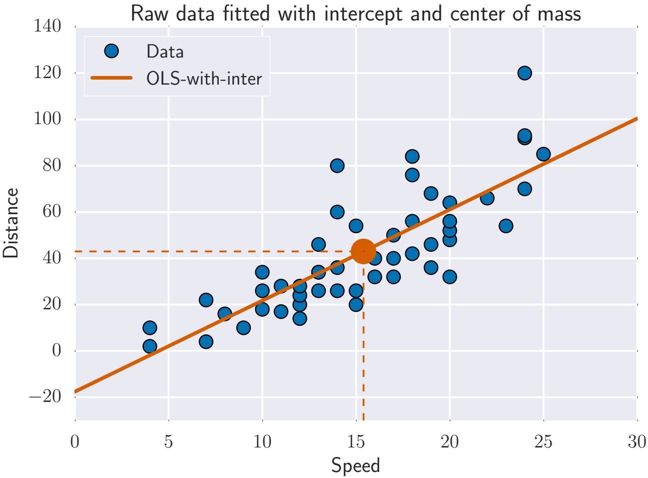
où $\quad \mathrm{corr}_n(\mathbf{x}, \mathbf{y}) = \dfrac{\frac{1}{n}\sum_{i=1}^n (x_i - \overline{x}_n)(y_i - \overline{y}_n)}{\sqrt{\mathrm{var}_n(\mathbf{x})}\sqrt{\mathrm{var}_n(\mathbf{y})}}$

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

respectively **empirical correlation empirical variances**

Back to the *cars* example

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



Outline

Centering

Centered model :

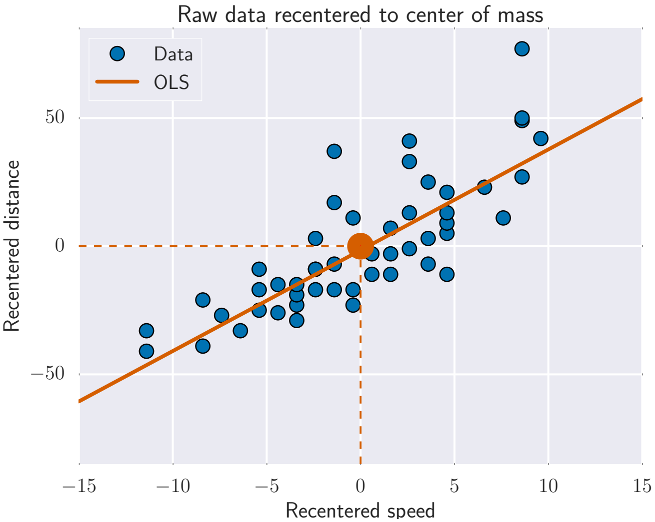
Write for any $i = 1, \ldots, n$: $\begin{cases} x'_i = x_i - \overline{x}_n \\ y'_i = y_i - \overline{y}_n \end{cases} \Leftrightarrow \begin{cases} \mathbf{x}' = \mathbf{x} - \overline{x}_n \mathbf{1}_n \\ \mathbf{y}' = \mathbf{y} - \overline{y}_n \mathbf{1}_n \end{cases}$

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

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

Rem: equivalent to choosing the points cloud 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 :

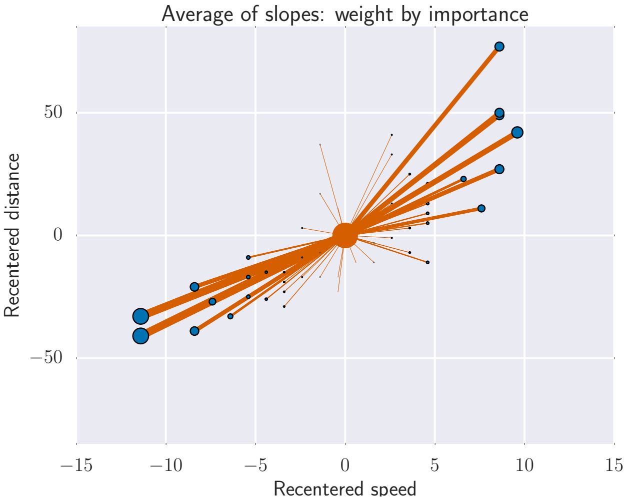
$$\widehat{\theta}'_1 \in \underset{\theta_1}{\arg\min} \sum_{i=1}^{n} (y'_i - \theta_1 x'_i)^2 = \underset{\theta'_1}{\arg\min} \sum_{i=1}^{n} x_i'^2 \left(\frac{y'_i}{x'_i} - \theta_1 \right)^2$$

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

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

Influence of extreme point : weights proportional to $x_i'^2$; connected to the **leverage** (: *levier*) effect

Extreme points – leverage effect



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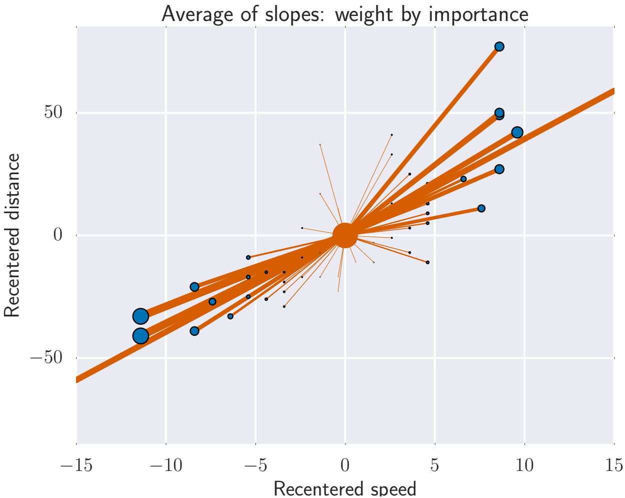

Extreme points – leverage effect (II)

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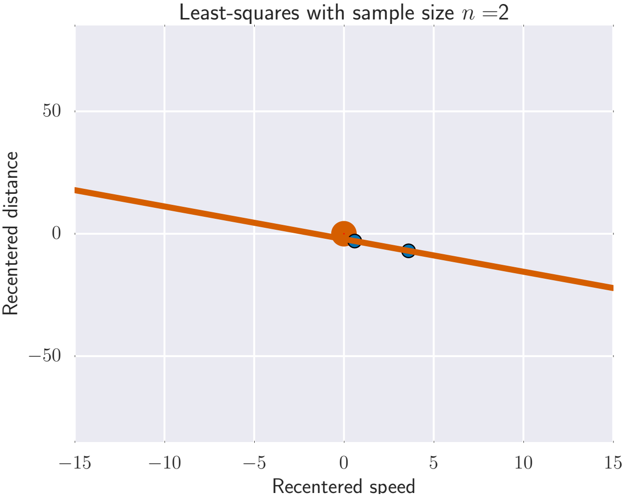

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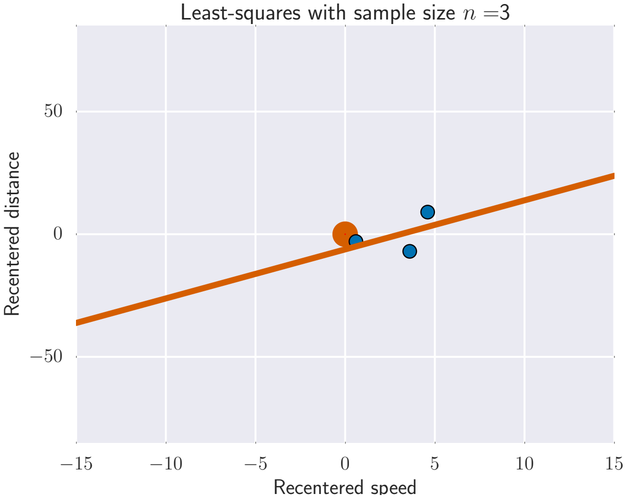

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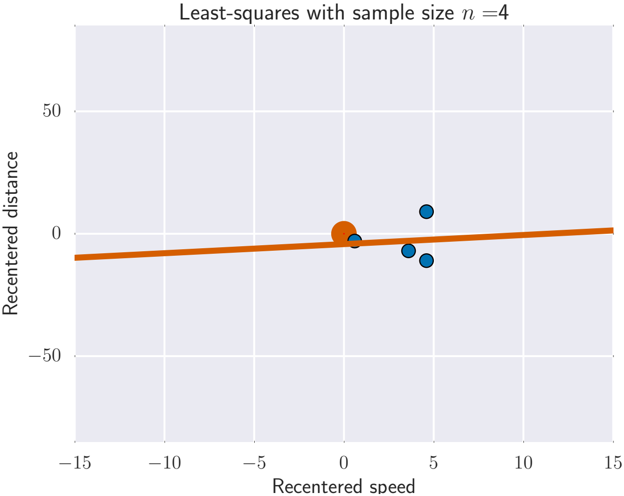

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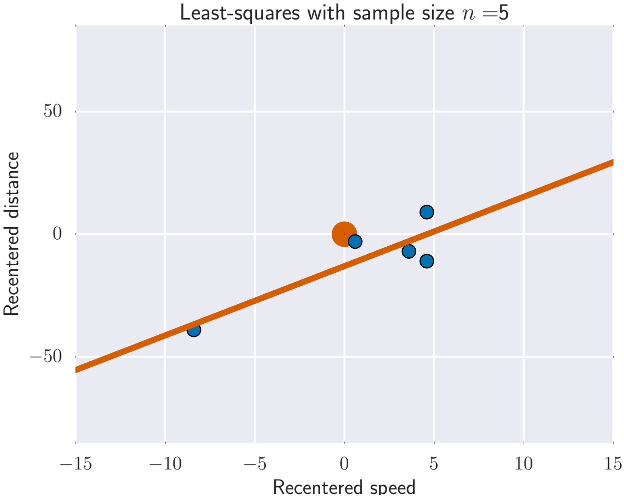

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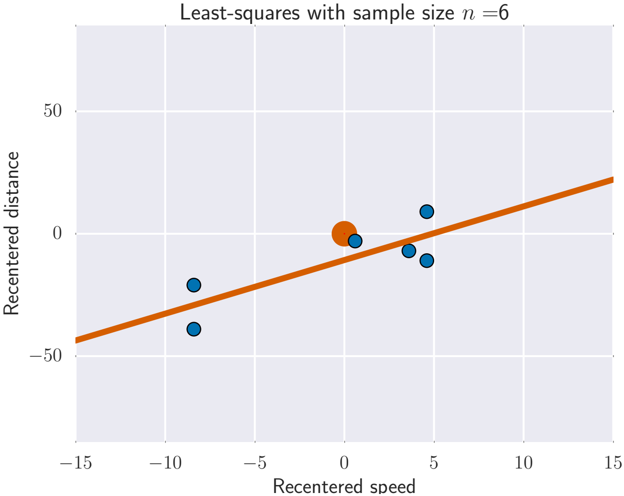

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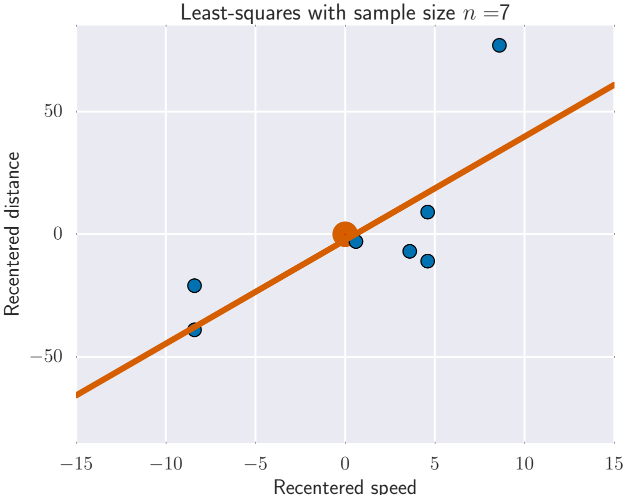

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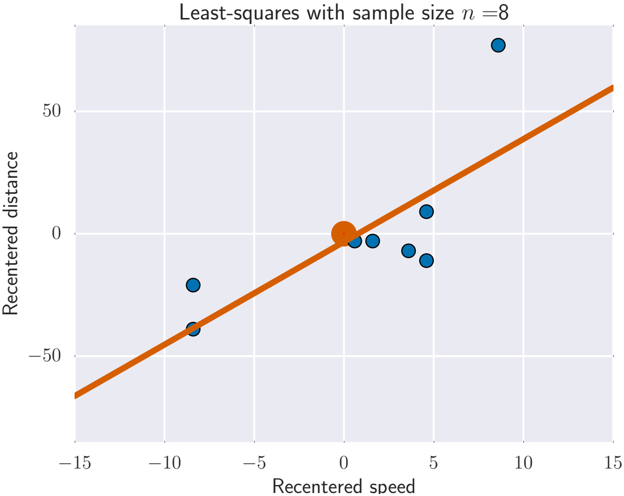

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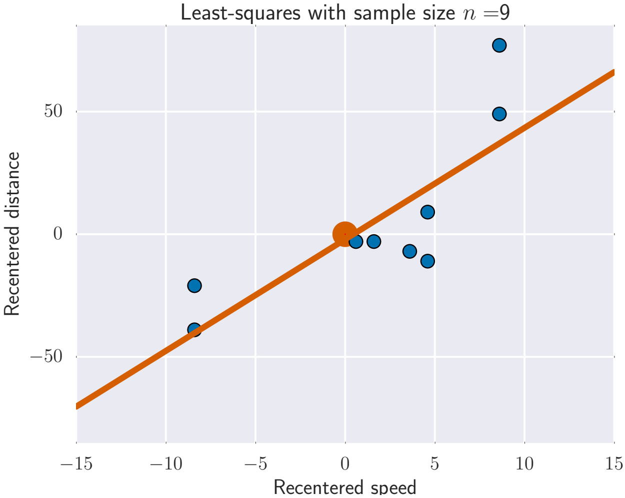

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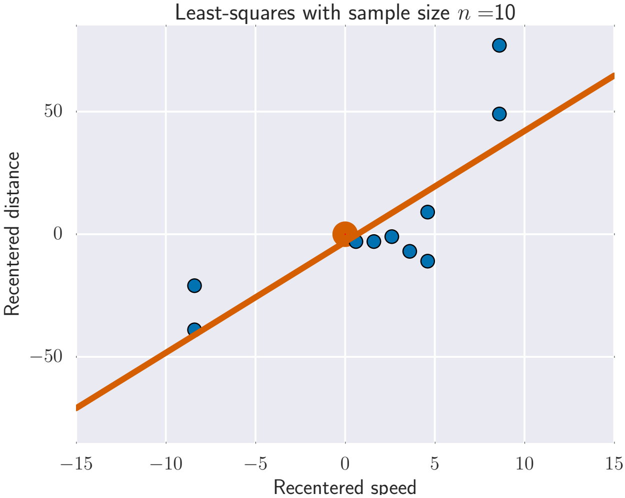

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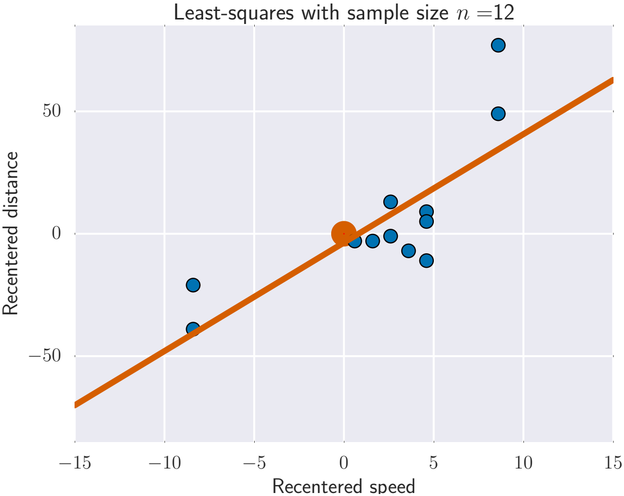

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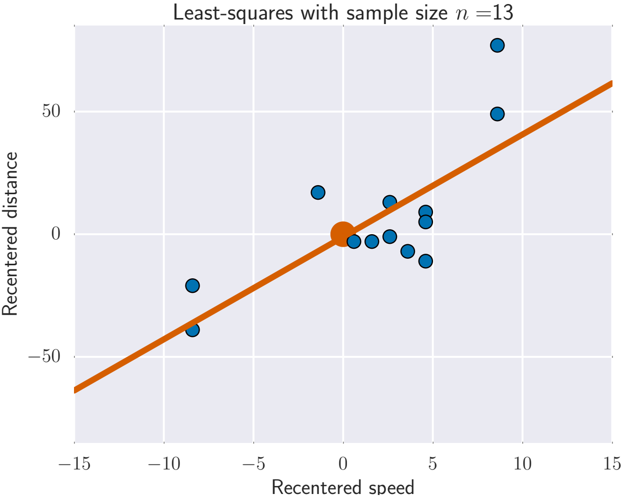

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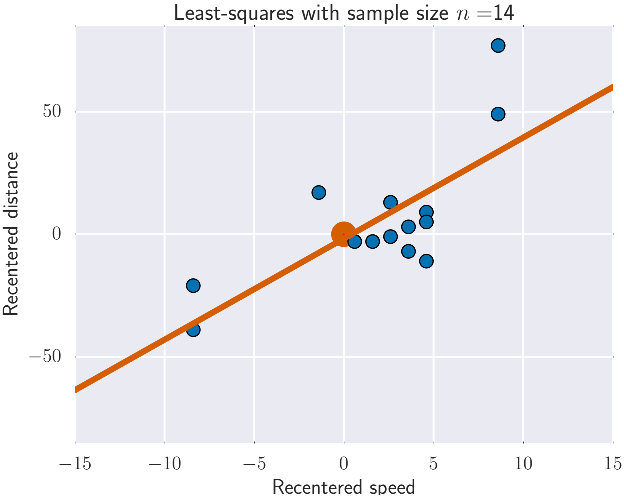

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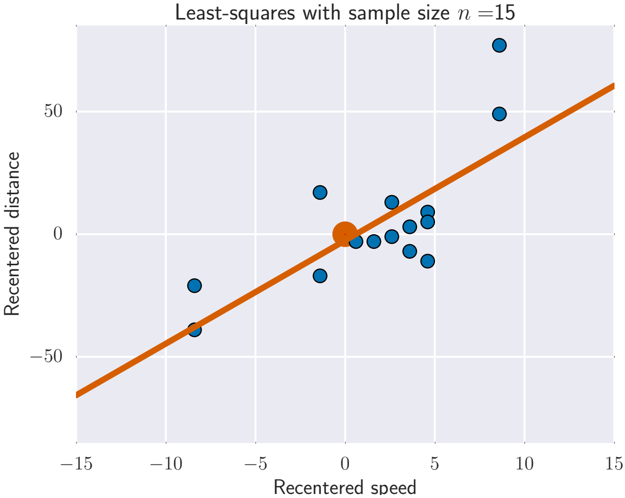

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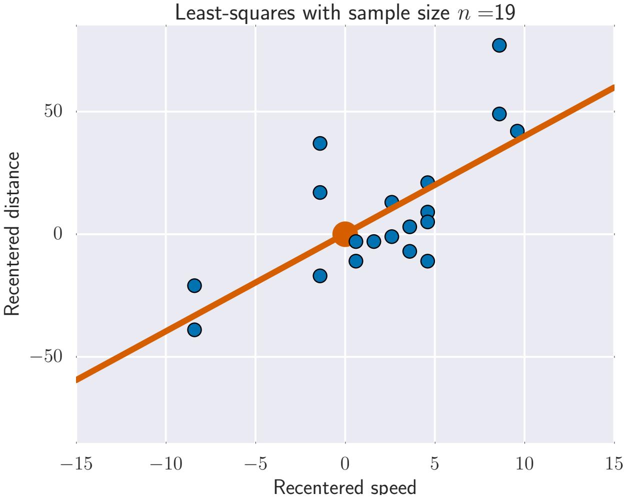

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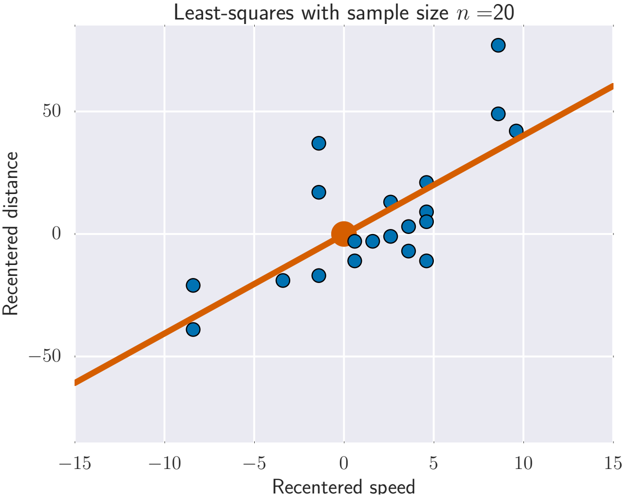

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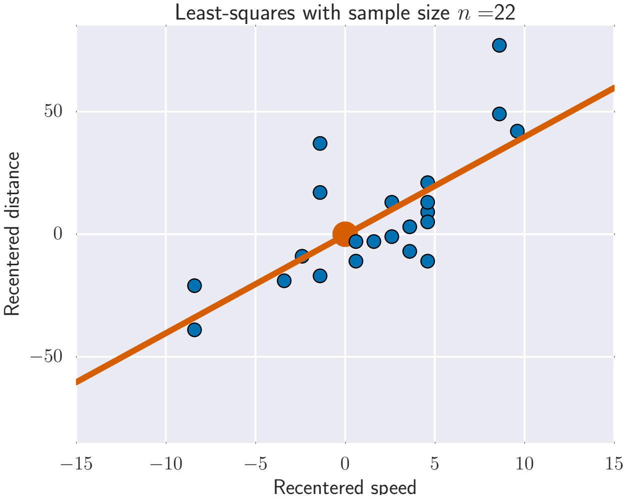

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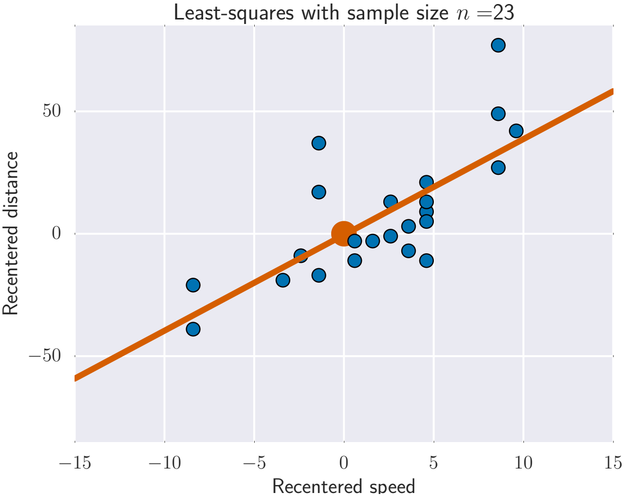

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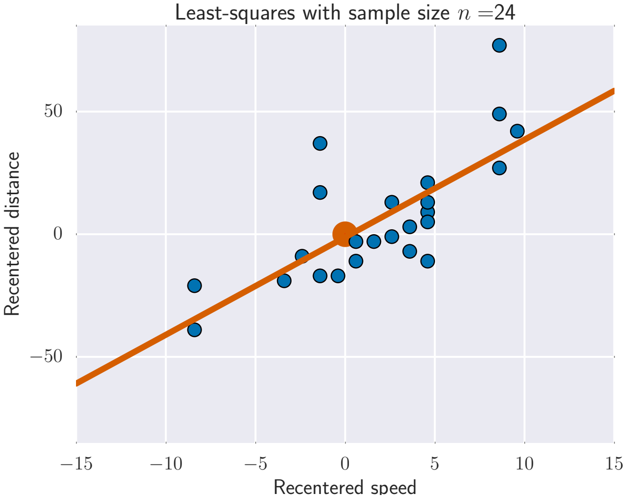

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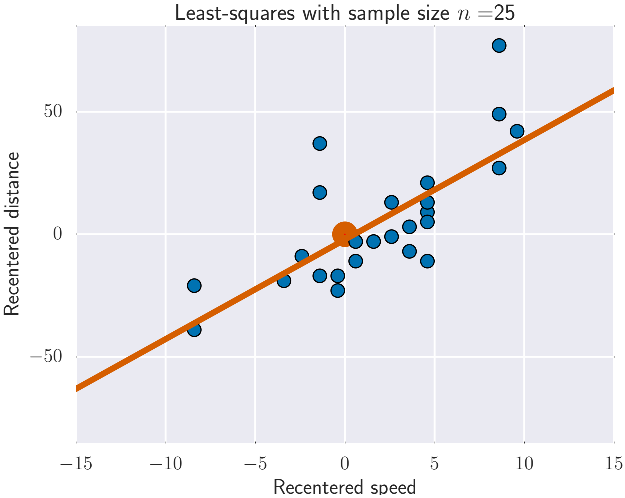

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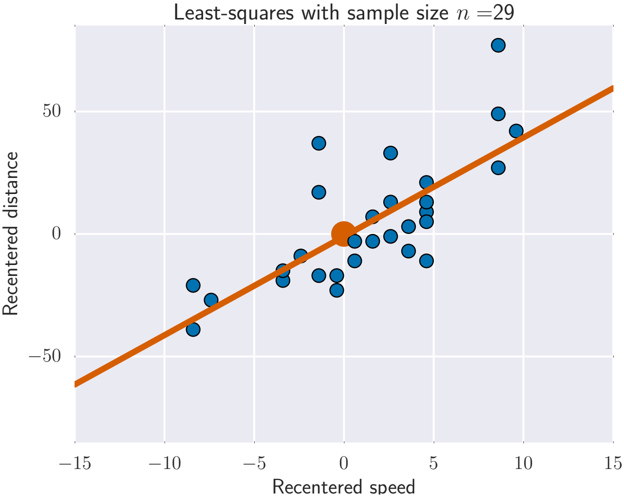

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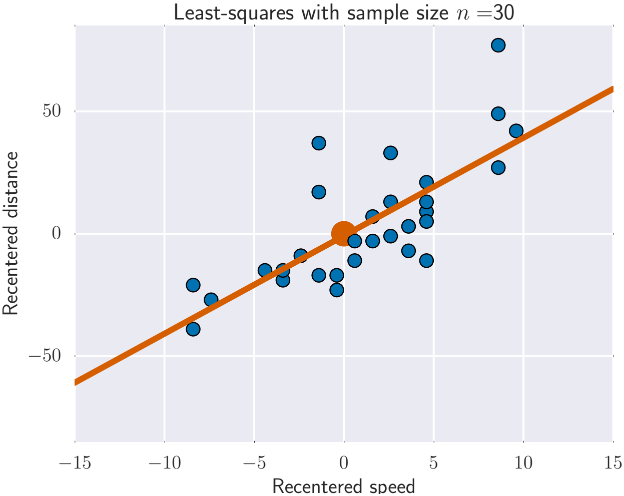

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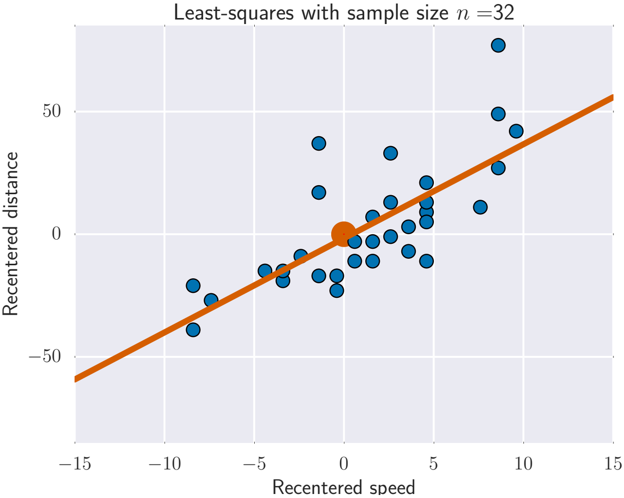

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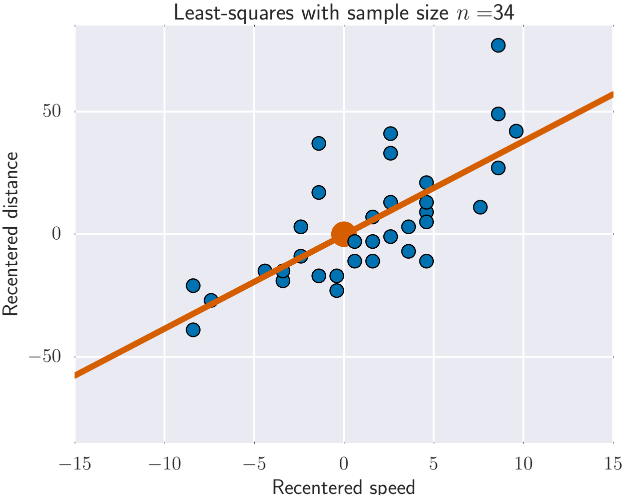

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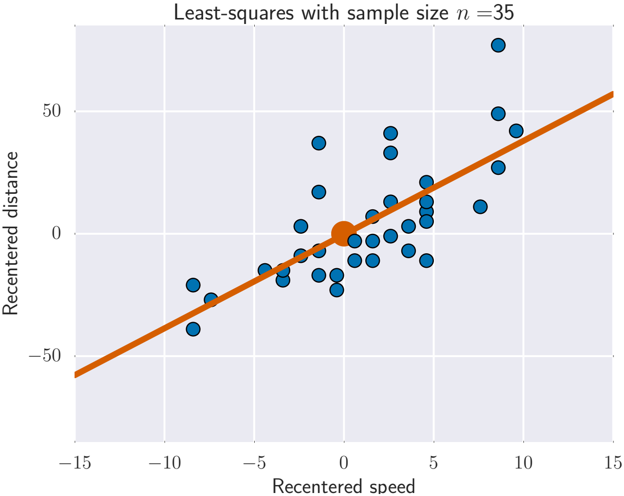

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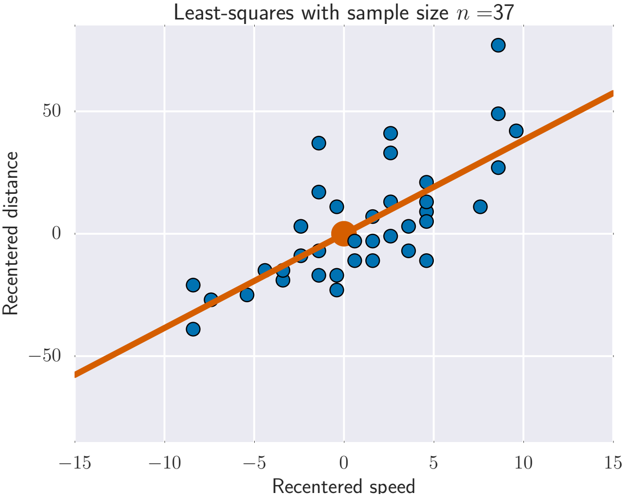

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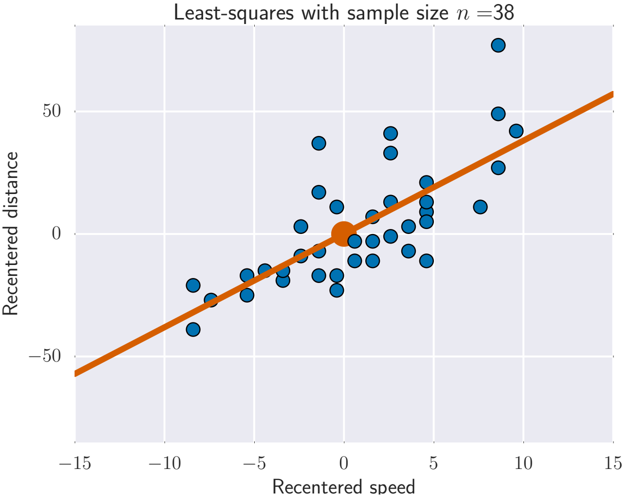

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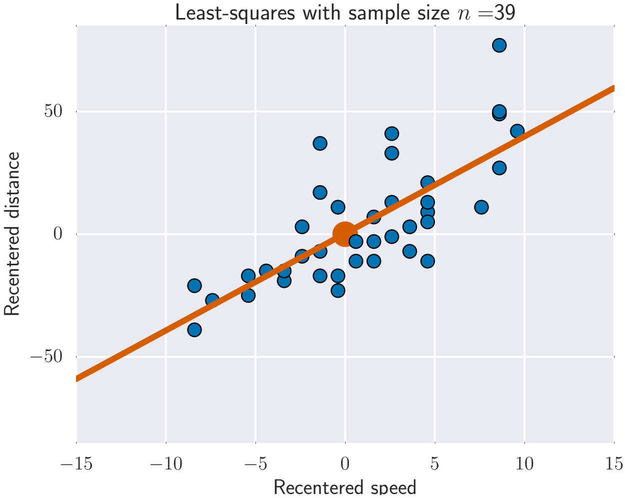

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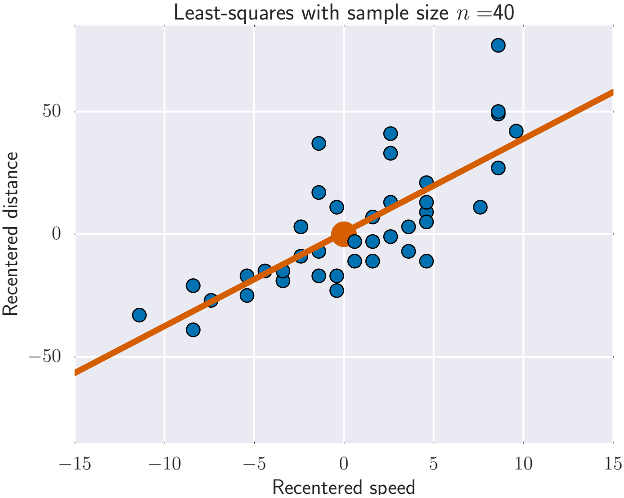

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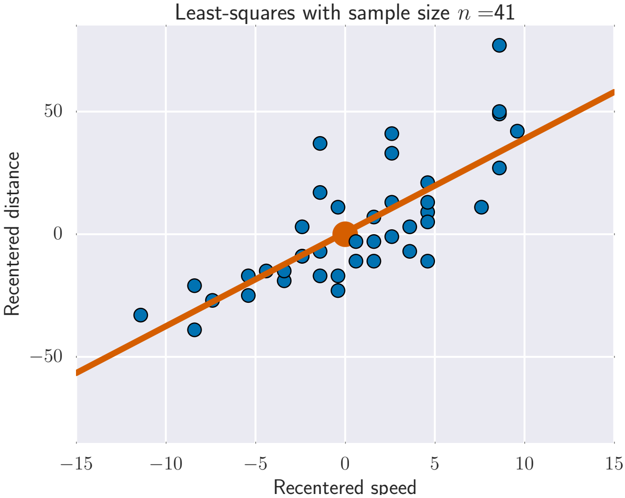

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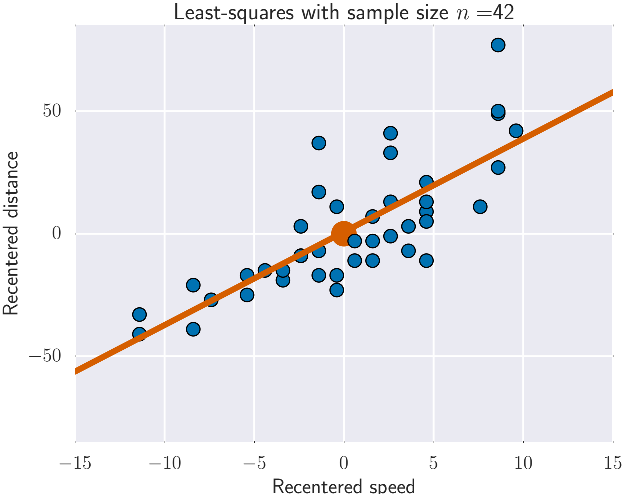

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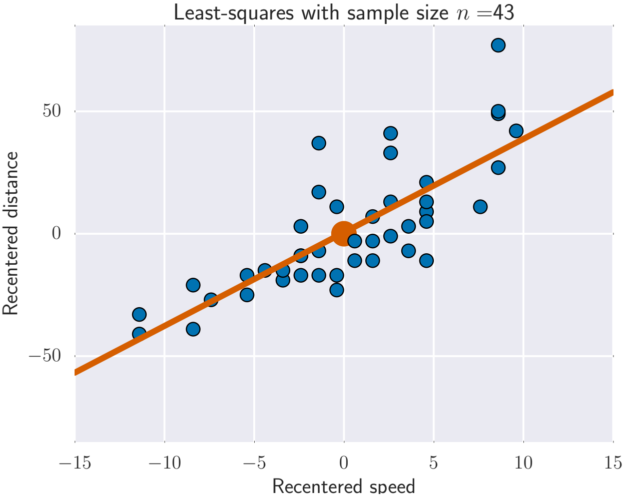

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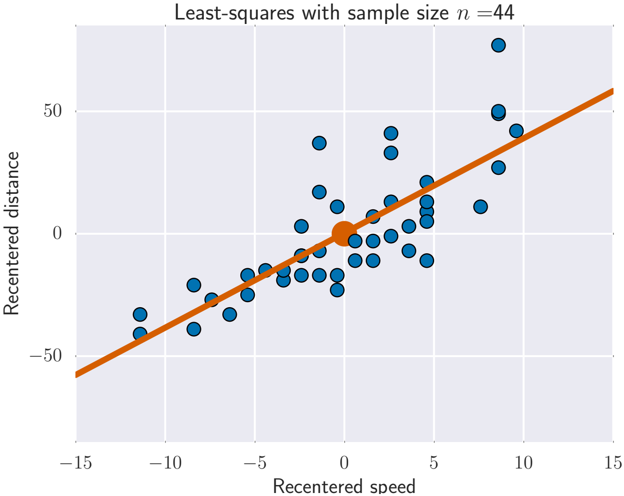

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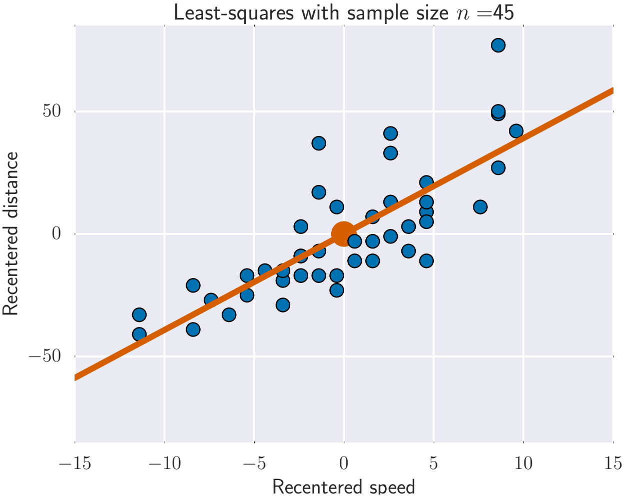

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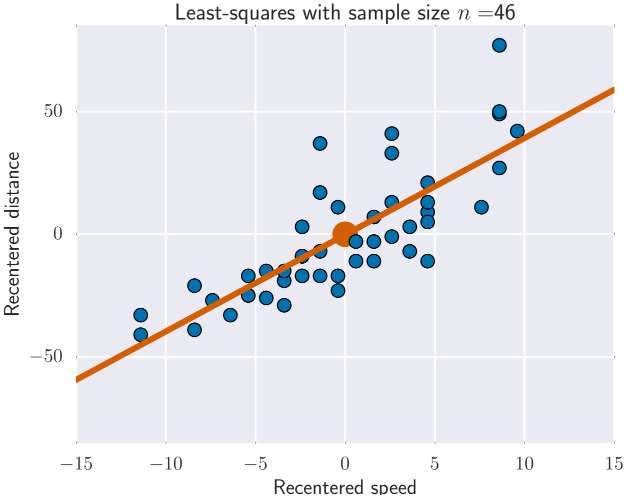

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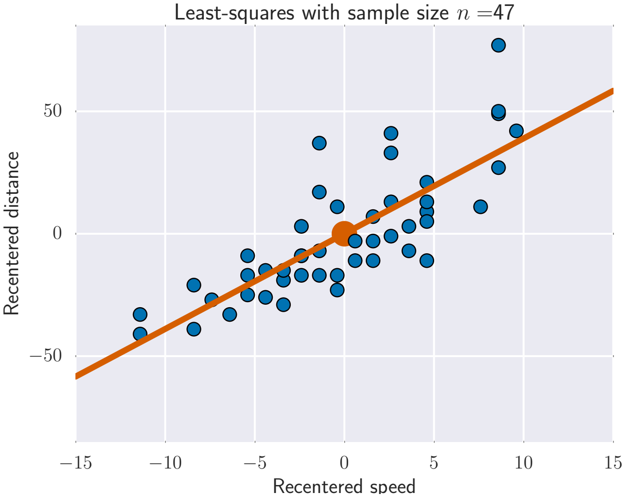

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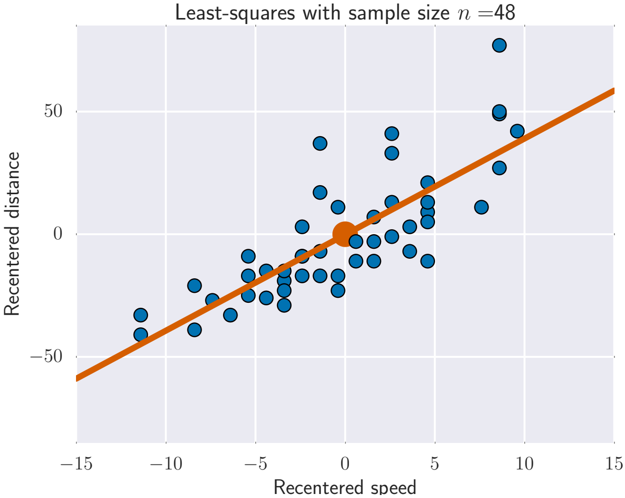

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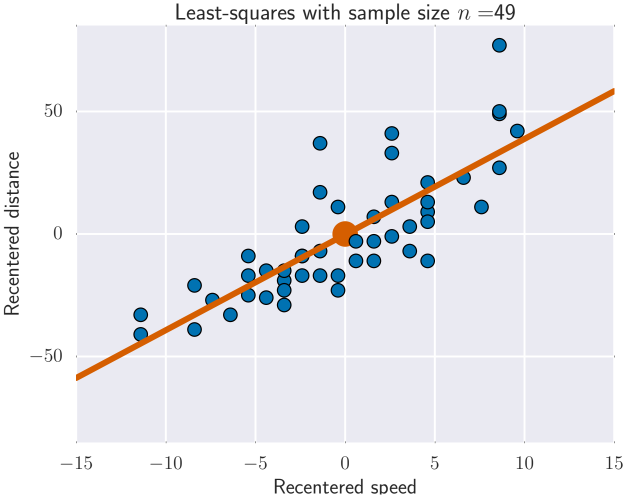

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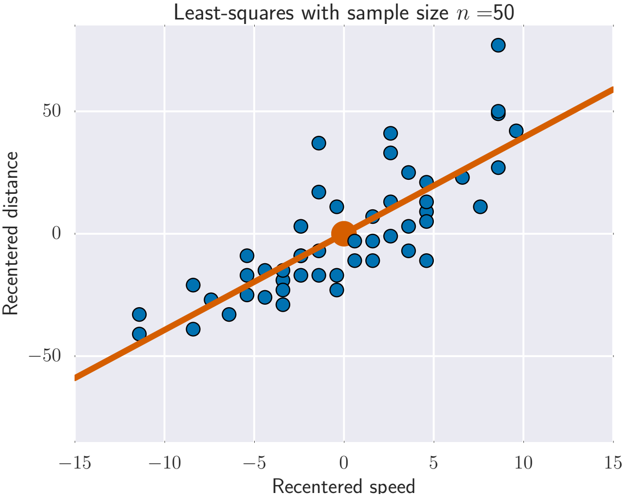


Centering + scaling

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

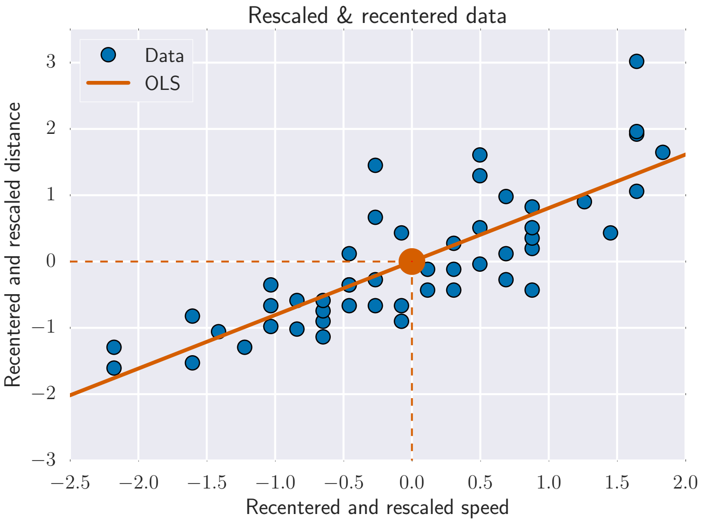
$$\begin{cases} \widehat{\theta}_0'' = 0 \\ \widehat{\theta}_1'' = \dfrac{1}{n} \displaystyle\sum_{i=1}^{n} x_i'' y_i'' \end{cases}$$

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

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

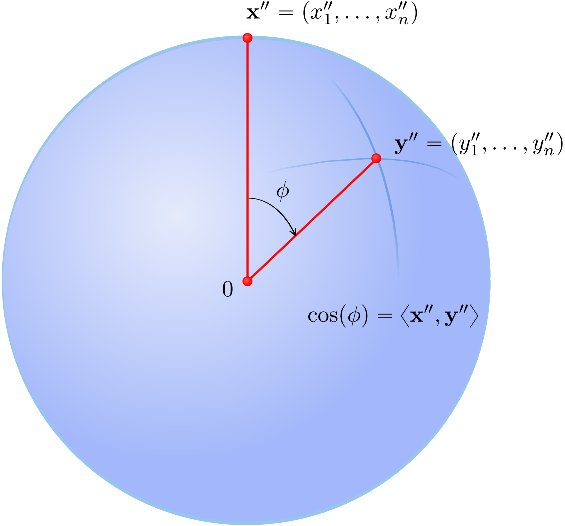
$$\|\mathbf{y}''\|_n^2 = \frac{1}{n} \sum_{i=1}^{n} (y_i'')^2 = 1$$

Centering + scaling



Correlation interpretation (centered-scaled case)

Example : $n = 3$ and $\|\mathbf{x}''\|_n^2 = \|\mathbf{y}''\|_n^2 = 1$



When/why preprocessing ?

Centering $\mathbf{y}$ or using an intercept (or adding a constant feature) is equivalent

Rem: for sparse (: *creux*) cases centering $\mathbf{y}$ adding a constant feature could be preferred

Scaling features is important :

- if you want to interpret coefficients amplitude in regression (better solution : t-tests)
- if you want to penalize or regularize coefficients (*cf.* Lasso, Ridge, etc.) a single scale is needed
- for computing reasons (*e.g.*, store scaling to improve efficiency, improve matrix conditioning, etc.)

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

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

Definitions

Prediction

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

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

Rem: often written $\hat{y}_{n+1}$ (implicit dependence on x_{n+1})

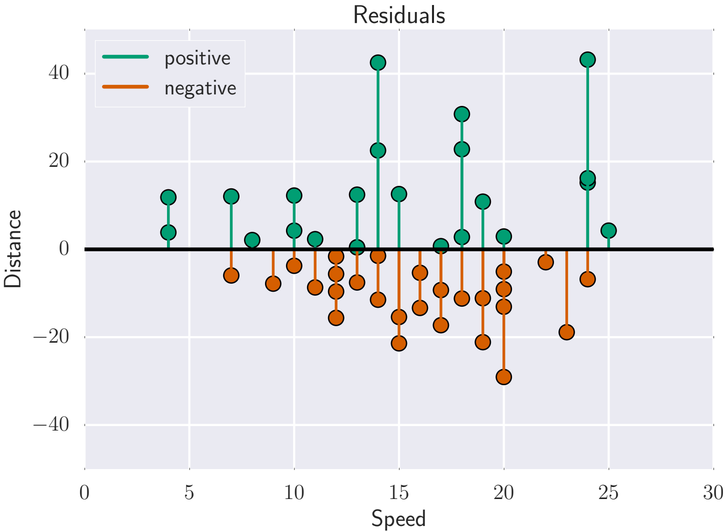
Residual

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

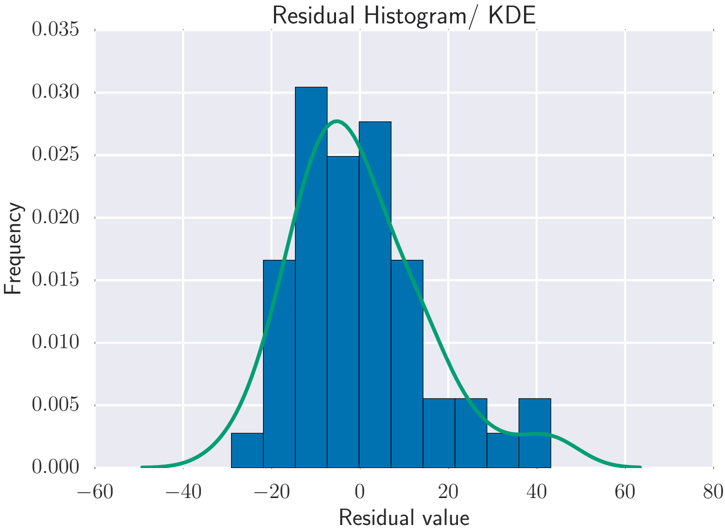
$$r_i = y_i - \mathrm{pred}(x_i) = y_i - \hat{y}_i = y_i - (\hat{\theta}_0 + \hat{\theta}_1 x_i)$$

Rem: observable estimate of the unobservable statistical error

Residuals (on cars)



Residual histograms



Residuals (continued)

Reminder : $r_i = y_i - \text{pred}(x_i) = y_i - \hat{y}_i = y_i - (\hat{\theta}_0 + \hat{\theta}_1 x_i)$

Properties

Residuals are **centered** : $$\frac{1}{n}\sum_{i=1}^{n} r_i = 0$$

Proof :

Residuals (continued)

Reminder : $r_i = y_i - \mathrm{pred}(x_i) = y_i - \hat{y}_i = y_i - (\hat{\theta}_0 + \hat{\theta}_1 x_i)$

Properties

Residuals are **centered** : $\frac{1}{n}\sum_{i=1}^{n} r_i = 0$

Proof :

$$\frac{1}{n}\sum_{i=1}^{n} r_i = \frac{1}{n}\sum_{i=1}^{n} (y_i - \mathrm{pred}(x_i))$$

Residuals (continued)

Reminder : $r_i = y_i - \mathrm{pred}(x_i) = y_i - \hat{y}_i = y_i - (\hat{\theta}_0 + \hat{\theta}_1 x_i)$

Properties

Residuals are **centered** : $\frac{1}{n}\sum_{i=1}^{n} r_i = 0$

Proof :

$$\begin{aligned}\frac{1}{n}\sum_{i=1}^{n} r_i &= \frac{1}{n}\sum_{i=1}^{n} (y_i - \mathrm{pred}(x_i)) \\ &= \frac{1}{n}\sum_{i=1}^{n} (y_i - \hat{y}_i)\end{aligned}$$

Residuals (continued)

Reminder : $r_i = y_i - \mathrm{pred}(x_i) = y_i - \hat{y}_i = y_i - (\hat{\theta}_0 + \hat{\theta}_1 x_i)$

Properties

Residuals are **centered** : $$\frac{1}{n}\sum_{i=1}^{n} r_i = 0$$

Proof :

$$\begin{aligned}
\frac{1}{n}\sum_{i=1}^{n} r_i &= \frac{1}{n}\sum_{i=1}^{n} (y_i - \mathrm{pred}(x_i)) \\
&= \frac{1}{n}\sum_{i=1}^{n} (y_i - \hat{y}_i) \\
&= \frac{1}{n}\sum_{i=1}^{n} \Big(y_i - (\hat{\theta}_0 + \hat{\theta}_1 x_i)\Big)
\end{aligned}$$

Residuals (continued)

Reminder : $r_i = y_i - \mathrm{pred}(x_i) = y_i - \hat{y}_i = y_i - (\hat{\theta}_0 + \hat{\theta}_1 x_i)$

Properties

Residuals are **centered** : $\frac{1}{n}\sum_{i=1}^{n} r_i = 0$

Proof :

$$
\begin{aligned}
\frac{1}{n}\sum_{i=1}^{n} r_i &= \frac{1}{n}\sum_{i=1}^{n} (y_i - \mathrm{pred}(x_i)) \\
&= \frac{1}{n}\sum_{i=1}^{n} (y_i - \hat{y}_i) \\
&= \frac{1}{n}\sum_{i=1}^{n} \Big(y_i - (\hat{\theta}_0 + \hat{\theta}_1 x_i)\Big) \\
&= \overline{y}_n - (\hat{\theta}_0 + \hat{\theta}_1 \overline{x}_n) = 0
\end{aligned}
$$

Outline

Least squares motivation

- Computing advantage : computationally heavy methods avoided before computers (*e.g.*, iterative methods)
- Theoretical advantage : least square analysis easy under simple hypothesis

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`)

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

Gaussian likelihood

Reminder : univariate probability density function (pdf)

We write $Y \sim \mathcal{N}(\mu, \sigma^2)$, for a random variable with pdf

$$\varphi_{\mu,\sigma}(y) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y-\mu)^2}{2\sigma^2}\right)$$

Assume : $y_i \sim \mathcal{N}(\theta_0^\star + \theta_1^\star x_i, \sigma^2)$, *i.e.*, $\varepsilon_i \sim \mathcal{N}(0, \sigma^2)$, then the most **likely** couple (θ_0, θ_1) based on the observations is maximizing the pdf of $(y_1, \dots, y_n)$

Under an independence hypothesis, this is achieved by solving :

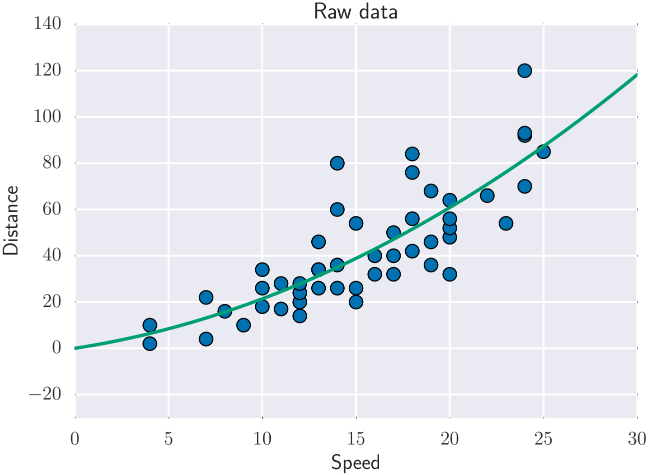
$$(\hat{\theta}_0, \hat{\theta}_1) \in \underset{(\theta_0,\theta_1)\in\mathbb{R}^2}{\arg\max} \prod_{i=1}^{n} \left(\frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(y_i - \theta_0 - \theta_1 x_i)^2}{2\sigma^2}\right)\right)$$

Exo: check that this is equivalent to the least squares formulation

---

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 as feature x_i^2 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)

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