

# Machine Learning

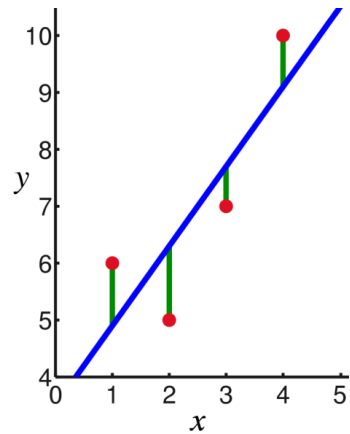
## 2. Linear regression

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# Part 1: Simple linear regression

# Regression problems (recall from last course)

## Linear regression (or curve fitting)



In linear regression, the observations (**red**) are assumed to be the result of random deviations (**green**) from an underlying relationship (**blue**) between a dependent variable ( $y$ ) and an independent variable ( $x$ ).

### Examples of methods:

- **Least square algorithms:** a method where the sum of the squares of the residuals made in the results of every single equation is minimized.
- **Bayesian linear regression:** an approach to linear regression in which the statistical analysis is undertaken within the context of Bayesian inference

$$\text{Posterior distribution} = \frac{\text{prior distribution} \times \text{likelihood}}{\text{model evidence}}$$

Ex. : maximum likelihood or maximum a posteriori estimation

This can also be made with multiple variables (and input  $x$  would become a vector)

*prior distribution*: initial set of parameters (things that you want to learn)

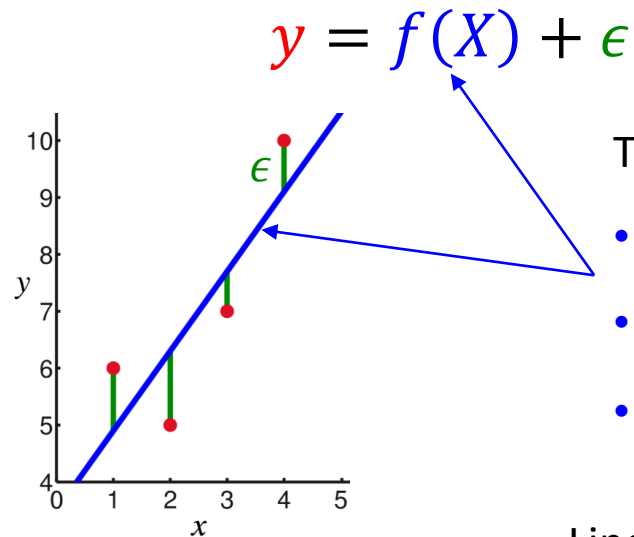
*likelihood*: similarity of the considered sample, from which you want to compute something, to the prior samples (to the prior distribution) considered, from which your algorithm has learned.

*model evidence*: represents how well it seems that the model is correct

*posterior distribution*: the new set of parameters

# Linear regression principia

Fixed equation from that relates  $X$  (input) to  $y$  (output) with the acceptance of  $\epsilon$  (an irreducible error)



The function that relates  $x$  to  $y$  could be:

- $f(X) = \alpha X + \beta$
- $f(X) = \alpha X + \theta X^2 + \beta$
- $f(X) = \alpha e^{-i\omega X} + \beta$

For the rest of the presentation, we will only focus on that simple case

Linear regression objective is to estimate the best matching  $f(X)$  which is called estimate, written  $\hat{y} = \widehat{f(X)}$

So the objective is to minimize the residual error  $e = y - \hat{y}$  for every sample  $X$

Don't confuse  $e$  with  $\epsilon$ :

$$\underline{e} = (\alpha X + \beta) + \epsilon - (\hat{\alpha} X + \hat{\beta}) = (\alpha - \hat{\alpha})X + (\beta - \hat{\beta}) + \underline{\epsilon}$$

# Linear regression least square resolution

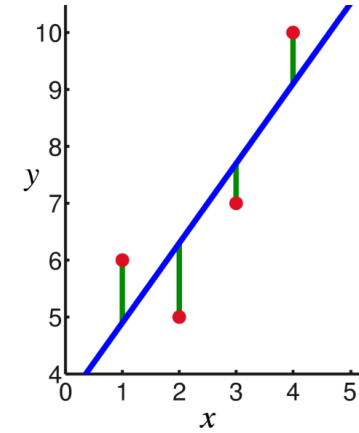
- Most used principle is to minimize the sum of squared residuals:

$$\text{minimize } \sum_{i=1}^n e_i^2 = \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

Number of observations

- Solution of that minimization is:

$$\hat{\beta} = \bar{y} - \hat{\alpha}\bar{X} \quad \text{and} \quad \hat{\alpha} = \frac{\sum_{i=1}^n X_i y_i - n\bar{X}\bar{y}}{\sum_{i=1}^n X_i^2 - n\bar{X}^2}$$



With  $\bar{X}$  the mean value of samples X and  $\bar{y}$  the mean value of observations.

This gives you the estimate function:  $\widehat{f(X)} = \hat{\alpha}X + \hat{\beta} = \hat{y}$  which allows to make predictions

GDP per capita

Amount of gold medals in Olympic games

GDP: gross domestic product

# A basic example of linear regression using least square method

X (input)	-2	-1	0	1	2	3	4
y (output)	-5	-3	-1	1	3	5	7

$$\widehat{f(X)} = \hat{\alpha}X + \hat{\beta}$$

- First let's compute  $\hat{\alpha}$ :

$$\hat{\alpha} = \frac{\sum_{i=1}^n X_i y_i - n \bar{X} \bar{y}}{\sum_{i=1}^n X_i^2 - n \bar{X}^2} = \frac{63 - 7}{35 - 7} = \frac{56}{28} = 2$$

$$\sum_{i=1}^n X_i y_i = (-2 \times -5) + (-1 \times -3) + \dots + (4 \times 7) = 10 + 3 + 0 + 1 + 6 + 15 + 28 = 63$$

$$\bar{X} = \frac{1}{n} \sum_{i=1}^n X_i = \frac{1}{7} (-2 + (-1) + \dots + 3 + 4) = 1$$

$$\bar{y} = 1$$

$$\sum_{i=1}^n X_i^2 = (-2 \times -2) + (-1 \times -1) + \dots + (4 \times 4) = 4 + 1 + 0 + 1 + 4 + 9 + 16 = 35$$

## A basic example of linear regression using least square method

X (input)	-2	-1	0	1	2	3	4
y (output)	-5	-3	-1	1	3	5	7

$$\widehat{f(X)} = \hat{\alpha}X + \hat{\beta}$$

- Then compute  $\hat{\beta}$ :

$$\hat{\beta} = \bar{y} - \hat{\alpha}\bar{X} = 1 - 2 = -1$$

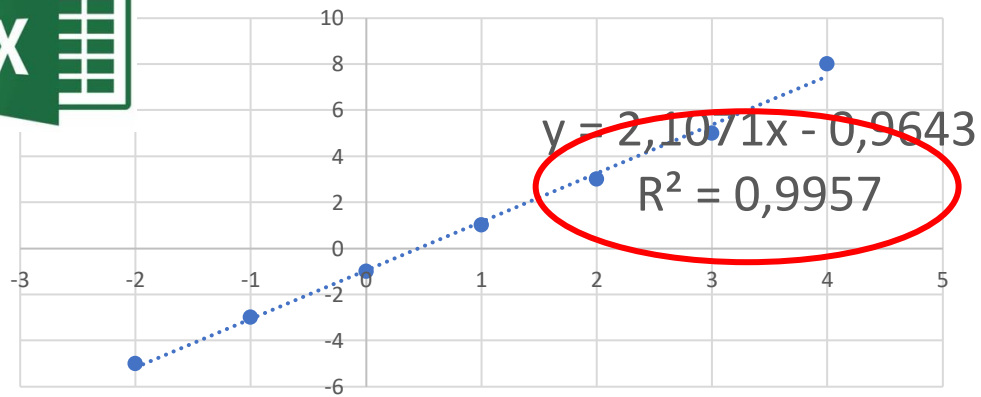
$\bar{X} = 1$ ,  $\bar{y} = 1$  and  $\hat{\alpha} = 2$

$$\widehat{f(X)} = 2X - 1$$

# Tools to analyze your results

X (input)	-2	-1	0	1	2	3	4
y (output)	-5	-3	-1	1	3	5	7

$$\widehat{f(X)} = 2X - 1$$



What is  $R^2$  ?

It indicates you a correlation score.

Best possible score is 1.0 which means perfect correlation.

Worst score is the lowest value (which can even be negative)

$$R^2(y, \hat{y}) = 1 - \frac{\sum_{i=1}^n (y_i - \hat{y}_i)^2}{\sum_{i=1}^n (y_i - \bar{y})^2}$$

Real values      Predicted values



## Tools to analyze your results

X (input)	-2	-1	0	1	2	3	4
y (output)	-5	-3	-1	1	3	5	7

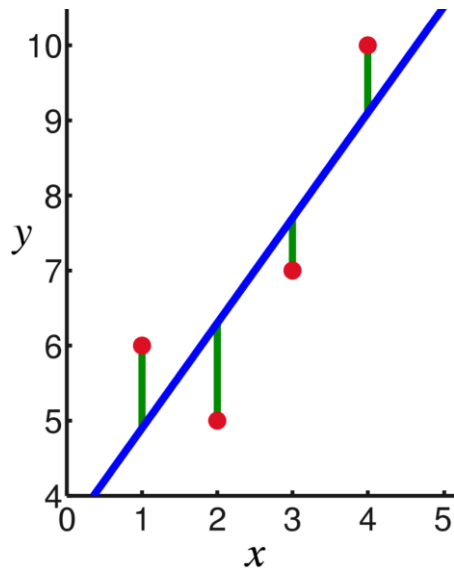
$$\widehat{f(X)} = 2X - 1$$

The mean squared error

$$\frac{1}{n} \sum_{i=1}^n (y_i - \hat{y}_i)^2$$

- Gives a value for the error
- Get the square root to have an order of magnitude of the potential error

# Assumptions for applying linear regression



- There is a linear relationship between the dependent variable ( $y$ ) and the independent variable ( $x$ ).
- The observations ( $y_i$ ) are selected independently and randomly from the population.
- For ordinary least squares or Bayesian regression :
  - Residuals should be normally distributed with a mean of 0 and variance  $\sigma$
  - If not the case some techniques allow the weighting of input data

# Videos

- For next class, please watch: <https://youtu.be/9saL47Nuguw>

## The Problem With Linear Regression | Data Analysis

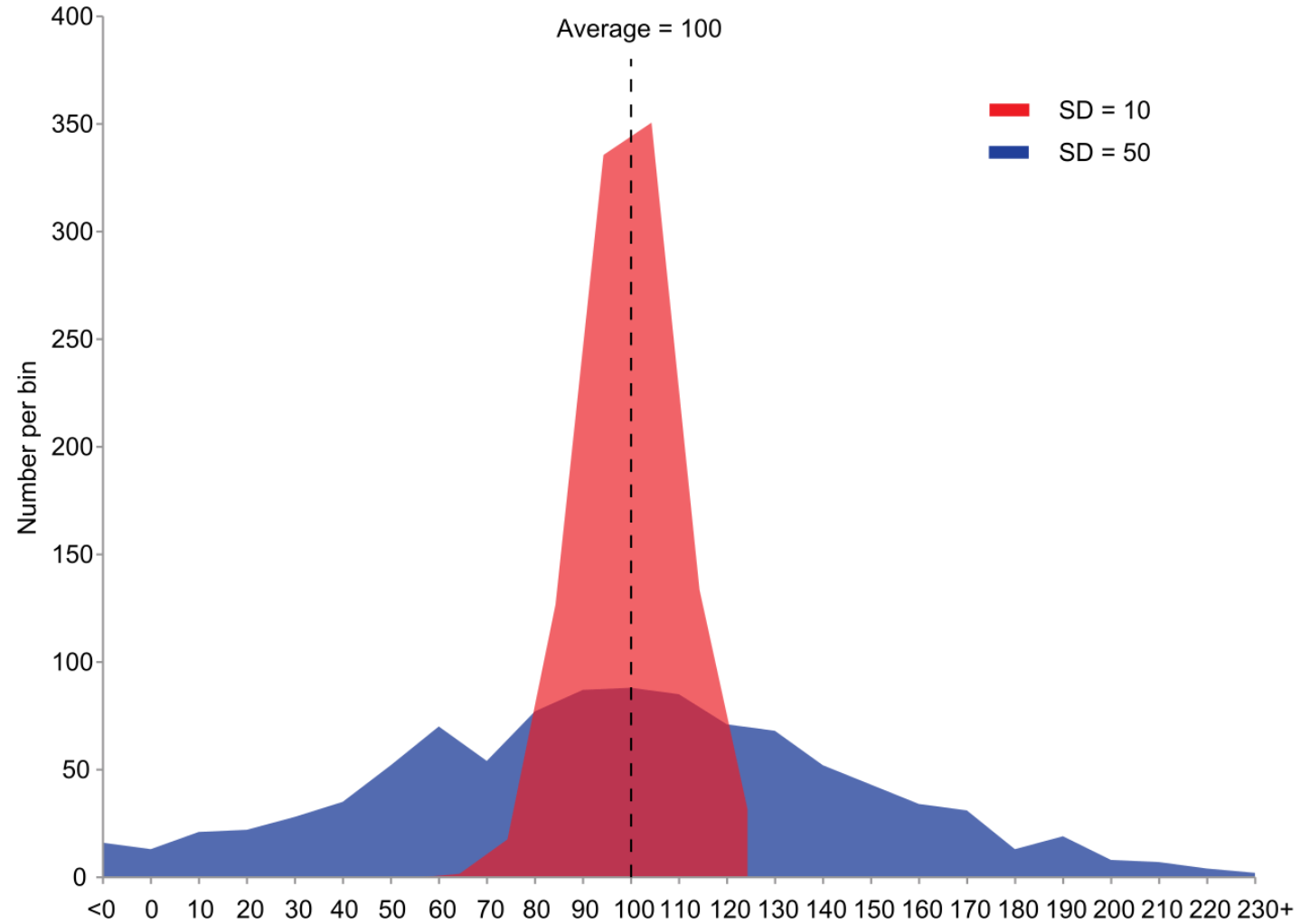
- Additionally, and **optionally**, you might have a look to: <https://youtu.be/eq7KF7JTinU>



- Only if you have time, maybe save it for later
- 9h course
- Very similar to what we will see in this class
- Can help you understand better

# Annex

# Variance



- A measure of the dispersion of the data
- It is the square of the standard deviation (SD)