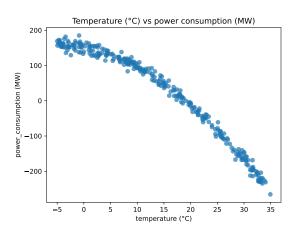
# Machine learning I, supervised learning: linear regression



#### Content

Linear regression in one dimension

General linear regression : Ordinary least squares

Overfitting, hyperparameters and ridge regression

## Linear regression

Linear regression is one of the most elementary methods used in ML regression problems. It is useful for many applications, and is often a component of more complex methods.

We will use is to illustrate several classical aspects of ML that are also encountered when using other methods (kernels, trees, neural networks, etc.)

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We want to predict the power that needs to be produced by a power plant in a city, as a function of the temperature only.

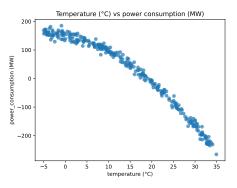


Figure - Dataset

## Exercice 1: Why are the samples not on a straight line?

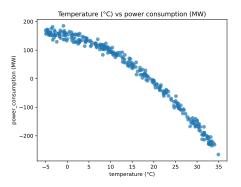


Figure - Dataset

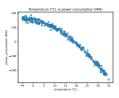


Figure – Dataset

The power consumption does not depend **only** on the temperature, but also on many other variables, that we do not have access to here:

- time in the day
- humidity, wind
- period of the year (holidays or not)
- other variables

However, our task is to predict the power consumption, only according to the temperature.

This is a **regression** problem, and we need to find a good **estimator** of the power consumed as a function of the temperature.

## Linear regression

#### Formalization:

- ightharpoonup input space (temperature) :  $\mathcal{X} = \mathbb{R}$
- lacktriangle output space (power consumption) :  $\mathcal{Y}=\mathbb{R}$
- ▶ dataset :  $D = \{(x_1, y_1), \dots, (x_n, y_n), i \in [1, n]\}.$

When doing linear regression in dimension 1 (as  $x \in \mathbb{R}$ ), our estimator is of the form :

$$h(x) = \theta x + b \tag{1}$$

with  $\theta \in \mathbb{R}$ ,  $b \in \mathbb{R}$ .

## Loss function

We will use the squared loss 1:

$$I(y_1, y_2) = (y_1 - y_2)^2$$
 (2)

# Empirical risk

With the squared loss, we define the empirical risk as :

$$R_n(\theta, b) = \sum_{i=1}^n (\theta x_i + b - y_i)^2$$
 (3)

We want to find  $\theta$  and b such that  $R_n(\theta, b)$  has the **smallest possible value**. (sometimes it is normalized by a division by n, but this does not change the problem)

# Numpy

Numpy demo.

# Computing empirical risks

#### Exercice 2:

cd code/linear\_regression /1D\_linear\_regression/ and fix utils.py in order to compute the empirical risk.

Launch main\_random\_params.py in order to test several values for  $\theta$  and b by evaluating their empirical risk.

## Analytic solutions

For some problems, like this one, it is possible to explicitely compute the optimal solution.

For some advanced reasons (convexity and differentiability of  $R_n(\theta)$ ), the points optimizing the empirical risk are obtained by finding  $(\theta^*, b^*)$  such that the gradient cancels (more on that tomorrow).

$$\nabla_{(\theta,b)}R_n(\theta^*,b^*)=0 \tag{4}$$

## **Derivatives**

$$\frac{\partial R_n}{\partial \theta}(\theta, b) = \sum_{i=1}^n 2(\theta x_i + b - y_i) x_i$$

$$= 2\left[\theta \sum_{i=1}^n x_i^2 + b \sum_{i=1}^n x_i - \sum_{i=1}^n x_i y_i\right]$$

$$\frac{\partial R_n}{\partial b}(\theta, b) = \sum_{i=1}^n 2(\theta x_i + b - y_i)$$

$$= 2\left[\theta \sum_{i=1}^n x_i + nb - \sum_{i=1}^n y_i\right]$$
(6)

Hence we have a system of 2 equations with 2 unknowns (dropping the  $\theta^*$  notation)

$$\theta \sum_{i=1}^{n} x_i^2 + b \sum_{i=1}^{n} x_i - \sum_{i=1}^{n} x_i y_i = 0$$
 (7)

$$\theta \sum_{i=1}^{n} x_i + nb - \sum_{i=1}^{n} y_i = 0$$
 (8)

#### Which means

$$b = \frac{1}{n} \left( \sum_{i=1}^{n} y_i - \theta \sum_{i=1}^{n} x_i \right)$$
 (9)

$$\theta \sum_{i=1}^{n} x_i^2 + \frac{1}{n} \left( \sum_{i=1}^{n} y_i - \theta \sum_{i=1}^{n} x_i \right) \sum_{i=1}^{n} x_i - \sum_{i=1}^{n} x_i y_i = 0$$
 (10)

#### Finally:

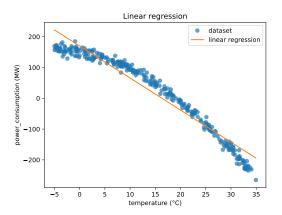
$$\theta(\sum_{i=1}^{n} x_i^2 - \frac{1}{n}(\sum_{i=1}^{n} x_i)^2) + \frac{1}{n} \sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} x_i y_i = 0$$
 (11)

or

$$\theta^* = \frac{\sum_{i=1}^n x_i y_i - \frac{1}{n} \sum_{i=1}^n x_i \sum_{i=1}^n y_i}{\sum_{i=1}^n x_i^2 - \frac{1}{n} [\sum_{i=1}^n x_i]^2}$$
(12)

#### Exercice 3:

Fix main\_optimal\_params.py in order to plot the linear regression found with the analytic solution on the same plot as the raw dataset.



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#### Generalization

Linear regression also works in higher dimensions, when the inputs are multidimensional. For instance in dimension 3,  $x = (x_1, x_2, x_3)$  and :

$$h(x) = \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + b \tag{13}$$

The parameter is now  $(\theta, b) = (\theta_1, \theta_2, \theta_3, b)$ .

Example: x contains the age, the profession, and the gender.

Now, the input data are stored in a matrix X with n lines and d columns.

The output data are stored in a vector y with n lines.

The empirical risk writes (adding back the normalization) :

$$R_n(\theta, b) = \frac{1}{n} ||X\theta - y + b||^2$$
 (14)

(more on the notion of norm later in the course)

## **OLS** estimator

It is possible to show, with some maths notions, that the  $\theta$  that minimizes the empirical risk is :

$$\hat{\theta} = (X^T X)^{-1} X^T y \tag{15}$$

 ${\cal T}$  is the transposition.

## Scikit

We can use scikit-learn in order to obtain the OLS estimator directly.

https://scikit-learn.org

## Scikit in 1D

main\_scikit.py computes the OLS for the previous power consumption example.

https://scikit-learn.org/stable/modules/generated/sklearn.linear\_model.LinearRegression.html

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# Overfitting

cd ../dD\_linear\_regression/ When d is of the same order of magnitude or larger than the number of samples n, it is possible to have a low train error and a high test error. This is known as overfitting.

- Example with OLS\_scikit.py
- You can experiment with the data used by changing generate\_data.py

## Ridge regression

Ridge regression is a variation of OLS. For some advanced reasons, it can reduce overfitting.

https://scikit-learn.org/stable/modules/generated/sklearn.linear\_model.Ridge.html

Example with Ridge\_scikit.py.

## Ridge regression

Ridge regression is a variation of OLS. For some advanced reasons, it can reduce overfitting.

https://scikit-learn.org/stable/modules/generated/sklearn.linear\_model.ridge.html

Example with ridge scikit.py.

Importantly, you can see that Ridge() has some parameters, called hyperparameters. Almost all machine learning algorithms have hyperparameters.

# Choice of the hyperparameters

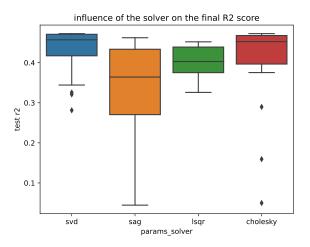
- ➤ The choice of the hyperparameters is very important. Most of the time, it is guided by experimentation and / or theoretical results.
- Some methods and libraries are helpful to look for good hyperparameters, such as optuna https://optuna.org/
- other classical methods : gridsearch, random search.

# Using optuna to tune Ridge regression

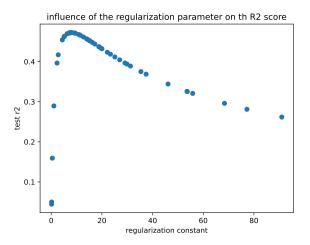
#### Exercice 4:

Use optuna\_ridge\_scikit.py in order to choose some good hyperparameters (alpha, solver) for ridge. You will need to study the optuna API and to edit the objective() function.

# Analysis of the hyperparameters

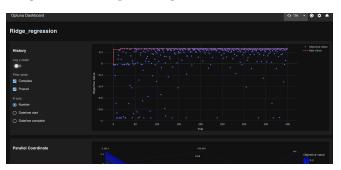


## Analysis of the hyperparameters



# Optuna dashboard

https://github.com/optuna/optuna-dashboard



## Multi-objective optimization

Optuna can be used to optimize several objectives, e.g. : optimize the score and minimize the computation time (both depend on the hyperparameters).

Notion of Pareto front.