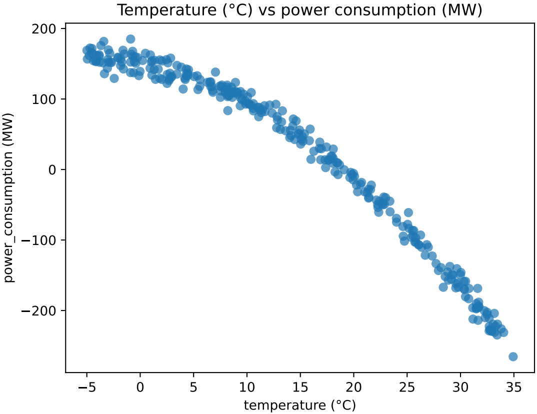
Machine learning I, supervised learning: linear regression



Content

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.)

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.

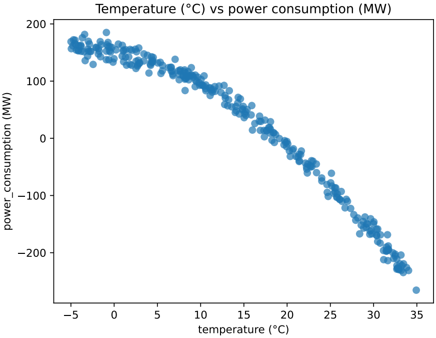


Figure – Dataset

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

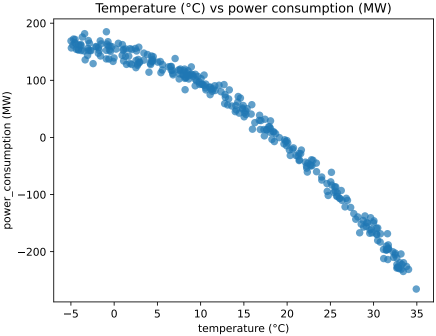


Figure – Dataset

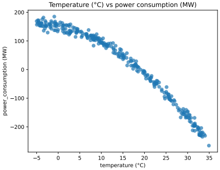


Figure – Dataset

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 :

- input space (temperature) : $\mathcal{X} = \mathbb{R}$
- 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 l :

$$l(y_1, y_2) = (y_1 - y_2)^2 \tag{2}$$

Empirical risk

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

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

We want to find θ and b such that $R_n(\theta, b)$ has the **smallest possible value**.

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 θ 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 (θ^*, b^*) such that the gradient cancels (more on that tomorrow).

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

Derivatives

We drop the $\frac{1}{n}$ as it does not change the final result :

$$\begin{aligned}\frac{\partial R_n}{\partial \theta}(\theta, b) &= \sum_{i=1}^{n} 2(\theta x_i + b - y_i)x_i \\ &= 2[\theta \sum_{i=1}^{n} x_i^2 + b \sum_{i=1}^{n} x_i - \sum_{i=1}^{n} x_i y_i]\end{aligned} \tag{5}$$

$$\begin{aligned}\frac{\partial R_n}{\partial b}(\theta, b) &= \sum_{i=1}^{n} 2(\theta x_i + b - y_i) \\ &= 2[\theta \sum_{i=1}^{n} x_i + nb - \sum_{i=1}^{n} y_i]\end{aligned} \tag{6}$$

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

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

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

Which means

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

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

Finally :

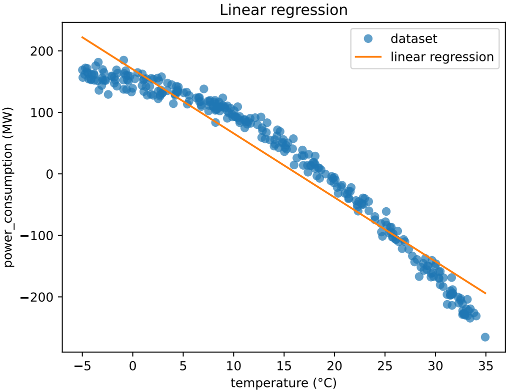
$$\theta(\sum_{i=1}^{n} x_i^2 - \frac{1}{n}(\sum_{i=1}^{n} x_i)^2) + \frac{1}{n}\sum_{i=1}^{n} x_i \sum_{i=1}^{n} y_i - \sum_{i=1}^{n} x_i y_i = 0 \qquad (11)$$

or

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

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.



Linear regression in one dimension

General linear regression : Ordinary least squares

Overfitting, hyperparameters and ridge regression

Generalization

Linear regression also works in higher dimenions, 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.

Empirical risk

The empirical risk now writes :

$$R_n(\theta, b) = \frac{1}{n} \sum_{i=1}^{n} (\langle \theta, x_i \rangle + b - y_i)^2 \tag{14}$$

Almost similarly to the 1D case ($\theta \in \mathbb{R}$, $x_i \in \mathbb{R}$), where it was :

$$R_n(\theta, b) = \frac{1}{n} \sum_{i=1}^{n} (\theta x_i + b - y_i)^2 \tag{15}$$

Matrix notations

If we store the input data in a matrix X with n lines and d columns, and the labels in a vector y with n lines, the empirical risk writes :

$$X = \begin{pmatrix} x_1^T \\ \dots \\ x_i^T \\ \dots \\ x_n^T \end{pmatrix} = \begin{pmatrix} x_{11}, \dots, x_{1j}, \dots x_{1d} \\ \dots \\ x_{i1}, \dots, x_{ij}, \dots x_{id} \\ \dots \\ x_{n1}, \dots, x_{nj}, \dots x_{nd} \end{pmatrix} \tag{16}$$

$$R_n(\theta, b) = \frac{1}{n} ||X\theta - y + b||^2 \tag{17}$$

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

OLS estimator

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

$$\hat{\theta} = (X^T X)^{-1} X^T y \tag{18}$$

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

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.
Example with **Ridge_scikit.py**.

- OLS risk :

$$R_{n,OLS}(\theta, b) = \sum_{i=1}^{n} (\theta x_i + b - y_i)^2 \tag{19}$$

- Ridge risk :

$$R_{n,Ridge}(\theta, b) = \sum_{i=1}^{n} (\theta x_i + b - y_i)^2 + \lambda ||\theta||^2 \tag{20}$$

with $\lambda > 0$ a real number (regularization parameter).

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

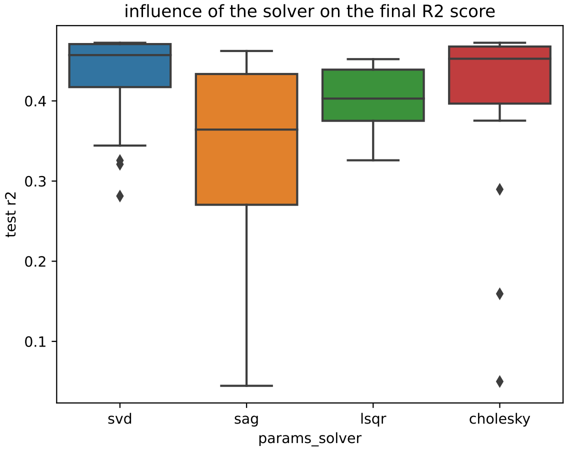
- The choice of the hyperparameters is very important. Most of the time, it is guided by experimentation and / or theoretical results.
- Some methods and libraries are helpful to look for good hyperparameters, such as **optuna** `https://optuna.org/`
- other classical methods : gridsearch, random search.

Using optuna to tune Ridge regression

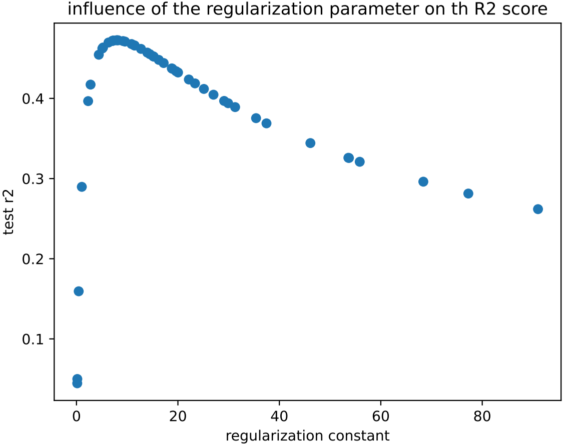
Exercice 4 :

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

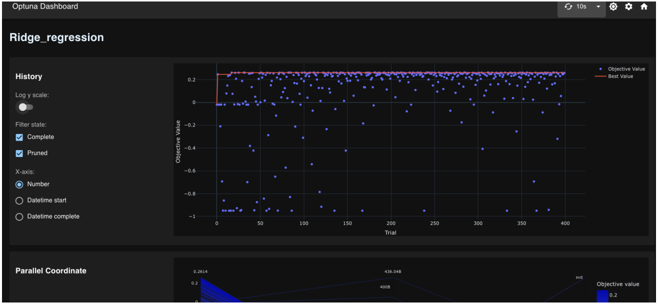


Analysis of the hyperparameters



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.