Exercise sheet 1: Gradient descent & statistical learning

- Please submit the solution as a single file, using the naming convention 'your_last_name.py', on the Moodle page of the course.
- Keep in mind to comment your code sufficiently and to include a demonstration.
- You should not import any packages that violate the spirit of the exercise.
- It should suffice to execute your Python script once to verify that the exercise has been solved.

The Michaelis-Menten model of enzyme kinetics

The Michaelis-Menten model describes the rate of formation of a product (x) by an enzyme with respect to the concentration of a substrate (y) that is processed by the enzyme. The more substrate there is, the higher the production-rate of the enzyme, but the processing capacity of the enzyme is also limited. The model posits the following relationship.

$$y = \frac{\theta_1 x}{\theta_2 + x}$$

The model is specified by the parameter vector $[\theta_1, \theta_2] \in \mathbb{R}^2$.

Data

x	0.05	0.1	0.25	0.5	1	2.5	5	8	20	30
y	4	7	16	32	50	90	115	119	142	166

The x-variable is substrate concentration (mM) and the y-variable is the reaction rate (muM/min).

Source: Aledo, Juan. Enzyme kinetic parameters estimation: A tricky task? Biochemistry and Molecular Biology Education 49:4, p. 663-638. 2021.

1 Implement gradient descent to fit the model

Implement gradient descent to solve the statistical learning problem of fitting the above model to the given data. Use the squared deviation loss on examples.

Hint: (i) Write down the function to be optimized by gradient descent (The arithmetic mean of the loss on examples). (ii) Compute the derivatives of this function with respect to the parameters. (iii) Implement gradient descent (using vectorization whenever possible).

2 Numerical experimentation

Illustrate numerically that you can fit the Michaelis-Menten model to the given data.