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DEPARTMENT  
OF CHEMISTRY MATERIALS  
AND CHEMICAL  
ENGINEERING

# Mono-dimensional optimization

Calcoli di Processo dell' Ingegneria Chimica

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# Exercises

# Mono dimensional optimization

In a one-dimensional optimization problem, it is necessary to identify the value of the variable  $x$  (also known as the degree of freedom) that optimizes the objective function  $f(x)$ .

The optimum of the problem can be represented by either the maximum or minimum of the objective function.

$$\max_x \{f(x)\} \quad \text{or} \quad \min_x \{f(x)\}$$

The two problems are entirely equivalent. Indeed, it is sufficient to change the sign of the objective function to transform a minimization problem into a maximization problem and vice versa:

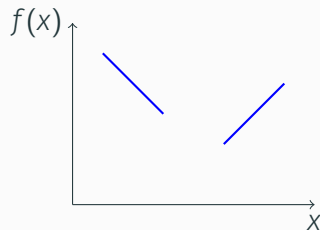
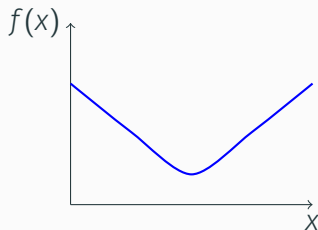
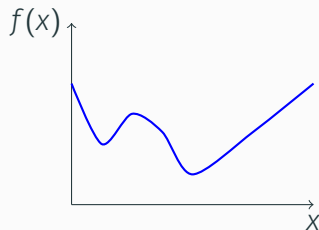
$$\max_x \{f(x)\} \equiv \min_x \{-f(x)\}$$

$$\min_x \{g(x)\} \equiv \max_x \{-g(x)\}$$

Using classical analysis knowledge incorrectly, one might think that to solve the problem:

$$\min_x \{f(x)\} \longrightarrow \frac{df(x)}{dx} = 0$$

Nothing could be more incorrect. It should be recalled that the aforementioned condition is necessary to identify an extremum point of a continuous and differentiable function. However, this condition does not cover specific cases such as the following examples:



In one-dimensional function optimization, two main families of solution methods can be identified:

- ▶ **Comparison Methods:** These methods rely exclusively on comparisons between objective function values.
- ▶ **Approximation Methods:** These methods approximate the objective function with simpler functions and seek to find the optimal point of these approximating functions.

An alternative classification can also be made:

**Sequential Methods:** The evaluation of the objective function is conducted sequentially. Each evaluation enables the determination of subsequent actions to be taken.

**Parallel Methods:** These methods allow multiple function evaluations to be performed before deciding on the next strategy. Generally, these methods require significantly more function evaluations. They become particularly relevant when utilizing multiprocessor computing systems.

# In Matlab

We are going to solve the following problem:

$$\min_x f(x) \text{ s.t. } \begin{cases} c(x) \leq 0 \\ ceq(x) = 0 \\ A \cdot x \leq b \\ Aeq \cdot x = beq \\ lb \leq x \leq ub \end{cases}$$

$$x = \textit{fmincon}(\textit{fun}, x0, A, b)$$

# Exercises

► **Exercise 1:** The task is to determine the optimal dimensions of a cylindrical pressure vessel with a specified volume of  $V = 100m^3$ . The following simplifying assumptions are made:

- Both ends (heads) are flat and closed.
- All vessel walls have constant thickness,  $t$ , and density,  $\rho$ .
- Manufacturing costs are equal for both heads and the lateral wall.
- Wall thickness,  $t$ , is independent of vessel pressure.
- There is no manufacturing waste.

The problem requires:

- Identification of possible objective function(s) to optimize
- Development of an analytical solution
- Proposal of an alternative numerical solution
- Determination of the optimal  $L/D$  ratio (height to diameter ratio of the cylinder)



► **Exercise 2:** By removing the simplifying assumptions expressed in Exercise 1, we arrive at a more complex objective function that takes into account the following considerations:

- The end caps are ellipsoidal, thus having a larger surface area compared to the flat surface assumption
- The end caps are more expensive to manufacture than the lateral surface
- The sheet metal thickness is a function of the vessel diameter.

In this case, the objective function to be optimized is:

$$f_{obj} = 0.0432V + 0.5\frac{V}{D} + 0.3041D^2 + 0.0263D^3$$

Determine the optimal diameter  $D$  and the height  $L$  knowing that:

$$V = \frac{\pi D^2}{4} \left( L + \frac{D}{2} \right).$$

- **Exercise 3:** In radiation, the spectral power emitted by a black body can be expressed using the following relation:

$$E_b(\lambda, T) = \frac{C_1}{\lambda^5 \exp\left(\frac{C_2}{\lambda T}\right)^{-1}}$$

Where:

$$C_1 = 3.742 \times 10^8 \text{ W} \cdot \mu\text{m}^4 / \text{m}^2$$

$$C_2 = 1.439 \times 10^4 \mu\text{m} \cdot \text{K}$$

Determine the peak power emission point of a black body at a temperature of 800 K by plotting the behavior of  $E_b$  versus electromagnetic radiation wavelength on a log-log graph. Compare the wavelength value found through numerical procedure with that obtained from Wien's Law:

$$\lambda_{\max} T = C_3 \quad C_3 = 2897.8 \mu\text{m} \cdot \text{K}$$

- **Exercise 4:** In a shock tube, autoignition delay times of a fuel are measured at a temperature of 1000 K under varying pressure conditions as reported in the following table:

P [atm]	tau [ms]
3	0.75
10	0.20
20	0.10
30	0.55
40	0.04
60	0.03

A model is to be formulated to estimate the autoignition delay time as a function of pressure, using the data point at 10 *atm* as a reference value, according to the formula:

$$\tau = \tau_0 \left( \frac{P}{P_0} \right)^\beta \quad \tau_0 = \tau(10 \text{ atm}) \quad P_0 = 10 \text{ atm}$$

Compute the parameter  $\beta$  using the method of the sum of the squared errors, in order to solve the problem:

- The definition of a model function that takes pressure and  $\beta$  as inputs and returns the value of  $\tau$ .
- The definition of an objective function that computes the sum of squared residuals  $f(x) = \sum_i (\tau_i - \tau_{mod_i})^2$ , taking  $\beta$  as input.

Thank you for your attention!