CHEM-E7225/2020-2021: Exercise 02

Task 1 (20 points). Consider the following uni-dimensional unconstrained optimisation problem

$$\min_{x \in \mathcal{R}} \quad \frac{x^2 - 5x + 6}{x^2 + 1}$$

1. Plot the objective function $f(x)$ and solve visually for the optimal value x^*;
2. Derive on paper the gradient $\nabla f(x)$ and the Hessian $\nabla^2 f(x)$ of the objective function;
3. Can you derive on paper the value x^* such that $\nabla f(x) = 0$? If positive, comment on $\nabla^2 f(x^*)$;
4. What would the minimiser be, had we included inequality constraints $x \in [0, 4]$,

$$\begin{aligned} \min_{x \in \mathcal{R}} \quad & \frac{x^2 - 5x + 6}{x^2 + 1} \\ \text{subject to} \quad & 4 \geq x \geq 0 \end{aligned}$$

5. Implement code to formulate both these problems and then solve them for the optimal values x^*;
6. Comment on the chosen solver and on the results of the optimisation.

Task 2 (40 points). Consider the following two-dimensional constrained optimisation problem

$$\begin{aligned} \min_{x,y \in \mathcal{R}} \quad & -20e^{-0.2\sqrt{0.5(x^2+y^2)}} - e^{(0.5(\cos(2\pi x)+\cos(2\pi y)))} + e + 20 \\ \text{subject to} \quad & x^2 + y^2 \leq 3 \end{aligned}$$

1. Plot the objective function $f(x, y)$ with the feasible set and solve for the optimal value (x^*, y^*);
2. Implement code to formulate this problem and then solve it for the optimal value (x^*, y^*). Show graphically and report the results when using 16 randomly chosen and different initial solutions;
3. Comment on the chosen solver and on the results of the optimisation.

Task 3 (40 points). Consider the constrained optimisation of the N-dimensional Rosenbrock function

$$\begin{aligned} \min_{x \in \mathcal{R}^{N+1}} \quad & \sum_{n=1}^{N} \left(100\left(x_{n+1} - x_n^2\right)^2 + (1 - x_n)^2\right) \\ \text{subject to} \quad & \sum_{n=1}^{N+1} (x_n - 1)^2 \leq 2 \end{aligned} \tag{1}$$

1. Implement code to formulate this problem for $N = 8$, then solve it from different initial solutions;
2. Solve for the optimal value x^* and comment on the chosen solver and on the results of the optimisation.

Errata

- Error in Task 2, item 1. Text should read 'Plot the objective function $f(x, y)$ ...', instead of $f(x^*, y^*)$.
- Error in Task 2, item 1. Removed the minus sign inside the square root.
- Errors in problem formulation in Eq. (1). The correct optimisation problem:

$$\begin{aligned} \min_{x \in \mathcal{R}^{N+1}} \quad & \sum_{n=1}^{N} \left(100\left(x_{n+1} - x_n^2\right)^2 + (1 - x_n)^2\right) \\ \text{subject to} \quad & \sum_{n=1}^{N+1} (x_n - 1)^2 \leq 2 \end{aligned}$$