CHEM-E7225/2022: Exercise 02

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

$$\min_{x \in \mathcal{R}} \frac{x^2 - 4x + 9}{x^2 + 2}$$

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 values 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 $x \in [-10, -1]$,

$$\begin{aligned} \min_{x \in \mathcal{R}} \quad & \frac{x^2 - 4x + 9}{x^2 + 2} \\ \text{subject to} \quad & -10 \leq x \leq -1 \end{aligned}$$

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

Task 2 (30 points). Consider the following two-dimensional constrained optimisation problem

$$\begin{aligned} \min_{x,y \in \mathcal{R}} \quad & \sin(y) e^{(1-\cos(x))^2} + \cos(x) e^{(1-\sin(y))^2} + (x - y)^2 \\ \text{subject to} \quad & (x+5)^2 + (y+5)^2 \leq 25 \end{aligned}$$

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 8 arbitrary chosen and different initial solutions. Choose one of results and show graphically the intermediate solutions for each iteration of the solver;
3. Comment on the results of the optimisation.

Task 3 (50 points). Consider the constrained optimisation of the N-dimensional Rosenbrock function

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

1. Implement code to formulate this problem for $N = 800$, then solve it from different initial solutions;
2. Comment on the results of the optimisation.

CasADi's Opti Stack tutorial

The **Opti Stack**[1] is a collection of helper functions from CasADi that allows us to construct nonlinear optimisation problems using the standard mathematical notation. Consider the optimization problem

$$
\begin{aligned}
\min_{x,y \in \mathcal{R}^N} \quad & (y - x^2)^2 \\
\text{subject to} \quad & x^2 + y^2 = 1 \\
& x + y \geq 1
\end{aligned}
$$

This problem is constructed and solved through the following script:

```
opti = casadi.Opti();                     % Creates an Opti Stack structure

x = opti.variable();                      % Creates a scalar decision variable (x)
y = opti.variable();                      % Creates a scalar decision variable (y)

opti.minimize( (y - x^2)^2 );             % Define the objective function to be minimized
opti.subject_to( x^2 + y^2 == 1 )         % Defines an equality constraint
opti.subject_to( x + y >= 1 )             % Defines an inequality constraint

opti.solver('ipopt')                      % Chooses a solver (IPOPT, qpOASES, ...)

% Adds callbacks to 'track' the value of (x,y)
x_iter = []; y_iter = [];
opti.callback(@(i) evalin('base',
        'x_iter = [x_iter opti.debug.value(x)]; y_iter = [y_iter opti.debug.value(y)];') )
% -

opti.set_initial([x  y], [-1 1])          % Sets an initial solution (default: 0)
opti.solve()                              % Executes the solver

x_sol = opti.value(x);                    % Retrieves the optimal solution of (x)
y_sol = opti.value(y);                    % Retrieves the optimal solution of (y)
```

The solver obtains the solution $(x^*, y^*) = (0.78615, 0.61803)$, associated to the optimal value $f(x^*, y^*) \approx 0$.

[1] Check the documentation in `https://web.casadi.org/docs/#document-opti` .