Instructions: (Please read carefully and follow them!)

Try to solve all problems on your own. If you have difficulties, ask the instructor or TAs.

In this session, we will discuss BFGS method to solve problems of the form $\min_{\mathbf{x}\in\mathbb{R}^n} f(\mathbf{x})$.

The implementation of the optimization algorithms in this lab will involve extensive use of the `numpy` Python package. It would be useful for you to get to know some of the functionalities of `numpy` package. For details on `numpy` Python package, please consult https://numpy.org/doc/stable/index.html

For plotting purposes, please use `matplotlib.pyplot` package. You can find examples in the site https://matplotlib.org/examples/.

Please follow the instructions given below to prepare your solution notebooks:

- Please use different notebooks for solving different Exercise problems.
- The notebook name for Exercise 1 should be `YOURROLLNUMBER_IE684_Lab5_Ex1.ipynb`.
- Similarly, the notebook name for Exercise 2 should be `YOURROLLNUMBER_IE684_Lab5_Ex2.ipynb`, etc.
- Please post your doubts in MS Teams Discussion Forum channel so that TAs can clarify.

There are only 2 exercises in this lab. Try to solve all problems on your own. If you have difficulties, ask the Instructors or TAs.

Only the questions marked **[R]** need to be answered in the notebook. You can either print the answers using `print` command in your code or you can write the text in a separate text tab. To add text in your notebook, click `+Text`. Some questions require you to provide proper explanations; for such questions, write proper explanations in a text tab. Some questions require the answers to be written in LaTeX notation. Please see the demo video (posted in Lab 1) to know how to write LaTeX in Google notebooks. Some questions require plotting certain graphs. Please make sure that the plots are present in the submitted notebooks. Please include all answers in your `.pynb` files.

After completing this lab's exercises, click File → Download .ipynb and save your files to your local laptop/desktop. Create a folder with name `YOURROLLNUMBER_IE684_Lab5` and copy your `.ipynb` files to the folder. Then zip the folder to create `YOURROLLNUMBER_IE684_Lab5.zip`. Then upload only the `.zip` file to Moodle. There will be extra marks for students who follow the proper naming conventions in their submissions.

Please check the **submission deadline announced in moodle.**

Exercise 1: BFGS Method

$k \leftarrow 0$;
Start with a suitable point $\mathbf{x}^k \in \mathbb{R}^n$;
while *not converged* **do**
  $\mathbf{p}^k \leftarrow -(B^k)\nabla f(\mathbf{x}^k)$;
  $\alpha^k \leftarrow \text{argmin}_{\alpha\geq 0} f(\mathbf{x}^k + \alpha\mathbf{p}^k)$;
  $\mathbf{x}^{k+1} \leftarrow \mathbf{x}^k + \alpha^k\mathbf{p}^k$;
  $\mathbf{s}^k = \mathbf{x}^{k+1} - \mathbf{x}^k$;
  $\mathbf{y}^k = \nabla f(\mathbf{x}^{k+1}) - \nabla f(\mathbf{x}^k)$;
  Implement the update rule to update B^{k+1}. ;
  $k \leftarrow k + 1$;
end

Algorithm 1: BFGS Method

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1. **[R]** What is a suitable initial choice of B (denoted by B^0)? Justify with proper reasons.
2. Implement the modules of BFGS method to solve the problem $\min_{\mathbf{x}\in\mathbb{R}^n} f(\mathbf{x})$ where we have $f(\mathbf{x}) = f(x_1, x_2, \ldots, x_n)$ $=\sum_{i=1}^{n-1}\left[4(x_i^2 - x_{i+1})^2 + (x_i - 1)^2)\right]$. Use backtracking line search with $\alpha^0 = 0.9, \rho = 0.5, \gamma = 0.5$ in the implementation of BFGS method. Take the starting point to be $\mathbf{x}^0 = (0, 0, \ldots, 0)$.
3. **[R]** Take $n \in \{1000, 2500, 5000, 7500, 10000\}$, find minimizer of the objective function in each case and compute the time taken by the BFGS method with backtracking line search. Tabulate the time taken by BFGS method for each n.
4. Use Newton's method to solve the problem $\min_{\mathbf{x}\in\mathbb{R}^n} f(\mathbf{x})$. In Newton's method implementation, use backtracking line search with $\alpha^0 = 0.9, \rho = 0.5, \gamma = 0.5$. Take the starting point to be $\mathbf{x}^0 = (0, 0, \ldots, 0)$ in the implementation of Newton's Method.
5. **[R]** Take $n \in \{1000, 2500, 5000, 7500, 10000\}$, find minimizer of the objective function in each case and compute the time taken by the Newton's method with backtracking line search. Tabulate the time taken by Newton's method for each n.
6. **[R]** Compare the time taken by BFGS method with backtracking line search against the time taken by Newton's method with backtracking line search for each value of n. Plot the time taken by both methods vs n using different colors. Comment on your observations.

Exercise 2:

In this exercise we shall consider the following problem:

$$\min_{\mathbf{x}=(x_1,x_2,\ldots,x_n)\in\mathbb{R}^n} q(x_1,x_2,\ldots,x_n) = \sum_{i=1}^{n}\left((x_i-1)^2 + (x_1 - x_i^2)^2\right).$$

1. Implement the required modules to compute the objective function value, gradient and Hessian for $q(\mathbf{x})$.
2. Use BFGS method to solve the problem $\min_{\mathbf{x}\in\mathbb{R}^n} q(\mathbf{x})$. Use backtracking line search with $\alpha^0 = 0.9, \rho = 0.5, \gamma = 0.5$ in the implementation of BFGS method. Take the starting point to be $\mathbf{x}^0 = (0,0,\ldots,0)$.
3. **[R]** Take $n \in \{1000, 2500, 5000, 7500, 10000\}$, find minimizer of the objective function in each case and compute the time taken by the BFGS method with backtracking line search. Tabulate the time taken by BFGS method for each n.
4. Use Newton's method to solve the problem $\min_{\mathbf{x}\in\mathbb{R}^n} q(\mathbf{x})$. In Newton's method implementation, use backtracking line search with $\alpha^0 = 0.9, \rho = 0.5, \gamma = 0.5$. Take the starting point to be $\mathbf{x}^0 = (0,0,\ldots,0)$ in the implementation of Newton's Method.
5. **[R]** Take $n \in \{1000, 2500, 5000, 7500, 10000\}$, find minimizer of the objective function in each case and compute the time taken by the Newton's method with backtracking line search. Tabulate the time taken by Newton's method for each n.
6. **[R]** Compare the time taken by BFGS method with backtracking line search against the time taken by Newton's method with backtracking line search for each value of n. Plot the time taken by both methods vs n using different colors. Comment on your observations.