Week 4 — Homework: Generalized minimal residual method

The goal of this exercise is to get familiar with scipy and numpy module by implementing an iterative solver and visualizing the results. We will use Python for this exercise. A README file has to be included and should describe how to execute the code as well as its structure and dependencies. The following points will be considered for the grading:

- Proper usage of git (meaningful comments, several commits with developments steps, use of .gitignore)
- Code works as intended
- Readability of the code (meaningful variable names, comments)
- Minimal documentation: README file

Exercise 1: Scipy optimization

In this exercise, we will use **Scipy** module. The goal of this exercise is to find the value of $\underline{x}^T = (x, y)$ which minimizes the quadratic function $S(\underline{x})$ defined by the equation:

$$S(\underline{x}) = \frac{1}{2} \underline{x}^T \underline{\underline{A}} \ \underline{x} - \underline{x}^T \underline{b}$$

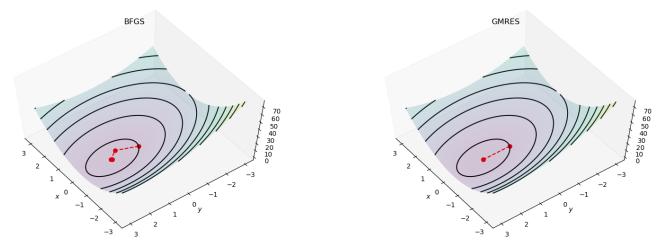
where

$$A = \begin{pmatrix} 8 & 1 \\ 1 & 3 \end{pmatrix} \text{ and } b = \begin{pmatrix} 2 \\ 4 \end{pmatrix}$$

The minimizer of the above function is also the solution of the linear system of equation:

$$\underline{A} \ \underline{x} = \underline{b}$$

Figure below shows the surface plot for $S(\underline{x})$. The red line shows the iterative path taken by BFGS and GMRES solvers to locate the minima of the function.



1. Create a **optimizer.py** file. In this file, create a function which takes $S(\underline{x})$ or (A,b) as a input argument in form of a python functor and returns the minimizer. Use scipy.optimize.minimize

scipy.sparse.linalg.lgmres routines to solve the minimization problem. The type of solver can be specified through method parameter. For more help, refer to the documentations: Scipy optimize and Scipy sparse linear algebra

2. Implement another routine which plots the $S(\underline{x})$ and the solution at each iteration step similar to figure shown above. Use **Matplotlib** module for plotting. To get the solution at each iterative step from scipy.optimize.minimize and scipy.sparse.linalg.lgmres, you will have to use the parameter callback.

Exercise 2: Generalized minimal residual method

The generalized minimal residual method (GMRES) is one of the many known iterative techniques for solving large sparse linear system. For this exercice, implement the GMRES method to find the solution of the equation:

$$\underline{A} \ \underline{x} = \underline{b}$$

- 1. Create a **GMRES.py** file which implements the GMRES method. Use **einsum** from the **Numpy** module to perform different matrix and vector operations such as inner product, dot product etc. The implementation should be independent of matrix and vector size. For help, please refer to the wikipedia page Generalized minimal residual method
- 2. Use argparse to input the coefficients A and b of the system defined in the previous exercise via the command-line. Use argparse also to specify which type of minimizer to be used (yours or the one from scipy.optimize/scipy.sparse.linalg).
- 3. Use the plotting routine developed in the previous exercise to plot the solution at each iteration step and compare the method with the **Scipy** optimization method chosen by you in the previous exercise. Use argparse to make the plot optional.