Homework assignment 2

Hand in on DTU Inside before 8 November 10pm. **The overall page limit exclude Appendix is 6.**

1 One-page report on the exercises for week 9 (40%)

In this one-page report, you should discuss the exercise that you did on the Powell's problem. In your discussion, you should focus on the following questions:

1. (5%) What makes the Powell's problem difficult to solve?
2. Comparisons of Newton's, Gauss-Newton, Levenberg-Marquardt.
   (a) (10%) What are the differences or similarities on these three methods?
   (b) (5%) What are the convergence rates?
   (c) (10%) What are the advantages and limitations on each method?
3. (10%) In the last method, we simply changed the variables, then what happened when we called the L-M method? Why?

For the report, you don't need the introduction and conclusion parts. You can illustrate your points by the figures, formulas, tables... But the page limit is **ONE**.

2 Rosenbrock problem (15%)

The Rosenbrock problem that we studied in 4-hour exercise in Week 5 can be formulated as a system of nonlinear equations:

$$\boldsymbol{r}(\boldsymbol{x}) = \sqrt{2}\begin{bmatrix} 10(x_2 - x_1^2) \\ 1 - x_1 \end{bmatrix}.$$

It is easy to see that this system has the unique solution $\boldsymbol{x}^* = [1, 1]^T$, and this is the unique minimizer for $f(\boldsymbol{x}) = \frac{1}{2}\|\boldsymbol{r}(\boldsymbol{x})\|_2^2$.

1. (by hand) Calculate the Jacobian J of $\boldsymbol{r}$.
2. Implement a Matlab function to calculate $\boldsymbol{r}$ and J with a given $\boldsymbol{x}$. You can start your function with

   ```
   function [r,J]=fun_rJ_Rosen(x)
   ```

   Please include this Matlab function in your answers.

3. Call the Matlab function `Levenberg_Marquardt_yq.m` to apply the Levenberg-Marquardt method to solve the minimization problem

$$\min_{\boldsymbol{x}} f(\boldsymbol{x}) = \frac{1}{2}\|\boldsymbol{r}(\boldsymbol{x})\|_2^2.$$

Set the starting point as $\boldsymbol{x}_0 = [-1.2, 1]^T$ and the initial λ as $10^{-3}\|J(\boldsymbol{x}_0)^T J(\boldsymbol{x}_0)\|_2$. Plot $\boldsymbol{e}_k = \|\boldsymbol{x}_k - \boldsymbol{x}^*\|_2$, $f(\boldsymbol{x}_k)$ and $\|\nabla f(\boldsymbol{x}_k)\|_2$ as functions of the iteration number. How many iterations did the method need until meeting the default stopping criteria? Which convergence rate did you observe?

3 Linear least squares with weights (15%)

In this exercise, we determine the parameters in the fit function

$$\phi(t) = x_1 e^{-27t} + x_2 e^{-8t} + x_3$$

to fit a NMR signal. We know that the exact parameters $\boldsymbol{x}^* = [1.27, 2.04, 0.3]^T$. In addition, we know that the first 10 data points was added larger Gaussian noise with mean 0 and standard deviation 0.5, and the rest data points was added Gaussian noise with mean 0 and standard deviation 0.1.

1. Load the data in `data_exe3.mat`. Compute the least squares fit without taking the difference in noise levels into account. What is the solutions of all three parameters? What is the 2-norm of the absolute error $\|\boldsymbol{e}\|_2 = \|\boldsymbol{x} - \boldsymbol{x}^*\|_2$?

2. Now, we take the difference of the noise levels into account and apply the linear weighted least squares fit. According to the standard deviations of the noise, how should we add weights to the problem, i.e, what is the weight matrix? Compute the weighted least squares solution and the 2-norm of the absolute error.

3. Compare the solutions without the weights and with the weights. Which one is more accurate?

4 Meyer's problem (30%)

This exercise illustrates that normally the algorithms for solving the least squares problems work best when the problem is scaled so that all the nonzero components of $\boldsymbol{x}$ are of the same order of magnitude.
Consider Meyer's problem:

$$r_i(\boldsymbol{x}) = y_i - x_1 \exp\left(\frac{x_2}{t_i + x_3}\right), \qquad i = 1, \cdots, 16,$$

with $t_i = 45 + 5i$ and

i	y_i	i	y_i	i	y_i
1	34780	7	11540	12	5147
2	28610	8	9744	13	4427
3	23650	9	8261	14	3820
4	19630	10	7030	15	3307
5	16370	11	6005	16	2872
6	13720				

1. (10%) Calculate the Jacobian J, and implement a Matlab function to return the residual $\boldsymbol{r}$ and J with given $\boldsymbol{x}$, $\boldsymbol{t}$ and $\boldsymbol{y}$. Please include this Matlab function in your answers.

2. (5%) Call the Matlab function `Levenberg_Marquardt_yq.m` to apply the Levenberg-Marquardt method to solve the minimization problem

$$\min_{\boldsymbol{x}} f(\boldsymbol{x}) = \frac{1}{2}\|\boldsymbol{r}(\boldsymbol{x})\|_2^2.$$

Set the starting point as $\boldsymbol{x}_0 = [0.02, 4000, 250]^T$ and the initial λ as $\|J(\boldsymbol{x}_0)^T J(\boldsymbol{x}_0)\|_2$. Plot $f(\boldsymbol{x}_k)$ and $\|\nabla f(\boldsymbol{x}_k)\|_2$ as functions of the iteration number. How many iterations did the method need until meeting the default stopping criteria?

Now we use an alternative formulation, which is

$$\rho_i(\boldsymbol{x}) = 10^{-3} y_i - z_1 \exp\left(\frac{10 z_2}{u_i + z_3} - 13\right), \qquad i = 1, \cdots, 16,$$

with $u_i = 0.45 + 0.05i$. The formulation corresponds to

$$\boldsymbol{z} = [10^{-3} e^{13} x_1, 10^{-3} x_2, 10^{-2} x_3]^T.$$

3. (5%) Calculate the Jacobian J_s, and implement a Matlab function to return the residual $\boldsymbol{\rho}$ and J_s with given $\boldsymbol{z}$, $\boldsymbol{u}$ and $\boldsymbol{y}$. Please include this Matlab function in your answers.

4. (5%) Call the Matlab function `Levenberg_Marquardt_yq.m` to apply the Levenberg-Marquardt method to solve the minimization problem

$$\min_{\boldsymbol{z}} f(\boldsymbol{z}) = \frac{1}{2}\|\boldsymbol{\rho}(\boldsymbol{z})\|_2^2.$$

Set the starting point as $\boldsymbol{z}_0 = [8.85, 4, 2.5]^T$ and the initial λ as $\|J(\boldsymbol{x}_0)^T J(\boldsymbol{x}_0)\|_2$. Plot $f(\boldsymbol{z}_k)$ and $\|\nabla f(\boldsymbol{z}_k)\|_2$ as functions of the iteration number. How many iterations did the method need until meeting the default stopping criteria?

5. (5%) Comparing both formulations, which need less iterations?