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Exercise session 10, 20 November, 2019

Numerical Methods in Informatics (L + E)

First part:

Exercise on PageRank (see Exercise session 9)

Exercise 1

Consider the following nonlinear system

$$\begin{aligned} &3x_1 - \cos(x_2 x_3) &&= 0.5 \\ &x_1^2 - 81(x_2 + 0.1)^2 + \sin x_3 &&= -1.06 \\ &e^{-x_1 x_2} + 20x_3 &&= -(10\pi - 3)/3 \end{aligned}$$

a. Write a MATLAB routine that implements the Newton's method to solve a system of non-linear equation, taking as inputs two function handles, one for the function and one for the Jacobian. Stop the algorithm when the euclidean norm of the difference between consecutive iterations is below an input threshold `tol`.

b. Which are the conditions under which the algorithm implemented in point **a.** is expected to converge?

c. Solve the given systems with initial guess $x^{(0)} = [0.1, 0.1, -0.1]^{\mathrm{T}}$ and $\texttt{tol} = 1 \cdot 10^{-8}$. Report the solution and the number of iterations.
Hint: π is defined in MATLAB as `pi`.

Exercise 2

Consider minimizing the function

$$f(\mathbf{x}) = \frac{1}{2}\left([1.5 - x_1(1 - x_2)]^2 + \left[2.25 - x_1(1 - x_2^2)\right]^2 + \left[2.65 - x_1(1 - x_2^3)\right]^2\right)$$

a. Formulate the minimization function as a zero-finding problem $\mathbf{F}(\mathbf{x}) = \boldsymbol{\nabla}\mathbf{f}(\mathbf{x}) = \mathbf{0}$.

b. Find the minimizer of this function using the Newton's method. Use $\mathbf{x}_a^{(0)} = [8, 0.2]^{\mathrm{T}}$ as initial guess.

c. Try to apply again the Newton's method, but now using $\mathbf{x}_b^{(0)} = [8, 0.8]^{\mathrm{T}}$ as initial guess. Does the method converge? Is the result an actual minimizer?

Exercise 3 Do at home!

Consider the nonlinear PDE in two dimensions given by

$$-\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) + \exp(u) = g(x, y)$$

Here $u = u(x, y)$ is an unknown function of 2 variables x and y, while $g(x, y)$ is a given function (usually called *source*)[1]. In this case, we consider $g(x, y) = \exp(1) = \text{const}$.
The problem is defined on the unit square on $0 < x, y < 1$, with boundary conditions $u(x, 0) = u(x, 1) = u(0, y) = u(1, y) = 0$. We can discretize this equation with centered differences on a uniform mesh (or grid), with a grid spacing $h = \frac{1}{(N+1)}$, obtaining the equations

$$\begin{aligned} 4u_{i,j} - u_{i+1,j} - u_{i-1,j} - u_{i,j+1} - u_{i,j-1} + h^2 e^{u_{i,j}} &= h^2 \exp(1), \quad && 1 \le i, j \le N, \\ u_{i,j} &= 0 && \text{otherwise.} \end{aligned} \tag{1}$$

where $u_{i,j}$ is the value of u at the grid node (i, j). Notice that without the term $h^2 \exp(u_{i,j})$, Eq. (1) can be written as a linear system (exactly the one reported on Page 5 of Lecture 7). In a similar way, we can now re-write the problem as a non-linear systems $\mathbf{F}(\mathbf{u}) = \mathbf{0}$ with

$$\mathbf{u} \in \mathbb{R}^n, \quad n = N^2, \qquad \text{and} \quad \mathbf{u} = [u_{1,1}, u_{2,1}, \ldots, u_{N,1}, u_{1,2}, u_{2,2}, \ldots, u_{N,2}, \ldots, u_{N,N}]^{\mathrm{T}}$$

The Jacobian matrix of this function $\mathbf{F}(\mathbf{x})$ is the sparse matrix obtained by summing the matrix A defined for the linear case and a diagonal matrix D with the exponential terms $D = \operatorname{diag}\left(h^2 \exp(\mathbf{u})\right)$, i.e., $J_{\mathbf{F}(\mathbf{u})} = A + D$. The matrix A can be viewed as tridiagonal block matrix, with block of size $N \times N$:

$$A = \left[\begin{array}{c|c|c|c} D_A & -I & & \\ \hline -I & D_A & -I & \\ \hline & \cdots & \cdots & \cdots \\ \hline & & -I & D_A \end{array}\right] \in \mathbb{R}^{n \times n}, \qquad \text{with} \quad D_A = \begin{bmatrix} 4 & -1 & & \\ -1 & 4 & -1 & \\ & \cdots & \cdots & \cdots \\ & & -1 & 4 \end{bmatrix} \in \mathbb{R}^{N \times N}$$

where the diagonal blocks D_A are tridiagonal matrices and the first upper and lower sub-diagonal blocks $-I$ are the negative identity matrices of size $N \times N$. Thus, we have

$$\mathbf{J}_{\mathbf{F}}(\mathbf{u}) = \left[\begin{array}{cccc|cccc|cccc|ccc} 4+d_{1,1} & -1 & & & -1 & & & & & & & & & & \\ -1 & 4+d_{2,1} & -1 & & & -1 & & & & & & & & & \\ & \cdots & \cdots & \cdots & & & \cdots & & & & & & & & \\ & & -1 & 4+d_{N,1} & & & & -1 & & & & & & & \\ \hline -1 & & & & 4+d_{1,2} & -1 & & & -1 & & & & & & \\ & -1 & & & -1 & 4+d_{2,2} & -1 & & & -1 & & & & & \\ & & \cdots & & & \cdots & \cdots & \cdots & & & \cdots & & & & \\ & & & -1 & & & -1 & 4+d_{N,2} & & & & -1 & & & \\ \hline & & & & \cdots & & & & \cdots & \cdots & & & \cdots & & \\ & & & & & \cdots & & & \cdots & \cdots & \cdots & & & & \cdots \end{array}\right]$$

where $d_{i,j} = h^2 \exp(u_{i,j})$.

Write a MATLAB program that solves this system of nonlinear equations using Newton's method developed in **Exercise 1** for $N = 8, 16, 32$. Start with an initial guess of all zeros, and stop the iteration when $\|\boldsymbol{\delta}\mathbf{u}^{(k)}\|_2 < 10^{-6}$. Plot the norms $\|\boldsymbol{\delta}\mathbf{u}^{(k)}\|_2$ explain the convergence behavior you observe.

[1] We have already seen a linear version of this problem, i.e., without the exponential terms, during the lecture 7 (see page 5 in slides of Lecture 7).