CAAM 454/554: Numerical Analysis II

Homework 5, April 2nd, 2019
Due: Friday 26th of April, 2019 8pm

- Unless specified, the problems should be solved by CAAM 454 and by CAAM 554 students.
- All MATLAB functions mentioned in this homework assignment can be found on the CAAM454/554 homepage, or come with MATLAB . You can use the MATLAB codes posted on the CAAM454/554 web-page. Turn in all MATLAB code that you have written/modified and turn in all output generated by your MATLAB functions/scripts. MATLAB functions/scripts must be commented, output must be formatted nicely, and plots must be labeled.
- Office hour Monday April 22nd (Mae and Nathaniel) at 5pm, room Duncan Hall 3076
- This set contains pledged problems.
- Work with your piers on non pledged problems!
- If you have questions, other than how to solve the homework problems, e-mail teemu.saksala@rice.edu or mdehoop@rice.edu.

Total points: CAAM 454 - 160points; CAAM 554 - 195points.

Problem 1 (**30 points**) We will determine parameters in a simple model for an electrical furnace.

The mathematical model for the oven involves the following quantities: t: time (seconds), T: temperature inside the oven (^{0}C), C: 'heat capacity' of the oven including load (joule/^{0}C), Q: rate of loss of heat inside the oven to the environment (joule/sec), V: voltage of the source of electricity (volt), I: intensity of the electric current (amp), R: resistance of the heating of the oven plus regulation resistance (ohm) ($R = \infty$ corresponds to the 'open' (disconnected) circuit). Then, according to the laws of Physics:

- $I = V/R$,
- $VI = V^2/R$ = power = heat generated per second,
- $Q = kT$, where k is a constant of loss of heat per second and per degree of temperature difference between oven and the environment,
- $(V^2/R) - Q$ = heat gain of the oven per second,
- $[(V^2/R) - kT]/C$ = rate of increase of temperature of the oven (^{0} C per second).

The temperature of the oven will then evolve according to the differential equation

$$T'(t) = \frac{(V^2/R(t)) - kT(t)}{C}. \tag{1}$$

With $\alpha = k/C > 0$, $\beta = V^2/C > 0$, and

$$u(t) = 1/R(t).$$

this equation is of the form

$$T'(t) = -\alpha T(t) + \beta u(t). \tag{2}$$

The model (2) depends on the parameters α, β, which depend on the particular oven (geometry, material, ...). Our goal is to determine the parameters from measurements using the least squares formulation.

First, we note that the solution of (2) for *constant* u is given by

$$T(t) = T(t_0)e^{-\alpha(t-t_0)} + \frac{\beta u}{\alpha}(1 - e^{-\alpha(t-t_0)}). \tag{3}$$

Assume $u \equiv 1$. Temperature measurements $\hat{T}_i$ at times t_i, $i = 0, \ldots, m$, are given in Table 1.

Table 1: Measurements for $u \equiv 1$.

i	t_i	$\hat{T}_i$
0	0.0	1.0000
1	0.1	1.0953
2	0.2	1.1813
3	0.3	1.2592
4	0.4	1.3298
5	0.5	1.3935
6	0.6	1.4512
7	0.7	1.5034
8	0.8	1.5508
9	0.9	1.5935
10	1.0	1.6322

i	t_i	$\hat{T}_i$
11	1.1	1.6672
12	1.2	1.6988
13	1.3	1.7275
14	1.4	1.7534
15	1.5	1.7770
16	1.6	1.7982
17	1.7	1.8174
18	1.8	1.8348
19	1.9	1.8505
20	2.0	1.8647

i. (5 points) Set up the least squares problem

$$\min_{\alpha,\beta,T_0 \in \mathbb{R}} \tfrac{1}{2}\|R(\alpha,\beta,T_0)\|_2^2, \tag{4}$$

i.e., determine R.

Note that since none of the temperature measurements above can assumed to be exact, we include $T_0 = T(t_0)$ as a variable into the least squares problem.

ii. (5 points) Determine the Jacobian of R.

iii. (20 points) Solve the least squares problem using Matlab's `lsqnonlin` `'levenberg-marquardt'` algorithm to solve the nonlinear least squares problem.

The matlab code fragment for computing the estimate of $p = (\alpha, \beta, T_0)$ should look like (i.e, you have to provide the code with the residual R and the Jacobian R')

```
lsqOpts = optimoptions('lsqnonlin', 'Display', 'iter', ...
                       'Algorithm', 'levenberg-marquardt', ...
                       'SpecifyObjectiveGradient',true);
pest    = lsqnonlin(@(p)furnace_res_jac(p, data), p0, [], [], lsqOpts);
```

Turn in the output generated by `lsqnonlin` as well as the estimated parameter $p = (\alpha, \beta, T_0)$.

Problem 2 (**30 points**) Consider the regularized linear least squares problem

$$\min \frac{1}{2}\|Ax-b\|_2^2 + \frac{\mu}{2}\|x\|_2^2, \tag{5}$$

where $A \in \mathbb{R}^{m\times n}$, $b \in \mathbb{R}^m$, and $\mu \geq 0$.

i. (5 points) Show that for each $\mu > 0$, (5) has a unique solution $x(\mu)$.

ii. (5+10+10 points) Let $\mu_2 > \mu_1 > 0$ and let $x_1 = x(\mu_1)$, $x_2 = x(\mu_2)$ be the solutions of (5) with $\mu = \mu_1$ and $\mu = \mu_2$, respectively.

   Show that

$$\begin{aligned} \frac{1}{2}\|Ax_1-b\|_2^2 + \frac{\mu_1}{2}\|x_1\|_2^2 &\leq \frac{1}{2}\|Ax_2-b\|_2^2 + \frac{\mu_2}{2}\|x_2\|_2^2, \\ \|x_2\|_2^2 &\leq \|x_1\|_2^2, \\ \frac{1}{2}\|Ax_1-b\|_2^2 &\leq \frac{1}{2}\|Ax_2-b\|_2^2. \end{aligned}$$

Problem 3 (**CAAM 554 only, optional, 40 points**) In many applications the linear least squares problem

$$\min \tfrac{1}{2}\|R'(x_k)s + R(x_k)\|_2^2$$

has to be solved iteratively using, e.g., the conjugate gradient method. We assume that the computed step s_k satisfies

$$\|R'(x_k)^T(R'(x_k)s + R(x_k))\|_2 \leq \eta_k \|R'(x_k)^T R(x_k)\|_2.$$

Formulate and prove an extension of the local convergence Theorem 7.4.2 for this inexact Gauss-Newton method.

Hint: Revisit Theorem 5.3.1.

Problem 4 (**Pledged 30 points**) Let $F : \mathbb{R}^n \to \mathbb{R}^n$ be Liptschitz-continuously differentiable (let L be the Liptschitz constant of the Jacobian F') and let $x_* \in \mathbb{R}^n$ be a point such that $F(x_*) = 0$ and $F'(x_*)$ is nonsingular. Assume that $\limsup_{k\to\infty} |1-\alpha_k| < 1$ and that the sequence $\{x_k\}$ generated by

$$x_{k+1} = x_k - \alpha_k F'(x_k)^{-1} F(x_k)$$

converges to x_*. This question explore the influence of the step size α_k on the local convergence.

i. (**10 points**) Prove that the convergence rate is at least q-linear and derive the q-linear factor

$$\limsup_{k\to\infty} \frac{\|x_{k+1}-x_*\|}{\|x_k - x_*\|}.$$

   (Hint: Show that $x_{k+1} - x_* = (1-\alpha_k)(x_k - x_*) + \alpha_k\big(x_k - x_* - F'(x_k)^{-1}F(x_k)\big)$.)

ii. (**15 points**) Prove that the convergence rate is at least superlinear if and only if $\lim_{k\to\infty} \alpha_k = 1$.

iii. (**5 points**) Let $\alpha_k \neq 1$ for all k. Is it possible for $\{x_k\}$ to converge quadratically? Prove your assertion.

Problem 5 (**Pledged 35 points**) Let $A \in \mathbb{R}^{n\times n}$ and assume there exist exist a diagonal matrix $D \in \mathbb{R}^{n\times n}$ and a nonsingular matrix $V \in \mathbb{R}^{n\times n}$ such that $A = VDV^{-1}$.

The problem of finding an eigenvalue λ_* and a corresponding eigenvector v_* with unit length of A can be formulated as a root finding problem

$$F(v,\lambda) = 0, \tag{6}$$

where

$$F : \mathbb{R}^n \times \mathbb{R} \to \mathbb{R}^n \times \mathbb{R}$$

is given by

$$F(v,\lambda) = \begin{pmatrix} Av - \lambda v \\ \frac{1}{2}v^T v - \frac{1}{2} \end{pmatrix}.$$

(i) (**5 points**) Formulate Newton's method for the computation of (v_*, λ_*).

(ii) (**10 points**) Show that the Jacobian $F'(v_*, \lambda_*)$ is nonsingular if λ_* is a simple eigenvalue. (You may assume that λ_* is the first eigenvalue.)

(iii) (**10 points**) Show that the Jacobian $F'(\cdot,\cdot)$ is Lipschitz continuous. (You can use any norm. The 1, the ∞ or the Frobenius matrix norm may be most conventient).

(iv) (**10 points**) Apply this method to compute an eigenvalue of

$$A = \frac{1}{h^2}\begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix} \in \mathbb{R}^{n\times n}, \qquad h = 1/(n+1).$$

Use $n = 100$, and starting values $v_0 = (1,\dots,1)^T/\sqrt{n}$, $\lambda_0 = 1$.

Stop the iteration when $\|F(v,\lambda)\|_2 < 10^{-6}/n$.

Output a table that shows the iteration number k, $\|F(v_k,\lambda_k)\|_2$, norm of the step, and λ_k.

What is the eigenvalue λ_k? What is the eigenvector (plot using `x = (h:h:1-h); plot(x,v);`)?

Problem 6 (Pledged 35 points)

The Chandrasekhar-H equation

$$H(\mu) - \left(1 - \frac{c}{2}\int_0^1 \frac{\mu H(\nu)}{\mu+\nu} d\nu\right)^{-1} = 0 \quad \mu \in [0,1], \tag{7}$$

is used to solve exit distributions problems in radiative transfer. The goal is to find a function H such that (7) is satisfied.

To solve the problem numerically, we discretize integrals by the composite mid-point rule,

$$\int_0^1 g(\nu) d\nu \approx \frac{1}{N}\sum_{j=1}^{N} g(\nu_j),$$

where $\nu_j = (j-1/2))/N$, $j = 1,\dots N$. With the integrals in (7) replaced the composite mid-point rule, we require (7) to hold at $\mu_j = (j-1/2))/N$, $j = 1,\dots N$. This leads to the discretization

$$H_i - \left(1 - \frac{c}{2N}\sum_{j=1}^{N} \frac{\mu_i H_j}{\mu_i+\mu_j}\right)^{-1} = 0 \quad i = 1,\dots N, \tag{8}$$

of (7), where $H_j \approx H(\nu_j)$. The equations (8) form a system $F(H) = 0$ of nonlinear equations in H_j, $j = 1,\dots N$.

i. (**10 points**) Solve this system numerically using Newton's method.

- Stop the iteration when
$$\|F(H^k)\|_2 < 10^{-10},$$
where H^k denotes the kth iterate, or if the number of iterations exceeds 100, or if
$$\|H^k - H^{k-1}\|_2 < 10^{-10},$$
- Perform two runs, one with $c = 0.9$ and the other with 0.9999. In both runs $N = 100$ subintervals for the discretization of the integral and use the starting value $H_j^0 = 1$, $j = 1,\dots N$.
- Output a table that shows the iteration number k, $\|H^k\|_2$, $\|F(H^k)\|_2$, α_k, where $\alpha_k \in (0,1]$ is the step size.
- Turn in program,source codes, tables generated by the program, and a plot of the approximate solution $H(\mu)$ of (7).

(Hint: Use the example code on http://www.caam.rice.edu/~caam454/lectures.html, Lecture 25, as a template).

ii. (**10 points**) Repeat Part i. using the finite difference Newton method.

Approximate the j-th column of the Jacobian as follows:

$$F'(H) \approx \begin{cases} \Big[F(H + t\|H\|_2 e_j) - F(H)\Big] / (t\|H\|_2) & \text{if } H \neq 0, \\ \Big[F(H + te_j) - F(H)\Big] / t & \text{if } H = 0, \end{cases}$$

where $t = \sqrt{\texttt{eps}}$ and `eps` is the relative floating point accuracy in Matlab. (Type `help eps` in Matlab.)

iii. (**5 points**) Repeat Part i. using Shamanskii's method (Algorithm 10.3.1) using $m = 10$.

iv. (**10 points**) Repeat Part i. using Broyden's method using the initial matrix $B_0 = I$.

Problem 7 (**Pledged CAAM 554 only, 35 points**) Let $A \in \mathbb{R}^{n \times n}$ be nonsingular and let $G : \mathbb{R}^n \to \mathbb{R}^n$ be Lipschitz continuous with Lipschitz constant $L > 0$, i.e., $\|G(x) - G(y)\|_2 \leq L\|x - y\|_2$ for all $x, y \in \mathbb{R}^n$.

Let x_* be a solution of

$$Ax + G(x) = 0. \tag{9}$$

(i) (**5 points**) Show that if $L\|A^{-1}\|_2 < 1$, then (9) has at most one solution.

(ii) (**5 points**) Show that if $L\|A^{-1}\|_2 < 1$, the iteration

$$\begin{aligned} s_k &= -A^{-1}(Ax_k + G(x_k)), \\ x_{k+1} &= x_k + s_k \end{aligned}$$

converges q-linearly to x_* with q-factor $L\|A^{-1}\|_2$.

If $L\|A^{-1}\|_2 \geq 1$, convergence of the iteration in Part ii is no longer guaranteed. We employ a line search

$$\begin{aligned} s_k &= -A^{-1}(Ax_k + G(x_k)), \\ x_{k+1} &= x_k + \alpha_k s_k \end{aligned}$$

with step length $\alpha_k > 0$.

From now on we assume that $A \in \mathbb{R}^{n \times n}$ is symmetric positive definite and that $G : \mathbb{R}^n \to \mathbb{R}^n$ is continuously differentiable with symmetric positive semidefinite Jacobian $G'(x)$. We define

$$F(x) = Ax + G(x) \quad \text{ and } \quad f(x) = \frac{1}{2} F(x)^T A^{-1} F(x).$$

(iii) (**10 points**) Show that s_k is a descent direction for f at x_k.

(iv) (**15 points**) We choose step lengths $\alpha_k > 0$ so that the sufficient decrease condition

$$f(x_k + \alpha_k s_k) \leq f(x_k) + c\,\alpha_k \nabla f(x_k)^T s_k$$

is satisfied for $c \in (0,1)$ independent of k. Suppose that the step lengths α_k are bounded away from zero, i.e., that $\alpha_k \geq \underline{\alpha} > 0$ for all k. Show that $\lim_{k\to\infty} Ax_k + G(x_k) = 0$.