CAAM 453/550: Numerical Analysis I - Fall 2021
Homework 7 - due by 5pm on Wednesday, October 20, 2021

Instructions: You may use any of the code on the Canvas page. Turn in all modified/new MATLAB/python code (scripts and functions) and all output generated by your code. All code must be commented, and it must be clear what your output is and why you are submitting it. Additionally, all plots must be labeled.

For any problems that do not require coding, either turn in handwritten work or typeset work using LaTeX or some other typsetting software. Please do not turn in math as commented MATLAB code or math that has been typed in a word processor!

MATLAB code fragments are provided in some problems. If you program in python, you may replace them corresponding numpy or scipy code.

CAAM 453 students are to complete problems 1, 2, 4. (110 points)
CAAM 550 students are to complete problems 1 - 4. (140 points)

CAAM 453 may complete additional problems "for fun," but you will not receive additional credit.

Problem 1 (30 points)

Use the relationship

$$b(t) = \frac{x_1}{t} + \frac{x_2}{t^2} + \frac{x_3}{t^3},$$

with $x_1^{\text{ex}} = x_2^{\text{ex}} = x_3^{\text{ex}} = 1$ to generate data (t_i, b_i), $b_i = b(t_i)$, $i = 1, \dots, 10$, where $t_i = t_0 + i$, $i = 1, \dots, 10$.

We want to identify x^{ex} from these data using the least squares approach

$$\min \|Ax - b\|_2,$$

where $A \in \mathbb{R}^{10\times 3}$ and $b \in \mathbb{R}^{10}$ are the matrix and the vector corresponding to the model and the data specified above.

i. (20 points) For $t_0 = 0, 50, 100, 150, 200$ compute the solution of the least squares problem using the normal equation approach and the QR decomposition. Let x^{norm} and x^{orth} denote the solutions computed with the two approaches. Print a table

t_0	$\kappa_2(A^TA)$	$\kappa_2(A)$	$\|x^{\text{norm}} - x^{\text{ex}}\|_2$	$\|x^{\text{orth}} - x^{\text{ex}}\|_2$

where $\kappa_2(X)$ is the 2-condition number of a matrix X computed by the MATLAB command `cond(X,2)`. (We have discussed the condition number only for square matrices, but it can be generalized to rectangular matrices.)

ii. (10 points) Interpret the behavior of $\|x^{\text{norm}} - x^{\text{ex}}\|_2$ and $\|x^{\text{orth}} - x^{\text{ex}}\|_2$ using Theorems 5.4.1 and 7.6.2 from the CAAM453/550 Notes.

Problem 2 (30 points)

i. (10 points) Show that the linear least squares problem $\min \|Ax - b\|_2^2$ is equivalent to the linear system

$$\begin{pmatrix} I & A \\ A^T & 0 \end{pmatrix} \begin{pmatrix} r \\ x \end{pmatrix} = \begin{pmatrix} b \\ 0 \end{pmatrix}. \tag{1}$$

(Hint: The first component r of the solution of (1) is the residual $b - Ax$ of the linear least squares problem.)

ii. (10 points) Assume that $rank(A) = n \leq m$ and that

$$AP = Q \begin{pmatrix} R \\ 0 \end{pmatrix}.$$

is the QR–decomposition with column pivoting of A.

Use this QR–decomposition of A to devise an algorithm for the solution of (1).

iii. (10 points) Suppose the singular value decomposition $A = U\Sigma V^T$ of A is known. Use the singular value decomposition of A to devise an algorithm for the solution of (1).

Problem 3 (30 points - CAAM 550 only) Fitting a linear function $b(t) = x_1 + x_2 t$ to the data (t_i, b_i), $b_i = b(t_i)$ leads to the least squares problem

$$\min \|Ax - b\|_2, \tag{2}$$

where $A \in \mathbb{R}^{m\times 2}$ and $b \in \mathbb{R}^m$. We solve it using the Householder QR–decomposition described in Section 3.4.2 of the CAAM 453/550 Notes. (In this problem we use QR–decomposition without pivoting.) In particular, Householder transformations Q_1, Q_2 are used to transform

$$Q_2 Q_1 A = \begin{pmatrix} R \\ 0 \end{pmatrix}. \tag{3}$$

i. (5 points) Now suppose that after fitting a linear function $b(t) = x_1 + x_2 t$ to the data, it was found that a quadratic function $b(t) = x_1 + x_2 t + x_3 t^2$ would better fit the data.

Describe how the least squares problem

$$\min \|\tilde{A}x - \tilde{b}\|_2,$$

obtained for the fitting of a quadratic function is related to the original least squares problem (2).

ii. (10 points) Describe how the QR–decomposition (3) can be reused to solve $\min \|\tilde{A}x - \tilde{b}\|_2$.

iii. (15 points) Implement your approach and apply it to the data (t_i, b_i), $b_i = 1 + t_i + t_i^2$, $t_i = i/5$, $i = 1, \ldots, 10$. Compare your solutions against MATLAB 's backslash or numpy's `numpy.linalg.lstsq`.

Problem 4 (50 points) We want to estimate the initial data $x_0 \in \mathbb{R}^n$ in a dynamical system from measurements of the solution $x(t)$ at times $t > 0$. This problem is also known as *Data Assimilation* and is, e.g., a basis for weather prediction. The weather (wind velocities, temperature, humidity, ..) can be modeled by systems of partial differential equations (PDEs). If the initial conditions for these PDEs were known at every point in space, the PDEs can be solved to produce weather forecasts. The problem is to determine the initial conditions from measurements of wind velocities, temperature, humidity, etc., at discrete points in space. We will study a simplified version of this problem:

$$\frac{\partial}{\partial t} x(\xi, t) - \alpha \frac{\partial^2}{\partial \xi^2} x(\xi, t) + \beta \frac{\partial}{\partial \xi} x(\xi, t) = 0, \qquad \xi \in (0,1),\ t > 0, \tag{4a}$$

$$x(0,t) = x(1,t), \quad \frac{\partial}{\partial \xi} x(0,t) = \frac{\partial}{\partial \xi} x(1,t), \qquad \xi \in (0,1),\ t > 0, \tag{4b}$$

$$x(\xi, 0) = x_0(\xi), \qquad \xi \in (0,1). \tag{4c}$$

The solution x can be thought of as the temperature at points in space $\xi \in [0,1]$ and time $t > 0$. Using a finite difference discretization in space on a uniform grid $0 = \xi_0 < \xi_1 < \ldots < \xi_n = 1$ with mesh size $h = 1/n$ and equidistant points $\xi_j = j/n = jh$, we arrive at dynamical system

$$x'(t) = Bx(t), \quad t > 0 \tag{5a}$$

$$x(0) = x_0, \tag{5b}$$

with

$$B = -h^{-2} \begin{pmatrix} 2\alpha + h\beta & -\alpha & & & -(\alpha + h\,\beta) \\ -(\alpha + h\,\beta) & 2\nu + h\beta & -\alpha & & \\ & \ddots & \ddots & \ddots & \\ & & -(\alpha + h\,\beta) & 2\alpha + h\beta & -\alpha \\ -\alpha & & & -(\alpha + h\,\beta) & 2\alpha + h\beta \end{pmatrix} \in \mathbb{R}^{n \times n}.$$

The vector $x(t)$ is an approximation of the solution $x(\xi_0, t), x(\xi_1, t), \ldots, x(\xi_{n-1}, t)$ of (4). (We abused notation a bit by using x for both the solution of (5) and (4). However, since in the following we only consider (5) we did not want to introduce extra notation for (4).)

For given initial data x_0, the solution of (5) is given by

$$x(t) = \exp(Bt)\, x_0.$$

Where $\exp(Bt) \in \mathbb{R}^{n \times n}$ is the *matrix exponential* of Bt. (You have used the matrix exponential already in Problem 4 of Homework 5.)

i. (10 points) Let $h = 1/(n+1)$, $\alpha = 0.01$, $\beta = 1$, and $n = 100$. Given the exact initial conditions

$$(x_0^{\text{ex}})_j = \exp(-(\xi_j - 0.3)^2/0.01), \quad j = 0, \ldots, n-1, \tag{6}$$

compute the solution of (5) and plot the solution. Your plot should look like the one in Figure 1.

ii. (10 points) Now, suppose that we do not know the initial value $x_0 \in \mathbb{R}^n$. We want to estimate x_0 from measurements of k components $x_{n/k}(t), x_{2n/k}(t), \ldots$ of the solution $x(t)$ at times $t_1, \ldots, t_m$. That is, we want to determine x_0 from measurements $z_1, \ldots, z_m$ of $Hx(t_1), \ldots, Hx(t_m)$, where x is the solution of (5) with the unknown initial condition and $H \in \mathbb{R}^{k \times n}$ is the matrix with entries

$$H_{ij} = 1 \quad \text{if } j = (n/k)i, \qquad H_{ij} = 0 \quad \text{else .}$$

($Hx(t)$ extracts the components $x(t)_{n/k}, x(t)_{2n/k}, \ldots, x(t)_n$ from $x(t) \in \mathbb{R}^n$.) Formulate the above problem as a least squares problem

$$\min_{\mathbf{x}} \|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2.$$

What are $\mathbf{A}$, $\mathbf{b}$ and $\mathbf{x}$ in this context?

iii. (10 points) Let $h = 1/(n+1)$, $\alpha = 0.01$, $\beta = 1$, and

$$n = 100, \quad k = 20.$$

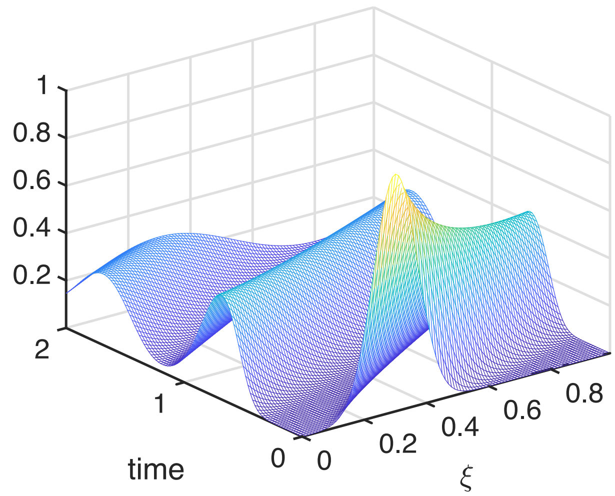

Figure 1: Solution of the dynamical system (5) with initial data (7).

Generate exact initial conditions

$$(x_0^{\mathrm{ex}})_j = \exp(-(\xi_j - 0.3)^2/0.01), \quad j = 0, \ldots, n-1, \tag{7}$$

and generate data $z_j = H\exp(Bt_j)x_0$, $t_1 = 0.02, t_2 = 0.04, \ldots, t_m = 0.5$. Now pretend that the exact initial data x_0 are not known. Use the data you have generated to solve the least squares problem.

Plot the exact solution x_0 and the solution of the least squares problem.

iv. (10 points) Repeat ii. with data (using MATLAB notation)

$$z_j = (1 + 0.1 * \mathrm{randn}(k, 1)). * (H * \mathrm{expm}(B * t_j) * x_0).$$

v. (10 points) Use the singular value decomposition of $\mathbf{A}$ to explain the differences in the computed solution due to measurement errors added in iv.