CAAM 453/550: Numerical Analysis I - Fall 2021
Homework 5 - due by 5pm on Wednesday, September 29, 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 - 4. (70 points)
CAAM 550 students are to complete problems 1 - 5. (100 points)

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

Problem 1 (25 points) For given integer n we want to evaluate the integral

$$\int_0^1 x^n e^x dx.$$

i. (10 points) Define $I_n = \int_0^1 x^n e^x dx$. Apply integration by parts to prove the recursion

$$I_{n+1} = e - (n+1)I_n, \quad n \in \mathbb{N}, \tag{1}$$

and prove that

$$I_1 > I_2 > \ldots > 0.$$

ii. (5 points) For $n = 0$, we can easily compute $I_0 = e - 1$. Apply the recursion in part i. starting with $I_1 = 1 (= e - I_0)$ to compute $\int_0^1 x^{20} e^x dx$. Print a table listing n and I_n, $n = 2, \ldots, 20$. Use the printing command (MATLAB , use analogous format in python)

```
fprintf(1,' %2d  %13.6e \n', n, I)
```

iii. (10 points) The recursion (1) is not well suited to compute the integral $\int_0^1 x^n e^x dx$ for large n, even if exact arithmetic is used. To show this consider the perturbed initial data $\widetilde{I}_1 = I_1 + \varepsilon$ and study the propagation of the error ε within (1).

Problem 2 (10points) Consider the matrix

$$A = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ 1 & 1 & 0 & 0 & \cdots & 0 \\ 1 & 0 & 1 & 0 & \cdots & 0 \\ 1 & 0 & 0 & 1 & \cdots & 0 \\ \vdots & & & & \ddots & \\ 1 & 0 & 0 & 0 & \cdots & 1 \end{pmatrix} \in \mathbb{R}^{n \times n}.$$

i. (5points) Show that

$$A^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 & \cdots & 0 \\ -1 & 1 & 0 & 0 & \cdots & 0 \\ -1 & 0 & 1 & 0 & \cdots & 0 \\ -1 & 0 & 0 & 1 & \cdots & 0 \\ \vdots & & & & \ddots & \\ -1 & 0 & 0 & 0 & \cdots & 1 \end{pmatrix} \in \mathbb{R}^{n \times n}.$$

ii. (5points) What is $\kappa_1(A)$? What is $\kappa_\infty(A)$?

Problem 3 (10 points) Consider the linear system

$$Ax = b,$$

where $A \in \mathbb{R}^{n \times n}$ is of the form

$$A = \begin{pmatrix} 1 & t_1 & t_1^2 & \cdots & t_1^{n-1} \\ 1 & t_2 & t_2^2 & \cdots & t_2^{n-1} \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & t_n & t_n^2 & \cdots & t_n^{n-1} \end{pmatrix} \in \mathbb{R}^{n \times n}. \tag{2}$$

A matrix of the form (2) is called a *Vandermonde matrix* and arises, e.g., in polynomial interpolation. We choose

$$t_i = -1 + 2\frac{i-1}{n-1}, \quad i = 1, \ldots, n,$$

The right hand side is constructed so that the exact solution is known. Do this by setting

$$x_{\text{ex}} = (1, 1, \ldots, 1)^T$$

and

$$b = Ax_{\text{ex}},$$

i.e.,

$$b_i = \sum_{j=1}^{n} a_{ij} = \sum_{j=1}^{n} t_i^{j-1} = \begin{cases} \frac{1-t_i^n}{1-t_i} & \text{if } t_i \neq 1, \\ n & \text{if } t_i = 1. \end{cases}$$

For systems of the size $n = 2, 4, \ldots, 40$ compute the solution of the linear system $Ax = b$ and tabulate the absolute and the relative errors between exact solution x_{ex} and computed solution x, as well as the condition numbers of the matrices A. In MATLAB you may use the backslash command to solve $Ax = b$. Your table should look like

n	$\|x - x_{comp}\|_2$	$\|x - x_{comp}\|_2 / \|x\|_2$	$\kappa_2(A)$
2	0	0	$1.0000E+00$
4	$3.3307E-16$	$1.6653E-16$	$8.0116E+00$
$\vdots$	$\vdots$	$\vdots$	$\vdots$

Interpret your results.

Problem 4 (25 points) For given $\alpha, \beta, \gamma, \delta \in \mathbb{R}$ consider the two point boundary value problem (BVP)

$$\frac{d^2}{dx^2}y(x) + \gamma\frac{d}{dx}y(x) + \delta y(x) = 0, \qquad x \in (0,10), \tag{3a}$$
$$y(0) = \alpha, \quad y(10) = \beta. \tag{3b}$$

This problem studies the so-called shooting method for solving (3), which reformulates (3) as a root finding problem governed by an initial value problem (IVP) derived from (3).

The (single) shooting method works as follows. Introduce an auxiliary variable $s \in \mathbb{R}$ and consider the IVP

$$\frac{d^2}{dx^2}y(x) + \gamma\frac{d}{dx}y(x) + \delta y(x) = 0, \qquad x \in (0,10), \tag{4a}$$
$$y(0) = \alpha, \quad \frac{d}{dx}y(0) = s. \tag{4b}$$

For each $s \in \mathbb{R}$ there is a unique solution of (6) which we denote by $y(\cdot; s)$. The value of this solution at x is $y(x; s)$. If s is such that

$$y(1; s) = \beta, \tag{5}$$

then $y(\cdot; s)$ solves the BVP (3). The problem (5) is a root finding problem in the variable $s \in \mathbb{R}$. Next we will examine the equation (5) in more detail.

Introducing the functions $y_1(x) = y(x)$ and $y_2(x) = \frac{d}{dx}y(x)$ the second order ODE (4) can be rewritten as a system of first order IVPs

$$\frac{d}{dx}\begin{pmatrix} y_1(x) \\ y_2(x) \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\delta & -\gamma \end{pmatrix}\begin{pmatrix} y_1(x) \\ y_2(x) \end{pmatrix}, \qquad x \in (0,10), \tag{6a}$$
$$\begin{pmatrix} y_1(0) \\ y_2(0) \end{pmatrix} = \begin{pmatrix} \alpha \\ s \end{pmatrix}. \tag{6b}$$

The solution of (6) is given via the *matrix exponential*,

$$\begin{pmatrix} y_1(x) \\ y_2(x) \end{pmatrix} = \exp\left(\begin{pmatrix} 0 & 1 \\ -\delta & -\gamma \end{pmatrix} x\right)\begin{pmatrix} \alpha \\ s \end{pmatrix}, \quad x \in (0,10). \tag{7}$$

In (7) the function exp is the matrix exponential. The MATLAB function `expm(M)` evaluates the matrix exponential of a square matrix M. (Note: `exp(M)` just applies the scalar exponential function to all entries of M, which is *not* the matrix exponential of a square matrix M!) In Python, `scipy.linalg.expm` evaluates the matrix exponential.

If we define

$$E = \exp\left(\begin{pmatrix} 0 & 1 \\ -\delta & -\gamma \end{pmatrix} 10\right),$$

let $E_1, E_2 \in \mathbb{R}^2$ denote the first and second column of E, and let $e_1 \in \mathbb{R}^2$ denote the first unit vector, then

$$\begin{pmatrix} y_1(10) \\ y_2(10) \end{pmatrix} = E\begin{pmatrix} \alpha \\ s \end{pmatrix},$$

and

$$y_1(10) = e_1^T E \begin{pmatrix} \alpha \\ s \end{pmatrix} = e_1^T E_1 \alpha + e_1^T E_2 s.$$

Thus, the root finding problem (5) can be written as $y(10;s) = y_1(10) = e_1^T E_1 \alpha + e_1^T E_2 s = \beta$, i.e., as the scalar linear equation

$$e_1^T E_2\, s = \beta - e_1^T E_1 \alpha. \tag{8}$$

i. (10 points) Set $\alpha = 0$, $\beta = 1$, and $\gamma = 1$, $\delta = 1$. Implement the single shooting approach. What is s? Plot the solution y_1.

   Now compute the solution from (7) with s replaced by $s + 10^{-8}$.

ii. (5 points) Repeat the computations in Part i. with γ, δ replaced by $\gamma = -2$, $\delta = -2$. You may want to use `semilogy` to plot the solution y_1 obtained with s and with $s + 10^{-8}$.

iii. (10 points) For the scalar IVP (6) we can compute the solution directly. Specifically, if $\gamma^2 - 4\delta \geq 0$, the solution is

$$y(x) = e^{\lambda_1 x}\, \frac{\lambda_2 \alpha - s}{\lambda_2 - \lambda_1} + e^{\lambda_2 x}\, \frac{s - \lambda_1 \alpha}{\lambda_2 - \lambda_1}, \tag{9}$$

   where

$$\lambda_{1,2} = -\frac{\gamma}{2} \pm \sqrt{\frac{\gamma^2 - 4\delta}{4}}.$$

   If $\gamma^2 - 4\delta < 0$, the solution is

$$y(x) = e^{\mu x} \sin(\theta x)\, \frac{s - \mu\alpha}{\theta} + e^{\mu x} \cos(\theta x)\, \alpha, \tag{10}$$

   where

$$\mu = -\frac{\gamma}{2}, \quad \theta = \sqrt{4\delta - \gamma^2}/2.$$

   Use the representations (9) or (10) for the solution y to explain the changes due to the perturbation $s + 10^{-8}$ in the initial condition.

   Note: For those who are curious, here are some details on how to derive (9) and (10). We use the Ansatz

$$y(x) = e^{\lambda_1 x} c_1 + e^{\lambda_2 x} c_2.$$

   Plugging this form into (6) gives

$$(\lambda_1^2 + \gamma\lambda_1 + \delta) e^{\lambda_1 x} c_1 + (\lambda_2^2 + \gamma\lambda_2 + \delta) e^{\lambda_2 x} c_2 = 0 \text{ for all } x \in (0, 10),$$

   which implies

$$\lambda_1^2 + \gamma\lambda_1 + \delta = 0 \quad \text{and} \quad \lambda_2^2 + \gamma\lambda_2 + \delta = 0.$$

   Thus,

$$\lambda_{1,2} = -\frac{\gamma}{2} \pm \sqrt{\frac{\gamma^2 - 4\delta}{4}}$$

   are the roots of $\lambda^2 + \gamma\lambda + \delta = 0$. The coefficients c_1, c_2 are determined by the initial conditions, $y(0) = c_1 + c_2 = \alpha$ and $\frac{d}{dx} y(0) = \lambda_1 c_1 + \lambda_2 c_2 = s$.

   The solution of (6) is given by

$$y(x) = e^{\lambda_1 x}\, \frac{\lambda_2 \alpha - s}{\lambda_2 - \lambda_1} + e^{\lambda_2 x}\, \frac{s - \lambda_1 \alpha}{\lambda_2 - \lambda_1}. \tag{11}$$

If $\gamma^2 - 4\delta < 0$, then the roots of $\lambda^2 + \gamma\lambda + \delta = 0$ are complex,

$$\lambda_{1,2} = \mu \pm i\theta \quad \text{with} \quad \mu = -\frac{\gamma}{2}, \quad \theta = \sqrt{4\delta - \gamma^2}/2$$

and $i = \sqrt{-1}$. The complex exponential is

$$e^{(\mu \pm i\theta)x} = e^{\mu x}\Big(\cos(\pm\theta x) + i\sin(\pm\theta x)\Big) = e^{\mu x}\Big(\cos(\theta x) \pm i\sin(\theta x)\Big).$$

In this case the solution of (6) is given by

$$y(x) = e^{\mu x}\sin(\theta x)\,\frac{s - \mu\alpha}{\theta} + e^{\mu x}\cos(\theta x)\,\alpha. \tag{12}$$

Problem 5 (30 points) (CAAM 550 Only)
In this problem we extend the single shooting approach from Problem 4 top the multiple shooting approach. Again, for given $\alpha, \beta, \gamma, \delta \in \mathbb{R}$ consider the two point boundary value problem (BVP)

$$\frac{d^2}{dx^2}y(x) + \gamma\frac{d}{dx}y(x) + \delta y(x) = 0, \qquad x \in (0, 10), \tag{13a}$$

$$y(0) = \alpha, \quad y(10) = \beta. \tag{13b}$$

and the equivalent reformulation of the second order BVP (13) into a system of first order BVPs

$$\frac{d}{dx}\begin{pmatrix} y_1(x) \\ y_2(x) \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\delta & -\gamma \end{pmatrix}\begin{pmatrix} y_1(x) \\ y_2(x) \end{pmatrix}, \qquad x \in (0, 10), \tag{14a}$$

$$y_1(0) = \alpha, \quad y_1(10) = \beta. \tag{14b}$$

Next for

$$0 = x_0 < x_1 < \ldots < x_N = 10$$

we consider the IVPs

$$\frac{d}{dx}\begin{pmatrix} y_{1,0}(x) \\ y_{2,0}(x) \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\delta & -\gamma \end{pmatrix}\begin{pmatrix} y_{1,0}(x) \\ y_{2,0}(x) \end{pmatrix}, \qquad x \in (0, x_1), \tag{15a}$$

$$\begin{pmatrix} y_{1,0}(0) \\ y_{2,0}(0) \end{pmatrix} = \begin{pmatrix} \alpha \\ s_{2,0} \end{pmatrix} \tag{15b}$$

and

$$\frac{d}{dx}\begin{pmatrix} y_{1,j}(x) \\ y_{2,j}(x) \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -\delta & -\gamma \end{pmatrix}\begin{pmatrix} y_{1,j}(x) \\ y_{2,j}(x) \end{pmatrix}, \qquad x \in (x_j, x_{j+1}), \tag{16a}$$

$$\begin{pmatrix} y_{1,j}(x_j) \\ y_{2,j}(x_j) \end{pmatrix} = \begin{pmatrix} s_{1,j} \\ s_{2,j} \end{pmatrix} \tag{16b}$$

for $j = 1, \ldots, N-1$.

The solutions of the IVPs (15) and (16) are given via the *matrix exponential*,

$$\begin{pmatrix} y_{1,0}(x) \\ y_{2,0}(x) \end{pmatrix} = \exp\left(\begin{pmatrix} 0 & 1 \\ -\delta & -\gamma \end{pmatrix} x \right) \begin{pmatrix} \alpha \\ s_{2,0} \end{pmatrix}, \qquad x \in (0, x_1), \tag{17a}$$

$$\begin{pmatrix} y_{1,j}(x) \\ y_{2,j}(x) \end{pmatrix} = \exp\left(\begin{pmatrix} 0 & 1 \\ -\delta & -\gamma \end{pmatrix} (x - x_j) \right) \begin{pmatrix} s_{1,j} \\ s_{2,j} \end{pmatrix}, \quad x \in (x_j, x_{j+1}), \quad j = 1, \dots, N-1. \tag{17b}$$

To generate the solution of (14) from (17) the auxiliary variables $s_{2,0}$, $s_{1,j}, s_{2,j}$, $j = 1, \dots, N-1$ must be chosen so that the subsolutions (17) are continuous at the domain boundaries $x_1, \dots, x_{N-1}$ which leads to

$$\exp\left(\begin{pmatrix} 0 & 1 \\ -\delta & -\gamma \end{pmatrix} x_1 \right) \begin{pmatrix} \alpha \\ s_{2,0} \end{pmatrix} = \begin{pmatrix} s_{1,1} \\ s_{2,1} \end{pmatrix}, \tag{18a}$$

$$\exp\left(\begin{pmatrix} 0 & 1 \\ -\delta & -\gamma \end{pmatrix} (x_{j+1} - x_j) \right) \begin{pmatrix} s_{1,j} \\ s_{2,j} \end{pmatrix} = \begin{pmatrix} s_{1,j+1} \\ s_{2,j+1} \end{pmatrix}, \qquad j = 1, \dots, N-2. \tag{18b}$$

and the right boundary condition (14b) is satisfies, which leads to

$$e_1^T \exp\left(\begin{pmatrix} 0 & 1 \\ -\delta & -\gamma \end{pmatrix} (x_N - x_{N-1}) \right) \begin{pmatrix} s_{1,N-1} \\ s_{2,N-1} \end{pmatrix} = \beta. \tag{18c}$$

The equations (18) form a system of $2(N-1)+1)$ linear equations for the $2(N-1)+1)$ unknowns $s_{2,0}$, $s_{1,j}, s_{2,j}$, $j = 1, \dots, N-1$.

i. (20 points) Let $x_j = j$ for $j = 0, \dots, N = 10$. Set $\alpha = 0$, $\beta = 1$, and $\gamma = 1$, $\delta = 1$. Implement the multiple shooting approach. What are $s_{2,0}$, $s_{1,j}, s_{2,j}$, $j = 1, \dots, N-1$? Plot the solutions $y_{1,j}(x)$, $x \in (x_j, x_{j+1})$, $j = 0, \dots, N-1$. (One plot).

   Now compute the solutions from (17) with the $s_{1,j}, s_{2,j}$ replaced by $s_{1,j} + 10^{-8}, s_{2,j} + 10^{-8}$.

ii. (5 points) Repeat the computations in Part i. with γ, δ replaced by $\gamma = -2$, $\delta = -2$.

iii. (5 points) Explain why the solutions $y_{1,j}(x)$, $x \in (x_j, x_{j+1})$, $j = 0, \dots, N-1$, less sensitive to perturbations in the initial data.