APMA E4300: Introduction to Numerical Methods

Final Project

INSTRUCTIONS: Please submit your completed project through `Gradescope`. Please contact the instructor immediately if you find any typos/mistakes or if you feel that a problem is not posed clearly enough. Note: The project is personalized. You should provide your own answer. We use $\alpha_1\alpha_2\alpha_3\alpha_4$ to denote the last four digits of your CU uni (e.g., if the uni is qdrsrt, then α_1=α_3=r, α_2=s, α_4=t). Important: Please work out problem 1 first, as the other problems in the project depend on your answer.

The project has three parts. Part I is similar to a homework assignment. Problems in Part II might appear unfamiliar at first. Thus, you are asked to complete the steps to transform them into those more familiar problems discussed in class. Part III involves largely conceptual reviews and discussions. Some of the concepts in Problem 10 are discussed in the final two weeks of class.

	1	2	3	4	5	6	7	8	9		10	Total
Points	30	30	30	30	30	25	50	30	15	EC	50	320
Scores												

Part I:

Problem 1. Let $p(x)$ be the polynomial with the smallest degree that interpolates the data $p(0) = \alpha_1$, $p(1)=\alpha_2$, $p'(1)=\alpha_3$, $p(2)=\alpha_4$. (Reminder, the α_i's are from your uni).
a) (10 points) Find the exact value of $\int_0^2 p(x)dx$ without tedious calculations.
b) (20 points) For the polynomial p, find its degree and the leading coefficient (of the term x^q).
(Note: the value of q is used in a number of problems posed later, make sure to get its correct value).

Problem 2. The minimum of the function $f(x, y) = (4-2.1x^2+x^4/3)x^2+xy+4(y^2-1)y^2$ is reached at two points in the square $[-2, 2]\times[-2, 2]$ with the minimum value approximately -1.0316. Implement an iterative method studied in class to find the minimum starting from $(\frac{2(q+4)}{q+5}, 0)$ and $(\frac{q}{q+5}, 0)$ respectively.
a) (10 points) Please state the method (and parameters, if any) used, and submit the code.
b) (20 points) Plot respectively the sequences of points $\{(x_n, y_n)\}$ generated by the iteration, and the associated values $\{f(x_n, y_n)\}$.

Problem 3. A data set $\{f_i\}_{i=1}^{N+1}$ may show fluctuations. To get a smoother representation $\{u_i\}_{i=1}^{N+1}$, we let $u_1=f_1$, $u_{N+1}=f_{N+1}$ and find $\{u_i\}_{i=2}^{N}$ as the minimizer of $\frac{1}{N}\sum_{i=2}^{N}(u_i - f_i)^2+\frac{N}{(q+7)}\sum_{i=1}^{N}(u_{i+1} - u_i)^2$.
a) (10 points) Find the matrix and right-hand side of the linear system satisfied by $\{u_i\}_{i=2}^{N}$.
b) (10 points) For N=7, let $\{f_i\}_{i=1}^{8}$ be the scores of your first 8 homework assignments (put 20 for any missing score), find $\{u_i\}_{i=2}^{7}$. Make a single plot to compare $\{(i, f_i)\}_{i=1}^{8}$ and $\{(i, u_i)\}_{i=1}^{8}$.
c) (10 points) Consider a large data set $\{f_i=f(\frac{i-1}{N})\}_{i=1}^{N+1}$ for some smooth function $f=f(x)$ defined on $0\le x\le 1$. What is the limit of $\{u_i\}_{i=1}^{N+1}$ representing as $N \to \infty$? State a brief reason.

Problem 4. The Lorenz system $x' = \sigma(y-x)$, $y' = (\rho-z)x-y$, $z' = xy-\beta z$ has had a profound impact on the study of the atmosphere and climate. Implement two different numerical methods studied in the class to solve the IVPs on the time interval $t \in (0, 100)$with σ=10, ρ=28 and $\beta=\frac{8}{3}$, and two sets of initial conditions $(x_0, y_0, z_0)=(-\alpha_1, -\alpha_2 - \alpha_3 - \alpha_4, \alpha_4)$ and $(x_0, y_0, z_0)=(\alpha_1, \alpha_2, \alpha_2 + \alpha_3 + \alpha_4)$ respectively.
a) (10 points) State the two methods and the parameters used respectively, and submit your codes.
b) (20 points) For each method and initial condition, present a single 3-dimensional plot of the trajectory of the numerical solution $\{(x_n, y_n, z_n)\}$. (Note: A total of 4 plots should be presented for all 4 cases).

Problem 5. Implement the power method $\mathbf{x}_{n+1}=\frac{\mathbf{A}\mathbf{x}_n}{\|\mathbf{A}\mathbf{x}_n\|}$ and inverse power method $\mathbf{x}_{n+1}=\frac{\mathbf{A}^{-1}\mathbf{x}_n}{\|\mathbf{A}^{-1}\mathbf{x}_n\|}$.
Run the codes to get two eigenvalues of $\mathbf{A}=\begin{bmatrix} 6 & 2 & 2 \\ 2 & 8 & -q \\ 2 & -q & 12 \end{bmatrix}$, starting with $\mathbf{x}_0=\frac{\mathbf{b}}{\|\mathbf{b}\|}$ where $\mathbf{b}=\begin{bmatrix} \alpha_1 + 1 \\ \alpha_2 + 1 \\ \alpha_3 + \alpha_4 \end{bmatrix}$.
Stop the iterations if the estimated eigenvalues between steps differ by less than 0.005 in magnitude.
a) (20 points) Please submit your codes and plot the sequence of estimated eigenvalues for each method.
b) (10 points) Use the fact that the sum of all eigenvalues of $\mathbf{A}$ is the same as the sum of all diagonal entries of $\mathbf{A}$ to find the remaining eigenvalue.

Problem 6. Implement the QR algorithm for computing matrix eigenvalues. Existing QR decomposition routines in Python/Matlab or other software libraries can be used to simplify the coding.
a) (10 points) Submit your code, and make sure that it records diag($\mathbf{A}_k$) obtained at the k-th step $\forall\, k$.
b) (15 points) Run your code on the 3×3 matrix $\mathbf{A}$ given in problem 5. Plot how the three recorded diagonal entries change with k respectively.

Part II

Problem 7. Consider the numerical solution to the initial-boundary value problem of the PARTIAL differential equation $u_t{=}u_{xx}$ on $0{<}t{<}10$ and $0{<}x{<}1$ for a function $u{=}u(t,x)$, with initial condition $u(0,x){=}\frac{1}{q+1}x(1-x)+\sin((q+1)\pi x)$ for $0{<}x{<}1$ and boundary condition $u(t,0){=}u(t,1){=}0$ for $0{<}t{<}10$. For an integer $N{>}0$, we first take a uniform grid $x_j{=}jh$ for $0{\le}j{\le}N{+}1$ with $h{=}\frac{1}{N+1}$, and let $u_j^h(t)$ represent the solution at (t,x_j). Replacing the 2nd order derivative u_{xx} by the 2nd order central difference at x_j, we get the following ODE system $\frac{d}{dt}u_j^h(t){=}\frac{1}{h^2}[u_{j-1}^h(t)-2u_j^h(t)+u_{j+1}^h(t)]$ with initial conditions $u_j^h(0){=}u(0,x_j)$ (for $1{\le}j{\le}N$), and $u_0^h(t){=}u_{N+1}^h(t){=}0$ for $0{<}t{<}10$.
a) (10 points) Applying the forward Euler method to solve the above ODE system on a uniform grid $\{t_i{=}ik\}_{i=0}^K$ in time with a time step $k{>}0$, and let $U_{i,j}$ denote the solution corresponding to (t_i,x_j). Please state how the solution $\{U_{i+1,j}\}_{j=0}^{N+1}$ can be computed from $\{U_{i,j}\}_{j=0}^{N+1}$.
b) (20 points) Implement the method and submit the code. Run the code by taking $N{+}1{=}16(q{+}2)$ and $N{+}1{=}32(q{+}2)$, and $k{=}h^2$ and $k{=}\frac{h^2}{q+2}$ respectively. For each of the four cases, present a plot of the evolution of numerical solutions as a two-dimensional surface (in time and space).
c) (20 points) Repeat b) but using the backward Euler method for the ODE system. State the method used to solve the linear system at each time step. Submit the code and the four plots.

Problem 8. Consider the BVP $-y''(t){=}\lambda(1+\frac{1}{q+2}\sin(2\pi t))y(t)$ on $0{<}t{<}1$ with boundary condition $y(0){=}y(1){=}0$ for an unknown constant λ. If for some value of λ, the BVP has a nonzero solution $y(t)$, then $y(t)$ is called an eigenfunction corresponding to the eigenvalue λ.
a) (10 points) Develop a numerical method to give an estimate of the smallest eigenvalue and the corresponding eigenfunction, present your method, and submit your computer code.
b) (10 points) Verify first that, without running the code, all eigenvalues are positive.
c) (10 points) Present the value of the smallest eigenvalue obtained from your code (accurate to at least the first three digits), along with a plot of the eigenfunction as a function of t.

Part III

Problem 9. (15 points) Give three examples where we used the idea of transformation to change a computational problem discussed in the later part of the semester to a problem studied earlier in class. Provide a brief description of the examples.
(Extra credit: 4 points) Give an example where you can use the idea of transformation to change a computational problem you encountered (but not discussed in class) to a problem studied in class.

Problem 10. Matrix computations are widely used in data and network/graph analysis. A few applications are briefly mentioned during the final two weeks of classes. Please present additional discussions on any TWO of the following three applications (25 points each, for a total of 50 points).
a) The Netflix problem and matrix completion.
b) The Pagerank and ranking of search results.
c) The Eigenvector centrality and influential nodes.
On each application, the discussions should include (but may not be limited to) i) a mathematical description of the problem (or the most relevant computational challenge) in terms of concepts studied in class, ii) how you would transform the problem into a computational problem that can be solved by the methods you have learned; iii) suggestions given by ChatGPT or other similar tools on how to solve the problem (be brief); iv) your personal assessment on the effectiveness of the suggestions; and v) a simple example (involving no more than 10 unknowns) to illustrate the problem and the solution.
