A11474W1

DEGREE OF MASTER OF SCIENCE

Mathematical Modelling and Scientific Computing

Numerical Linear Algebra and Numerical Solution of Differential Equations

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Hilary TERM 2021

FRIDAY, 15 January 2021

Opening Time: 9:30am GMT

You have 2 hours and 30 minutes of writing time to complete the paper and up to 30 minutes technical time to upload your answer file.

This exam paper contains two sections. You may attempt as many questions as you like but you must answer at least one question in each section. Your best answer in each section will count, along with your next best two answers, making a total of four answers.

Numerical Linear Algebra

1. 1. Let $A \in \mathbb{R}^{m\times n}, m \geqslant n$, and denote by $\sigma_1(A) \geqslant \sigma_2(A) \geqslant \cdots \geqslant \sigma_n(A)$ its singular values.

   (a) (i) [3 marks] Prove that the eigenvalues of a real symmetric matrix are real.

   (ii) [2 marks] Show that the eigenvalues of A^TA are real and nonnegative.

   (b) [5 marks] Prove the existence of the SVD, i.e., $A = U\Sigma V^T$ where $U^TU = I_n$, $V^TV = VV^T = I_n$ and $\Sigma = \mathrm{diag}(\sigma_1(A), \dots, \sigma_n(A))$.

   (c) [5 marks] Prove the Courant–Fisher maxmin theorem for singular values: $\sigma_i(A) = \max_{\dim \mathcal{S}=i} \min_{x\in\mathcal{S}, \|x\|_2=1} \|Ax\|_2$.

   (d) Let $A = \begin{bmatrix} A_1 \\ A_2 \end{bmatrix} \in \mathbb{R}^{4\times 2}$ where $A_1 = \begin{bmatrix} 2 & \\ & 1 \end{bmatrix}$ and $A_2 \in \mathbb{R}^{2\times 2}$ is some matrix whose entries are unknown.

   (i) [5 marks] Prove that $\sigma_1(A) \geqslant 2$. Give an example of A_2 for which this bound is tight, and another example where it is not tight.

   (ii) [5 marks] Derive a lower bound for $\sigma_2(A)$ and give an example of A_2 for which the bound is attained, and another where it is not.

2. (a) [5 marks] Householder reflectors are matrices of the form $H = I - 2vv^T$, where v is a vector of unit norm $\|v\|_2 = 1$. Prove that for any u, w of the same norms, there exists a Householder reflector such that $Hu = w$ and $Hw = u$.

(b) [5 marks] What are the eigenvalues and eigenvectors of the Householder reflector $H = I - 2vv^T$ with $\|v\|_2 = 1$?

(c) [5 marks] Explain how to use Householder reflectors to form a full QR factorisation of $A \in \mathbb{R}^{m \times n}$, $m \geqslant n$.

(d) Consider a least-squares problem $\min_x \|Ax - b\|_2$, $A \in \mathbb{R}^{m \times n}$, $m \geqslant n$, where $\operatorname{rank}(A) = n$.

(i) [5 marks] Explain how to obtain a solution using a (full or thin) QR factorisation of A.

(ii) [5 marks] Let $b_0 = Ax_0$ where $x_0 \in \mathbb{R}^n$, and $A = [Q, Q_\perp] \begin{bmatrix} R \\ 0 \end{bmatrix}$ be a full QR factorisation, so that $[Q, Q_\perp] \in \mathbb{R}^{m \times m}$ is orthogonal and R is upper triangular. Now let $b_1 = Q_\perp c$ for some vector $c \in \mathbb{R}^{m-n}$.
What is the solution x_* for $\min_x \|Ax - (b_0 + b_1)\|_2$? And with this x_*, what is the value of $\|Ax_* - (b_0 + b_1)\|_2$?

Numerical Solution of Differential Equations

3. Consider the initial-value problem $y'(x) = 2[y(x)]^{1/2}$, $y(0) = b$, where b is a nonnegative real number and $x \in [0, \infty)$, and where y' denotes the derivative of the real-valued function y with respect to the independent variable x.

(a) [4 marks] Show that if $b > 0$ then the initial-value problem has a unique positive solution.
Show further that if $b = 0$ then, in addition to the trivial solution $y(x) \equiv 0$, the initial-value problem has at least one other nonnegative solution.

(b) (i) [2 marks] Formulate Euler's explicit and implicit methods for the approximate solution of the initial-value problem $y'(x) = 2[y(x)]^{1/2}$, $y(0) = b$, where b is a nonnegative real number, for $x \in [0, 1]$, on the mesh $\{x_n : x_n = nh,\ n = 0, 1, \ldots, N\}$, $h = 1/N$, $N \geqslant 1$, with starting value $y_0 = b$.

(ii) [2 marks] Show that if $b = 0$ then the explicit Euler approximations coincide with the values of the trivial solution $y(x) \equiv 0$ of the initial-value problem at the mesh points.

(iii) [2 marks] Show further that Euler's implicit method generates the sequence of approximations $(y_n)_{n=1}^{N}$ defined by

$$y_{n+1} = \left(h \pm \sqrt{h^2 + y_n}\right)^2, \qquad n = 0, 1, \ldots, N-1. \tag{1}$$

Hence deduce that if $b = 0$ and the $-$ sign is chosen in this expression for all $n \in \{0, 1, \ldots, N-1\}$ then the implicit Euler approximations coincide with the values of the trivial solution $y(x) \equiv 0$ of the initial-value problem at the mesh points.

(iv) [8 marks] Show that if $b = 0$ and the $+$ sign is chosen in the expression (1) for all $n \in \{0, 1, \ldots, N-1\}$ then Euler's implicit method approximates the function $y : x \in [0, 1] \mapsto x^2$, in the sense that $|y(x_1) - y_1| = 3h^2$ and

$$\lim_{\substack{n \to \infty,\, h \to 0 \\ nh \to x}} |y(x) - y_n| = 0.$$

[Hint: You may find it helpful to show first that $y_n \geqslant x_n^2$ for all $n = 0, 1, \ldots, N$, and hence deduce that

$$\left(1 - \frac{1}{n+1}\right) |y(x_{n+1}) - y_{n+1}| \leqslant |y(x_n) - y_n| + h|T_n|, \qquad n = 0, 1, \ldots, N-1,$$

where T_n is the consistency error of Euler's implicit method.]

(c) [7 marks] Let $b = 4$. Find a positive integer $N_0 \geqslant 1$ (as small as possible) such that the global error of the implicit Euler approximation of the solution to the initial value problem $y'(x) = 2[y(x)]^{1/2}$, $y(0) = 4$, on the interval $[0, 1]$, with mesh spacing $h = 1/N$ and starting value $y_0 = 4$, is bounded above by $\texttt{TOL} = 10^{-4}$ for all $N \geqslant N_0$.

4. Consider the ordinary differential equation $y'(x) = f(x, y(x))$, where f is a real-valued continuous function defined for all $(x, y) \in \mathbb{R}^2$, which, for each $x \in \mathbb{R}$ satisfies the Lipschitz condition with respect to y, with a Lipschitz constant that is independent of x. Here, y' denotes the derivative of the real-valued function y with respect to the independent variable x.

(a) [2 marks] Let $x_0, y_0 \in \mathbb{R}$. State the general form of a linear k-step method for the numerical solution of the initial-value problem $y'(x) = f(x, y(x))$, $y(x_0) = y_0$, on the mesh $\{x_n : x_n = x_0 + nh,\ n = 0, 1, \dots\}$ of uniform spacing $h > 0$.

(b) [6 marks] Consider the two-parameter family of implicit linear two-step methods defined by

$$y_{n+2} - a y_{n+1} = \frac{h}{12}\left(b f_{n+2} + 8 f_{n+1} - f_n\right), \qquad n = 0, 1, \dots, \tag{2}$$

where $f_j = f(x_j, y_j)$, and a and b are real numbers. Show that this two-step method is zero-stable if, and only if, $|a| \leqslant 1$.

(c) [6 marks] Now suppose that $a = 1$ in the previous part of the question. Show that there exists a unique choice of b such that the two-step method (2) is third-order consistent; show further that for this value of b the two-step method (2) is third-order convergent.
[If Dahlquist's Theorem is used, it must be stated carefully.]

(d) [11 marks] Suppose that $a = 1$ and b is such that the two-step method (2) is third-order convergent. Show that the stability polynomial $\pi(\cdot, \bar{h})$ of the linear multistep method (2) is then of the form

$$\pi(r, \bar{h}) = \left(1 - \frac{5\bar{h}}{12}\right) z^2 - \left(1 + \frac{8\bar{h}}{12}\right) z + \frac{\bar{h}}{12},$$

where $\bar{h} := h\lambda$ and λ is a negative real number.
Find the interval of absolute stability of the two-step method (2) for these values of a and b using Schur's criterion.

5. Consider the initial-boundary-value problem

$$\frac{\partial u}{\partial t} + u^3 = \frac{\partial^2 u}{\partial x^2}, \qquad 0 < x < 1, \quad 0 < t \leqslant T,$$

$$u(x,0) = u_0(x), \qquad 0 < x < 1,$$

subject to homogeneous Dirichlet boundary conditions at $x = 0$ and $x = 1$, where T is a fixed positive real number, and u_0 is a real-valued continuous function of $x \in [0,1]$ such that $u_0(0) = u_0(1) = 0$.

(a) [5 marks] Show that if a solution to this initial-boundary-value problem exists, then it must be unique. You may find it helpful to note that $(a^3 - b^3)(a - b) \geqslant 0$ for all $a, b \in \mathbb{R}$.

(b) [10 marks] Formulate the implicit Euler scheme for the numerical solution of this initial-boundary-value problem on a mesh with uniform spacings $\Delta x = 1/N$, $N \geqslant 2$, and $\Delta t = T/M$, $M \geqslant 1$, in the x and t coordinate directions, respectively.
Show that if a solution to the implicit Euler scheme exists, then it must be unique.
You may find it helpful to note that $a^2 + ab + b^2 \geqslant 0$ for all $a, b \in \mathbb{R}$.

(c) [10 marks] Let U_j^m denote the implicit Euler approximation to $u(j\Delta x, m\Delta t)$, $0 \leqslant m \leqslant M$, $j = 0, \ldots, N$, where $M \geqslant 1$ and $N \geqslant 2$. Assuming that the solution u to the initial-boundary-value problem exists and possesses as many partial derivatives with respect to x and t as are required by your argument, and that these partial derivatives are continuous on $[0,1] \times [0,T]$, show that there exists a positive constant C, independent of Δx and Δt, such that

$$\max_{1 \leqslant m \leqslant M} \max_{1 \leqslant j \leqslant N-1} |u(j\Delta x, m\Delta t) - U_j^m| \leqslant C(\Delta t + (\Delta x)^2).$$

6. (a) [4 marks] Suppose that v is a real-valued function, defined and three times continuously differentiable on $(-\infty, \infty)$. Show that for each $x \in (-\infty, \infty)$ and $\Delta x > 0$ there exists a real-number $\xi = \xi(x, \Delta x)$, contained in the interval $(x - \Delta x, x + \Delta x)$, such that

$$\frac{v(x+\Delta x) - v(x-\Delta x)}{2\Delta x} = v'(x) + \frac{1}{6}(\Delta x)^2 v'''(\xi),$$

where v' and v''' denote the first and third derivative of v with respect to the independent variable x, respectively.

(b) [7 marks] Let a be a real number and κ a positive real number. Consider the time-dependent advection-diffusion equation

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = \kappa \frac{\partial^2 u}{\partial x^2}$$

on the space-time domain $(-\infty, \infty) \times (0, T]$, where $T > 0$, subject to the initial condition $u(x, 0) = \mathrm{e}^{-x^2}$.
Denoting by U_j^m the numerical approximation to $u(j\Delta x, m\Delta t)$ for $j = 0, \pm 1, \pm 2, \ldots$ and $m = 0, 1, \ldots, M$, formulate the explicit Euler finite difference scheme for the numerical solution of this initial-value problem on a mesh of spacing $\Delta x > 0$ in the x-direction and $\Delta t = T/M$, with $M \geqslant 1$, in the t-direction, so that the consistency error of the scheme is $\mathcal{O}(\Delta t + (\Delta x)^2)$.

(c) [14 marks] Let $\nu = a\Delta t/\Delta x$ and $\mu = \kappa \Delta t/(\Delta x)^2$. By representing U_j^m in terms of its inverse semidiscrete Fourier transform $\hat{U}^m(k)$, $k \in [-\pi/\Delta, \pi/\Delta x]$, as

$$U_j^m = \frac{1}{2\pi}\int_{-\pi/\Delta x}^{\pi/\Delta x} \mathrm{e}^{\imath k j \Delta x} \hat{U}^m(k)\, dk$$

and using the discrete version of Parseval's identity, show that if $\nu^2 \leqslant 2\mu \leqslant 1$ then the explicit Euler finite difference scheme from part (b) of the question is practically stable.