A18289W1

DEGREE OF MASTER OF SCIENCE

Mathematical Modelling and Scientific Computing

Numerical Solution of Partial Differential Equations and Numerical Linear Algebra

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Hilary Term 2023

Friday, 13 January 2023, 9:30am to 12.00pm

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.

Candidates may bring a summary sheet into this exam consisting of (both sides of) one sheet of A4 paper containing material prepared in advance in accordance with the guidance given by the Mathematical Institute.

Please start the answer to each question in a new booklet.

Do not turn this page until you are told that you may do so

Numerical Linear Algebra

1. Let $A \in \mathbb{R}^{m\times n}$ $(m \geqslant n)$ and let $A = U\Sigma V^T$ be its SVD (singular value decomposition), where U has orthonormal columns (so that $U^TU = I_n$), V is orthogonal, and $\Sigma = \mathrm{diag}(\sigma_1, \ldots, \sigma_n)$, with $\sigma_1 \geqslant \sigma_2 \geqslant \cdots \geqslant \sigma_n \geqslant 0$. Let $\|A\|_2 = \sigma_1$ denote the spectral norm.

   (a) [13 marks] Suppose that the SVD, $A = U\Sigma V^T$, is given.

      (i) Find the SVD of AA^TA.

      (ii) Show that $\|AA^TAx\|_2 \geqslant (\sigma_n(A))^3\|x\|_2$ for any $x \in \mathbb{R}^n$.

      (iii) Find the matrix B such that $AB = U\Sigma^2V^T$.

      (iv) Let $\sigma_1u_1v_1^T$ be a best rank-1 approximation to A in the spectral norm, where $\|u_1\|_2 = \|v_1\|_2 = 1$. Find a best rank-1 approximation to AA^T.

   (b) [12 marks] Let $A = \begin{bmatrix}1 & 1\\ 1 & 0\\ 0 & 1\end{bmatrix}\begin{bmatrix}1 & \\ & 10^{-10}\end{bmatrix}\begin{bmatrix}1 & 1 & 0\\ 1 & 0 & 1\end{bmatrix} \left(= \begin{bmatrix}1 & 1\\ 1 & 0\\ 0 & 1\end{bmatrix}\begin{bmatrix}1 & \\ & 10^{-10}\end{bmatrix}\begin{bmatrix}1 & 1\\ 1 & 0\\ 0 & 1\end{bmatrix}^T\right)$.

      (i) Prove that A is positive semidefinite, e.g. by showing that $x^TAx \geqslant 0$ for any $x \in \mathbb{R}^3$.

      (ii) Find a rank-1 matrix A_1 such that $\|A - A_1\|_2 \leqslant 2 \times 10^{-10}$.
      [*The matrix A_1 can be found without lengthy calculations.*]

      (iii) Prove that there exists a rank-1 matrix $\tilde{A}_1$ such that $\|A - \tilde{A}_1\|_2 < 2 \times 10^{-10}$.
      [*You may use the fact that in the QR factorisation* $\begin{bmatrix}1 & 1\\ 1 & 0\\ 0 & 1\end{bmatrix} = QR$, $R = \begin{bmatrix}\sqrt{2} & \sqrt{\frac{1}{2}}\\ 0 & \sqrt{\frac{3}{2}}\end{bmatrix}$.]

2. (a) [13 marks] Consider the LU factorisation $A = LU \in \mathbb{R}^{n\times n}$.

   (i) Suppose that a pivoted LU factorisation $PA = LU$ is known, where P is a permutation matrix. Describe an algorithm that can be used to solve the linear system $Ax = b$.

   (ii) What is the computational complexity of the algorithm in (i)? Answer in the big-O notation, e.g. $O(n^3), O(n \log n)$, and justify your answer.

   (iii) Give an example of a 2×2 matrix, A, that does not have an LU factorisation.

   (iv) Show that $A \in \mathbb{R}^{n\times n}$ has a pivoted LU factorisation $PA = LU$ if A is nonsingular.

   (b) [12 marks] Recall that a Householder reflector is a matrix of the form $H = I - 2vv^T \in \mathbb{R}^{n\times n}$ where $v \in \mathbb{R}^n$ is a vector of unit norm $\|v\|_2 = 1$.

   (i) Let $a, b \in \mathbb{R}^n$ be vectors such that $a \neq b$ and $\|a\|_2 = \|b\|_2$. Find a Householder reflector H such that $Ha = b$.

   (ii) Using Householder reflectors, show that any $A \in \mathbb{R}^{m\times n}$ has a QR factorisation $A = QR$, where Q has orthonormal columns and R is upper triangular. (Discuss both cases $m \geqslant n$, and $m < n$.)

   (iii) Show that any orthogonal matrix $Q \in \mathbb{R}^{n\times n}$ can be written as a product of Householder reflectors, $Q = H_1 H_2 \cdots H_\ell$, where $\ell \leqslant n$.

Numerical Solution of Partial Differential Equations

3. Let $f \in C([0,1])$ and suppose that $u \in C^2([0,1])$ is the unique solution of the boundary-value problem

$$-u''(x) + a(x)u'(x) + c(x)u(x) = f(x), \quad x \in (0,1), \qquad u(0) = 0, \quad u(1) = 0, \tag{1}$$

where $a \in C^1([0,1])$ is a monotonically non-increasing function and $c \in C([0,1])$, with $c(x) \geqslant 1$ for all $x \in [0,1]$.

(a) [7 marks] Show that

$$\int_0^1 (u'(x))^2 \,\mathrm{d}x - \frac{1}{2}\int_0^1 a'(x)(u(x))^2 \,\mathrm{d}x + \int_0^1 c(x)(u(x))^2 \,\mathrm{d}x = \int_0^1 f(x)u(x)\,\mathrm{d}x.$$

Hence deduce that

$$\int_0^1 (u'(x))^2 \,\mathrm{d}x + \int_0^1 (u(x))^2 \,\mathrm{d}x \leqslant \int_0^1 (f(x))^2 \,\mathrm{d}x.$$

(b) [7 marks] Suppose, in addition, that $a(x) \geqslant 0$ for all $x \in [0,1]$. On a finite difference mesh $\overline{\Omega}_h := \{x_i := ih : i = 0, \ldots, N\}$ of spacing $h := 1/N$, where $N \geqslant 2$, construct a finite difference scheme for the numerical solution of the boundary-value problem (1), where the term u'' has been approximated by a second-order central difference and the term u' has been approximated by a first-order backward difference. Denoting by U the finite difference approximation of u on the mesh $\overline{\Omega}_h$, show that

$$\|D_x^- U]|_h^2 + a(x_N)U_{N-1}^2 + \|U\|_h^2 \leqslant \|f\|_h^2,$$

where D_x^- denotes the first-order backward difference operator, and the norms $\|\cdot]|_h$ and $\|\cdot\|_h$ are defined by $\|V]|_h := (V,V]_h^{1/2}$ and $\|V\|_h := (V,V)_h^{1/2}$, respectively, with

$$(V,W]_h := \sum_{i=1}^{N} hV_iW_i \quad \text{and} \quad (V,W)_h := \sum_{i=1}^{N-1} hV_iW_i.$$

(c) [7 marks] Still assuming that $a \in C^1([0,1])$ is monotonically non-increasing, now suppose that a can be of either sign on the interval $[0,1]$. Define $a^+(x) := \max(a(x),0)$ and $a^-(x) := \min(a(x),0)$. By noting that $a^+(x) \geqslant 0$, $a^-(x) \leqslant 0$ and $a(x)u'(x) = a^+(x)u'(x) + a^-(x)u'(x)$, construct a finite a difference scheme for the numerical solution of the boundary-value problem (1). In the finite difference scheme the term $u''(x_i)$ should be approximated by $D_x^+D_x^-U_i$ and the term $a(x_i)u'(x_i)$ should be approximated by $a^+(x_i)D_x^-U_i + a^-(x_i)D_x^+U_i$. Here, D_x^+ denotes the first-order forward difference operator. Show that

$$\|D_x^- U]|_h^2 + (-a^-(x_0))U_1^2 + a^+(x_N)U_{N-1}^2 + \|U\|_h^2 \leqslant \|f\|_h^2.$$

(d) [4 marks] Adopt the same assumptions as in part (c), and denote by φ_i the consistency error of the finite difference scheme constructed in part (c) at the mesh point x_i, $i = 1, \ldots, N-1$. Show that

$$\|U - u\|_{1,h} \leqslant \|\varphi\|_h,$$

where $\|\cdot\|_{1,h}$ is a discrete Sobolev norm that you should carefully define.

4. Suppose that $\Omega := (0,1)^2$ and $f \in C(\overline{\Omega})$, and let $u \in C^2(\overline{\Omega})$ denote the unique solution of the elliptic boundary-value problem

$$\begin{aligned} -\Delta u + u + u^3 + u^5 &= f \quad \text{in } \Omega, \\ u &= 0 \quad \text{on } \partial\Omega. \end{aligned} \tag{1}$$

(a) [6 marks] On the finite difference mesh

$$\overline{\Omega}_h := \{(x_i, y_j) \,:\, x_i := ih,\ y_j := jh,\ i,j = 0,\dots,N\},$$

of spacing $h := 1/N$ in both coordinate directions, where $N \geqslant 2$, construct a five-point finite difference scheme for the numerical solution of the boundary-value problem (1).

(b) [6 marks] For a mesh-function V defined on $\Omega_h := \overline{\Omega}_h \setminus \partial\Omega$ consider the discrete maximum norm $\|\cdot\|_{\infty,h}$ defined by

$$\|V\|_{\infty,h} := \max_{1 \leqslant i,j \leqslant N-1} |V_{i,j}|.$$

Show that

$$\|U\|_{\infty,h} \leqslant \|f\|_{\infty,h}.$$

(c) [6 marks] Define the consistency error $\varphi_{i,j}$ of the finite difference scheme constructed in part (a) at the mesh point (x_i, y_j), $i,j = 1,\dots,N-1$.
Show that

$$\|u - U\|_{\infty,h} \leqslant \|\varphi\|_{\infty,h}.$$

Suppose that $u \in C^4(\overline{\Omega})$. Deduce that there exists a positive constant C, independent of h, which you should specify, such that

$$\|u - U\|_{\infty,h} \leqslant Ch^2.$$

[*You may wish to note that, for any* $a, b \in \mathbb{R}$,

$$a^3 - b^3 = (a-b)(a^2 + ab + b^2) \quad \textit{and} \quad a^5 - b^5 = (a-b)(a^4 + a^3b + a^2b^2 + ab^3 + b^4)$$

and that, since $x \mapsto x^3$ *and* $x \mapsto x^5$ *are monotonically increasing functions,* $a^2+ab+b^2 \geqslant 0$ *and* $a^4 + a^3b + a^2b^2 + ab^3 + b^4 \geqslant 0$ *for all* $a, b \in \mathbb{R}$.]

(d) [7 marks] Show that if $f(x_i, y_j) \geqslant 0$ for all $i,j = 1,\dots,N-1$, then $U_{i,j} \geqslant 0$ for all $i,j = 0,\dots,N$.

5. Consider the initial-value problem

$$\begin{aligned} \frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} &= a\frac{\partial^2 u}{\partial x^2}, \qquad && -\infty < x < \infty, \quad t > 0, \\ u(x,0) &= u_0(x), && -\infty < x < \infty, \end{aligned} \tag{1}$$

where $a \geqslant 0$ is a real number, and u_0 is a real-valued, bounded and continuous function of $x \in (-\infty, \infty)$.

Let $\mathbb{Z}$ denote the set of all integers and consider a finite difference mesh of spacing $\Delta x > 0$ in the x-direction and $\Delta t > 0$ in the positive t-direction.

(a) [4 marks] Formulate an implicit finite difference scheme for the numerical solution of the initial-value problem (1), with U_j^m denoting the finite difference approximation of $u(j\Delta x, m\Delta t)$ for $j \in \mathbb{Z}$ and $m = 0, 1, \ldots$, where $\frac{\partial^2 u}{\partial x^2}(j\Delta x, m\Delta t)$ is approximated by

$$D_x^+ D_x^- U_j^m := (U_{j+1}^m - 2U_j^m + U_{j-1}^m)/(\Delta x)^2,$$

and where $\frac{\partial u}{\partial x}(j\Delta x, m\Delta t)$ is approximated by the backward difference

$$D_x^- U_j^m := (U_j^m - U_{j-1}^m)/(\Delta x).$$

(b) [8 marks] Suppose further that $U_j^0 := u_0(x_j)$, $j \in \mathbb{Z}$, and that

$$\|U^0\|_{\ell_2} := \left(\Delta x \sum_{j \in \mathbb{Z}} |U_j^0|^2 \right)^{1/2},$$

is finite. Show that the implicit scheme from part (a) is unconditionally practically stable in the ℓ_2 norm.

(c) [4 marks] Formulate an explicit finite difference scheme for the numerical solution of the initial-value problem (1), with U_j^m denoting the finite difference approximation of $u(j\Delta x, m\Delta t)$ for $j \in \mathbb{Z}$ and $m = 0, 1, \ldots$, where $\frac{\partial^2 u}{\partial x^2}(j\Delta x, m\Delta t)$ is approximated by $D_x^+ D_x^- U_j^m$ and where $\frac{\partial u}{\partial x}(j\Delta x, m\Delta t)$ is approximated by $D_x^- U_j^m$.

(d) [9 marks] Let $\nu := \Delta t/\Delta x$, $\mu := \Delta t/(\Delta x)^2$ and suppose that U_j^0 is as in part (b). Show that if

$$\nu + 2a\mu \leqslant 1,$$

then the explicit finite difference scheme from part (c) is practically stable in the ℓ_2 norm.

[*The discrete version of Parseval's identity for the semidiscrete Fourier transform may be used without proof.*]

6. Consider the initial-boundary-value problem

$$
\begin{aligned}
\frac{\partial u}{\partial t} + (1+u^2)\frac{\partial u}{\partial x} &= 0, && 0 < x < \infty, \quad t > 0, \\
u(x,0) &= u_0(x), && 0 \leqslant x < \infty, \\
u(0,t) &= 0, && 0 \leqslant t < \infty,
\end{aligned}
\tag{1}
$$

where u_0 is a real-valued continuous function of x such that $u_0(0) = 0$ and

$$\lim_{x\to\infty} |u_0(x)| = 0.$$

Consider a finite difference mesh of spacing $\Delta x > 0$ in the positive x-direction and $\Delta t > 0$ in the positive t-direction.

(a) [4 marks] With U_j^m denoting the finite difference approximation of $u(j\Delta x, m\Delta t)$ for $j = 0, 1, \ldots$ and $m = 0, 1, \ldots$, construct an explicit finite difference scheme, involving U_j^{m+1}, U_j^m and U_{j-1}^m for $j = 1, 2, \ldots$ and $m = 0, 1, \ldots$, for the numerical solution of the initial-boundary-value problem (1).

(b) [7 marks] Let $m \geqslant 0$. Show that if $\sup_{j\geqslant 0} |U_j^m| < \infty$ and

$$(1 + \sup_{j\geqslant 0}(U_j^m)^2)\Delta t \leqslant \Delta x,$$

then

$$\sup_{j\geqslant 0} |U_j^{m+1}| \leqslant \sup_{j\geqslant 0} |U_j^m|.$$

(c) [7 marks] Show that, under the stated assumptions on u_0, $A := \max_{x\in[0,\infty)} |u_0(x)| < \infty$. Hence deduce that if $(1 + A^2)\Delta t \leqslant \Delta x$, then

$$\sup_{j\geqslant 0} |U_j^{m+1}| \leqslant \sup_{j\geqslant 0} |U_j^m|, \qquad \text{for all } m = 0, 1, \ldots.$$

(d) [7 marks] Show that if $(1+A^2)\Delta t \leqslant \Delta x$, with A defined as in part (c), then $\lim_{j\to\infty} |U_j^m| = 0$ for each $m \geqslant 0$ and that, therefore, in each of the inequalities above $\sup_{j\geqslant 0}$ can be replaced by $\max_{j\geqslant 0}$.

Suppose that $u_0(x) \geqslant 0$ for all $x \in [0, \infty)$. Show that, if $(1 + A^2)\Delta t \leqslant \Delta x$, with A as defined in part (c), then

$$0 \leqslant U_j^m \leqslant A, \qquad \text{for all } j, m = 0, 1, \ldots.$$