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 2024

Friday 12 January, 9:30am - 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.
Please begin each question in a new answer booklet.

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

Numerical Linear Algebra

1. (a) [7 marks] Vector and matrix p-norms are related by various inequalities, often involving the dimension of the vectors and matrices. For each of the following, verify the inequality and give an example of a nonzero m-vector x or $m \times n$ matrix A (for general m and n) for which equality is achieved.

    1. $\|x\|_\infty \leqslant \|x\|_1 \leqslant m\|x\|_\infty$
    2. $\|A\|_\infty \leqslant n^{1/2}\|A\|_2$

    For inequality 2 you can use without proof that $\|x\|_\infty \leqslant \|x\|_2 \leqslant m^{1/2}\|x\|_\infty$.

   (b) [4 marks] The matrix max norm is defined as $\|A\|_{max} = \max_{i,j} |a_{ij}|$. Show that the matrix max norm is not sub-multiplicative; that is, give an example of matrices A and B for which $\|AB\|_{max} > \|A\|_{max} \cdot \|B\|_{max}$.

   (c) [8 marks] Any matrix $A \in \mathbb{R}^{m\times n}$ with $m > n$ has the singular value decomposition $A = U\Sigma V^T$ where $U^TU = I_m \in \mathbb{R}^{m\times m}$, $V^TV = I_n \in \mathbb{R}^{n\times n}$ and $\Sigma \in \mathbb{R}^{m\times n}$ with diagonal entries $\sigma_{11} \geqslant \sigma_{22} \geqslant \cdots \sigma_{nn} \geqslant 0$ and all other entries in Σ equal to zero. Prove the aforementioned decomposition exists by considering that the matrix AA^T is positive semi-definite with eigen-decomposition $AA^T = U\Lambda U^T$ where $U^TU = I_m$ and Λ is a diagonal matrix.

   (d) [6 marks] Prove that for every matrix A there exists a matrix E, with $\|E\|_2$ small enough such that $\sigma_i(A+E) = \sigma_i(A) + \sigma_i(E)$, where $\sigma_i(C)$ is the i^{th} singular value of a matrix C.

2. (a) [6 marks] Below is pseudo-code for the modified Gram-Schmidt algorithm of a matrix $A \in \mathbb{R}^{m\times n}$ whose i^{th} column is denoted a_i. Determine the exact, not just leading order, number of floating point operations (additions, subtractions, multiplications, divisions, and square-roots) of the modified Gram-Schmidt algorithm defined as:

for $i = 1$ to n
  $\nu_i = a_i$
for $i = 1$ to n
  $r_{ii} = \|\nu_i\|_2$
  $q_i = \nu_i / r_{ii}$
  for $j = i+1$ to n
    $r_{ij} = \nu_j^* q_i$
    $\nu_j = \nu_j - r_{ij} q_i$

(b) [6 marks] Let A be an $m \times n$ matrix with $m \geqslant n$, and let $A = QR$ be its QR factorization with R of size $n \times n$.

1. Show that A has rank n if and only if all the diagonal entries of R are nonzero.
2. Suppose R has k nonzero diagonals for some $0 \leqslant k < n$. What does this imply about the rank of A?

(c) [7 marks] Let $A \in \mathbb{R}^{2\times 2}$ be a matrix with two repeated eigenvalues but without two independent eigen-vectors; that is $\lambda_1 = \lambda_2$, has algebraic multiplicity 2 and geometric multiplicity 1. Consequently, $A = VJV^{-1}$ where J is of the form

$$J = \begin{pmatrix} \lambda_1 & 1 \\ 0 & \lambda_1 \end{pmatrix}.$$

Show that the power method applied to this matrix, with initial vector $\nu^{(0)} = Vc$ and $c_i \neq 0$ for all i, converges to the leading eigenvalue λ_1 at a rate at least as fast as k^{-1} at the k^{th} iteration.

(d) [6 marks] We refer to a matrix as being strictly column diagonally dominant (SCDD) if the modulus of the diagonal entry on each column is strictly greater than the sum of the modulus of the off diagonal entries in the same column; that is $A \in \mathbb{R}^{n\times n}$ with entries a_{ij} is SCDD if $|a_{jj}| > \sum_{i=1}^{j-1} |a_{ij}| + \sum_{i=j+1}^{n} |a_{ij}|$. Show that the LU factorization of a SCDD matrix A has all subdiagonal entries of L strictly less than one.

Numerical Solution of Differential Equations

3. Let $\Omega = (0,1)$ and $b, f \in C(\bar{\Omega})$ be given functions and $u_L, u_R \in \mathbb{R}$ be given nonnegative constants. Consider the elliptic partial differential equation

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

(a) [3 marks] On the uniform finite difference mesh

$$\bar{\Omega}_h := \{x_i := ih,\ i = 0, \dots, N\}$$

of spacing $h := 1/N$, where $N \geqslant 2$, formulate a finite difference approximation $\{U_i : 0 \leqslant i \leqslant N\}$ to (1) of the form

$$\mathcal{L}_h U_i = f_i, \qquad 1 \leqslant i \leqslant N-1,$$

using the three-point stencil for the second-order term $-u''$ and the two-point central difference operator for the first order term u'.

(b) [6 marks] Show that if $f < 0$ on $\bar{\Omega}$ and $\|b\|_{C(\bar{\Omega})}h \leqslant 2$, then U satisfies

$$\max_{0 \leqslant i \leqslant N} U_i = \max\{u_L, u_R\}.$$

(c) [6 marks] Suppose that there exists $\delta > 0$ such that $\|b\|_{C(\bar{\Omega})}h \leqslant 2 - \delta$. Show that there exists $\lambda > 0$ such that the mesh function $W_i := e^{\lambda x_i}$ satisfies

$$\mathcal{L}_h W_i < 0 \qquad 1 \leqslant i \leqslant N-1.$$

Then, under the same assumptions, show that if $f \leqslant 0$, then U satisfies

$$\max_{0 \leqslant i \leqslant N} U_i = \max\{u_L, u_R\}.$$

(d) [4 marks] Suppose that $u_L = u_R = 0$. Show that if $\|b\|_{C(\bar{\Omega})}h \leqslant 2$, then U satisfies

$$\max_{1 \leqslant i \leqslant N-1} |U_i| \leqslant \max_{1 \leqslant i \leqslant N-1} |f(x_i)|.$$

[*Hint: Do not use parts (b) or (c).*]

(e) [6 marks] Define the consistency error φ_i of your scheme in (a) at the mesh-point x_i, $i = 1, 2, \dots, N-1$. Assuming that $u \in C^4(\bar{\Omega})$, show that

$$\max_{1 \leqslant i \leqslant N-1} |\varphi_i| \leqslant Ch^2 \left(\|b\|_{C(\bar{\Omega})} \|u'''\|_{C(\bar{\Omega})} + \|u''''\|_{C(\bar{\Omega})} \right),$$

where C is a positive constant that you should specify. Conclude that if $\|b\|_{C(\bar{\Omega})}h \leqslant 2$, then

$$\max_{0 \leqslant i \leqslant N} |u(x_i) - U_i| \leqslant Ch^2 \left(\|b\|_{C(\bar{\Omega})} \|u'''\|_{C(\bar{\Omega})} + \|u''''\|_{C(\bar{\Omega})} \right).$$

4. Let $\Omega := (0,1)^2$, $b \in \mathbb{R}$ be a given constant, and $c, f \in C(\bar{\Omega})$ be given functions. Consider the elliptic partial differential equation

$$-\Delta u + b\frac{\partial u}{\partial y} + c(x,y)u = f, \qquad \text{in } \Omega, \tag{1a}$$

$$u = 0, \qquad \text{on } \partial\Omega. \tag{1b}$$

(a) [7 marks] Suppose that $u \in C^2(\bar{\Omega})$. Show that

$$\int_\Omega |\nabla u(x,y)|^2 \,\mathrm{d}x\,\mathrm{d}y = \int_\Omega \{f(x,y)u(x,y) - c(x,y)u^2(x,y)\} \,\mathrm{d}x\,\mathrm{d}y.$$

[*Hint: The identity* $\frac{\partial(u^2)}{\partial y} = 2u\frac{\partial u}{\partial y}$ *may be helpful.*]
Then, find a positive constant $M_0 > 0$ such that if

$$\|c\|_{C(\bar{\Omega})} \leqslant M_0, \tag{2}$$

then any solution $u \in C^2(\bar{\Omega})$ to the partial differential equation (1) satisfies

$$\|u\|_{H^1(\Omega)} \leqslant C_0 \|f\|_{L^2(\Omega)},$$

where C_0 is a constant you should specify. Conclude that if (2) holds, then $C^2(\bar{\Omega})$ solutions to (1) are unique.
[*You may use the Poincaré-Friedrichs inequality without proof.*]

(b) [3 marks] On the uniform finite difference mesh

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

of spacing $h := 1/N$ in both coordinate directions, where $N \geqslant 2$, formulate a finite difference approximation to (1) using the five-point stencil for the second-order term $-\Delta u$ and the two-point central difference operator for the first-order term $\frac{\partial u}{\partial y}$.

(c) [7 marks] Find a positive constant $M_1 > 0$ independent of h such that if

$$\|c\|_{C(\bar{\Omega})} \leqslant M_1, \tag{3}$$

then any solution U to the finite difference scheme in (b) satisfies

$$\|U\|_{1,h} \leqslant C_1 \|f\|_h,$$

where C_1 is a constant you should specify and $\|\cdot\|_{1,h}$ is a discrete H^1 norm that you should specify.
Conclude that your finite difference scheme has a solution and that the solution is unique.
[*You may use the discrete Poincaré-Friedrichs inequality without proof.*]

(d) [8 marks] Define the consistency error $\varphi_{i,j}$ of your scheme in (b) at the mesh-point (x_i, y_j), $i,j = 1,2,\dots,N-1$. Assuming that $u \in C^4(\bar{\Omega})$, show that

$$\max_{1\leqslant i,j\leqslant N-1} |\varphi_{i,j}| \leqslant C_2 h^2 \left(|b| \left\|\frac{\partial^3 u}{\partial y^3}\right\|_{C(\bar{\Omega})} + \left\|\frac{\partial^4 u}{\partial x^4}\right\|_{C(\bar{\Omega})} + \left\|\frac{\partial^4 u}{\partial y^4}\right\|_{C(\bar{\Omega})} \right),$$

where C_2 is a positive constant that you should specify. Then, show that there exists a positive constant C_3, that you should specify in terms of C_1 and C_2, such that if (3) holds, then

$$\|u - U\|_{1,h} \leqslant C_3 h^2 \left(|b| \left\|\frac{\partial^3 u}{\partial y^3}\right\|_{C(\bar{\Omega})} + \left\|\frac{\partial^4 u}{\partial x^4}\right\|_{C(\bar{\Omega})} + \left\|\frac{\partial^4 u}{\partial y^4}\right\|_{C(\bar{\Omega})} \right).$$

5. Consider the initial value problem

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} + u = \kappa\frac{\partial^2 u}{\partial x^2}, \qquad -\infty < x < \infty,\ 0 < t \leqslant T, \tag{1a}$$

$$u(x,0) = u_0(x), \qquad -\infty < x < \infty, \tag{1b}$$

where a, κ, and T are strictly positive real numbers, and u_0 is a real-valued, bounded, and continuous function of $x \in (-\infty, \infty)$.

(a) [5 marks] Suppose that $\theta \in [0,1]$. Formulate the θ-scheme, with $\theta = 1$ corresponding to the backward Euler scheme, for the numerical solution of (1) on a mesh with uniform spacings $\Delta x = 1/N$ and $\Delta t = T/M$ in the x and t coordinate directions, respectively, where $N \geqslant 2$ and $M \geqslant 1$ are integers. Use the two-point backward difference operator for the first order spatial derivative and denote the solution by U_j^m.

(b) [10 marks] Suppose that

$$\|U^0\|_{\ell^2} := \left(\Delta x \sum_{j=-\infty}^{\infty} |U_j^0|^2\right)^{1/2}$$

is finite. Find a complex valued function λ such that

$$\hat{U}^m(k) = [\lambda(k)]^m \hat{U}^0(k), \qquad k \in [-\pi/\Delta x, \pi/\Delta x],$$

for all $m = 0, 1, \ldots, M$, where $\hat{U}^m$ is the semi-discrete Fourier transform of $\{U_j^m\}$:

$$\hat{U}^m(k) := \Delta x \sum_{j=-\infty}^{\infty} U_j^m e^{-\mathrm{i}kx_j}, \qquad k \in [-\pi/\Delta x, \pi/\Delta x].$$

Then, show that the backward Euler scheme ($\theta = 1$) satisfies

$$\|U^m\|_{\ell^2} \leqslant \left(\frac{1}{1+\Delta t}\right)^m \|U^0\|_{\ell^2}, \qquad 1 \leqslant m \leqslant M,$$

for any choice of Δx and Δt.

[*You may use the discrete version of Parseval's identity for the semidiscrete Fourier transform without proof.*]

(c) [10 marks] Suppose that u is smooth in space and time. Define the consistency error T_j^m for the θ-scheme in (a) and show that that the backward Euler scheme ($\theta = 1$) has consistency error

$$T_j^m = \mathcal{O}(\Delta t + \Delta x), \qquad j \in \mathbb{Z},\ m = 0, 1, \ldots, M-1.$$

Modify the finite difference scheme in (a) so that the Crank-Nicolson scheme ($\theta = 1/2$) has consistency error

$$T_j^m = \mathcal{O}((\Delta t)^2 + (\Delta x)^2), \qquad j \in \mathbb{Z},\ m = 0, 1, \ldots, M-1.$$

Prove that your modification has the above consistency error.

6. Consider the advection equation

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0, \qquad -\infty < x < \infty,\ 0 < t \leqslant T, \tag{1a}$$

$$u(x,0) = u_0(x), \qquad -\infty < x < \infty, \tag{1b}$$

where a and T be a positive constants and u_0 is a real-valued, bounded, continuous function of $x \in (-\infty, \infty)$.

We discretize space-time $(-\infty,\infty) \times [0,T]$ with uniform spacings $\Delta x = 1/N$ and $\Delta t = T/M$ in the x and t coordinate directions, respectively, where $N \geqslant 2$ and $M \geqslant 1$ are integers. The so-called *Beam-Warming scheme* for (1) is

$$\frac{U_j^{m+1} - U_j^m}{\Delta t} + \frac{a}{2\Delta x}\left(3U_j^m - 4U_{j-1}^m + U_{j-2}^m\right) = \frac{a^2\Delta t}{2(\Delta x)^2}\left(U_j^m - 2U_{j-1}^m + U_{j-2}^m\right), \tag{2a}$$

$$U_j^0 = u_0(j\Delta x), \tag{2b}$$

where $j \in \mathbb{Z}$ and $m = 0, 1, \ldots, M-1$.

(a) [10 marks] Show that

$$u_j^{m+1} - \frac{(a\Delta t)^2}{2(\Delta x)^2}\left(u_j^m - 2u_{j-1}^m + u_{j-2}^m\right) = \left[u - a(\Delta t)\frac{\partial u}{\partial x}\right]_j^m + \mathcal{O}((\Delta t)^3 + (\Delta t)^2(\Delta x)), \tag{3}$$

where $u_j^m := u(j\Delta x, m\Delta t)$, $j \in \mathbb{Z}$, and $0 \leqslant m \leqslant M-1$. You may assume that u has as many bounded derivatives as necessary for your arguments.
[*Hint: You may want to relate* $\frac{\partial^2 u}{\partial t^2}$ *to* $\frac{\partial^2 u}{\partial x^2}$.]

(b) [5 marks] Define the consistency error T_j^m, $j \in \mathbb{Z}$, $0 \leqslant m \leqslant M-1$, for the scheme (2) and show that it satisfies

$$T_j^m = \mathcal{O}((\Delta t)^2 + (\Delta x)^2 + (\Delta t)(\Delta x)), \qquad j \in \mathbb{Z},\ 0 \leqslant m \leqslant M-1. \tag{4}$$

You may assume that u has as many bounded derivatives as necessary for your arguments and that (3) holds regardless of your answer for part (a).

(c) [10 marks] Find a complex valued function λ of the form

$$\lambda(k) = \alpha + \beta e^{-\mathrm{i}k\Delta x} + \gamma e^{-2\mathrm{i}k\Delta x},$$

such that

$$\hat{U}^m(k) = [\lambda(k)]^m \hat{U}^0(k), \qquad k \in [-\pi/\Delta x, \pi/\Delta x],$$

for all $m = 0, 1, \ldots, M$, where α, β, and γ are constants that you should specify. Here, $\hat{U}^m$ is the semi-discrete Fourier transform of $\{U_j^m\}$:

$$\hat{U}^m(k) := \Delta x \sum_{j=-\infty}^{\infty} U_j^m e^{-\mathrm{i}kx_j}, \qquad k \in [-\pi/\Delta x, \pi/\Delta x].$$

Show that

$$|\lambda(k)|^2 = \alpha^2 + \beta^2 + \gamma^2 + 2\beta(\alpha+\gamma)\cos(k\Delta x) + 2\alpha\gamma\cos(2k\Delta x),$$

and

$$\frac{d}{dk}|\lambda(k)|^2 = 2(\Delta x)\mu(\mu-2)(\mu-1)^2\sin(k\Delta x)(1-\cos(k\Delta x)), \quad \text{where } \mu = \frac{a\Delta t}{\Delta x}.$$

Conclude that the Beam-Warming scheme is practically stable if $0 \leqslant \mu \leqslant A$, where A is a positive constant you should specify.

[*You may use without proof the result that if* $|\lambda(k)| \leqslant 1$ *for* $k \in [-\pi/\Delta x, \pi/\Delta x]$, *then the scheme is practically stable.*]