Degree Master of Science in Mathematical Modelling and Scientific Computing

Numerical Solution of Differential Equations & Numerical Linear Algebra

HILARY TERM 2009
Thursday 15th January, 2:00 p.m. – 4:00 p.m.

Candidates should submit answers to a maximum of four questions that include an answer to at least one question in each section.

Please start the answer to each question on a new page.

All questions will carry equal marks.

Do not turn over until told that you may do so.

Section A —Numerical Solution of Differential Equations

Question 1

Consider the initial value problem $y' = f(x, y)$, $y(x_0) = y_0$, on the closed interval $[x_0, X]$ of the real line, where f is a smooth function of its arguments and y_0 is a given real number. On a uniform mesh

$$\{x_n : x_n = x_0 + nh\,,\ n = 0, \ldots, N\}$$

of spacing $h = (X - x_0)/N$, $N \geq 1$, the solution y to the initial value problem is approximated at the mesh points $(x_n)_{n=0,\ldots,N}$ by the sequence $(y_n)_{n=0,\ldots,N}$, defined by the one-step method

$$y_{n+1} = y_n + ahf(x_n, y_n) + bhf(x_n + ch, y_n + chf(x_n, y_n))\,, \quad n = 0, \ldots, N-1, \qquad (1)$$

where a, b and c are real parameters and y_0 is as above.

(a) Define the truncation error T_n of this method. Show that

$$T_n = (1 - a - b)y'(x_n) + \tfrac{1}{2}(1 - 2bc)hy''(x_n) + \mathcal{O}(h^2)\,, \quad \text{as } h \to 0\,.$$

Hence deduce that the method is consistent if, and only if, $a + b = 1$.

Show further that there exists a one-parameter family of second-order accurate methods of the form (1).

[8 marks]

(b) By considering the method (1) applied to the problem $y' = y$, $y(0) = 1$, show that there is no choice of a, b and c such that the order of convergence exceeds 2.

[8 marks]

(c) Suppose that a second-order method of the form (1) is applied to the initial value problem $y' = \lambda y$, $y(0) = 1$, where $\lambda < 0$ is a fixed constant. The solution $y(x) = \mathrm{e}^{\lambda x}$ to this initial value problem is monotonic decreasing. Find the set of all $h > 0$ such that the corresponding sequence of numerical approximations $(y_n)_{n=0,\ldots,N}$, with $y_0 = 1$, is monotonic decreasing.

Discuss the practical implications of the resulting restriction when λ is negative and $|\lambda| \gg 1$.

[9 marks]

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Question 2

Write down the general form of a linear k–step method for the numerical solution of the initial value problem $y' = f(x, y)$, $y(x_0) = y_0$, on the mesh $\{x_n : x_n = x_0 + nh,\ n = 0, 1, 2, \dots\}$ of uniform spacing $h > 0$.

(a) What does it mean to say that a linear k–step method is *zero-stable*? State an equivalent characterisation of zero-stability in terms of the roots of a certain polynomial.

[8 marks]

(b) Determine all values of the real parameter α such that the linear 2-step method given by the formula

$$y_{n+2} - \alpha y_{n+1} + (\alpha - 1)y_n = \frac{h}{12}\left[(4+\alpha)f_{n+2} + 8(2-\alpha)f_{n+1} + (4-5\alpha)f_n\right]$$

is zero stable.

[9 marks]

(c) Show that for $\alpha = 0$ the method is fourth order accurate. Is the method convergent for:

(i) $\alpha = 0$;

(ii) $\alpha = 2$?

[Justify your answers.]

[8 marks]

Question 3

Consider the system of linear algebraic equations

$$-a_j U_{j-1} + b_j U_j - c_j U_{j+1} = d_j \,, \qquad j = 1, \dots, J-1 \,,$$

with $J \geq 2$, and

$$U_0 = 0 \,, \qquad U_J = 0 \,,$$

where $a_j > 0$, $b_j > 0$, $c_j > 0$ and $b_j > a_j + c_j$ for all $j \in \{1, \dots, J-1\}$.

(a) Show that

$$U_j = e_j U_{j+1} + f_j \,, \qquad j = J-1, J-2, \dots, 1 \,,$$

where

$$e_j = \frac{c_j}{b_j - a_j e_{j-1}} \,, \qquad f_j = \frac{d_j + a_j f_{j-1}}{b_j - a_j e_{j-1}} \,, \qquad j = 1, 2, \dots, J-1 \,,$$

with $e_0 = 0$ and $f_0 = 0$.

How would you use these formulae to formulate an algorithm for the solution of the system of linear equations? Explain in particular the *forward elimination* and *back substitution* steps of the algorithm.

[8 marks]

(b) Show by induction that $0 < e_j < 1$ for $j = 1, 2, \dots, J-1$. Comment on the practical significance of this result in relation to the sensitivity of the computed values of U_j to rounding errors in the back-substitution step of the algorithm. You may assume that the values f_j, $j = 0, \dots, J-1$, are free of rounding error.

[8 marks]

(c) Consider the heat equation $u_t = u_{xx} + u_{yy}$ for (x, y) contained in the unit square $\Omega = (0,1)^2$ and for $t \in (0, T]$, subject to homogeneous Dirichlet boundary conditions and the initial condition $u(x, y, 0) = u_0(x, y)$, where u_0 is a given continuous function of two variables defined on $\overline{\Omega}$ and vanishing on the boundary of Ω.

Set up an ADI scheme, based on the Crank–Nicolson method, for the numerical solution of this initial boundary value problem, on a uniform mesh of spacings $\Delta x = 1/K$, $\Delta y = 1/L$ and $\Delta t = T/M$ in the x, y, and t co-ordinate directions, respectively; K, $L \geq 2$, $M \geq 1$.

Explain how the results of part (a) of this question can be exploited in this scheme.

[9 marks]

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Question 4

Define the characteristic curves of the linear advection equation

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0\,, \qquad -\infty < x < \infty\,, \quad t > 0\,,$$

where a is a given real number.

(a) Suppose that the partial differential equation is supplemented by the initial condition $u(x, 0) = u_0(x)$. Show that $u(x, t) = u_0(x - at)$.

What is the domain of dependence of the point (x, t)?

[10 marks]

(b) Now suppose that this initial value problem has been approximated by the finite difference scheme

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} + a\frac{U_j^n - U_{j-1}^n}{\Delta x} = 0\,, \quad j = \ldots, -1, 0, 1, \ldots\,, \quad n \geq 0\,,$$

$$U_j^0 = u_0(j\Delta x)\,.$$

Formulate the Courant–Friedrichs–Lewy (CFL) condition relating the domain of dependence of the finite difference scheme to that of the differential equation.

Find all values of a such that the above difference scheme obeys the CFL condition.

Show further that when the CFL condition holds, the difference scheme is stable in the ℓ_∞ norm in the sense that

$$\max_{n\geq 0} \|U^n\|_{\ell_\infty} \leq \|U^0\|_{\ell_\infty}\,,$$

where $\|U^n\|_{\ell_\infty} = \max_j |U_j^n|$.

[15 marks]

Section B — Numerical Linear Algebra

Question 5

(a) What axioms are required for $\langle \cdot, \cdot \rangle : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$ to define an inner product?

[4 marks]

(b) How is the vector norm $\|\cdot\|_2$ defined? Given a vector norm, how is a corresponding (subordinate) matrix norm defined?

[4 marks]

(c) What is the Singular Value Decomposition (SVD) of a matrix $A \in \mathbb{R}^{m\times n}$? (You do not need to prove that it exists). Show that $\|A\|_2 = \sigma_1$ where σ_1 is the largest singular value of A.

[7 marks]

(d) How might the SVD of $A \in \mathbb{R}^{m\times n}$, $m > n$, be used to solve a linear least squares problem

$$\min_{x\in\mathbb{R}^n} \|Ax - b\|_2$$

for given $b \in \mathbb{R}^m$? You should assume that A has full rank.

[4 marks]

(e) Now $(x_i, y_i, z_i), i = 1, \ldots, m$, are points in $\mathbb{R}^3$ and it is required to find the plane $\mathbf{r}\cdot\mathbf{n} = c$ which fits best through these points in the least squares sense. Here $\mathbf{r} = (x, y, z)$ and $\mathbf{n} = (n_1, n_2, n_3)$ is a unit normal vector to the plane; note that any two of n_1, n_2, n_3 could be zero. Formulate this problem as a linear least squares problem $\min_{x\in\mathbb{R}^n} \|Ax - b\|_2$ together with the constraint $n_1^2 + n_2^2 + n_3^2 = 1$, giving explicit expressions for A, b and x. You do not need to solve this problem.

[6 marks]

Question 6

This question is about the solution of the linear system $Ax = b$ given $A \in \mathbb{R}^{n \times n}$ which is nonsingular and $b \in \mathbb{R}^n$.

(a) Give an algorithm for Gaussian Elimination (GE). Why is 'pivoting' possibly required? Show that all of the multipliers in GE are in absolute value less than or equal to 1 when partial pivoting is employed. To what matrix factorization is GE equivalent to and how is pivoting represented?

[11 marks]

(b) What is Gauss-Seidel iteration? If $D = diag(A)$, L is the strictly lower triangular part of A and U is the strictly upper triangular part of A, write Gauss-Seidel iteration in matrix form.

State but do not prove a theorem giving necessary and sufficient conditions for the convergence of the sequence of iterates $\{x^{(k)}\}$ computed by the simple iteration

$$Mx^{(k)} = Nx^{(k-1)} + b, \quad k = 1, 2, \ldots, \qquad x^{(0)} \text{ arbitrary},$$

where $A = M - N$. Prove that if A is strictly row diagonally dominant, then Gauss-Seidel iteration converges.

[14 marks]