Degree Master of Science in Mathematical Modelling and Scientific Computing

Numerical Solution of Differential Equations & Numerical Linear Algebra

Thursday, 11th January 2007, 2:00 p.m. – 4:00 p.m.

Candidates may attempt as many questions as they wish. The best four solutions will count.
Solutions to questions 1–4 and 5–6 should be handed in separately.

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.

Numerical Solution of Differential Equations

Question 1

Consider the initial-value problem $y' = f(x, y)$, $y(0) = y_0$, where f is a smooth function of its arguments and y_0 is a given real number. Suppose that $h > 0$, $x_n = nh$ for $n = 0, 1, \ldots$, and let y_n be an approximation to $y(x_n)$, $n = 0, 1, \ldots$, defined successively by the one-step method

$$y_{n+1} = y_n + h\,\{c_1 f(x_n, y_n) + c_2 f(x_n + ah, y_n + ahf(x_n, y_n))\}\,, \qquad n = 0, 1, \ldots, \qquad (\star)$$

where c_1, c_2 and a are parameters.

(a) Apply the method ($\star$) to the initial-value problem $y' = \lambda y$, $y(0) = y_0$, where $\lambda > 0$ is a real number and $y_0 > 0$.

(i) Show that
$$y_n = \left(1 + (c_1 + c_2)\lambda h + (c_2 a)(\lambda h)^2\right)^n y_0, \qquad n = 0, 1, \ldots.$$

(ii) Show that if $c_1 + c_2 = 1$ and $c_2 a = \frac{1}{2}$ then

$$|y(x_n) - y_n| \le y_0\, n \mathrm{e}^{\lambda x_{n-1}} \sum_{k=3}^{\infty} \frac{1}{k!}(\lambda h)^k.$$

Hence deduce that
$$|y(x_n) - y_n| \le \frac{y_0}{3!}\left(x_n \mathrm{e}^{\lambda x_n} \lambda^3\right) h^2.$$

(iii) Show, further, that:

- if $c_1 + c_2 \neq 1$ then the method is not consistent;
- if $c_1 + c_2 = 1$ and $c_2 a \neq \frac{1}{2}$ then there is no $r > 1$ such that $|y(x_n) - y_n| = \mathcal{O}(h^r)$.

[You may use without proof that if $\alpha > \beta > 0$ then $n\beta^{n-1}(\alpha - \beta) \le \alpha^n - b^n \le n\alpha^{n-1}(\alpha - \beta)$.]

[4+8+8 marks]

(b) Now, apply the method ($\star$) to the initial-value problem $y' = \lambda y$, $y(0) = y_0$, where $\lambda \in \mathbb{C}$ with $\mathrm{Re}(\lambda) < 0$, over the mesh $\{x_n \,:\, x_n = nh,\ n = 0, 1, \ldots\}$, $h > 0$, with $y_n \in \mathbb{C}$ denoting the numerical approximation to $y(x_n) \in \mathbb{C}$ at $x = x_n$, $n = 0, 1, \ldots$.

Show that $\lim_{x \to +\infty} y(x) = 0$.

Supposing that $c_1 + c_2 = 1$ and $c_2 a = \frac{1}{2}$, specify carefully the set $\mathcal{H}$ of all complex numbers $\bar{h} = \lambda h$ such that $\lim_{n \to \infty} y_n = 0$. Give a rough sketch the set $\mathcal{H}$ in the complex plane. [2+3 marks]

Question 2

(a) State 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 $\{x_n : x_n = x_0 + nh,\ n = 0, 1, \dots\}$ of uniform spacing $h > 0$. [2 marks]

(b) Define the *truncation error* of a linear k-step method. What is meant by saying that a linear k-step method is *consistent*? What is meant by saying that a linear multistep method is *second-order accurate*? [6 marks]

(c) What is meant by saying that a linear k-step method is *zero-stable*? Formulate an equivalent characterisation of zero-stability in terms of the roots of a certain polynomial of degree k. [6 marks]

(d) Consider the three-parameter family of linear two-step methods defined by

$$y_{n+2} - a y_{n+1} + b y_n = h\, c\, f_{n+2},$$

where $f_j = f(x_j, y_j)$, and a, b and c are real numbers. Show that there exists a unique choice of a, b and c such that the method is second-order accurate; show further that, for these values of a, b and c, the method is second-order convergent. [If Dahlquist's Theorem is used, it must be stated carefully.] [11 marks]

Question 3

Consider the initial-value problem

$$\frac{\partial u}{\partial t} + u = \frac{\partial^2 u}{\partial x^2}, \qquad -\infty < x < \infty, \quad 0 < t \leq T,$$

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

where $T > 0$ is a fixed real number, and u_0 is a real-valued, bounded and continuous function of the variable $x \in (-\infty, \infty)$.

(a) Formulate the implicit (backward) Euler scheme for the numerical solution of this initial-value problem on a mesh with uniform spacings $\Delta x > 0$ and $\Delta t = T/M$ in the x and t co-ordinate directions, respectively, where M is a positive integer. [4 marks]

(b) Define the truncation error of the scheme and show that it is of size $\mathcal{O}((\Delta x)^2 + \Delta t)$ as $\Delta x, \Delta t \to 0$. [You may assume that u has as many bounded and continuous partial derivatives with respect to x and t as are required by your proof.] [5 marks]

(c) Let U_j^m denote the implicit (backward) Euler approximation to $u(j\Delta x, m\Delta t)$, $0 \leq m \leq M$, $j \in \mathbb{Z}$, where $\mathbb{Z}$ denotes the set of all integers. Suppose, further, that $\|U^0\|_{\ell_2} = \left(\Delta x \sum_{j \in \mathbb{Z}} |U_j^0|^2\right)^{1/2}$ is finite. Show that

$$\|U^m\|_{\ell_2} \leq (1 + \Delta t)^{-m} \, \|U^0\|_{\ell_2}$$

for all m, $1 \leq m \leq M$. [8 marks]

(d) Show, further, that

$$\max_{j \in \mathbb{Z}} |U_j^m| \leq (1 + \Delta t)^{-m} \max_{j \in \mathbb{Z}} |U_j^0|$$

for all m, $1 \leq m \leq M$. [8 marks]

Question 4

Suppose that a is a nonzero real number, $T > 0$, and u_0 is a real-valued continuous function of $x \in (-\infty, \infty)$ which is equal to zero outside a bounded subinterval of $(-\infty, \infty)$. Consider the initial-value problem

$$u_t + au_x = 0, \quad -\infty < x < \infty, \quad 0 < t \leq T, \qquad\qquad u(x,0) = u_0(x), \quad -\infty < x < \infty.$$

Let $\mathbb{Z}$ denote the set of all integers and suppose that $\Delta x > 0$, $\Delta t = T/M$, where M is a positive integer, and let $\mu = a\Delta t/\Delta x$.

(a) Show that if $|\mu| \leq 1$ then the *Lax–Friedrichs scheme*

$$\frac{U_j^{m+1} - \frac{1}{2}(U_{j+1}^m + U_{j-1}^m)}{\Delta t} + a\frac{U_{j+1}^m - U_{j-1}^m}{2\Delta x} = 0, \quad \left\{ \begin{array}{l} 0 \leq m \leq M-1, \\ j \in \mathbb{Z}, \end{array} \right.$$

$$U_j^0 = u_0(x_j), \qquad j \in \mathbb{Z},$$

is stable in the ℓ_2 norm $\|\cdot\|_{\ell_2}$. [7 marks]

(b) Define the truncation error T_j^m of the Lax–Friedrichs scheme. Show that

$$\max_{0 \leq m \leq M-1} \max_{j \in \mathbb{Z}} |T_j^m| \leq K,$$

where $K = C_1(\Delta t) + C_2(\Delta x)^2 + C_3\frac{(\Delta x)^2}{\Delta t}$ and C_1, C_2, C_3 are constants which you should define in terms of a and upper bounds on absolute values of certain partial derivatives of the solution u.

[You may assume that u has as many bounded and continuous partial derivatives with respect to x and t as are required by your proof.] [6 marks]

(c) Now consider a modification of the Lax–Friedrichs scheme, called the *central difference scheme*, where the arithmetic average $\frac{1}{2}(U_{j+1}^m + U_{j-1}^m)$ is replaced by U_j^m:

$$\frac{U_j^{m+1} - U_j^m}{\Delta t} + a\frac{U_{j+1}^m - U_{j-1}^m}{2\Delta x} = 0, \quad \left\{ \begin{array}{l} 0 \leq m \leq M-1, \\ j \in \mathbb{Z}, \end{array} \right.$$

$$U_j^0 = u_0(x_j), \qquad j \in \mathbb{Z}.$$

By writing

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

where $\hat{U}^m$ denotes the semidiscrete Fourier transform of the mesh-function $j \in \mathbb{Z} \mapsto U_j^m$ defined by the central difference scheme, show that

$$\hat{U}^{m+1}(k) = \lambda(k)\hat{U}^m(k), \qquad k \in [-\pi/\Delta x, \pi/\Delta x], \quad m = 0, 1, \ldots, M-1,$$

where $k \mapsto \lambda(k)$ is a function that you should define on the interval $[-\pi/\Delta x, \pi/\Delta x]$ in terms of μ, the wave number k and the spatial mesh-size Δx.

Show that $|\lambda(k)|^2 = 1 + \mu^2 \sin^2(k\Delta x)$ for all $k \in [-\pi/\Delta x, \pi/\Delta x]$.

Hence deduce the existence of an initial condition U^0 such that $\|U^m\|_{\ell_2}^2 \geq (1 + \frac{1}{2}\mu^2)^m \|U^0\|_{\ell_2}^2$.

What does this inequality imply about the stability, or otherwise, of the central difference scheme in the ℓ_2 norm for μ fixed? [3+3+3+3 marks]

Numerical Linear Algebra

Question 5

(a) What is an orthogonal matrix? If $Q \in I\!R^{m \times n}$ is the first n columns of an orthogonal matrix (with $n < m$), show that $Q^T Q = I \in I\!R^{n \times n}$. [2+2 marks]

(b) What does it mean to say that $A = U \Sigma V^T$ is the Singular Value Decomposition (SVD) of the matrix $A \in I\!R^{m \times n}$? Suppose that $m > n$ and that A is of rank n. If $Q \in I\!R^{m \times n}$ is the first n columns of U, show that the columns of Q are a basis for the range of A. [4+4 marks]

(c) It is now desired to use this singular value decomposition of A to compute the solution of the linear least squares problem

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

for some given $b \in I\!R^m$. Explain how the solution may be computed without any other factorisation of A, proving any results that you need. What is the linear least squares error? [7+1 marks]

(d) If the rank of A was known to be $r < n$ rather than n, can the singular value decomposition still be used to solve the linear least squares problem? If so, what is a solution in terms of the SVD: is it unique? What is the linear least squares error? [5 marks]

Question 6

(a) What is Gauss-Seidel iteration for the solution of a linear system of equations $Ax = b$ where $A \in I\!R^{n \times n}$ is nonsingular? What is a necessary condition on A in order that this method can be applied? Show that if the Gauss-Seidel iterates converge then they must converge to the solution x of the linear system. State without proof a necessary and sufficient condition for convergence. [3+1+3+2 marks]

(b) If D is the diagonal part of A, L the strictly lower triangular part of A and U the strictly upper triangular part of A show that iterates which satisfy

$$x^{(k)} = (D+U)^{-1}\left(I - L(D+L)^{-1}\right)b + (D+U)^{-1}L(D+L)^{-1}Ux^{(k-1)} \qquad (1)$$

can be calculated by the *symmetric* Gauss-Seidel method. Show that the iteration (1) is the simple iteration related to the splitting $A = M - N$ with $M = (D+L)D^{-1}(D+U)$ and $N = LD^{-1}U$. [5+6 marks]

(c) Deduce a necessary and sufficient condition in terms of the eigenvalues of the matrix

$$D(D+L)^{-1}LD^{-1}U(D+U)^{-1}$$

for the iteration (1) to be convergent. [5 marks]