Degree Master of Science in Mathematical Modelling and Scientific Computing

Numerical Solution of Differential Equations & Numerical Linear Algebra

Friday, 14th January 2011, 9:30 p.m. – 11:30 a.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 $y' = f(y)$, $y(0) = 1$, where f is a twice continuously differentiable function defined on the real line, such that $|f(s)| \le 1$, $|f'(s)| \le 1$ and $|f''(s)| \le 1$ for all $s \in \mathbb{R}$.

[You may assume that this initial-value problem has a unique solution $x \mapsto y(x)$, defined for all $x \in \mathbb{R}$, such that the functions $x \mapsto y'(x)$, $x \mapsto y''(x)$ and $x \mapsto y'''(x)$ are defined and continuous for all $x \in \mathbb{R}$.]

i) Show that the function f satisfies the following Lipschitz condition:

$$|f(u) - f(v)| \le |u - v| \qquad \forall u, v \in \mathbb{R}\,.$$

Show further that $|y''(x)| \le 1$ and $|y'''(x)| \le 2$ for all $x \in \mathbb{R}$. **[4 marks]**

ii) The trapezium rule approximation y_n to $y(x_n)$ on the mesh $\{x_n \,:\, x_n = nh,\, n = 0, 1, \dots\}$ of uniform spacing $h \in (0, 1)$ is obtained from the formula

$$\frac{y_n - y_{n-1}}{h} = \frac{1}{2}\left[f(y_n) + f(y_{n-1})\right], \quad n = 1, 2, \dots, \qquad y_0 = 1.$$

Let $g(s) := s - \frac{h}{2} f(s)$. Show that the function $s \mapsto g(s)$ is strictly monotonic increasing and $\lim_{s\to\pm\infty} g(s) = \pm\infty$. By rewriting the trapezium rule method as $g(y_n) = y_{n-1} + \frac{h}{2} f(y_{n-1})$, deduce that, given $y_{n-1} \in \mathbb{R}$, the trapezium rule approximation y_n is uniquely defined in $\mathbb{R}$.

[8 marks]

iii) Show that the truncation error T_n of the method applied to the initial-value problem under consideration satisfies

$$T_n = h^2\left(\frac{1}{6} y'''(\xi_n) - \frac{1}{4} y'''(\eta_n)\right), \qquad n = 1, 2, \dots,$$

where $\xi_n, \eta_n \in (x_{n-1}, x_n)$. Hence deduce that $|T_n| \le \frac{5}{6} h^2$. **[4 marks]**

Show further that

$$|y(x_n) - y_n| \le \frac{2+h}{2-h} |y(x_{n-1}) - y_n| + \frac{2h}{2-h} |T_n|, \qquad n = 1, 2, \dots,$$

and deduce that

$$|y(x_n) - y_n| \le \frac{5}{6} h^2 \left[\left(1 + \frac{2h}{2-h}\right)^n - 1\right], \qquad n = 1, 2, \dots.$$

Show that there exists $h_0 \in (0, 1)$ such that if $h \le h_0$, then $|y(x_n) - y_n| \le \frac{1}{2} 10^{-2}$ for all $x_n \in [0, 1]$. **[9 marks]**

[The actual value of h_0 is not required for a complete answer.]

Question 2

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 a nonempty closed interval $[x_0, X]$ of the real line. **[2 marks]**

i) Define the *truncation error* T_n of the method. **[2 marks]**

ii) What does it mean to say that the method is:

   a) *consistent*; **[2 marks]**

   b) *zero-stable*; **[2 marks]**

   c) *convergent*? **[2 marks]**

iii) State the *root condition*, relating zero-stability of a linear k-step method to the roots of a certain kth degree polynomial. **[2 marks]**

iv) Show using Dahlquist's theorem, which you must clearly state, that there is a unique value of the parameter $\alpha \in \mathbb{R}$ such that the three-step method

$$y_{n+3} = y_{n+2} + \frac{h}{12}\left[\,23f(x_{n+2}, y_{n+2}) - 16f(x_{n+1}, y_{n+1}) + \alpha f(x_n, y_n)\,\right]$$

is convergent. **[13 marks]**

Question 3

Consider the initial-value problem

$$\begin{aligned} \frac{\partial u}{\partial t} &= \frac{\partial^2 u}{\partial x^2} - u, \qquad && -\infty < x < \infty, \quad 0 < t \leq T, \\ u(x,0) &= u_0(x), && -\infty < x < \infty, \end{aligned}$$

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

i) Formulate the θ-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 and $\theta \in [0,1]$. You should state the scheme so that $\theta = 1$ corresponds to the implicit (backward) Euler scheme. **[7 marks]**

ii) Let U_j^m denote the numerical approximation to $u(j\Delta x, m\Delta t)$ computed by the θ-scheme, $0 \leq m \leq M$, $j \in \mathbb{Z}$, where $\mathbb{Z}$ denotes the set of all integers. Suppose that $\|U^0\|_{\ell_2} = \left(\Delta x \sum_{j\in\mathbb{Z}} |U_j^0|^2\right)^{1/2}$ is finite. Show that if $\theta \in [\frac{1}{2}, 1]$, then

$$\|U^m\|_{\ell_2} \leq \|U^0\|_{\ell_2}$$

for all m, $1 \leq m \leq M$, for any Δt and Δx.

Now, suppose that $\theta \in [0, \frac{1}{2})$. Show that $\|U^m\|_{\ell_2} \leq \|U^0\|_{\ell_2}$ for all m, $1 \leq m \leq M$, provided that $(1-2\theta)\Delta t \leq \frac{2(\Delta x)^2}{4+(\Delta x)^2}$.

Deduce that both the implicit (backward) Euler scheme and the Crank–Nicolson scheme are *unconditionally stable* in the $\|\cdot\|_{\ell_2}$ norm.

[9 marks]

iii) Let U_j^m denote the numerical approximation to $u(j\Delta x, m\Delta t)$ computed by the θ-scheme, $0 \leq m \leq M$, $j \in \mathbb{Z}$, where $\mathbb{Z}$ denotes the set of all integers. Suppose that $\|U^0\|_{\ell_\infty} = \max_{j\in\mathbb{Z}} |U_j^0|$ is finite. Show that if $\theta \in [0,1]$, then

$$\|U^m\|_{\ell_\infty} \leq \left(\frac{1-(1-\theta)\Delta t}{1+\theta\Delta t}\right)^m \|U^0\|_{\ell_\infty}$$

for all m, $1 \leq m \leq M$, provided that $(1-\theta)\Delta t \leq \frac{(\Delta x)^2}{2+(\Delta x)^2}$.

Deduce that the implicit (backward) Euler scheme is *unconditionally stable* in the $\|\cdot\|_{\ell_\infty}$ norm. Show, further, that the Crank–Nicolson scheme is *conditionally stable* in the $\|\cdot\|_{\ell_\infty}$ norm and state the condition on Δt and Δx that ensures stability.

[9 marks]

Question 4

Suppose that a is a non-zero real number, $T > 0$, and u_0 is a real-valued, bounded and continuous function of $x \in (-\infty, \infty)$. The initial-value problem

$$\begin{aligned} &u_t + au_x - u = 0, \qquad -\infty < x < \infty, \quad 0 < t \le T, \\ &u(x,0) = u_0(x), \qquad -\infty < x < \infty, \end{aligned}$$

has been approximated by the central difference scheme

$$\begin{aligned} &\frac{U_j^{m+1} - U_j^m}{\Delta t} + a\frac{U_{j+1}^m - U_{j-1}^m}{2\Delta x} - U_j^m = 0, \qquad j \in \mathbb{Z}, \quad 0 \le m \le M-1, \\ &U_j^0 = u_0(x_j), \qquad j \in \mathbb{Z}, \end{aligned}$$

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

i) Define the truncation error T_j^m of the scheme, and show that $T_j^m = \mathcal{O}((\Delta x)^2 + \Delta t)$ as $\Delta x \to 0$ and $\Delta t \to 0$. **[7 marks]**

[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.]

ii) Show that if $\mu = a\Delta t/\Delta x$ is held fixed as $\Delta t \to 0$, then the difference scheme is *not* stable in the ℓ_2 norm in von Neumann's sense. **[9 marks]**

iii) Show that if $\nu = a\Delta t/(\Delta x)^2$ is held fixed as $\Delta t \to 0$, then the scheme is stable in the ℓ_2 norm in von Neumann's sense. **[9 marks]**

Section B — Numerical Linear Algebra

Question 5

(a) Let $\|\cdot\|$ and $\|\cdot\|_*$ be two norms on $\mathbb{R}^n$. Show that

$$\|A\| := \sup_{\mathbf{x}\in\mathbb{R}^n\setminus\{\mathbf{0}\}} \frac{\|A\mathbf{x}\|}{\|\mathbf{x}\|_*}, \qquad A \in \mathbb{R}^{n\times n},$$

defines a norm on the vector space of all $n \times n$ matrices. **[3 marks]**

(b) The ℓ_p norms on $\mathbb{R}^n$ are defined as

$$\|\mathbf{x}\|_p := \begin{cases} \left(\sum_{j=1}^n |x_j|^p\right)^{1/p} & \text{for } 1 \le p < \infty, \\ \max_{1\le j\le n} |x_j| & \text{for } p = \infty. \end{cases}$$

Following (a), we can introduce the *induced matrix norm*

$$\|A\|_{p,q} := \sup_{\mathbf{x}\in\mathbb{R}^n\setminus\{\mathbf{0}\}} \frac{\|A\mathbf{x}\|_q}{\|\mathbf{x}\|_p}, \qquad A \in \mathbb{R}^{n\times n}.$$

Give explicit formulas (without proof) for $\|A\|_{\infty,\infty}$, $\|A\|_{1,1}$ and $\|A\|_{2,2}$ and compute these norms for

$$A = \begin{pmatrix} 2 & 1 \\ 0 & 1 \end{pmatrix}.$$

[6 marks]

(c) Using the same notation, show that

$$\|A\|_{1,\infty} = \sup_{\mathbf{x}\in\mathbb{R}^n\setminus\{\mathbf{0}\}} \frac{\|A\mathbf{x}\|_\infty}{\|\mathbf{x}\|_1} = \max_{1\le i,j\le n} |a_{ij}|.$$

[6 marks]

(d) Show that $\|A\|_{2,2} \le \sqrt{\|A\|_{1,1}\|A\|_{\infty,\infty}}$. **[5 marks]**

(e) Define the condition number $\kappa(A)$ of an invertible matrix $A \in \mathbb{R}^{n\times n}$. Show that, if using the matrix norm induced by the Euclidean norm,

$$\kappa(A^T A) = \kappa(A)^2 \ge \kappa(A).$$

[5 marks]

Question 6

(a) Define what the LU factorisation of a matrix $A \in \mathbb{R}^{n\times n}$ is. Use Gaussian elimination (without pivoting) to compute the LU factorisation of the matrix

$$A = \begin{pmatrix} 2 & 1 & 2 \\ 0 & 3 & -1 \\ 4 & 5 & 4 \end{pmatrix}.$$

[5 marks]

(b) Define the Cholesky factorisation of a symmetric matrix $A \in \mathbb{R}^{n\times n}$. Suppose A allows an LU factorisation $A = \widetilde{L}\widetilde{U}$, where $\widetilde{U}$ has only positive diagonal entries show that A possesses a Cholesky factorisation. **[8 marks]**

(c) Suppose the invertible matrix $A \in \mathbb{R}^{n\times n}$ possesses a Cholesky factorisation. Show that A is symmetric and positive definite. **[4 marks]**

(d) Suppose $A \in \mathbb{R}^{n\times n}$ is a tridiagonal matrix with diagonal elements $a_1, \dots, a_n$, subdiagonal elements $b_2, \dots, b_n$ and superdiagonal elements $c_1, \dots, c_{n-1}$, i.e.

$$A = \begin{pmatrix} a_1 & c_1 & & & \\ b_2 & a_2 & c_2 & & \\ & \ddots & \ddots & \ddots & \\ & & b_{n-1} & a_{n-1} & c_{n-1} \\ & & & b_n & a_n \end{pmatrix}.$$

Assume that

$$\begin{aligned} |a_1| &> |c_1| > 0, \\ |a_i| &\geq |b_i| + |c_i|, \quad b_i \neq 0, c_i \neq 0, \qquad 2 \leq i \leq n-1, \\ |a_n| &> |b_n| > 0. \end{aligned}$$

Consider the following algorithm to generate two vectors $\boldsymbol{\ell} = (\ell_j) \in \mathbb{R}^{n-1}$ and $\mathbf{r} = (r_j) \in \mathbb{R}^n$:

- $r_1 = a_1$,
- for $i = 2, \dots, n$
  - $\ell_i = b_i / r_{i-1}$
  - $r_i = a_i - \ell_i c_{i-1}$.

Show by induction on $1 \leq i \leq n-1$ that $r_i \neq 0$ and $|c_i / r_i| < 1$ such that the algorithm is indeed well defined.

Conclude that A possesses the LU factorisation

$$A = \begin{pmatrix} 1 & & & \\ \ell_2 & 1 & & \\ & \ddots & \ddots & \\ & & \ell_n & 1 \end{pmatrix} \begin{pmatrix} r_1 & c_1 & & \\ & r_2 & \ddots & \\ & & \ddots & c_{n-1} \\ & & & r_n \end{pmatrix}$$

and that A is invertible. **[8 marks]**