Degree Master of Science in Mathematical Modelling and Scientific Computing

Numerical Solution of Differential Equations & Numerical Linear Algebra

Friday, 13th January 2012, 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

The function $u(t)$, $t \geq 0$, with $u(0) = u_0$, is determined by

$$\frac{\mathrm{d}u}{\mathrm{d}t} = f(t, u), \quad t > 0,$$

where f is a uniformly continuous function of its arguments and where f satisfies a Lipshitz condition

$$|f(t, u) - f(t, v)| \leq L|u - v|, \quad \forall u, v \in \mathbb{R}, t > 0.$$

The system is discretised at points $t_n = n\Delta t$, $n = 0, 1, \ldots$ where $\Delta t > 0$ by

$$U_{n+1} = U_n + \Delta t \Phi(t_n, U_n; \Delta t),$$

where Φ is uniformly continuous in its arguments and U_n is an approximation to $u_n = u(t_n)$.

a) Define a truncation error (denoted by T_n) and show that the error, $e_n = u_n - U_n$ satisfies

$$|e_{n+1}| \leq (1 + \Delta t L)|e_n| + \Delta t|T_n|.$$

Deduce that provided initial data is $U_0 = u_0$ then

$$|e_n| \leq \frac{1}{L}(\mathrm{e}^{Lt_n} - 1) \max_{0 \leq p < n} |T_p|.$$

[8 marks]

b) Define consistency for, and order of accuracy of, the discrete scheme. Show that for the discrete scheme to be consistent it is necessary that

$$\Phi(t, u; 0) = f(t, u).$$

[5 marks]

c) Suppose

$$\Phi(t_n, U_n; \Delta t) = c_1 k_1 + c_2 k_2 + c_3 k_3,$$

where c_1, c_2, c_3 are constants and

$$\begin{aligned} k_1 &= f(t_n, U_n), \\ k_2 &= f(t_n + \frac{1}{2}\Delta t, U_n + \frac{1}{2}\Delta t k_1), \\ k_3 &= f(t_n + \alpha\Delta t, U_n + \alpha\Delta t k_2), \end{aligned}$$

where c_1, c_2, c_3 and α are real constants.

Determine the constants c_1, c_2, c_3, α so that the scheme is third order accurate.

You may find useful to use

$$\frac{\mathrm{d}^2 u}{\mathrm{d}t^2} = f_t + f f_u, \quad \frac{\mathrm{d}^3 u}{\mathrm{d}t^3} = f_u(f_t + f f_u) + f_{tt} + 2f f_{ut} + f^2 f_{uu}.$$

[12 marks]

Question 2

The function $u(t)$, $t \geq 0$ is determined by

$$\frac{\mathrm{d}u}{\mathrm{d}t} = f(t,u), \;\; t > 0,$$

where f is a uniformly continuous function of its arguments and $u(0) = u_0$,
A linear multistep method for numerical approximation of this equation at the points $t_r = r\Delta t,\ r = 0, 1, 2, \ldots$, with $\Delta t > 0$ is defined for integer $k > 0$ by

$$\sum_{r=0}^{k} \alpha_r U_{n+r} = \Delta t \sum_{r=0}^{k} \beta_r F_{n+r},\ n = 0, 1, \ldots,$$

where U_n is an approximation to $u_n = u(t_n)$, $F_n = f(t_n, U_n)$, $\alpha_k \neq 0$ and $\alpha_0^2 + \beta_0^2 > 0$. Define polynomials

$$\rho(z) = \sum_{r=0}^{k} \alpha_r z^r, \;\; \sigma(z) = \sum_{r=0}^{k} \beta_r z^r.$$

a) Define zero stability for a linear multistep method.

[3 marks]

b) Prove that a necessary condition for zero stability is that the roots of ρ lie on the unit disc with any root on the unit circle being simple.

[9 marks]

c) The truncation error is defined by

$$T_n = \frac{1}{\Delta t \sigma(1)} \left[\sum_{r=0}^{k} \alpha_r u_{n+r} - \Delta t \sum_{r=0}^{k} \beta_r f_{n+r} \right],$$

where $f_n = f(t_n, u_n)$.

[3 marks]

Show that

$$\rho(1) = 0 \text{ and } \rho'(1) = \sigma(1)$$

are necessary conditions for the scheme to be consistent.

d) Define an interval of absolute stability for the linear multistep method.

Determine the interval of absolute stability for the scheme

$$2U_{n+2} - 2U_{n+1} = \Delta t[3F_{n+1} - F_n].$$

[10 marks]

Question 3

The function $u(x,t)$, defined for $x \in \mathbb{R}$ and $t \geq 0$, satisfies for real β

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} - \beta^2 u, \;\; t > 0,$$

with initial data $u(x,0) = u_0(x)$ where $|u_0| \to 0$ as $|x| \to \infty$.

The continuous system is discretised on a uniform mesh $x_r = rh$, $r = 0, \pm 1, \pm 2, \cdots$, and $t_n = n\Delta t$, $n = 1, 2, \cdots$ with $h > 0$ and $\Delta t > 0$ such that U_r^n is an approximation for $u_r^n = u(x_r, t_n)$, by a theta-method:

$$\frac{U_r^{n+1} - U_r^n}{\Delta t} = \theta\Big[\frac{1}{h^2}\delta_x^2 U_r^{n+1} - \beta^2 U_r^{n+1}\Big] + (1-\theta)\Big[\frac{1}{h^2}\delta_x^2 U_r^n - \beta^2 U_r^n\Big],$$

where $0 \leq \theta \leq 1$ and δ_x^2 is the standard second order space difference operator.

a) Define practical stability for the discrete method in terms of the l_2-norm

$$||U^n||_{l_2} = \big(h \sum_{r=-\infty}^{\infty} |U_r^n|^2\big)^{1/2}.$$

[2 marks]

b) Determine the amplification factor $\lambda(k)$ for this scheme so that

$$\hat{U}^{n+1}(k) = \lambda(k)\hat{U}^n(k),$$

where $\hat{U}^n(k)$ is the semi-discrete Fourier transform

$$\hat{U}^n(k) = h \sum_{r=-\infty}^{\infty} \mathrm{e}^{-\mathrm{i}krh} U_r^n.$$

Show that the scheme is practically stable provided

$$\max_k |\lambda(k)| \leq 1.$$

You may use without proof Parseval's Identity

$$||U^n||_{l_2} = \frac{1}{\sqrt{2\pi}}||\hat{U}^n||_{L_2}.$$

[5 marks]

c) Determine conditions on Δt such that the scheme is practically stable when $0 \leq \theta \leq 1$.

[8 marks]

d) Show that if the space domain is restricted to $0 \leq x \leq 1$ with $u(0,t) = u(1,t) = 0, \; t > 0$ then the discrete scheme satisfies a maximum principle for $0 \leq \theta \leq 1$ provided

$$\Delta t \leq \frac{h^2}{(1-\theta)(2 + h^2\beta^2)}.$$

[10 marks]

Question 4

The function $u(x,t)$, defined for $x \in \mathbb{R}$ and $t \geq 0$, satisfies

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0, \;\; t > 0,$$

where $a > 0$ is constant, and initial data $u(x,0) = u_0(x)$ where u_0 is bounded on $\mathbb{R}$.

This hyperbolic equation is discretised on a uniform mesh $x_r = rh$, $r = 0, \pm 1, \pm 2, \cdots$, and $t_n = n\Delta t$, $n = 1, 2, \cdots$ with $h > 0$ and $\Delta t > 0$ such that U_r^n is an approximation for $u_r^n = u(x_r, t_n)$.

a) Show that a time-explicit, space-central difference scheme

$$\frac{U_r^{n+1} - U_r^n}{\Delta t} + a\frac{U_{r+1}^n - U_{r-1}^n}{2h} = 0,$$

is unconditionally unstable.

[3 marks]

b) Let $\nu = a\Delta t/h$ and show that

$$u(rh, (n+1)\Delta t) = u((r-\nu)h, n\Delta t).$$

[3 marks]

c) Derive a quadratic polynomial, denoted $p(x)$, which interpolates U_{r-1}^n, U_r^n and U_{r+1}^n at $x_{r-1},\ x_r,\ x_{r+1}$ respectively. By applying the result for part (b) to the polynomial $p(x)$ derive the explicit difference scheme

$$U_r^{n+1} = [1 - \nu\Delta_0 + \frac{1}{2}\nu^2\delta^2]U_r^n,$$

where $\Delta_0 U_r^n = (U_{r+1}^n - U_{r-1}^n)/2$, $\delta^2 U_r^n = U_{r+1}^n - 2U_r^n + U_{r-1}^n$.

[8 marks]

d) Show that this scheme is practically stable provided $|\nu| \leq 1$. Let T_r^n be the truncation error at $(rh, n\Delta t)$. Show that provided sufficiently high derivatives of u are bounded on $\mathbb{R}$ then there exists a positive constant C such that, as $\Delta t,\ h \to 0$,

$$|T_r^n| \leq C(\Delta t^2 + h^2).$$

[11 marks]

Section B — Numerical Linear Algebra

Question 5

Let $\|\cdot\| : \mathbb{R}^n \to \mathbb{R}$ be a vector norm. State the definition of the associated or induced matrix norm.

[2 marks]

Let $A \in \mathbb{R}^{n\times n}$ be symmetric and positive definite with *Cholesky factorisation* $A = LL^T$. Show that

$$\|\mathbf{x}\|_A = (\mathbf{x}^T A\mathbf{x})^{1/2}, \qquad \mathbf{x} \in \mathbb{R}^n,$$

defines a norm on $\mathbb{R}^n$ and that the induced matrix norm can be expressed as

$$\|B\|_A = \|L^T B(L^T)^{-1}\|_2.$$

[8 marks]

Let $A \in \mathbb{R}^{n\times n}$ be symmetric and positive definite. Let $\epsilon > 0$. Show that the problem

$$\min_{\mathbf{x}\in\mathbb{R}^n} \left\{\|A\mathbf{x} - \mathbf{b}\|_2 + \epsilon\|\mathbf{x}\|_A^2\right\}$$

has a unique solution, which can be computed by solving a linear system.
How does the condition number in the 2-norm of the matrix of this system relate to the eigenvalues of A?

[10 marks]

Consider the linear system $A\mathbf{x} = \mathbf{b}$ with

$$A = \begin{pmatrix} 1 & 2 & 0 \\ 1 & 2 & 2 \\ 0 & 2 & 4 \end{pmatrix}, \qquad \text{and } \mathbf{b} = \begin{pmatrix} 3 \\ 2 \\ 5 \end{pmatrix}.$$

Examine whether the system can be solved using

1. Gaussian elimination without pivoting,
2. Gaussian elimination with partial pivoting,
3. Cholesky method.

Explain your answer in each case.

[5 marks]

Question 6

Define what is meant by saying that a square matrix A has a QR factorisation.

[2 marks]

Show that a matrix $Q \in \mathbb{R}^{n \times n}$ is orthogonal if and only if $\|Q\mathbf{x}\|_2 = \|\mathbf{x}\|_2$ for all $\mathbf{x} \in \mathbb{R}^n$.

[5 marks]

Let $H = I - 2\frac{\mathbf{u}\mathbf{u}^T}{\mathbf{u}^T\mathbf{u}}$ be an $n \times n$-Householder matrix ($\mathbf{u} \neq \mathbf{0}$). Determine the eigenvalues and eigenvectors of H.

[8 marks]

Let

$$A = \begin{pmatrix} 1 & 5 & 4 \\ -2 & 1 & 3 \\ 2 & 0 & -2 \end{pmatrix}, \qquad \text{and} \qquad \mathbf{b} = \begin{pmatrix} -1 \\ 4 \\ 3 \end{pmatrix}.$$

Using Householder transformations, compute a QR factorisation of the matrix A and determine the set of points $\mathbf{x} \in \mathbb{R}^3$ which minimise the expression $\|A\mathbf{x} - \mathbf{b}\|_2$.

[10 marks]