Degree Master of Science in Mathematical Modelling and Scientific Computing

Numerical Solution of Differential Equations & Numerical Linear Algebra

Friday 16th January 2015, 9:30 a.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 $u(0) = u_0$, $u'(0) = v_0$,is determined for $t > 0$ by

$$u'' = f(u),$$

where f is a uniformly continuous function of its argument satisfying a Lipshitz condition

$$|f(u_1) - f(u_2)| \leq L|u_1 - u_1|, \ \ \forall u_1, u_2 \in \mathbb{R}.$$

(a) A discrete solution is determined by writing:

$$\begin{aligned} u' &= v, \\ v' &= f(u), \end{aligned}$$

with $u(0) = u_0$, $v(0) = v_0$ and discretising on a uniform mesh $t_n = n\Delta t$, $n = 0, 1, 2, \ldots$ according to the Explicit Euler method: for $n = 0, 1, 2, \ldots,$

$$\begin{aligned} U_{n+1} &= U_n + \Delta t V_n, \\ V_{n+1} &= V_n + \Delta t f(U_n), \end{aligned}$$

with $U_0 = u_0$ and $V_0 = v_0$. Use the notation that $u_n = u(t_n)$, $v_n = v(t_n)$.

Determine the truncation error

$$\mathbf{T}_n = \begin{bmatrix} \dfrac{u_{n+1} - u_n}{\Delta t} - v_n \\ \dfrac{v_{n+1} - v_n}{\Delta t} - f(u_n) \end{bmatrix}.$$

Hence show that the scheme is consistent and first order accurate. **[5 marks]**

Let

$$\mathbf{e}_n = \begin{bmatrix} u_n - U_n \\ v_n - V_n \end{bmatrix}.$$

Determine a matrix $\mathbf{B}_n$ such that

$$\mathbf{e}_{n+1} = (\mathbf{I} + \mathbf{B}_n)\mathbf{e}_n + \Delta t \mathbf{T}_n.$$

Hence deduce that $||\mathbf{e}_n||_\infty \to 0$ as $\Delta t \to 0$ with $n\Delta t \to t > 0$.

[10 marks]

(b) Show that when $\Delta t > 0$ is fixed and $f(u) = -u$, then the method in (a) gives a solution which becomes unbounded. Show that the method

$$\begin{aligned} U_{n+1} &= U_n + \Delta t V_n, \\ V_{n+1} &= V_n + \Delta t f(U_{n+1}), \end{aligned}$$

when applied to $f = -u$ with fixed $\Delta t > 0$ gives a solution which remains bounded.

[10 marks]

Question 2

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

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

where f is a uniformly differentiable function of u.

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 $\beta_0 \neq 0$. The polynomials $\rho(z)$ and $\sigma(z)$ are given by

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

a) Define zero stability and the root condition for a linear multistep method.

[4 marks]

b) Prove that the root condition is a necessary condition for convergence. **[6 marks]**

c) Determine constants a and b such that the

$$U_{n+2} - (1 + a)U_{n+1} + aU_n = b\Delta t F_{n+2}$$

is a second order multistep method. **[5 marks]**

d) Define absolute stability for the case $f(u) = \lambda u$ and determine the interval of absolute stability for the method in (c). **[5 marks]**

e) Show that the method is A-stable. **[5 marks]**

[You may use without proof that the order $p - 1$ error constant of this linear k-step method is given by $C_p/\sigma(1)$, $p = 0, 1, 2, \ldots$, where

$$\begin{aligned} C_0 &= \sum_{j=0}^{k} \alpha_j, \qquad C_1 = \sum_{j=1}^{k} j\alpha_j - \sum_{j=0}^{k} \beta_j, \\ C_p &= \sum_{j=1}^{k} \frac{j^p}{p!}\alpha_j - \sum_{j=1}^{k} \frac{j^{p-1}}{(p-1)!}\beta_j \qquad \text{for } p \geq 2.] \end{aligned}$$

Question 3

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

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

with initial data $u(x,0) = u_0(x) \geq 0$ where $|u_0| \to 0$ as $|x| \to \infty$.
The partial differential 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 $u_r^n = u(x_r, t_n)$ and $U_r^0 = u_0(x_r)$. Denote $u^n = \{u_r^n\}$ and $U^n = \{U_r^n\}$. For data $\{U_r\}$ let $\delta^2 U_r = U_{r+1} - 2U_r + U_{r-1}$ and define a semi-discrete Fourier transform by

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

Let $\mu = \Delta t / h^2$. It is given that the contunous function $u(x,t)$, when restricted to the mesh, satisfies

$$\hat{u}^{n+1} = \Lambda(k)\hat{u}^n, \ \ \Lambda(k) = \mathrm{e}^{-\mu(kh)^2}.$$

a) Define von Neumann stability and practical stability. **[2 marks]**

b) A discrete approximation is found for $n = 0, 1, \ldots$, $r = 0, \pm 1, \pm 2, \ldots$, using:

$$U_r^* = U_r^n + \mu\delta^2 U_r^n,$$

$$U_r^{n+1} = U_r^n + \frac{1}{2}\mu(\delta^2 U_r^* + \delta^2 U_r^n).$$

i) Determine $\lambda(k)$ such that $\hat{U}^{n+1} = \lambda(k)\hat{U}^n$. **[5 marks]**

ii) Determine the range of μ for which this scheme is practically stable in the l_2-norm. **[4 marks]**

c) The scheme is replaced by

$$U_r^* = U_r^n + \frac{1}{2}\mu\delta^2 U_r^n,$$
$$U_r^{n+1} = U_r^n + \mu\delta^2 U_r^*.$$

Deduce that this scheme has the same accuracy and stability constraint as the scheme in (b) and explain how this is possible. **[4 marks]**

d) Show that for both schemes that

$$||u^n - U^n||_{l_2} \leq K_n ||u^0||_{l_2},$$

and estimate K_n when $\mu = 0.25$. **[10 marks]**
You may use without proof Parseval's Identity

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

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

This 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 $u_r^n = u(x_r, t_n)$. Let $\nu = a\Delta t/h$.

a) A general form for an explicit finite difference scheme is written

$$U_r^{n+1} = \sum_{s=-\alpha}^{s=\gamma} \beta_s(\nu) U_{r+s}^n,$$

where α and γ are integers, $n = 0, 1, \ldots$, and $r = 0, \pm 1, \pm 2, \ldots$.

Define

$$c(z) = \sum_{s=-\alpha}^{s=\gamma} \beta_s(\nu) z^s.$$

Show that for the scheme to be consistent it is necessary that

$$c(1) = 1, \quad \text{and} \quad c'(1) = -\nu.$$

Derive conditions on the coefficients β_s for the truncation error to be order p. **[8 marks]**

b) Determine the order of the truncation error in the Lax–Freidrichs scheme

$$U_r^{n+1} = \frac{1}{2}(1+\nu)U_{r-1}^n + \frac{1}{2}(1-\nu)U_{r+1}^n.$$

[4 marks]

c) Show that the truncation error for the Lax–Wendroff scheme

$$U_r^{n+1} = \frac{1}{2}(\nu^2+\nu)U_{r-1}^n + (1-\nu^2)U_r^n + \frac{1}{2}(\nu^2-\nu)U_{r+1}^n,$$

is second order. **[4 marks]**

d) Prove that there is no other second order scheme of this form with $\alpha = \gamma = 1$. **[3 marks]**

d) Derive the third order scheme of this form when $\alpha = 2$, $\gamma = 1$. **[6 marks]**

Section B — Numerical Linear Algebra

Question 5

(a) Show that matrix matrix multiplication from the left is stable with bound

$$\frac{\|(A+\delta A)B - AB\|}{\|AB\|} \leq \min(\kappa(A), \kappa(B))\frac{\|\delta A\|}{\|A\|}$$

where $\kappa(C) = \|C\| \cdot \|C^{-1}\|$ is the condition number of a matrix.

[5 marks]

(b) Let H be an $m \times m$ upper Hessenberg matrix; that is $H_{ij} = 0$ for $i > j+1$. State an algorithm using Givens rotations to compute the QR decomposition of H. Determine, to leading order, the number of floating point operations taken by the algorithm.

[10 marks]

(c) Orthomin(2) is given, as in lecture, by

Input: $A \in \mathbb{R}^{n\times n}$, $b \in \mathbb{R}^n$, and estimate $x^{(0)}$ of $Ax = b$

Initialization: Set $p^{(0)} = r^{(0)} = b - Ax^{(0)}$, $\alpha_0 = \frac{(r^{(0)})^* A r^{(0)}}{\|Ar^{(0)}\|_2^2}$, $x^{(1)} = x^{(0)} + \alpha_0 r^{(0)}$, and $r^{(1)} = b - Ax^{(1)}$

for $k = 1$ until termination (say $\|r^{(k)}\| \leq \epsilon \|b\|$)

$\beta_{k-1} = \frac{(Ar^{(k)})^* Ap^{(k-1)}}{\|Ap^{(k-1)}\|_2^2}$

$p^{(k)} = r^{(k)} - \beta_{k-1} p^{(k-1)}$

$\alpha_k = \frac{(r^{(k)})^* Ap^{(k)}}{\|Ap^{(k)}\|_2^2}$

$x^{(k+1)} = x^{(k)} + \alpha_k p^{(k)}$

$r^{(k+1)} = b - Ax^{(k+1)}$

Show that if A is Hermitian, $A^* = A$ that

$$(r^{(k)})^* Ap^{(j)} = 0 \quad \text{and} \quad (Ap^{(k)})^* Ap^{(j)} = 0 \quad \text{for all } j < k.$$

[10 marks]

Question 6

(a) State the Householder reflector $H_j(u_j)$ with the property that for any $m \times m$ matrix A, the matrix $H_j(u_j)A$ has its (i,j) entries are equal to zero for $i > j$. State an algorithm for computing the QR factorization of a matrix using Householder reflections. Why is this algorithm preferable to Gram-Schmidt both in terms of stability and floating point operations (be quantitative, but you don't need to prove these reasons are true).

[9 marks]

(b) Consider the iteration $x^{(k+1)} = x^{(k)} + \alpha_k r^{(k)}$ where $r^{(k)} = b - Ax^{(k)}$ and A is positive definite. Derive a formula for α_k so that $\|x^{(k+1)} - A^{-1}b\|_A$ is minimized. Show that this algorithm converges to $A^{-1}b$ at a linear rate; that is $\|x^{(k+1)} - A^{-1}b\|_A \leq \gamma \|x^{(k)} - A^{-1}b\|_A$ for $\gamma < 1$, and state a formula of γ for this algorithm.

[8 marks]

(c) The iterates for Conjugate gradient were defined in lecture as:

for $k = 1$ until termination

$$\beta_{k-1} = \frac{(r^{(k)})^* A p^{(k-1)}}{\|p^{(k-1)}\|_A^2}$$

$$p^{(k)} = r^{(k)} - \beta_{k-1} p^{(k-1)}$$

$$\alpha_k = \frac{(r^{(k)})^* p^{(k)}}{\|p^{(k)}\|_A^2}$$

$$x^{(k+1)} = x^{(k)} + \alpha_k p^{(k)}$$

$$r^{(k+1)} = b - Ax^{(k+1)}$$

Show that alternatively α_k and β_{k-1} are equal to

$$\alpha_k = \frac{\|r^{(k)}\|_2^2}{\|p^{(k)}\|_A^2}.$$

$$\beta_{k-1} = -\frac{\|r^{(k)}\|_2^2}{\|r^{(k-1)}\|_2^2}$$

You may assume that the residuals are orthogonal, $(r^{(i)})^* r^{(j)} = 0$ for $i \neq j$.

[8 marks]