JMAT 7302

M.Sc. in Mathematical Modelling and Scientific Computing

Paper B (Numerical Analysis)

Friday 28 April, 2000, 9.30 a.m. – 12.30 p.m.

Candidates may attempt as many questions as they wish. All questions will carry equal marks.

Do not turn this page until you are told that you may do so

Numerical Linear Algebra

1. (a) What is a QR factorisation of a matrix $A \in \mathbb{R}^{m\times n}$? Show that such a factorisation always exists. If PS is a QR factorisation of $A \in \mathbb{R}^{m\times n}$ deduce that the singular values of A and of S are the same.

If the factorisation PS of A is available, how might one readily solve $Ax = b$ when A is square and invertible? Briefly say what factorisation is usually used for solving linear systems.

(b) If for square matrices $A \in \mathbb{R}^{n\times n}$ with entries $\{a_{i,j}, i, j = 1, \ldots, n\}$, $\mathrm{Trace}(A) = \sum_{i=1}^{n} a_{i,i}$, verify that $\langle A, B\rangle = \mathrm{Trace}(A^T B)$ is an inner product on the vector space of real $n \times n$ matrices. Show that any skew-symmetric matrix A ($a_{i,j} = -a_{j,i}, i, j = 1, \ldots, n$) and any symmetric matrix B ($b_{i,j} = b_{j,i}, i, j = 1, \ldots, n$) are orthogonal to one another in this inner product. Given an arbitrary $A \in \mathbb{R}^{n\times n}$, find the best approximation to A (with respect to the norm associated with this inner product) from the vector subspace of real symmetric matrices.

Numerical Solution of Ordinary Differential Equations

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 $\{x_n : x_n = x_0 + nh,\ n = 0, 1, 2, \ldots\}$ of uniform spacing $h > 0$.

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.

Define the *truncation error* of a linear k-step method.

Determine all values of the real parameter α such that the linear two-step method given by the formula

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

is zero-stable. Show that there exists a value of α for which the order of the method is 4. Is the method convergent for this value of α?

What is meant by saying that a linear multistep method, applied to the initial value problem $y' = \lambda y$, $y(x_0) = y_0$, $\lambda < 0$, is *absolutely stable*? Assuming that $\alpha = -1$ in the two-step method above, characterise the set of h such that the method is absolutely stable.

[You may use without proof that the error constants of the linear k-step method $\sum_{j=0}^{k} \alpha_j y_{n+j} = h \sum_{j=0}^{k} \beta_j f_{n+j}$ are given by the formulae

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

Numerical Solution of Partial Differential Equations

3. The Poisson equation

$$u_{xx} + u_{yy} = f(x,y), \qquad u = 0 \text{ on the boundary}$$

is posed on the unit square $0 \le x, y \le 1$. It is decided to discretise this problem on a regular square grid indexed from 0 to J in each direction using a 9-point stencil in the shape of a cross instead of the usual 5-point stencil. That is, $u_{r,s}$ will be coupled to $u_{r-2,s}$, $u_{r-1,s}$, $u_{r+1,s}$, $u_{r+2,s}$, $u_{r,s-2}$, $u_{r,s-1}$, $u_{r,s+1}$ and $u_{r,s+2}$.

(a) Derive coefficients for the optimal finite difference formula based on this stencil (i.e., the one with highest order of accuracy).

(b) Explain the problem that arises near the boundary, and describe a solution to it. (There is more than one acceptable answer to this part.)

(c) Assume that the unknowns are ordered in the usual 'typewriter' or 'lexicographic' fashion. Describe the structure of the matrix involved in your discretisation, making clear exactly where the nonzero entries are located.

4. Suppose the usual Lax-Wendroff model of $u_t = u_x$ is applied on an infinite grid with $\Delta x = 0.01$ to compute an approximate solution at $t = 1$. The computation is carried out for two different initial conditions. For each initial condition two time steps are used.

The initial data at $t = 0$ are

$$u_1(x) = \cos(\pi x) \qquad \text{and} \qquad u_2(x) = \max\{0, 1 - |x|\}.$$

The time steps are $\Delta t = \sigma \Delta x$ with

$$\sigma_a = \frac{4}{5} \qquad \text{and} \qquad \sigma_b = \frac{4}{3}.$$

Thus we have four computations: 1a, 1b, 2a, 2b. Let E_{1a}, E_{1b}, E_{2a}, E_{2b} denote the corresponding maximum errors over the grid at $t = 1$.

(a) The numbers E_{1a}, E_{1b}, E_{2a}, E_{2b} will be of varying sizes. Which will be less than 1, and which will be greater than 1? Which of the four will be biggest, second biggest, third biggest, and smallest? Explain your reasoning in each case, giving rough estimates of the numbers involved (within a few orders of magnitude) where possible.

(b) One of these four numbers will depend significantly on the floating point precision of the computer ('machine epsilon'). Which one, and why?

Finite Element Methods

5. Given that α is a non-negative real number, consider the boundary value problem

$$-(\mathrm{e}^x u')' + x^2 u = 0 \quad \text{for } x \in (0,1), \qquad u(0) = 0, \quad \alpha u(1) + \mathrm{e}u'(1) = 1.$$

Using continuous piecewise linear basis functions on a uniform mesh of size $h = 1/N$, $N \geq 2$, write down the finite element approximation to this problem and show that this has a unique solution u_h. Expand u_h in terms of the finite element basis functions ϕ_i, where $\phi_i(x) = (1 - |x - x_i|/h)_+$ and $x_i = ih$, $i = 1, \ldots, N$, by writing

$$u_h(x) = \sum_{i=1}^{N} U_i \phi_i(x)$$

to obtain a system of linear equations for the vector of unknowns $(U_1, \ldots, U_N)^T$. Comment on the structure of the matrix of this linear system, and give expressions for all nonzero entries of this matrix in terms of the finite element basis functions, without evaluating the integrals.

Now, consider the unsteady diffusion equation

$$\frac{\partial u}{\partial t} - \frac{\partial}{\partial x}\left(\mathrm{e}^x \frac{\partial u}{\partial x}\right) + x^2 u = 0$$

on the space-time domain $Q = (0,1) \times (0,T]$ with final time $T > 0$, subject to the same boundary conditions for u at $x = 0$ and $x = 1$ as above, and initial condition $u(x,0) = u_0(x)$ with $u_0 \in L_2(0,1)$ given.

How would you adapt the finite element discretisation developed in the first part of the question to this initial boundary value problem using the backward Euler method as your time discretisation scheme?

6. Consider the quadratic energy functional

$$J(v) = \frac{1}{2}\int_{\Omega}\left[a_1\left(\frac{\partial v}{\partial x}\right)^2 + a_2\left(\frac{\partial v}{\partial y}\right)^2 + a_3\left(\frac{\partial v}{\partial x} - \frac{\partial v}{\partial y}\right)^2 - fv\right]\mathrm{d}x\,\mathrm{d}y,$$

where a_1 and a_2 are positive real numbers, a_3 is a nonnegative real number, $\Omega = (0,2)^2$, and $f \in L_2(\Omega)$.

Denoting by u the minimiser of J over $H_0^1(\Omega)$ and given that

$$\lim_{\lambda \to 0}\left(J(u+\lambda v) - J(u)\right)/\lambda = 0 \qquad \text{for all } v \in H_0^1(\Omega),$$

deduce the Euler-Lagrange equation associated with minimising J over $H_0^1(\Omega)$.

Consider a triangulation of Ω which has been obtained from a square mesh of spacing $h = 1/N$, $N \geq 2$, in both co-ordinate directions by subdividing each square into two triangles with the diagonal of negative slope. Using continuous piecewise linear basis functions on this triangulation, state the finite element approximation to the energy minimisation problem.

It is known from the theory of partial differential equations that $u \in H^2(\Omega) \cap H_0^1(\Omega)$. Denoting by u_h the piecewise linear finite element approximation to u, show that

$$\|u - u_h\|_a \leq Ch|u|_{H^2(\Omega)},$$

where $\|\cdot\|_a$ is a suitable energy norm that you should define and C is a positive constant, independent of h.

[You may use without proof the inequality $|v - I_h v|_{H^1(\Omega)} \leq Ch|v|_{H^2(\Omega)}$, where $v \in H^2(\Omega) \cap H_0^1(\Omega)$, $I_h v$ is the piecewise linear finite element interpolant of v and C is a positive constant, independent of h.]

Suppose now that $\Omega = (0,2)^2$ has been replaced by the L-shaped domain $\Omega' = (0,2)^2 \setminus (1,2)^2$. Numerical experiments indicate that the error in the $H^1(\Omega')$ seminorm, $|\cdot|_{H^1(\Omega')}$, between the energy minimiser $u \in H_0^1(\Omega')$ and its piecewise linear finite element approximation u_h, on a uniform partition of Ω' of size h, $h \ll 1$, is $O(h^{2/3})$. Explain briefly why the observed rate of convergence is less than 1?