DEGREE OF MASTER OF SCIENCE

MATHEMATICAL MODELLING AND SCIENTIFIC COMPUTING

B1 Numerical Linear Algebra and Numerical Solution of Differential Equations

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HILARY TERM 2019

FRIDAY, 11 JANUARY 2019, 9.30am to 12.00pm

You may attempt as many questions as you like but you must answer at least one question in each section. Your best answer in each section will count, along with your next best answer(s), making a total of four answers.

Please start the answer to each question in a new booklet.
All questions will carry equal marks.

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

Section A: Numerical Solution of Differential Equations

1. (a) [6 marks] Write the definition of a *one-step method* and of a *consistent one-step method.*

   (b) [6 marks] Write the definition of *consistency error* and *consistency order* of a one-step method. Is it true that, if a one-step method is consistent and sufficiently smooth, then its consistency order is at least 1?

   (c) [7 marks] Consider the Runge-Kutta method with Butcher table

$$\begin{array}{c|c} 2/3 & 2/3 \\ \hline & 1 \end{array} \,. \tag{1}$$

   Use Taylor expansion to determine the consistency order of this Runge-Kutta method.

   (d) [6 marks] Let $\mathbf{f}(t, \mathbf{x}) = \mathbf{f}(\mathbf{x})$, and let $\boldsymbol{\Psi}(t, \mathbf{x}, h, \mathbf{f}) = \mathbf{x} + h\mathbf{k}$ denote one step of the Runge-Kutta method with Butcher table (1). The stage $\mathbf{k}$ can be equivalently rewritten as $\mathbf{f}(\mathbf{g})$, where $\mathbf{g}$ satisfies

$$\mathbf{g} = \mathbf{x} + \frac{2h}{3}\mathbf{f}(\mathbf{g})\,.$$

   Let $\tilde{\mathbf{g}}$ be an approximation of $\mathbf{g}$ obtained using two steps of the fixed-point iteration algorithm with initial value $\tilde{\mathbf{g}}^{(0)} = \mathbf{x}$, and let $\tilde{\mathbf{k}} := \mathbf{f}(\tilde{\mathbf{g}})$. Write the Butcher table of the Runge-Kutta method $\tilde{\boldsymbol{\Psi}}(t, \mathbf{x}, h, \mathbf{f}) := \mathbf{x} + h\tilde{\mathbf{k}}$.

2. (a) [5 marks] Linear multi-step methods can be derived using the *shift operator* E, the *difference operator* Δ, the *identity operator* $\mathbf{I}$, and the *differential operator* D. Give the definitions of these four operators. Use the symbol h to denote the step size.

(b) [10 marks] By formal computations, it is possible to show that

$$hD = \left(\Delta + \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 + \dots\right). \tag{2}$$

Write the formula of the linear 3-step method that arises from truncating (2) and show that this linear 3-step method has consistency order 3.

(c) [10 marks] The linear 2-step method associated to (2) reads

$$\frac{3}{2}\mathbf{y}_n - 2\mathbf{y}_{n-1} + \frac{1}{2}\mathbf{y}_{n-2} = h\mathbf{f}(t_n, \mathbf{y}_n). \tag{3}$$

(i) Give the definition of the *stability polynomial* and of the *stability domain* of a linear multi-step method.

(ii) Specify the stability polynomial of (3).

(iii) It is known that (3) is A-stable. Show directly (without using the definition of A-stability) that the negative real line $\mathbb{R}^- := \{z : \operatorname{Re} z \leqslant 0 \text{ and } \operatorname{Im} z = 0\}$ is included in the stability domain of (3).

3. (a) [5 marks] Give the definition of a *linear k-step method.*

(b) [5 marks] Determine the consistency order of the linear multi-step method

$$\mathbf{y}_2 - \mathbf{y}_1 = h\left(-\frac{1}{12}\mathbf{f}(t_0, \mathbf{y}_0) + \frac{2}{3}\mathbf{f}(t_1, \mathbf{y}_1) + \frac{5}{12}\mathbf{f}(t_2, \mathbf{y}_2)\right). \tag{4}$$

(c) [9 marks] Let the initial values $\mathbf{y}_0$ and $\mathbf{y}_1$ be given, and let the function $\mathbf{f}$ be sufficiently smooth. Use the Banach fixed-point theorem to show that, if $h > 0$ is sufficiently small, the linear multi-step formula (4) has a unique solution $\mathbf{y}_2$. In your proof, specify the upper bound on h.

(d) [6 marks] Let

$$h = 0.1\,, \quad \mathbf{y}_0 = \begin{pmatrix} 2 \\ 2.7 \end{pmatrix}, \quad \mathbf{y}_1 = \begin{pmatrix} 2 \\ 1.1 \end{pmatrix}, \quad \text{and} \quad \mathbf{f}(t, \mathbf{y}) = \begin{pmatrix} 0 & 0 \\ 0 & -10 \end{pmatrix} \mathbf{y}\,.$$

Let $\{\mathbf{y}_n\}_{n \geqslant 0}$ be the sequence defined by (4). Compute $\lim_{n\to\infty} \|\mathbf{y}_n\|$.

4. Consider the following initial boundary value problem:

$$u_t(t,x) - u_{xx}(t,x) = 0 \text{ for } (t,x) \in \mathbb{R}^+ \times (0,1)\,, \tag{5a}$$

$$u_x(t,0) = 0\,, \quad u(t,1) = e^{-(2\pi)^2 t}, \quad u(0,x) = \cos(2\pi x)\,. \tag{5b}$$

(a) [5 marks] Show that $u(t,x) = e^{-(2\pi)^2 t}\cos(2\pi x)$ is a solution to (5).

(b) [7 marks] Let $N \in \mathbb{N}$ and $\Delta x := 1/N$. Derive a linear system of ODEs and its initial condition by semi-discretizing (5) in space with the finite difference approximations

$$u_{xx}(x) \approx \frac{u(x+\Delta x) - 2u(x) + u(x-\Delta x)}{\Delta x^2}$$

and

$$u_x(x) \approx \frac{-3u(x) + 4u(x+\Delta x) - u(x+2\Delta x)}{2\Delta x}\,.$$

(c) [6 marks] Show that, if the function v is sufficiently regular, then

$$v_{xx}(x) = \frac{v(x+\Delta x) - 2v(x) + v(x-\Delta x)}{\Delta x^2} + \mathcal{O}(\Delta x^2)$$

and

$$v_x(x) = \frac{-3v(x) + 4v(x+\Delta x) - v(x+2\Delta x)}{2\Delta x} + \mathcal{O}(\Delta x^2)$$

(d) [7 marks] Let $\mathbf{A} \in \mathbb{R}^{N\times N}$ be a given matrix and consider the linear system of ODEs $\mathbf{y}' = \mathbf{A}\mathbf{y}$. Let $\{\mathbf{y}_n\}_{n\geqslant 0}$ be its numerical solution computed with a linear k-step method with a sufficiently small step size $h > 0$ and initial values $\{\mathbf{y}_m\}_{m=0}^{k-1}$. Show that $\{\mathbf{y}_n\}_{n\geqslant 0}$ satisfies

$$\mathbf{y}_n = (\alpha_k \mathbf{I} - h\beta_k \mathbf{A})^{-1}\left(h\mathbf{A}\mathbf{Y}_n \begin{pmatrix} \beta_{k-1} \\ \beta_{k-2} \\ \vdots \\ \beta_0 \end{pmatrix} - \mathbf{Y}_n \begin{pmatrix} \alpha_{k-1} \\ \alpha_{k-2} \\ \vdots \\ \alpha_0 \end{pmatrix} \right),$$

where $\mathbf{I}$ is the identity matrix, $\mathbf{Y}_n \in \mathbb{R}^{N\times k}$ is a matrix with columns $\mathbf{y}_{n-1}, \mathbf{y}_{n-2}, \ldots, \mathbf{y}_{n-k}$, and $\{\alpha_i\}_{i=0}^{k}$ and $\{\beta_i\}_{i=0}^{k}$ are the coefficients of the linear multi-step method.

Section B: Numerical Linear Algebra

5. In this question $x \in \mathbb{R}^n$ denotes a generic vector and $A \in \mathbb{R}^{m\times n}$ a generic matrix.

(a) [3 marks] Define $\|x\|_1$. Define the *operator norm* $\|A\|_1$ and the *Frobenius norm* $\|A\|_F$.

(b) [3 marks] Use the operator norm definition of $\|A\|_1$ to show that

$$\|A\|_1 = \max_{j\in\{1,\dots,n\}} \sum_{i=1}^{m} |a_{i,j}|,$$

where $\{a_{i,j}, i = 1, \dots, m, j = 1, \dots, n\}$ are the entries of A.

(c) [4 marks] Prove that

$$\frac{1}{\sqrt{m}}\|A\|_1 \leqslant \|A\|_F.$$

(d) [4 marks] Give the definition of an *orthogonal matrix*. Show that if Q is an orthogonal matrix, then $\|AQ\|_F = \|A\|_F$.

(e) [3 marks] Let $D \in \mathbb{R}^{m\times n}$ be a diagonal matrix. Show that

$$\|D\|_1 = \|D\|_2.$$

(f) [8 marks] For $C \in \mathbb{R}^{n\times n}$, what is an *LU factorization with partial pivoting* of C? For this factorization, why is $\|L\|_1 \leqslant n$ for any C? For the matrix

$$C = \begin{bmatrix} 1 & 0 & \dots & \dots & 0 & 1 \\ -1 & 1 & 0 & \dots & 0 & 1 \\ \vdots & \ddots & \ddots & \ddots & \vdots & \vdots \\ -1 & \dots & -1 & 1 & 0 & 1 \\ -1 & \dots & \dots & -1 & 1 & 1 \\ -1 & \dots & \dots & \dots & -1 & 1 \end{bmatrix}$$

why would no row swaps be required even if partial pivoting was employed? Show that

$$\|U\|_1 = \sum_{j=0}^{n-1} 2^j$$

for this matrix.

6. (a) [4 marks] Calculate the iterate vectors $\mathbf{x}^{(1)}$ and $\mathbf{x}^{(2)}$ obtained by Jacobi iteration for the system

$$Wx = \begin{bmatrix} 4 & 1 & 0 & \cdots & 0 \\ 1 & 4 & 1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & 1 \\ 0 & \cdots & 0 & 1 & 4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{n-1} \\ x_n \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix} \qquad (1)$$

starting from $\mathbf{x}^{(0)} = (1, 1, \ldots, 1)^T$.

(b) [4 marks] Show that the vector $\mathbf{v}^{(r)} \in \mathbb{R}^n$ that has entries

$$v_j^r = \sin \frac{rj\pi}{n+1}, \qquad j = 1, 2, \ldots, n$$

is an eigenvector of W with corresponding eigenvalue

$$\lambda^r = 4 + 2\cos \frac{r\pi}{n+1}$$

for each $r = 1, 2, \ldots, n$.

(c) [6 marks] Let $\{\mathbf{x}^{(k)}, k = 0, 1, 2, \ldots\}$ be the sequence of vectors computed by Jacobi iteration for (1). By quoting (but not proving) a relevant theorem involving eigenvalues, show that $\mathbf{x}^{(k)}$ will tend to the zero vector as $k \to \infty$.

After how many iterations can you guarantee that the 2-norm of the error, $\|\mathbf{x}^{(k)}\|_2$, is necessarily less than 10^{-5} if $n = 10^4$? (Note that $2^{10} = 1024 \approx 10^3$).

(d) [2 marks] Consider the problem

$$Ax = \begin{bmatrix} 2 & -1 & 0 & \cdots & 0 \\ -1 & 2 & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -1 \\ 0 & \cdots & 0 & -1 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_{n-1} \\ x_n \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 0 \end{bmatrix}. \qquad (2)$$

By writing the Jacobi iteration matrix, J_A, for A in term of the Jacobi iteration matrix, J_W, for W, find the largest eigenvalue in absolute value of J_A. Deduce that Jacobi iteration for (2) will define a sequence of iterates converging to the zero vector for any starting vector.

(e) [5 marks] The matrix A can be written as $A = D + L + U$ where D is a diagonal matrix, L a strictly lower triangular matrix and U a strictly upper triangular matrix. Show that the symmetric Gauss-Seidel iteration

$$\begin{aligned} (D+L)x^{(k-\frac{1}{2})} &= b - Ux^{(k-1)} \\ (D+U)x^{(k)} &= b - Lx^{(k-\frac{1}{2})} \end{aligned}$$

for $Ax = b$ can be written as

$$Mx^{(k)} = Nx^{(k-1)} + b \qquad \text{where} \qquad M = (D+L)D^{-1}(D+U).$$

(f) [4 marks] Prove that the eigenvalues of M must lie in the real interval $[\frac{1}{2}, \frac{9}{2}]$ for the specific matrix A as given above in part (d). State and prove any theorem that you use.