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 2018

FRIDAY, 12 JANUARY 2018, 9.30am to 11.30am

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 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. The solution $[t_0, T] \ni t \to \mathbf{y}(t)$ to the initial value problem

$$\mathbf{y}' = \mathbf{f}(t, \mathbf{y}), \quad \mathbf{y}(t_0) = \mathbf{y}_0, \tag{1}$$

satisfies

$$\mathbf{y}(t+h) = \mathbf{y}(t) + \int_t^{t+h} \mathbf{f}(\tau, \mathbf{y}(\tau))\, \mathrm{d}\tau\,. \tag{2}$$

To devise a one-step method to solve (1), one can replace the integral on the right-hand side of (2) with

$$h(1-\theta)\mathbf{f}(t, \mathbf{y}(t)) + h\theta\mathbf{f}(t+h, \mathbf{y}(t+h))$$

where $\theta \in [0, 1]$ is a real parameter. The resulting scheme reads

$$\mathbf{\Psi}(t, t+h, \mathbf{y}) = \mathbf{y} + h(1-\theta)\mathbf{f}(t, \mathbf{y}) + h\theta\mathbf{f}(t+h, \mathbf{\Psi}(t, t+h, \mathbf{y}))\,.$$

(a) [6 marks] Derive the Butcher table of this family of Runge-Kutta methods and write the formulas of its Runge-Kutta stages. For which values of θ is the method explicit?

(b) [4 marks] Give the definition of consistency error and *consistency order* of a one-step method.

(c) [10 marks] In the case that $\mathbf{f}$ is autonomous (so that $\mathbf{f}(t, \mathbf{y}) = \mathbf{f}(\mathbf{y})$), use Taylor expansion to verify that the Runge-Kutta scheme obtained by setting $\theta = 1$ has consistency order 1.

(d) [5 marks] In the case that $\mathbf{f}(t, \mathbf{y}) = \mathbf{A}\mathbf{y}$ for a given matrix $\mathbf{A}$, show that the scheme obtained by setting $\theta = 1/2$ preserves quadratic invariants. State clearly any results you quote.

2. We consider the following family of quadrature rules

$$\int_a^b f(\tau)\,\mathrm{d}\tau \approx (b-a) f\big(a+\theta(b-a)\big)\,,$$

where $\theta \in [0,1]$ is a real parameter. In particular, note that $\int_0^1 f(\tau)\,\mathrm{d}\tau \approx f(\theta)$.

(a) [7 marks] Show that the Butcher table of the family of collocation Runge-Kutta methods based on these quadratures reads

$$\begin{array}{c|c} \theta & \theta \\ \hline & 1 \end{array}\,.$$

[Hint: Let $s \geqslant 1$ and $i \in \{1,2,\dots,s\}$. The i-th Lagrange polynomial associated to s distinct points $c_1,\dots,c_s$ is the polynomial of degree $s-1$ that satisfies $L_i(c_j) = \delta_{ij}$.]

(b) [4 marks] Derive the stability function of this family of Runge-Kutta methods (keeping θ generic).

(c) [4 marks] Give the definition of: (i) *stability domain* of a Runge-Kutta method, (ii) *A-stability*, and (iii) *L-stability.*

(d) [4 marks] Consider the IVP

$$y'(t) = (-10^9 + 4i)y\,, \quad y(0) = 1\,.$$

and denote by $\{y_k\}_{k\in\mathbb{N}}$ a sequence of approximations obtained by employing: (i) an explicit Runge-Kutta method, (ii) an A-stable (but not L-stable) Runge-Kutta method, and (iii) an L-stable Runge-Kutta method. For each case, describe the qualitative behaviour of $\{y_k\}_{k\in\mathbb{N}}$ and compare it to the qualitative behaviour of the exact solution to this IVP.

(e) [6 marks] Show that, if the stability domain $S_{\boldsymbol{\Psi}}$ of a Runge-Kutta method $\boldsymbol{\Psi}$ satifies $S_{\boldsymbol{\Psi}} = \mathbb{C}^-$, then that Runge-Kutta $\boldsymbol{\Psi}$ method cannot be L-stable.

3. The first and second characteristic polynomials of the linear multi-step method BDF2 are

$$\rho(z) = z^2 - \frac{4}{3}z + \frac{1}{3} \quad \text{and} \quad \sigma(z) = \frac{2}{3}z^2\,,$$

respectively.

(a) [4 marks] Write the update formula of BDF2 in terms of $h, \mathbf{y}_n, \mathbf{y}_{n+1}, \mathbf{y}_{n+2}, \mathbf{f}(t_n,\mathbf{y}_n)$, $\mathbf{f}(t_{n+1},\mathbf{y}_{n+1})$, and $\mathbf{f}(t_{n+2},\mathbf{y}_{n+2})$.

(b) [7 marks] Give the definition of *zero-stability* of a linear k-step method and describe how to verify this property using the root condition. Is BDF2 zero-stable?

(c) [7 marks] Show that

$$\rho(\mathrm{e}^h) - h\sigma(\mathrm{e}^h) = \mathcal{O}(h^3)\,.$$

What can you conclude about the consistency order of BDF2?

(d) [7 marks] The linear multi-step method

$$\frac{11}{6}\mathbf{y}_n - 3\mathbf{y}_{n-1} + \frac{3}{2}\mathbf{y}_{n-2} - \frac{1}{3}\mathbf{y}_{n-3} = h\mathbf{f}(t_n,\mathbf{y}_n)\,.$$

is implicit. Describe how to use Newton's method to approximate $\mathbf{y}_n$ provided that $\mathbf{y}_{n-1}, \mathbf{y}_{n-2}$, and $\mathbf{y}_{n-3}$ are available.

4. Consider the following parabolic boundary value problem

$$u_t(t,x) = u_{xx}(t,x)\,, \quad \text{for } (t,x) \in (0,1] \times (0,1)$$

with homogeneous Dirichlet boundary conditions.

(a) [8 marks] Following the method of lines, discretize this equation in space using a central difference scheme and derive the associate system of ODEs.

(b) [4 marks] Show that for any $k, \Delta x \in \mathbb{R}$ and $j \in \mathbb{N}$,

$$\sin\big(k(j+1)\Delta x\big) - 2\sin\big(kj\Delta x\big) + \sin\big(k(j-1)\Delta x\big) = 2\big(\cos(k\Delta x) - 1\big)\sin\big(kj\Delta x\big)\,.$$

(c) [6 marks] Let $N = 1/\Delta x$. Show that the eigenvectors of the matrix

$$\mathbf{K} = \begin{pmatrix} -2 & 1 & & \\ 1 & -2 & 1 & \\ & \ddots & \ddots & 1 \\ & & 1 & -2 \end{pmatrix} \in \mathbb{R}^{N-1,N-1}$$

are given by

$$\mathbf{z}_p^\top = (\sin(p\pi\Delta x), \sin(2p\pi\Delta x), \ldots, \sin((N-1)p\pi\Delta x))\,, \quad p = 1, \ldots, N-1\,.$$

What are the corresponding eigenvalues?

(d) [7 marks] Show that Runge-Kutta methods are affine covariant when applied to a linear system of ODEs $\mathbf{y}(t)' = \mathbf{M}\mathbf{y}(t)$, where $\mathbf{y} \in \mathbb{R}^d$ and $\mathbf{M} \in \mathbb{R}^{d,d}$. State clearly any results you quote.

Section B: Numerical Linear Algebra

5. Throughout this question we consider a rectangular matrix $A \in \mathbb{R}^{m\times n}$ and a nonsingular matrix $B \in \mathbb{R}^{n\times n}$.

   (a) [4 marks] What is a QR factorisation of A? You do not need to show that such a factorisation exists.

   What is an LU factorisation of B? You do not need to show that such a factorisation exists.

   (b) [4 marks] If $m > n$, the columns of the given matrix A are linearly independent and $b \in \mathbb{R}^m$ is also given, explain how to solve the linear least squares problem

$$\min_{x\in\mathbb{R}^n} \|Ax - b\|_2$$

   using a QR factorisation.

   (c) [2 marks] If $QR = B = LU$, identify an LU factorisation of Q.

   (d) [3 marks] Supposing that all the required factorisations exist, let $B = B_1$ and

   `for` $k = 1, 2, \ldots$
   $L_k U_k = B_k - \mu_k I$ (ie. perform an LU factorisation of $B_k - \mu_k I$)
   $B_{k+1} = U_k L_k + \mu_k I$ (ie. define B_{k+1} by matrix multiplication and addition of $\mu_k I$)
   `end`

   where $\mu_k \in \mathbb{R}$ is such that $B_k - \mu_k I$ is invertible for every $k = 1, 2, \ldots$. Prove that all of the matrices $\{B_k, k = 1, 2, \ldots\}$ are mathematically *similar* to $B_1 = B$.

   (e) [5 marks] If the matrix B is perturbed to $B + \delta B$, prove that

$$\frac{\|\delta x\|_2}{\|x + \delta x\|_2} \leqslant \|B\|_2 \|B^{-1}\|_2 \frac{\|\delta B\|_2}{\|B\|_2}$$

   where $Bx = b$ and $(B + \delta B)(x + \delta x) = b$ with $x \neq -\delta x$. What is the relevance of this inequality to the computational solution of a linear system of equations?

   (f) [7 marks] Calculate $\|B\|_2 \|B^{-1}\|_2$ for the matrix

$$B = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 4 & 0 \\ 0 & 0 & 0 & 0 & 5 \end{bmatrix}.$$

   Identify $\|C\|_2 \|C^{-1}\|_2$ for the matrix

$$C = \begin{bmatrix} 1 & 1 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 & 0 \\ 0 & 0 & 3 & 1 & 0 \\ 0 & 0 & 1 & 4 & 0 \\ 0 & 0 & 0 & 0 & 5 \end{bmatrix}?$$

   Give your reasoning.

6. If $A = M - N \in \mathbb{R}^{m\times m}$ with A and M nonsingular, a *simple iteration* for the solution of $A\mathbf{x} = \mathbf{b}$ based on this splitting is:
choose $\mathbf{x}_0$ and solve $M\mathbf{x}_k = N\mathbf{x}_{k-1} + \mathbf{b}$ for $k = 1, 2, \ldots$.

   (a) [9 marks] For a general matrix $A = \{a_{i,j},\ i, j = 1, \ldots, m\}$, what is Gauss-Seidel iteration? Calculate the first two Gauss-Seidel iterate vectors, $\mathbf{x}_1, \mathbf{x}_2$ for the problem

$$\begin{bmatrix} \frac{1}{2} & 2 \\ 0 & \frac{1}{2} \end{bmatrix} \mathbf{x} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

   starting with $\mathbf{x}_0 = [0, 1]^T$. Does the iteration converge to the solution $\mathbf{x}$? Does the sequence $\{\|\mathbf{x}_k - \mathbf{x}\|_2, k = 0, 1, 2, \ldots\}$ reduce monotonically?

   (b) [8 marks] What is a *Jordan canonical form*?
   [You may assume that any square matrix has a Jordan canonical form.]
   If for any particular splitting $A = M - N$ we have that all of the eigenvalues of $M^{-1}N$ lie strictly inside the unit disc, prove that the simple iteration based on this splitting must generate a sequence of iterates that converge to the solution for any $\mathbf{x}_0$.
   Further prove that if additionally $M^{-1}N$ is symmetric, then

$$\|\mathbf{x}_k - \mathbf{x}\|_2 \leqslant \|\mathbf{x}_{k-1} - \mathbf{x}\|_2 \qquad \text{for each} \quad k = 1, 2, \ldots.$$

   [Hint: Any symmetric matrix is orthogonally diagonalisable, so that there exists an orthonormal basis of eigenvectors.]

   (c) [8 marks] Consider the nonsingular matrix

$$A = \begin{bmatrix} B & -I & 0 & \cdots & 0 \\ -I & B & -I & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -I \\ 0 & \cdots & 0 & -I & B \end{bmatrix}, \text{ where } B = \begin{bmatrix} 4+\epsilon & -1 & 0 & \cdots & 0 \\ -1 & 4+\epsilon & -1 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & -1 \\ 0 & \cdots & 0 & -1 & 4+\epsilon \end{bmatrix}$$

   is a tridiagonal matrix with $B \in \mathbb{R}^{n\times n}$, $A \in \mathbb{R}^{n^2\times n^2}$ and ϵ a positive constant.
   Prove that the simple iteration based on the splitting $A = M - N$ with

$$M = \begin{bmatrix} B & 0 & 0 & \cdots & 0 \\ 0 & B & 0 & \ddots & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 0 & B \end{bmatrix} \in \mathbb{R}^{n^2\times n^2}.$$

   will generate a sequence that will converge to the solution of $A\mathbf{x} = \mathbf{b}$ for any $\mathbf{b}$ and any $\mathbf{x}_0$. Quote, but do not prove, any results that you use.