MA2501

NUMERICAL METHODS

NTNU, SPRING 2023

Exam 2, 17-08-2023, 09:00-13:00

Grading document

In the exam one could obtain 100 points and the grade follows the usual grading scheme, that is

A	B	C	D	E	F
100-89	88-77	76-65	64-53	52-41	40-0

Date: August 17, 2023.

Problem 1. *(QR factorisation)*

10 points *Consider the* 4×2*-matrix*

$$A = \begin{pmatrix} 2 & 1 \\ 2 & -3 \\ -2 & -1 \\ -2 & 3 \end{pmatrix}.$$

(1) *(4 points) Determine the upper triangular* 2×2*-matrix* $R = (r_{ij})$ *with* $r_{ii} > 0$, $i = 1, 2$, *from the equation* $A^T A = R^T R$.

(2) *(4 points) Determine the matrix* Q *such that* $A = QR$.

(3) *(2 points) Verify that this is a QR factorisation of* A.

Solution

(1) (1 point) We see that

$$A^T A = \begin{pmatrix} 16 & -8 \\ -8 & 20 \end{pmatrix}.$$

(3 points) From $A^T A = R^T R$ we deduce R with positive diagonal entries

$$R = \begin{pmatrix} r_{11} & r_{12} \\ 0 & r_{22} \end{pmatrix} = \begin{pmatrix} 4 & -2 \\ 0 & 4 \end{pmatrix}.$$

(2) (1 points) The matrix R is non-singular. We compute its inverse

$$R^{-1} = \begin{pmatrix} 1/4 & 1/8 \\ 0 & 1/4 \end{pmatrix}.$$

(3 points) From $A = QR$ we deduce

$$Q = AR^{-1} = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ -1 & -1 \\ -1 & 1 \end{pmatrix}.$$

(3) (2 points) We need to verify that $A = QR$ is a QR factorisation of A, that is, that R is upper triangular and $Q^T Q = I_2$. The latter is checked by computation

$$\frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ -1 & -1 \\ -1 & 1 \end{pmatrix}^T \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ -1 & -1 \\ -1 & 1 \end{pmatrix} = \frac{1}{4} \begin{pmatrix} 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ -1 & -1 \\ -1 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$$

Problem 2. *(Iteration methods)*

15 points

Let A be a non-singular $n \times n$-matrix. Consider the sequence of matrices $\{X^{(k)}\}_{k\geq 0}$ computed from the iteration method

$$X^{(k+1)} = X^{(k)}\big(2I - AX^{(k)}\big), \quad k \geq 0,$$

with initial matrix $X^{(0)}$. Show that the sequence $\{X^{(k)}\}_{k\geq 0}$ converges to the inverse A^{-1} if and only if the spectral radius of the matrix $I - AX^{(0)}$ is smaller than one, $\rho(I - AX^{(0)}) < 1$.

Hint: Given a matrix Y, recall that the sequence of matrix powers $\{Y^k\}$ converges to the zero matrix if and only if the spectral radius $\rho(Y) < 1$.

Solution (5 points) From $X^{(k+1)} = X^{(k)}\big(2I - AX^{(k)}\big)$ we can deduce that

$$I - AX^{(k+1)} = I - AX^{(k)}\big(2I - AX^{(k)}\big) = I - 2AX^{(k)} + AX^{(k)}AX^{(k)} = (I - AX^{(k)})^2.$$

(7 points) Now we see that

$$I - AX^{(k+1)} = (I - AX^{(k)})^2 = (I - AX^{(k-1)})^4 = (I - AX^{(k-2)})^8 = \cdots = (I - AX^{(0)})^{2^{k+1}}$$

(3 points) Hence, convergence of $I - AX^{(k+1)}$ to zero, i.e., $X^{(k+1)} \to A^{-1}$, if and only if $\rho(I - AX^{(0)}) < 1$.

Problem 3. *(Runge–Kutta methods)*

10 points

Suppose that $f(x, y)$ satisfies a Lipschitz condition in the second variable, y, on $[t_0, T] \times \mathbb{R}^d$, with Lipschitz constant L. Consider the fourth-order Runge–Kutta method

$$y_{next} = y + h\Phi(t, y; h),$$

with

$$\begin{aligned} k_1 &= f(t, y) \\ k_2 &= f(t + \frac{1}{2}h, y + \frac{1}{2}hk_1) \\ k_3 &= f(t + \frac{1}{2}h, y + \frac{1}{2}hk_2) \\ k_4 &= f(t + h, y + hk_3) \\ \Phi(t, y; h) &= \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4). \end{aligned}$$

(1) *Write down the Butcher tableau.*
(2) *Show that the function Φ satisfies a Lipschitz condition for $t + h \in [t_0, T]$.*
(3) *Determine a respective Lipschitz constant $\tilde{L}$.*

Solution

(1) (1 point) Butcher tableau:
- (1 point)

$$\begin{array}{c|cccc} c_1 & a_{11} & a_{12} & a_{13} & a_{14} \\ c_2 & a_{21} & a_{22} & a_{23} & a_{24} \\ c_3 & a_{31} & a_{32} & a_{33} & a_{34} \\ c_4 & a_{41} & a_{42} & a_{43} & a_{44} \\ \hline & b_1 & b_2 & b_3 & b_4 \end{array} = \begin{array}{c|cccc} 0 & 0 & 0 & 0 & 0 \\ 1/2 & 1/2 & 0 & 0 & 0 \\ 1/2 & 0 & 1/2 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 \\ \hline & 1/6 & 1/3 & 1/3 & 1/6 \end{array}$$

(2) (8 points) Lipschitz condition:
- (1 points) Consider $k_i = k_i(t, y; h)$ and $k_i' = k_i'(t, y'; h)$, for $i = 1, \dots, 4$. Then

$$\begin{aligned} k_1 - k_1' &= f(t, y) - f(t, y') \\ k_2 - k_2' &= f(t + \frac{1}{2}h, y + \frac{1}{2}hk_1) - f(t + \frac{1}{2}h, y' + \frac{1}{2}hk_1') \\ k_3 - k_3' &= f(t + \frac{1}{2}h, y + \frac{1}{2}hk_2) - f(t + \frac{1}{2}h, y' + \frac{1}{2}hk_2') \\ k_4 - k_4' &= f(t + h, y + hk_3) - f(t + h, y' + hk_3'). \end{aligned}$$

- (3 points) Using that $f(t, y)$ satisfies a Lipschitz condition in the y-variable yields

$$\begin{aligned} ||k_1 - k_1'|| &= ||f(t, y) - f(t, y')|| \\ &\leq L||y - y'|| \\ ||k_2 - k_2'|| &= ||f(t + h, y + hk_1) - f(t + h, y' + hk_1')|| \\ &\leq L(1 + \frac{1}{2}hL)||y - y'|| \\ ||k_3 - k_3'|| &= ||f(t + h, y + hk_2) - f(t + h, y' + hk_2')|| \\ &\leq L(1 + \frac{1}{2}hL + \frac{1}{4}h^2L^2)||y - y'|| \\ ||k_4 - k_4'|| &= ||f(t + h, y + hk_3) - f(t + h, y' + hk_3')|| \\ &\leq L(1 + hL + \frac{1}{2}h^2L^2 + \frac{1}{4}h^3L^3)||y - y'||. \end{aligned}$$

- (1 points) This implies for

$$\Phi(t, y; h) - \Phi(t, y'; h) = \frac{1}{6}\Big((k_1 - k_1') + 2(k_2 - k_2') + 2(k_3 - k_3') + (k_4 - k_4')\Big)$$

- (3 points) the estimate

$$\begin{aligned} ||\Phi(t, y; h) - \Phi(t, y'; h)|| &\leq \frac{1}{6}L\Big(1 + (2 + hL) + (2 + hL + \frac{1}{2}h^2L^2) \\ &\qquad + (1 + hL + \frac{1}{2}h^2L^2 + \frac{1}{4}h^3L^3)\Big)||y - y'|| \\ &= L\Big(1 + \frac{1}{2}hL + \frac{1}{6}h^2L^2 + \frac{1}{24}h^3L^3\Big) \end{aligned}$$

(3) (1 point) Lipschitz constant

$$\tilde{L} = L\Big(1 + \frac{1}{2}hL + \frac{1}{6}h^2L^2 + \frac{1}{24}h^3L^3\Big)$$

Problem 4. *(Norms)*

15 points

Assume that $||\cdot||$ *is a matrix-norm on the space* $\mathbb{R}^{n\times n}$ *of* $n\times n$*-matrices with real entries, which is sub-multiplicative* ($||AB|| \le ||A||\,||B||$). Let $A \in \mathbb{R}^{n\times n}$ be non-singular. Suppose that the matrix X is an approximation of the inverse A^{-1}. Define $R := AX - I$, where $I \in \mathbb{R}^{n\times n}$ is the identity matrix.

(1) (10 points) Show that

$$\frac{||X - A^{-1}||}{||A^{-1}||} \le ||R||.$$

(2) (5 points) Show that

$$||XA - I|| \le \kappa(A)||R||,$$

where $\kappa(A) := ||A||\,||A^{-1}||$.

Solution

(1) (4 points) From A being non-singular and $R = AX - I$ we deduce that $A^{-1}R = X - A^{-1}$.
(4 points) Sub-multiplicativity gives $||X - A^{-1}|| = ||A^{-1}R|| \le ||A^{-1}||\,||R||$.
(2 points) This implies the inequality $\frac{||X-A^{-1}||}{||A^{-1}||} \le ||R||$.

(2) (3 points) We see that from $A^{-1}R = X - A^{-1}$ we can deduce that $A^{-1}RA = XA - I$.
(2 points) Sub-multiplicativitiy gives $||XA - I|| = ||A^{-1}RA|| \le ||A^{-1}||\,||R||\,||A|| = \kappa(A)||R||$

Problem 5. *(Lagrange interpolation)*

15 points

Consider the function $f(x) = e^{ax} - 1$ *with* $x \ge 0$*, where* a *is a real, positive number.*

(1) (7 points) *Using Lagrange interpolation construct a polynomial of degree at most* 2 *that interpolates the function at* $x_0 = 0$*,* $x_1 = 2$ *and* $x_2 = 4$*.*

(2) (5 points) *Calculate the sharp error bound of the interpolation for* $x \in [0, 4]$*.*

$$E(a) = |f(x) - p_2(x)|$$

Reminder: The interpolation error bound is given by

$$\frac{M_3}{3!}|\omega_3(x)|, \quad M_3 = \max_{\zeta\in[0,2]}(f^{(3)}(\zeta)) \quad \textit{and} \quad \omega_3(x) = \prod_{i=0}^{2}(x - x_i).$$

(3) (3 points) *Using the Taylor expansion of* $f(x)$ *around* $x_0 = 0$*, construct a smooth approximating polynomial,* $g_2(x)$ *of degree* 2*. What is the error* $|f(x) - g_2(x)|$*?*

Solution

(1) (7 points) Using Lagrange interpolation polynomials we have:

$$\begin{aligned} p_2(x) &= L_0(x)f(0) + L_1(x)f(1) + L_2(x)f(2) \\ &= \frac{1}{8}\left(e^{4a} - 2e^{2a} + 1\right)x^2 - \frac{1}{4}\left(e^{4a} - 4e^{2a} + 3\right)x. \end{aligned}$$

(2) (5 points) The n^{th} derivative of $e^{ax}-1$ is $f^{(n)}=a^n e^{ax}$.

$$\begin{aligned} E(a) &= \frac{M_3}{3!}|\omega_3(x)| \\ &= \frac{a^3e^{4a}}{3!}|x^3-6x^2+8x|. \end{aligned}$$

The polynomial $\omega_3(x)=x^3-6x^2+8x$ has extrema at $x=2\pm\frac{2}{\sqrt{3}}$ and value $|\omega_3(x)|=\frac{16}{3\sqrt{3}}$, hence the error bound reads:

$$E(a)=\frac{8a^3e^{4a}}{9\sqrt{3}}.$$

(3) (3 points) The Taylor expansion of $e^{ax}-1$ reads:

$$g_n(x)=\sum_{i=1}^{n}a^i\frac{x^i}{i!},$$

truncating it we get

$$g_2(x)=ax+a^2\frac{x^2}{2}.$$

The error $E_g(a) \coloneqq |f(x)-g_2(x)|$ is given by the truncation error, $|\sum_{i=3}^{\infty}\frac{(4a)^i}{i!}|$.

Problem 6. *(Numerical integration)*

15 points

Consider a function $f(x)$, $x\in[-1,1]$, which is approximated by a quadratic Lagrange interpolation polynomial, $p_2(x)$, with equidistant interpolation nodes, i.e. $x_0=-1$, $x_1=0$ and $x_2=1$. Construct the corresponding (closed) Newton-Cotes quadrature rule for the integral

$$I(f) \coloneqq \int_{-1}^{1} f(x)dx.$$

What is the order of exactness for the constructed quadrature rule?

Solution

(4 points) The function is approximated by a quadratic Lagrange polynomial, hence $n=2$ and $L_i=\prod_{\substack{j=0,\\ j\neq i}}^{2}\frac{x-x_j}{x_i-x_j}$. The Newton-Cotes quadrature is Simpson's (1/3) rule.

(4 points) The quadrature rule is given by

$$Q(f)=\sum_{i=0}^{i=2}W_if(x_i),$$

where

$$W_0=\int_{-1}^{1}\frac{x(x-1)}{2}dx=\frac{1}{3}.$$

Similarly, one can find that

$$W_1=\frac{4}{3}$$

and from symmetry $W_2 = W_0 = \frac{1}{3}$.
(4 points) The resulting rule reads: $Q(f) = \frac{1}{3}(f(-1) + 4f(0) + f(1))$.
(3 points) The level of exactness of Newton-Cotes formulae for n being even is $n+1$, in this case 3.

Problem 7. *(Boundary value problems)*

20 points

Consider the homogeneous Dirichlet boundary value problem

$$u_{xx} - 2u_x = f(x), \qquad 0 < x < 1$$
$$u(0) = 0,$$
$$u(1) = 0.$$

(1) (12 points) *Construct a central difference scheme such that* $u_x = \sum_{n=1}^{N} \alpha_n u(x_i) + \mathcal{O}(h^4)$, *i.e. a central difference scheme for the first derivative,* u_x, *that is* 4^{th} *order accurate.*
(2) (5 points) *Using the proposed scheme and second-order accurate central difference for* u_{xx} *write the algebraic form of the boundary value problem:*

$$A_h \mathbf{U} = \mathbf{f}.$$

Hint: *You may drop to lower order of accuracy near the boundaries.*

(3) (3 points) *What is the resulting order of consistency?*

Solution

(1) Multiple solutions available.

(4 points) We take the Taylor expansion of $u(x+h)$, $u(x-h)$ and $u(x+2h)$, $u(x-2h)$:

$$u(x+h) = \sum_{n=0}^{\infty} \frac{u^{(n)}(x)}{n!} h^n \tag{1}$$

$$u(x-h) = \sum_{n=0}^{\infty} \frac{u^{(n)}(x)}{n!} (-h)^n \tag{2}$$

$$u(x+2h) = \sum_{n=0}^{\infty} \frac{u^{(n)}(x)}{n!} (2h)^n \tag{3}$$

$$u(x-2h) = \sum_{n=0}^{\infty} \frac{u^{(n)}(x)}{n!} (-2h)^n \tag{4}$$

(4 points) Taking the linear combination 8((1)-(2)) − ((3)-(4)) we get the following 4^{th}-order accurate scheme:

$$u'(x) = \frac{-u(x+2h) + 8u(x+h) - 8u(x-h) + u(x-2h)}{12h} - 4\frac{h^4 u^{(5)}}{5!} + \mathcal{O}(h^6) \tag{5}$$

(4 points)

(2) We assume discretisation of space using $\mathrm{M}+2$ equidistant grid points, with $x_0 = 0, x_1 = h, \ldots, x_{\mathrm{M}+1} = 1$ and $h = \frac{1}{\mathrm{M}+1}$.
(2 points) Central differencing for the second derivative reads:

$$u_{xx} = \frac{u_{m-1} - 2u_m + u_{m+1}}{h^2}.$$

Assuming we drop to a 2^{nd} order accurate scheme for the first derivative on the neighbouring grid points of the boundaries, $m = 1$ and $m = \mathrm{M}$,

$$u_x = \frac{u_{m+1} - u_m}{2h},$$

we get the following scheme:

$$\frac{(1+h)U_0 - 2U_1 + (1-h)U_2}{h^2} = f_1$$

and

$$\frac{(1+h)U_{\mathrm{M}-1} - 2U_{\mathrm{M}} + (1-h)U_{\mathrm{M}+1}}{h^2} = f_{\mathrm{M}}$$

.
(2 points) On the internal grid points, x_m, with $m = 2, 3, \ldots, \mathrm{M}-1$, we use the constructed 4^{th}-order scheme, hence:

$$\frac{-\frac{h}{6}U_{m-2} + (1+\frac{8h}{6})U_{m-1} - 2U_i + (1-\frac{8h}{6})U_{m+1} + \frac{h}{6}U_{m+2}}{h^2} = f_m$$

(1 point) Taking into account the homogenious boundary conditions, we get:

$$\frac{1}{h^2}\begin{bmatrix} -2 & 1-h & & & & \\ 1+\frac{8h}{6} & -2 & 1-\frac{8h}{6} & \frac{h}{6} & & \\ -\frac{h}{6} & 1+\frac{8h}{6} & -2 & 1-\frac{8h}{6} & \frac{h}{6} & \\ & \ddots & \ddots & \ddots & \ddots & \ddots \\ & & -\frac{h}{6} & 1+\frac{8h}{6} & -2 & 1-\frac{8h}{6} \\ & & & & 1+h & -2 \end{bmatrix} \begin{bmatrix} U_1 \\ U_2 \\ U_3 \\ \vdots \\ U_{\mathrm{M}-1} \\ U_{\mathrm{M}} \end{bmatrix} = \begin{bmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \\ f_{\mathrm{M}-1} \\ f_{\mathrm{M}} \end{bmatrix}$$

(3) (3 points) The truncation error for any discretisation h is defined as:

$$\tau(h) \coloneqq A_h u + \frac{1}{4}f.$$

Considering the points x_m, with $m = 1$ and M, it reads:

$$\tau_m(h) = \frac{1}{h^2}((1+h)u_{m-1} - 2u_m + (1-h)u_{m+1}) - f_m.$$

The numerical scheme for the first and second derivatives is second-order accurate, i.e.

$$u_{xx}(x_m) = \frac{u(x_{m-1}) - 2u(x_m) + u(x_{m+1})}{h^2} - \frac{h^2}{12}u^{(4)} + \mathcal{O}(h^4)$$

and

$$u_x(x_m) = \frac{u(x_{m+1}) - u(x_{m-1})}{2h} - \frac{h^2}{6}u^{(3)} + \mathcal{O}(h^4).$$

Combining the three and the system, we get

$$\tau_m(h) = u_{xx_m} - 2u_{x_m} - f_m + \mathcal{O}(h^2) = \mathcal{O}(h^2).$$

Therefore, the system is second-order accurate.
Similar result is observed when checking the intermediate points.