MA2501

NUMERICAL METHODS

NTNU, SPRING 2023

Exam 1, 26-05-2023, 9:00–13:00

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: June 16, 2023.

Problem 1. *(LU decomposition)*

10 points

Verify that the matrices

$$M := \begin{pmatrix} 3 & 0 & 0 \\ 1 & 6 & 0 \\ 2 & 3 & 1 \end{pmatrix} \qquad \textit{and} \qquad N := \begin{pmatrix} 2 & 6 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

give a LU decomposition of the matrix

$$A := \begin{pmatrix} 6 & 18 & 3 \\ 2 & 12 & 1 \\ 4 & 15 & 3 \end{pmatrix}.$$

Use the LU decomposition of the matrix A to solve the linear system

$$Ax = (3, 19, 0)^T.$$

⋆ **Solution**:

• (2 points) We check that

$$MN = \begin{pmatrix} 3 & 0 & 0 \\ 1 & 6 & 0 \\ 2 & 3 & 1 \end{pmatrix} \begin{pmatrix} 2 & 6 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} = \begin{pmatrix} 6 & 18 & 3 \\ 2 & 12 & 1 \\ 4 & 15 & 3 \end{pmatrix} = A.$$

Next we want to find the solution of $Ax = (3, 19, 0)^T$.

• (2 points) First, we set

$$y = (y_1, y_2, y_3)^T := Nx.$$

• (3 points) Then we solve

$$My = (3, 19, 0)^T,$$

which gives: $y_1 = 1$, $y_2 = 3$, $y_3 = -11$.

• (3 points) Next we return to $y = Nx$ and solve for x

$$\begin{pmatrix} 2 & 6 & 1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} x = (1, 3, -11)^T,$$

which gives: $x_1 = -3$, $x_2 = 3$, $x_3 = -11$.

We may check that

$$A(-3, 3, -11)^T = \begin{pmatrix} 6 & 18 & 3 \\ 2 & 12 & 1 \\ 4 & 15 & 3 \end{pmatrix} (-3, 3, -11)^T = (3, 19, 0)^T.$$

Problem 2. *(Householder transformation)*

10 points

Given the 4×4 *matrix*

$$A = \begin{pmatrix} 0 & \mathbf{1}_3 \\ \alpha & 0 \end{pmatrix},$$

where $\alpha \in]0,1[$ *and* $\mathbf{1}_3$ *is the* 3×3 *unit-matrix. Find a Householder transformation* P *such that the* 4×4 *matrix*

$$\tilde{A} = PAP = \begin{pmatrix} 0 & 0 & 0 & 1 \\ \alpha & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

(Hint: consider the Householder transformation defined in terms of $p = (-\alpha, 0, \alpha)^T$*.)*

⋆ **Solution**: We are looking for a Householder transformation P mapping $x = (0,0,\alpha)^T$ to $y = (\alpha, 0, 0)^T$.

• (5 points) Ansatz: using the hint, the Householder transformation defined in terms of $p = x - y = (-\alpha, 0, \alpha)^T$ is

$$\tilde{P} = \mathbf{1}_3 - 2\frac{pp^T}{p^T p} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}.$$

• (4 points) Then we define the 4×4 matrix

$$P := \begin{pmatrix} 1 & 0_3^T \\ 0_3 & \tilde{P} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}$$

where $0_3^T := (0,0,0)$.

• (1 point) Then we verify that indeed

$$PAP = \begin{pmatrix} 0 & 0 & 0 & 1 \\ \alpha & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{pmatrix}.$$

Problem 3. *(Initial value problems)*

10 points

(1) (2 points)

Consider the following system of ordinary differential equations:

$$u_1^{(2)}(t) - t^2 + u_1^{(1)}(t) + u_2^2(t) = 0$$
$$u_2^{(2)}(t) - t - u_2^{(1)}(t) - u_1^3(t) = 0,$$

with initial values $u_1(0) = 0$, $u_2(0) = 1$, $u_1^{(1)}(0) = 1$, $u_2^{(1)}(0) = 0$. *Transform it into a first order initial value problem.*

(2) (8 points)

Suppose that $f(t, y)$ *satisfies a Lipschitz condition in the* y*-variable, on* $[t_0, T] \times \mathbb{R}^d$, *with Lipschitz constant* L. *Consider the 2nd-order Runge–Kutta method*

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

with

$$k_1 = f(t, y)$$
$$k_2 = f(t + h, y + hk_1)$$
$$\Phi(t, y; h) = \frac{1}{2}(k_1 + k_2).$$

i) Write down the Butcher tableau.

ii) Show that the function Φ *also satisfies a Lipschitz condition for* $t + h \in [t_0, T]$ *and*

iii) determine the respective Lipschitz constant $\tilde{L}$.

⋆ **Solution**:

(3.1)

• (1 point) Define

$$y_1(t) := u_1(t) \qquad y_2(t) := u_2(t) \qquad y_3(t) := u_1^{(1)}(t) \qquad y_4(t) := u_2^{(1)}(t).$$

• (1 point) Then the linear system

$$(y_1^{(1)}(t), y_2^{(1)}(t), y_3^{(1)}(t), y_4^{(1)}(t))^T = \begin{pmatrix} y_3(t) \\ y_4(t) \\ -y_2^2(t) - y_3(t) + t^2 \\ y_1^3(t) + y_4(t) + t \end{pmatrix}.$$

with initial values

$$(y_1(0), y_2(0), y_3(0), y_4(0))^T = (0, 1, 1, 0)^T$$

is a first order initial value problem.

(3.2)

i) Butcher tableau:

• (1 point)

$$\begin{array}{c|cc} c_1 & a_{11} & a_{12} \\ c_2 & a_{21} & a_{22} \\ \hline & b_1 & b_2 \end{array} = \begin{array}{c|cc} 0 & 0 & 0 \\ 1 & 1 & 0 \\ \hline & 1/2 & 1/2 \end{array}$$

ii) Lipschitz condition for $t + h \in [t_0, T]$:

• (2 points) Consider $k_i = k_i(t, y; h)$ and $k'_i = k'_i(t, y'; h)$, for $i = 1, 2$. Then

$$k_1 - k'_1 = f(t, y) - f(t, y')$$

and

$$k_2 - k'_2 = f(t + h, y + hk_1) - f(t + h, y' + hk'_1).$$

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

$$||k_1 - k'_1|| = ||f(t, y) - f(t, y')|| \leq L||y - y'||$$

and

$$\begin{aligned} ||k_2 - k'_2|| &= ||f(t + h, y + hk_1) - f(t + h, y' + hk'_1)|| \\ &\leq L||y - y' + h(k_1 - k'_1)) \\ &\leq L(1 + hL)||y - y'||. \end{aligned}$$

• (2 points) This implies that

$$\begin{aligned} ||\Phi(t, y; h) - \Phi(t, y'; h)|| &= \frac{1}{2}||(k_1 - k'_1) + (k_2 - k'_2)|| \\ &\leq \frac{1}{2}\big(L + L(1 + hL)\big)||y - y'|| \\ &\leq (L + \frac{h}{2}L^2)||y - y'||. \end{aligned}$$

iii) Lipschitz constant for Φ

• (1 point)

$$\tilde{L} = L + \frac{h}{2}L^2$$

Problem 4. *(Norms)*

20 points

We consider a non-singular $n \times n$ matrix $A = (a_{rs})_{\substack{1\leq r\leq n \\ 1\leq s\leq n}}$ with entries in $\mathbb{R}$, which satisfies

$$\sum_{q=1}^{n} |a_{jq}| = 1,$$

for every $j = 1, \dots, n$. Show that for every invertible diagonal matrix $D \in \mathbb{R}^{n\times n}$ the following holds

$$\kappa(A) \leq \kappa(DA).$$

Here, κ is the condition number defined with respect to the ∞-norm ($\|A\|_\infty = \max_{1\leq j\leq n}(\sum_{q=1}^{n}|a_{jq}|)$).

⋆ **Solution**:

Denote the $n \times n$ diagonal matrix $D = \mathrm{diag}(d_1, d_2, \dots, d_n)$.

• (5 points) Compute

$$||DA||_\infty = \max_{1\leq i\leq n}\Big(\sum_{k=1}^{n}|d_i|\;|a_{ik}|\Big) = \max_{1\leq i\leq n}\Big(|d_i|\;\sum_{k=1}^{n}|a_{ik}|\Big) = \max_{1\leq i\leq n}\big(|d_i|\big).$$

Here we used that $\sum_{q=1}^{n} |a_{rq}| = 1$, for all $1 \leq r \leq n$.

• (10 points) As A is a non-singular matrix, we denote its inverse $A^{-1} = (b_{rs})_{\substack{1\leq r\leq n\\ 1\leq s\leq n}}$. Note that D is supposed to be invertible, i.e., $d_r \neq 0$, for all $1 \leq r \leq n$. Then

$$\begin{aligned} ||(DA)^{-1}||_\infty &= ||A^{-1}D^{-1}||_\infty \\ &= \max_{1\leq i\leq n} \left(\sum_{k=1}^{n} |b_{ik}| \, |\frac{1}{d_k}| \right) \\ &\geq \frac{||A^{-1}||_\infty}{\max_{1\leq i\leq n} |d_i|}. \end{aligned}$$

• (5 points) From this we deduce:

$$\begin{aligned} \kappa(DA) &= ||DA||_\infty ||(DA)^{-1}||_\infty \\ &\geq ||A||_\infty ||A^{-1}||_\infty = \kappa(A). \end{aligned}$$

Problem 5. *(Lagrange interpolation)*

15 points

Consider the function $f(x) = \ln(ax + 1)$ with $x \geq 0$, where a is a real, positive number.

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

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

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

(Reminder: The interpolation error bound is given by $|f(x) - p_2(x)| = \frac{M_3}{3!}|\omega_3(x)|$, $M_3 = \max_{\zeta\in[0,2]}(f^{(3)}(\zeta))$ and $\omega_3(x) = \prod_{i=0}^{2}(x - x_i)$.)

(3) (3 points) *Consider interpolation with a larger number of equidistant nodes ($n \gg 2$) in the interval $[0, 2]$. Under which condition for the coefficient "a" is the error bound $E(a, n) := |f(x) - p_n(x)|$ guaranteed to decrease?*

⋆ **Solution**:

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

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

(2) (5 points) The n^{th} derivative of $\ln(ax + 1)$ is $f^{(n)} = (-1)^{n-1}\frac{(n-1)!a^n}{(ax+1)^n}$.

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

The polynomial $\omega_3(x) = x^3 - 3x^2 + 2x$ has extrema at $x = 1 \pm \frac{1}{\sqrt{3}}$ and value $|\omega_3(x)| = \frac{2}{3\sqrt{3}}$, hence the error bound reads:

$$E(a) = \frac{2a^3}{9\sqrt{3}}$$

(3) (3 points) As we indefinitely increase the number of equidistant interpolation nodes the error bound reads:

$$\begin{aligned} E(a) &= \lim_{n\to\infty} \frac{M_{n+1}}{(n+1)!}|\omega_{n+1}(x)| \\ &= \lim_{n\to\infty} \frac{n!a^{n+1}}{(n+1)!}|\omega_{n+1}(x)| \\ &= \lim_{n\to\infty} \frac{a^{n+1}}{n+1}2^{n+1} \\ &= \lim_{n\to\infty} \frac{(2a)^{n+1}}{n+1} \end{aligned}$$

Using l'Hospital's rule the limit exists, and is equal to 0, iff $a \leq \frac{1}{2}$.

Problem 6. *(Numerical integration)*

15 points

Consider an integral of the form $I(f) := \int_0^1 f(x)dx$. The Gaussian quadrature rule for said integral reads:

$$Q_n(f) := \sum_{i=0}^{n} W_i f(x_i),\ n \geq 0$$

(1) (5 points) *If $\{\phi_0, \phi_1, \phi_2\}$ is a system of orthogonal polynomials on (a,b) with respect to $w(x) \equiv 1$, and $\phi_0 \equiv 1$, construct ϕ_2 and find the corresponding quadrature nodes x_0, x_1.*

(2) (5 points) *Calculate the first 2 quadrature weights W_0, W_1 and construct the quadrature rule $Q_1(f)$.*

(3) (5 points) *Using the constructed quadrature rule and $f(x) = \sqrt{3}x^3 - x^2$, calculate the integral*

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

.

⋆ **Solution**:

(1) (5 points) Using the Gram-Schmidt method, we construct the orthogonal polynomials:

$$\phi_1(x) = x - a_0\phi_0(x), \qquad \phi_2(x) = x^2 - b_1\phi_1(x) - b_0\phi_0(x)$$

with $a_0 = \frac{\langle x,\phi_0\rangle}{\langle \phi_0,\phi_0\rangle} = \frac{1}{2}$. Hence, $\phi_1(x) = x - \frac{1}{2}$.
Similarly, we find $b_0 = \frac{1}{3}$ and $b_1 = 1$, resulting in $\phi_2(x) = x^2 - x + \frac{1}{6}$.
The quadrature nodes are the roots of $\phi_2(x)$, or $x_{0,1} = \frac{1}{2} \pm \sqrt{\frac{1}{12}}$.

(2) (5 points) The quadrature weights read:

$$W_i = \int_0^1 L_i^2(x)dx$$

Using the quadrature nodes $x_{0,1}$ we get:

$$W_0 = W_1 = \frac{1}{2}$$

and the quadrature rule reads:

$$Q_1(f) = \frac{1}{2} f\left(\frac{1}{2} - \sqrt{\frac{1}{12}}\right) + \frac{1}{2} f\left(\frac{1}{2} + \sqrt{\frac{1}{12}}\right)$$

(3) (5 points) Using a change of interval we move from $x \in [-1, 1]$ to $\xi \in [0, 1]$:

$$x = 2\xi - 1$$

Starting from $\xi_{0,1} = \frac{1}{2} \pm \sqrt{\frac{1}{12}}$, the new quadrature nodes are $x_{0,1} = 2\xi_{0,1} - 1 = \pm\frac{1}{\sqrt{3}}$ and based on the constructed quadrature rule we get:

$$\begin{aligned}\int_{-1}^{1} f(x)dx &= \int_0^1 f(2\xi - 1)2d\xi \\ &\approx 2\left(W_0 f\left(-\frac{1}{\sqrt{3}}\right) + W_1 f\left(\frac{1}{\sqrt{3}}\right)\right) \\ &= -\frac{2}{3}\end{aligned}$$

Problem 7. *(Boundary value problems)*

20 points

Consider the Dirichlet boundary value problem

$$\begin{aligned}-4u_{xx} + 16u &= f(x), \qquad 0 < x < 1 \\ u(0) &= 0, \\ u(1) &= 0.\end{aligned}$$

(1) (7 points) *Using central difference schemes, construct the finite difference method:*

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

(2) (3 points) *What is the order of accuracy of the resultant system? In other words, what is the order of the truncation error?*

(3) (10 points) *Prove that the discretised system is stable in the 2-norm. You may use, without proof, that the following holds:*

The eigenvalues of a tridiagonal matrix of size $M \times M$,

$$A = \begin{bmatrix} a & b & & & \\ c & a & b & & \\ & \ddots & \ddots & \ddots & \\ & & c & a & b \\ & & & c & a \end{bmatrix},$$

read

$$\lambda_m = a + 2\sqrt{bc}\cos\phi_m, \qquad \phi_m = \frac{m\pi}{M+1},$$

for $m = 1, \dots, M$.

⋆ **Solution**:

(1) (7 points) The problem can also be written as

$$\begin{aligned} u_{xx} - 4u &= -\frac{1}{4} f(x), \qquad 0 < x < 1 \\ u(0) &= 0, \\ u(1) &= 0 \end{aligned}$$

Assuming $M+2$ equidistant grid points, with $x_0 = 0, x_1 = h, \dots, x_{M+1} = 1$ and $h = \frac{1}{M+1}$, the central difference scheme for the second derivative reads:

$$u_{xx}(x_m) \approx \frac{u(x_{m-1}) - 2u(x_m) + u(x_{m+1})}{h^2}.$$

Then A_h is the $M \times M$ tridiagonal matrix, $A_h = \frac{1}{h^2}\text{tridiag}_{\text{M}\times\text{M}}(2, -4h^2 - 1, 2)$. The unknown is $\mathbf{U} \coloneqq [U_1, U_2, \dots, U_M]^\intercal$, and the source term is $\mathbf{F} \coloneqq -\frac{1}{4}\left[F_1, F_2, \dots, F_M\right]^\intercal$.

(2) (3 points) The truncation error for any discretisation h is defined as:

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

For any specific point, x_m, it reads:

$$\tau_m(h) = \frac{1}{h^2}(u_{m-1} - (2 - 4h^2)u_m + u_{m+1}) + \frac{1}{4} f.$$

The numerical scheme for the second derivative is second-order accurate, i.e.

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

Combining the two and the system, we get

$$\tau_m(h) = u_{xx_m} - 4u_m + \frac{1}{4} f + \mathcal{O}(h^2) = \mathcal{O}(h^2).$$

Therefore, the system is second-order accurate.

(3) (10 points) The tridiagonal matrix A_h has non-zero diagonal and $bc > 0$. It has M distinct eigenvalues that read:

$$\lambda_m = a + 2\sqrt{bc}\cos\left(\frac{m\pi}{M+1}\right) = \frac{2}{h^2}\left(-1 - 2h^2 + \cos\left(m\pi h\right)\right).$$

Taking the Taylor expansion of $\cos(x)$ around 0, $\cos(x) = 1 - \frac{x^2}{2} + \frac{x^4}{4!} + \mathcal{O}(h^6)$ and plugging it in the eigenvalue expression, we get:

$$\lambda_m = -4 - m^2\pi^2 + \mathcal{O}(h^2).$$

Moreover, A_h is symmetric, hence $\|A_h\|_2 = \rho(A_h) = \max_{\lambda\in\sigma(A_h)}|\lambda|$. For A_h^{-1} we have

$$\|A_h^{-1}\|_2 = \max_{\lambda\in\sigma(A_h)} |\lambda^{-1}| = \frac{1}{\min_{\lambda\in\sigma(A_h)}|\lambda|} = \frac{1}{4 + \pi^2 + \mathcal{O}(h^2)}$$

and as $h \to 0$, $\|A_h^{-1}\|_2 = \frac{1}{4+\pi^2}$. So, there exists a $C > 0$ and $H > 0$, such that for any $h < H$, $\|A_h^{-1}\|_2 < C$, proving stability of the discretised system in the 2-norm.