Final exam, Numerical Analysis (WISB251)

Tuesday, 11 April 2023, 17:00-20:00, BBG 023, 061

- Write your name on each page you turn in, and additionally, on the first page, write your student number and the *total number of pages submitted.*
- You may use one A4 sheet with notes while working the problems.
- For each question, motivate your answer. You may make use of results from previous subproblems, even if you have been unable to prove them.
- The maximum number of points per subproblem are given between square brackets. Your grade is the total earned points divided by 4. The final exam weighs 50% in your grade for the course.

`Solution.` In small type-font letters.

Problem 1. [*Nonlinear systems of algebraic equations*]

Consider the following system of nonlinear equations for x and y. Write $r = (x, y)^T$.

$$f(r) = \begin{pmatrix} x + \frac{1}{2}y - \frac{\pi}{2} \\ y - \frac{1}{2}\sin(x + \frac{1}{2}y) \end{pmatrix} = 0$$

Suppose we attempt to solve this system using the fixed point iteration

$$r_{k+1} = r_k - \alpha f(r_k).$$

(a) [2pts] Find (by hand) a solution $r^* = (x^*, y^*)^T$, $f(r^*) = 0$ of the nonlinear system.

[2] Solution. From $f(r^*) = 0$ we find $x^* + \frac{1}{2}y^* = \frac{\pi}{2}$ and $y^* = \frac{1}{2}\sin(\frac{\pi}{2}) = \frac{1}{2}$, whence $x^* = \frac{\pi}{2} - \frac{1}{4}$.

(b) [4pts] What is the Jacobian matrix $f'(r^*) = Df(r^*)$ at r^*? What are its eigenvalues?

[4] Solution. The Jacobian matrix is

$$f'(r^*) = \begin{bmatrix} \frac{\partial f_1}{\partial x} & \frac{\partial f_1}{\partial y} \\ \frac{\partial f_2}{\partial x} & \frac{\partial f_2}{\partial y} \end{bmatrix}(r^*) = \begin{bmatrix} 1 & \frac{1}{2} \\ -\frac{1}{2}\cos\frac{\pi}{2} & 1 - \frac{1}{4}\cos\frac{\pi}{2} \end{bmatrix} = \begin{bmatrix} 1 & \frac{1}{2} \\ 0 & 1 \end{bmatrix}.$$

The eigenvalues are $\lambda_1 = \lambda_2 = 1$.

(c) [4pts] For what range of values α does the fixed-point iteration converge to r^*?

[4] Solution. The fixed point iteration is $r_{k+1} = g(r_k)$, where $g(r) = r - \alpha f(r)$. The Jacobian of g at the fixed point r^* is

$$g'(r^*) = I - \alpha f'(r^*) = \begin{bmatrix} 1-\alpha & -\frac{1}{2}\alpha \\ 0 & 1-\alpha \end{bmatrix}.$$

Its eigenvalues are $\mu_1 = \mu_2 = 1 - \alpha$. The fixed point r^* is stable if $|\mu_i| < 1$ for $i = 1, 2$. For this we need $0 < \alpha < 2$.

Problem 2. [*Numerical integration*]

We wish to approximate the definite integral

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

using the values $f(c)$ and $f(-c)$ for $0 < c \leq 1$.

(a) [3pt] Construct the interpolating polynomial $p(x)$ through the points $(c, f(c))$ and $(-c, f(-c))$.

[3] Solution. The Newton divided difference formula gives $p(x) = f[-c] + f[-c, c](x + c)$. Using Lagrange polynomials, one finds $p(x) = \frac{1}{2c}\left[f(c)(x + c) - f(-c)(x - c)\right]$.

(b) [2pt] Show that the associated quadrature formula is given by

$$\bar{I} = \int_{-1}^{1} p(x)\, dx = f(c) + f(-c).$$

[2] Solution. Integrating the expression for $p(x)$ gives

$$\bar{I} = \int_{-1}^{1} f[-c] + f[-c, c](x + c)\, dx = f(-c)\int_{-1}^{1} dx + \frac{f(c) - f(-c)}{c - (-c)}\int_{-1}^{1}(x + c)\, dx = f(-c) + f(c).$$

(c) [3pt] Derive an expression for the error $E = I - \bar{I}$ for the case $f(x)$ is a polynomial of degree n.

[3] Solution. Because the limits of integration are symmetric about x=0, the uneven monomials integrate to zero ($\int_{-1}^{1} x^k\, dx = 0$ for uneven k.) Without loss of generality, assume n is even. Let $f(x) = a_0 + a_1 x + a_2 x^2 + \ldots a_n x^n$. Then

$$I = \int_{-1}^{1} f(x)\, dx = 2a_0 + \frac{2}{3}a_2 + \cdots + \frac{2}{n+1}a_n$$

For the approximant,

$$\bar{I} = f(-c) + f(c) = 2a_0 + 2a_2c^2 + 2a_4c^4 + \cdots + 2a_nc^n$$

(again, uneven monomials terms vanish). The error is

$$E = (\frac{2}{3} - 2c^2)a_2 + (\frac{2}{5} - 2c^4)a_4 + \ldots (\frac{2}{n+1} - 2c^n)a_n = 2\sum_{k=1}^{n/2}(\frac{1}{2k+1} - c^{2k})a_{2k}.$$

(d) [2pt] The formula is exact for polynomials up to a certain degree n. For what carefully chosen value of c can you maximize this degree n?

[2] Solution. The formula is exact for polynomials up to $n = 1$. By choosing $c = \frac{1}{\sqrt{3}}$ the formula is exact for polynomials up to $n = 3$.

Problem 3. [*Numerical integration of ODEs*]

Consider the following numerical method for solving an initial value problem $y'(t) = f(y(t))$, $y(0) = y_0$, $y(t) \in \mathbf{R}^d$, $f : \mathbf{R}^d \to \mathbf{R}^d$, $t \in [0, T]$:

$$y_{n+1} = y_n + hf\left((1-\theta)y_n + \theta y_{n+1}\right),$$

where $y_n \approx y(t_n)$, $n = 0, \ldots, N$, $t_n = nh$, $h = T/N$.

(a) [5pts] Determine the truncation error for this method in the form

$$\text{trunc. error} = Ch^q + \mathcal{O}(h^{q+1})$$

(i.e. determine q and and expression for C). What choice of θ gives the best accuracy? (*Hint:* Define $\bar{y}(t) = (1-\theta)y(t) + \theta y(t+h)$, and derive the Taylor expansion of $\bar{y}(t)$ about $y(t)$. Then determine the Taylor expansion of $f(\bar{y}(t))$ about $y(t)$.)

[5] Solution. For $y(t)$ a solution of the differential equation, Taylor expansion of $y(t+h)$ gives

$$\begin{aligned} y(t+h) &= y(t) + hy'(t) + \frac{h^2}{2}y''(t) + \frac{h^3}{6}y'''(t) + \mathcal{O}(h^4) \\ &= y(t) + hf(y) + \frac{h^2}{2}f'(y)f(y) + \frac{h^3}{6}(f'(y)f'(y)f(y) + f''(y)(f(y(t)), f(y)) + \mathcal{O}(h^4), \end{aligned}$$

where all terms on the right are evaluated at $y(t)$ and using shorthand notation:

$$f'f = \sum_j \frac{\partial f_i}{\partial y_j} f_j, \qquad f'f'f = \sum_{j,k} \frac{\partial f_i}{\partial y_j}\frac{\partial f_j}{\partial y_k} f_k, \qquad f''(f,f) = \sum_{j,k} \frac{\partial^2 f_i}{\partial y_j \partial y_k} f_j f_k.$$

Using the above, the expansion of $\bar{y}(t)$ is

$$\bar{y}(t) = y(t) + \theta h f(y(t)) + \theta\frac{h^2}{2}f'(y(t))f(y(t)) + \mathcal{O}(h^3).$$

Now expanding $f(\bar{y}(t)$ gives

$$f(\bar{y}(t)) = f(y(t)) + f'(y(t))\left[\theta hf(y(t)) + \theta\frac{h^2}{2}f'(y(t))f(y(t))\right] + f''(y(t))(\theta hf(y(t)), \theta hf(y(t))) + \mathcal{O}(h^3).$$

Substituting the above expansions into the formula for the method:

$$\text{trunc. error} = y(t+h) - y(t) - hf(\bar{y}(t)) = (\frac{1}{2} - \theta)h^2 f'(y(t))f(y(t)) + \mathcal{O}(h^3)$$

Consequently we can bound the truncation error by Ch^2 where

$$C = (\frac{1}{2} - \theta)\max\|y''(t)\|.$$

Choosing $\theta = \frac{1}{2}$ improves the truncation error to $\mathcal{O}(h^3)$.

(b) [3pts] Compute the stability function $R(z)$ such that $y_{n+1} = R(h\lambda)y_n$ when the method is applied to the test problem $y'(t) = \lambda y(t)$ for λ a complex number.

[3] Solution. Applying the method to $y' = \lambda y$ gives

$$y_{n+1} = y_n + h\lambda((1-\theta)y_n + \theta y_{n+1})$$

Solving for y_{n+1} yields

$$y_{n+1} = R(h\lambda)y_n, \qquad R(z) = \frac{1 + (1-\theta)z}{1 - \theta z}.$$

(c) [2pts] Sketch the stability regions $S = \{z \in \mathbb{C}; |R(z)| < 1\}$ for $\theta = 0$, $\theta = 1$, and $\theta = 1/2$.

[2] Solution. The stability regions are those of ($\theta = 0$) Euler's (explicit) method (i.e. the unit disc centered at $z = -1$ in the complex plane); ($\theta = 1$) the Implicit Euler method (everything outside the unit disc centered at $z = +1$); and Trapezoidal Rule (precisely $\mathbb{C}^-$.)

Problem 4. [*Numerical differentiation formula*]

In some applications it is necessary to evaluate a numerical difference formula at the midpoint between two nodes.

(a) [2pts] Write the Newton divided difference polynomial $p_1(x)$ for the points $(x_0, f(x_0))$ and $(x_1, f(x_1))$ with $x_1 = x_0+h$, and give an expression for the error $e(x) = f(x)-p_1(x)$.

[2] Solution. The divided difference formula is

$$p_1(x) = f[x_0] + f[x_0, x_1](x - x_0)$$

The error is

$$f(x) - p_1(x) = f[x_0, x_1, x](x - x_0)(x - x_1).$$

(b) [3pts] Show that the approximation of the derivative $f'(x) = p_1'(x)$ is given by the difference formula

$$f'(x) \approx \frac{f(x_0 + h) - f(x_0)}{h},$$

(independent of x) and derive an upper bound on the error $e'(x) = f'(x) - p_1'(x)$ for $x \in [x_0, x_1]$.

[3] Solution. The differentiation formula is given by the derivative of $p_1(x)$:

$$p_1'(x) = f[x_0, x_1] = \frac{f(x_1) - f(x_0)}{x_1 - x_0} = \frac{f(x_0 + h) - f(x_0)}{h}.$$

Differentiating the error formula gives

$$e'(x) = f[x_0, x_1, x, x'](x - x_0)(x - x_1) + f[x_0, x_1, x](x - x_0 + x - x_1)$$

This can be bounded by

$$|e'(x)| \leq \frac{|f'''(\xi)|}{3!}h^2 + \frac{|f''(\eta)|}{2!}h, \qquad \xi, \eta \in [x_0, x_1].$$

(c) [2pts] By directly expanding $f(x_0+h)$ in a Taylor series about x_0, derive an error bound for the above difference formula at x_0.

[2] Solution. Taylor gives

$$f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2}f''(\zeta), \qquad \zeta \in [x_0, x_1].$$

Substitution yields

$$\left| \frac{f(x_0 + h) - f(x_0)}{h} - f'(x_0) \right| \leq \frac{h}{2}|f''(\zeta)|.$$

(d) [3pts] Instead, expand both $f(x_0 + h)$ and $f(x_0)$ in a Taylor series about the midpoint $\widehat{x} = x_0 + \frac{h}{2}$, and derive an error bound for the difference formula at $\widehat{x}$. How does the error of the approximation at the midpoint compare with your earlier bounds?

[3] `Solution.` `Here, Taylor gives`

$$f(\widehat{x} \pm \frac{h}{2}) = f(\widehat{x}) \pm \frac{h}{2} f'(\widehat{x}) + \frac{h^2}{8} f''(\widehat{x}) \pm \frac{h^3}{48} f'''(\widehat{x}) + \mathcal{O}(h^4), \qquad \zeta' \in [x_0, x_1].$$

`Subtracting and dividing by` h `gives`

$$\frac{f(x_0 + h) - f(x_0)}{h} = f'(\widehat{x}) + \frac{h^2}{24} f'''(\widehat{x}) + \mathcal{O}(h^4).$$

`So the error is` $\mathcal{O}(h^2)$ `at the midpoint.`