INDIAN INSTITUTE OF TECHNOLOGY GUWAHATI
DEPARTMENT OF MATHEMATICS

MA 322: SCIENTIFIC COMPUTING

Mid-Semester Examination (Answer Key), Semester II, Academic Year 2022-23

Duration: 120 minutes **Total Marks: 30**

1. (**Choose the correct option(s)**) Assume $f : \mathbb{R} \to \mathbb{R}$ is a twice continuously differentiable function such that $f(x) = f(x+T)$, $\forall x \in \mathbb{R}$ and $T > 0$. The quadrature formula

$$\frac{1}{T}\int_1^{T+1} f(x)\mathrm{d}x \approx \frac{1}{n}\sum_{j=1}^{n} f(x_j),$$

where $x_j (j = 0, 1, \ldots n)$ are $n+1$ equidistant nodes, is exact for

(a) every piecewise linear function $f(x)$,
(b) every piecewise constant function $f(x)$,
(c) every linear function $f(x)$
(d) none of the above.

[2]

Answer: Piecewise functions are not differentiable; every linear function is not periodic. Therefore, the correct option is **(d)**.

2. If we interpolate the function $f(x) = e^{2x-3}$ with a polynomial p_n of degree 11 using 12 nodes in $[-3/2, 3/2]$, what is a good upper bound for $|f(x) - p_n(x)|$ on $[-3/2, 3/2]$? **[2]**

Answer:

$$|f(x) - p_n(x)| = \left|\frac{1}{(n+1)!}\prod_{j=0}^{n}(x - x_j) f^{(n+1)}(\eta)\right|, \qquad \eta \in [x_0, x_n]$$

$$\therefore \max_{x_n \le x \le x_n} |f(x) - p_n(x)| = \max_{\substack{x_n \le x \le x_n \\ x_0 \le \eta \le x_n}} \left|\frac{1}{(n+1)!}\prod_{j=0}^{n}(x - x_j) f^{(n+1)}(\eta)\right|.$$

$$\Rightarrow \max_{x_n \le x \le x_n} |f(x) - p_n(x)| \le \frac{1}{(n+1)!}\max_{x_0 \le \eta \le x_n} |f^{(n+1)}(\eta)| \max_{x_n \le x \le x_n}\left|\prod_{j=0}^{n}(x - x_j)\right|.$$

For $f(x) = e^{2x-3}$,

$$f^{(n+1)}(x) = 2^{(n+1)} f(x), \quad \text{and} \quad \max_{x_n \le x \le x_n} |f(x)| = 1.$$

$$\therefore \max_{x_n \le x \le x_n} |f(x) - p_n(x)| \le \frac{2^{(n+1)}}{(n+1)!} M_{n+1}, \quad M_{n+1} :=| \max_{x_0 \le x \le x_n} \left| \prod_{j=0}^{n} (x - x_j) \right|.$$

For $n = 11$,

$$\max_{x_n \le x \le x_1 1} |f(x) - p_1 1(x)| \le \frac{2^{12}}{12!} M_{12}, \quad M_{12} :=| \max_{x_0 \le x \le x_n} \left| \prod_{j=0}^{11} (x - x_j) \right|.$$

The desired upper bound is $\frac{2^{12}}{12!} M_{12}$.

3. Does there exist a quadrature formula

$$\int_0^\infty f(x) e^{-x} \mathrm{d}x \approx w_1 f(2 - \sqrt{2}) + w_2 f(2 + \sqrt{2})$$

that is exact for polynomials of degree $\le n (\in \mathbb{N})$? If yes, find the weights w_1 and w_2. Determine the degree of precision of the quadrature rule — **show detailed calculations and justify your claim**. **[8]**

Answer: We know (you have to prove this),

$$\int_0^\infty x^n e^{-x} \mathrm{d}x = n!, \quad n \ge 0.$$

Therefore, for $f(x) = x^0$, we have from the quadrature formula

$$w_1 + w_2 = 1,$$

and, for $f(x) = x$, we have from the quadrature formula

$$w_1(2 - \sqrt{2}) + w_2(2 + \sqrt{2}) = 1.$$

Solving these two equations we obtain

$$w_1 = \frac{2 + \sqrt{2}}{4}, \quad w_2 = \frac{2 - \sqrt{2}}{4}.$$

For $f(x) = x^2$,

$$w_1(2-\sqrt{2})^2 + w_2(2+\sqrt{2})^2 = \frac{2+\sqrt{2}}{4}(2-\sqrt{2})^2 + \frac{2-\sqrt{2}}{4}(2+\sqrt{2})^2 = \frac{1}{2}(2-\sqrt{2}+2+\sqrt{2}) = 2.$$

For $f(x) = x^3$,

$$w_1(2-\sqrt{2})^3 + w_2(2+\sqrt{2})^3 = \frac{2+\sqrt{2}}{4}(2-\sqrt{2})^3 + \frac{2-\sqrt{2}}{4}(2+\sqrt{2})^3 = \frac{1}{2}(6-4\sqrt{2}+6+4\sqrt{2}) = 6.$$

For $f(x) = x^4$,

$$w_1(2-\sqrt{2})^4 + w_2(2+\sqrt{2})^4 = \frac{2+\sqrt{2}}{4}(2-\sqrt{2})^4 + \frac{2-\sqrt{2}}{4}(2+\sqrt{2})^4 = 20.$$

Therefore, the quadrature formula is exact for x^n, $n \le 3$, but not for x^4. **Therefore, the degree of precision is** 3.

4. Determine the value of (a, b, c) that makes the function

$$f(x) = \begin{cases} x^3, & x \in [0,1]. \\ \frac{1}{2}(x-1)^3 + a(x-1)^2 + b(x-1) + c, & x \in [1,2] \end{cases}$$

a cubic spline. Is it a natural cubic spline? **[4]**

Answer: For $f(x)$ to be a cubic spline on $[0, 2]$ is required to satisfy,

- $f(x)$ is a cubic polynomial on each of the sub-intervals $[0, 1]$ and $[1, 2]$.
- $f(x)$ is continuous at the knot $x = 1$.
- $f'(x)$ is continuous at the knot $x = 1$.
- $f''(x)$ is continuous at the knot $x = 1$.

Furthermore, it is a natural cubic spline if $f''(0) = 0 = f''(2)$.
Let us denote,

$$f(x) = \begin{cases} S_1(x), & x \in [0,1]. \\ S_2(x), & x \in [1,2] \end{cases}$$

First condition is satisfied as $S_1(x)$ and $S_2(x)$ are cubic polynomials. Second condition,

$$\lim_{x \to 1^-} S_1(x) = \lim_{x \to 1^+} S_2(x) \Rightarrow c = 1.$$

Third condition,

$$\lim_{x \to 1^-} \frac{S_1(x) - S_1(1)}{x-1} = \lim_{x \to 1^+} \frac{S_2(x) - S_2(1)}{x-1} \Rightarrow b = 3,$$

where

$$S_1'(x) = \begin{cases} 0, & x = 0. \\ 3x^2, & x \in (0,1) \\ 3, & x = 1 \end{cases}$$

and

$$S_2'(x) = \begin{cases} 3, & x = 1. \\ \frac{3}{2}(x-1)^2 + 2a(x-1) + 3, & x \in (1,2) \\ \frac{3}{2} + 2a + 3, & x = 1 \end{cases}$$

Fourth condition,

$$\lim_{x \to 1^-} \frac{S_1'(x) - S_1'(1)}{x-1} = \lim_{x \to 1^+} \frac{S_2'(x) - S_2'(1)}{x-1} \Rightarrow a = 3,$$

Now,

$$f''(0) = \lim_{x \to 0^+} \frac{S_1'(x) - S_1'(0)}{x-0} = 0,$$

and

$$f''(2) = \lim_{x \to 2^-} \frac{S_2'(x) - S_2'(0)}{x-2} = 3 + 2a = 9 \neq 0.$$

Therefore, it is not a natural cubic spline.

5. Approximate

$$\int_0^1 e^x \mathrm{d}x$$

using Trapezoidal rule using 5 nodes. Determine the relative error. Compare your results with the approximation obtained using corrected trapezoidal rule. **[4]**

Answer: We have (correct up to six decimal places),

$$I(f) = \int_0^1 e^x \mathrm{d}x = e - 1 = 1.718282.$$

Using 5-point trapezoidal rule (correct up to six decimal places),

$$I_n(f) = \frac{1/4}{2}\left[e^1 + e^0 + 2\left(e^{1/4} + e^{1/2} + e^{3/4}\right)\right] = 1.727222.$$

Relative error (correct up to six decimal places),

$$\left|\frac{I(f) - I_n(f)}{I(f)}\right| = 0.005203.$$

Corrected trapezoidal rule (correct up to six decimal places),

$$CT_n(f) - I_n(f) - \frac{h^2}{12}[f'(1) - f'(0)] = 1.727222 - \frac{1}{192}(e-1) = 1.718272.$$

Therefore, the relative error is (correct up to six decimal places),

$$\left|\frac{I(f) - CT_n(f)}{I(f)}\right| = 0.000006.$$

6. (**True/False** – Justify your answer) The function F defined by $F(x) = 4x(1-x)$ maps the interval $[0, 1]$ into itself and is not a contraction. **[2]**

Answer: Given $F(x) = 4x(1-x)$. Therefore, $F\prime(x) = 4 - 8x$ and $F''(x) = -8 < 0$. $F'(x) = 0 \Rightarrow x = 1/2$. $F(x)$ has a maximum at $x = 1/2$ and the maximum value is 1. Also, $F(x) \geq 0, \quad x \in [0, 1]$.

$$\therefore 0 \leq F(x) \leq 1 \quad \forall x \in [0, 1].$$

For $F(x)$ to be a contraction, we require

$$|F(x) - F(y)| \leq \lambda |x - y|, \quad 0 < \lambda < 1, \text{ and } \forall x, y \in [0, 1].$$

For $x = 1/2$ and $y = 0$ the above inequality does not hold for any $0 < \lambda < 1$. Therefore, $F(x)$ is not a contraction.

The statement is TRUE.

7. Prove that the asymptotic error formula for Simpson's 1/3-rule is

$$\widetilde{E}_n = -\frac{h^4}{180}\left[f^{(3)}(b) - f^{(3)}(a)\right].$$

[3]

Answer: The error in Simpson's rule is given by

$$\begin{aligned}
E_n(f) &= -\frac{h^5}{90}\sum_{j=1}^{n/2} f^{(iv)}(\eta_j) \quad \eta_j \in [x_{2j-2}, x_{2j}],\ h = \frac{x_{2j} - x_{2j-2}}{2}, \\
&= -\frac{h^4}{180}\sum_{j=1}^{n/2}\left(\frac{b-a}{n/2}\right) f^{(iv)}(\eta_j) \quad (b - a = nh) \\
\therefore \frac{E_n(f)}{-h^4/180} &= \sum_{j=1}^{n/2}\left(\frac{b-a}{n/2}\right) f^{(iv)}(\eta_j). \\
\Rightarrow \lim_{n\to\infty}\left(\frac{E_n(f)}{-h^4/180}\right) &= \lim_{n\to\infty}\sum_{j=1}^{n/2}\left(\frac{b-a}{n/2}\right) f^{(iv)}(\eta_j) \\
&= \int_a^b f^{(iv)}(x)\mathrm{d}x \\
&= f^{(3)}(b) - f^{(3)}(a). \qquad (1)
\end{aligned}$$

Asymptotic error is defined as

$$\widetilde{E}_n = \lim_{n\to\infty} E_n.$$

Therefore, the asymptotic error formula is

$$\widetilde{E}_n = -\frac{h^4}{180}\left[f^{(3)}(b) - f^{(3)}(a)\right].$$

□

8. The equation $x - 25^{-x} = 0$ has a solution in $[0, 1]$. Find the interpolation polynomial on $x_0 = 0,\ x_1 = 0.5,\ x_2 = 1$ for the function on the left side of the equation. By setting the interpolation polynomial equal to 0 and solving the equation, find an approximate solution to the equation correct up to 4 decimal places. **[4]**

Answer: Let $f(x) = x - 25^{-x}$. Therefore, $f(0) = -1$, $f(1/2) = 3/10$, and $f(1) = 24/25$. Lagrange polynomial interpolation gives

$$\begin{aligned}
p_2(x) &= \frac{(x-1/2)(x-1)}{(-1/2)(-1)}(-1) + \frac{(x-0)(x-1)}{(1/2)(-1/2)}\frac{3}{10} + \frac{(x-0)(x-1/2)}{1(1/2)}\frac{24}{25} \\
&= -(2x-1)(x-1) - \frac{6}{5}x(x-1) + \frac{24}{25}x(2x-1) \\
&= \frac{1}{25}(-32x^2 + 81x - 25).
\end{aligned}$$

Equating $p_2(x)$ to zero, i.e., $p_2(x) = 0$ gives

$$x_{1,2} = \frac{81 \pm \sqrt{81^2 - 3200}}{64} = \frac{81 \pm \sqrt{3361}}{64}.$$

The root corresponding to the $+ve$ sign is outside the interval [0, 1]. Therefore, the desired root of $f(x) = 0$ is obtained corresponding to the $-ve$ sign and the **root is** 0.3598 (correct up to four decimal places).

9. (**Fill in the blanks**) The degree of precision of the following quadrature formula to approximate the average of $f(x)\cos x$ over the interval $[-\pi, \pi]$:

$$\frac{1}{2\pi}\int_{-\pi}^{\pi} f(x)\cos x \mathrm{d}x \approx -\frac{4}{\pi^2}\left[f\left(-\frac{\pi}{2}\right) + f\left(\frac{\pi}{2}\right)\right]$$

is .... **[1]**

Answer: The quadrature is not exact for any polynomial of degree $\leq n$ for some positive integer n. Therefore, the degree of precision is **UNDEFINED**.