Homework 4 of Computational Mathematics

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Problem 1. Use the following data and the knowledge that the first five derivatives of f are bounded on $[1, 5]$ by 2, 3, 6, 12, and 23, respectively, to approximate $f'(3)$ as accurately as possible. Find a bound for the error.

x	1	2	3	4	5
$f(x)$	2.4142	2.6734	2.8974	3.0976	3.2804

Solution. By the five-point midpoint formula,

$$\begin{aligned} f'(3) &= \frac{1}{12 \cdot 1}\left(f(1) - 8 \cdot f(2) + 8 \cdot f(4) - f(5)\right) + \frac{h^4}{30} \cdot f^{(5)}(\xi) \\ &= \frac{1}{12}\left(2.4142 - 8 \cdot 2.6734 + 8 \cdot 4.0976 - 3.2804\right) + \frac{(0.1)^4}{30} \cdot f^{(5)}(\xi) \\ &= 0.8773 + \frac{(0.1)^4}{30} \cdot f^{(5)}(\xi), \end{aligned}$$

where $\xi \in (1, 5)$. The bound for the error is

$$\begin{aligned} \left|\frac{(0.1)^4}{30} \cdot f^{(5)}(\xi)\right| &\leq \frac{(0.1)^4}{30} \cdot 23 \\ &= 7.667 \cdot 10^{-5}. \end{aligned}$$

□

Problem 2. Let $f(x) = 3xe^x - \cos x$. Use the following data and equation (4.9) to approximate $f''(1.3)$ with $h = 0.1$ and with $h = 0.01$.

x	1.20	1.29	1.30	1.31	1.40
$f(x)$	11.59006	13.78176	14.04276	14.30741	16.86187

Compare your results to $f''(1.3)$.

Solution. We first deal with the case $h = 0.1$. By the second derivative midpoint formula,

$$\begin{aligned} f''(1.3) &= \frac{1}{(0.1)^2}\left(f(1.20) - 2\cdot f(1.30) + f(1.40)\right) - \frac{(0.1)^2}{12}\cdot f^{(4)}(\xi_1) \\ &= \frac{1}{0.01}\cdot(11.59006 - 2\cdot 14.04276 + 16.86187) - \frac{0.01}{12}\cdot f^{(4)}(\xi_1) \\ &= 36.641 - \frac{0.01}{12}\cdot f^{(4)}(\xi_1), \end{aligned}$$

where $\xi_1 \in (1.20, 1.40)$. We now deal with the case $h = 0.01$. Again by the second derivative midpoint formula,

$$\begin{aligned} f''(1.3) &= \frac{1}{(0.01)^2}\left(f(1.29) - 2\cdot f(1.30) + f(1.31)\right) - \frac{(0.01)^2}{12}\cdot f^{(4)}(\xi_2) \\ &= \frac{1}{0.0001}\cdot(13.78176 - 2\cdot 14.04276 + 14.30741) - \frac{0.0001}{12}\cdot f^{(4)}(\xi_2) \\ &= 36.5 - \frac{0.0001}{12}\cdot f^{(4)}(\xi_2), \end{aligned}$$

where $\xi_2 \in (1.29, 1.31)$. The actual value of $f''(1.3)$ can be calculated as follows:

$$\begin{aligned} & f'(x) = 3e^x + 3xe^x + \sin x \\ \Longrightarrow\ & f''(x) = 6e^x + 3xe^x + \cos x \\ \Longrightarrow\ & f''(1.3) = 6e^{1.3} + 3\cdot 1.3\cdot e^{1.3} + \cos(1.3) \\ & \qquad = 36.59354. \end{aligned}$$

The case with $h = 0.01$ is closed to the true value, and the other is farther to the true value. $\square$

Problem 3. Derive an $\mathcal{O}(h^4)$ five-point formula to approximate $f'(x_0)$ that uses $f(x_0 - h)$, $f(x_0)$, $f(x_0 + h)$, $f(x_0 + 2h)$, and $f(x_0 + 3h)$. [Hint: Consider the expression $A \cdot f(x_0 - h) + B \cdot f(x_0 + h) + C \cdot f(x_0 + 2h) + D \cdot f(x_0 + 3h)$. Expand in fourth Taylor polynomials, and choose A, B, C, and D, appropriately.]

Solution.

Problem 4. The following data give approximations to the integral

$$M = \int_0^{\pi} \sin x \, \mathrm{d}x.$$

$$N_1(h) = 1.570796, \quad N_1\left(\frac{h}{2}\right) = 1.896119, \quad N_1\left(\frac{h}{4}\right) = 1.974232, \quad N_1\left(\frac{h}{8}\right) = 1.993570.$$

Assuming $M = N_1(h) + K_1 h^2 + K_2 h^4 + K_3 h^6 + K_4 h^8 + \mathcal{O}(h^{10})$, construct an extrapolation table to determine $N_4(h)$.

Solution. By the formula for the $\mathcal{O}(h^{2j})$ approximation

$$N_j(h) = N_{j-1}\left(\frac{h}{2}\right) + \frac{N_{j-1}\left(\frac{h}{2}\right) - N_{j-1}(h)}{4^{j-1} - 1},$$

we can have the following table:

$\mathcal{O}(h^2)$	$\mathcal{O}(h^4)$	$\mathcal{O}(h^6)$	$\mathcal{O}(h^8)$
1.570796			
1.896119	2.004560		
1.974232	2.000270	1.999984	
1.993570	2.000016	1.999837	1.999834

□

Problem 5. The forward-difference formula can be expressed as

$$f'(x_0) = \frac{1}{h}\left(f(x_0+h) - f(x_0)\right) - \frac{h}{2}f''(x_0) - \frac{h^2}{6}f'''(x_0) + \mathcal{O}(h^3).$$

Use extrapolation to derive an $\mathcal{O}(h^3)$ formula for $f'(x_0)$.

Solution.

Problem 6. Find the degree of precision of the quadrature formula

$$\int_{-1}^{1} f(x)\,\mathrm{d}x = f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right).$$

Solution. For $f(x) = P_0(x) = 1$, it is clear that

$$\int_{-1}^{1} 1\,\mathrm{d}x = f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right) = 2.$$

For $f(x) = P_1(x) = x$, it is also clear that

$$\int_{-1}^{1} x\,\mathrm{d}x = f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right) = 0.$$

For $f(x) = P_2(x) = x^2$,

$$\int_{-1}^{1} x^2\,\mathrm{d}x = \frac{2}{3}$$

and

$$f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right) = \frac{1}{3} + \frac{1}{3} = \frac{2}{3}.$$

For $f(x) = P_3(x) = x^3$, it is clear that

$$\int_{-1}^{1} x^3\,\mathrm{d}x = f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right) = 0.$$

For $f(x) = P_4(x) = x^4$,

$$\int_{-1}^{1} x^4\,\mathrm{d}x = \frac{2}{5}$$

and

$$f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right) = \frac{1}{9} + \frac{1}{9} = \frac{2}{9}.$$

Hence, the degree of precision of this quadrature formula is 3. □

Problem 7. Find the constants x_0, x_1, and c_1 so that the quadrature formula

$$\int_0^1 f(x)\,\mathrm{d}x = \frac{1}{2}f(x_0) + c_1 f(x_1)$$

has the highest possible degree of precision.

Solution. Set $f(x) = P_0(x) = 1$. Then

$$1 = \frac{1}{2} + c_1.$$

This implies that c_1 must be $\frac{1}{2}$. Set $f(x) = P_1(x) = x$. Then

$$\frac{1}{2} = \frac{1}{2}x_0 + \frac{1}{2}x_1.$$

Set $f(x) = P_2(x) = x^2$. Then

$$\frac{1}{3} = \frac{1}{2}{x_0}^2 + \frac{1}{2}{x_1}^2.$$

Since there are two unknowns and two equations, two unknowns may be solved:

$$\begin{aligned}\frac{1}{3} &= \frac{1}{2}\left(1 - x_1\right)^2 + \frac{1}{2}{x_1}^2 \\ 2 &= 3(1 - x_1)^2 + 3{x_1}^2 \\ x_1 &= \frac{3 \pm \sqrt{3}}{6}.\end{aligned}$$

Choose $x_0 < x_1$. Then $(x_0, x_1, c_1) = \left(\frac{3-\sqrt{3}}{6}, \frac{3+\sqrt{3}}{6}, \frac{1}{2}\right)$. $\square$

Problem 8. Determine the values of n and h required to approximate

$$\int_0^2 e^{2x} \sin 3x \,\mathrm{d}x$$

to within 10^{-4} . Use

a. composite trapezoidal rule;

b. composite Simpson's rule; and

c. composite midpoint rule.

Solution.

Problem 9. Determine to within 10^{-6} the length of the graph of the ellipse with $4x^2 + 9y^2 = 36$.

Solution.

Problem 10. Show that the error $E(f)$ for composite Simpson's rule can be approximated by

$$-\frac{h^4}{180}\left(f'''(b) - f'''(a)\right).$$

[Hint: $\displaystyle\sum_{j=1}^{n/2} f^{(4)}(\xi_j)(2h)$ is a Riemann sum for $\displaystyle\int_a^b f^{(4)}(x)\,\mathrm{d}x$.]

Solution.

Problem 11. Use the following data to approximate $\int_1^5 f(x)\,\mathrm{d}x$ as accurately as possible.

x	1	2	3	4	5
$f(x)$	2.4142	2.6734	2.8974	3.0976	3.2804

Solution.

Problem 12. Show that the approximation obtained from $R_{k,2}$ is the same as that given by the composite Simpson's rule described in Theorem 4.4 with $h = h_k$.

Solution.

Problem 13. Use composite Simpson's rule with $n = 4, 6, 8, \ldots,$ until successive approximations to the following integrals agree to within 10^{-6}. Determine the number of nodes required. Use the adaptive quadrature algorithm to approximate the integral to within 10^{-6}, and count the number of nodes. Did Adaptive quadrature produce any improvement?

a. $\displaystyle\int_0^{\pi} x\sin(x^2)\,\mathrm{d}x$; and

b. $\displaystyle\int_0^{\pi} x^2\sin x\,\mathrm{d}x$.

Solution.

Problem 14. Approximate the following integral using Gaussian quadrature with $n = 2, 3, 4$. Compare your answers with the exact values of the integral.

$$\int_1^{1.6} \frac{2x}{x^2 - 4}\,\mathrm{d}x.$$

Solution. We first transform the interval $[1, 1.6]$ to $[-1, 1]$ by using $t = \dfrac{2x - 2.6}{0.6}$. Hence the integral becomes

$$\int_{-1}^{1} \frac{1.2t + 5.2}{\left(\frac{0.6t+2.6}{2}\right)^2 - 4} \cdot \frac{0.6}{2}\,\mathrm{d}t = \int_{-1}^{1} \frac{12t + 52}{3t^2 + 26t - 77}\,\mathrm{d}t.$$

We now deal with the case $n = 2$. Using Table 4.12, the approximation is

$$1 \cdot \frac{12 \cdot 0.5773502692 + 52}{(0.5773502692)^2 + 26 \cdot 0.5773502692 - 77} + 1 \cdot \frac{12 \cdot (-0.5773502692) + 52}{(-0.5773502692)^2 + 26 \cdot (-0.5773502692) - 77}$$

$$= -1.4474.$$

The exact value of the integral is

$$\begin{aligned}\int_1^{1.6} \frac{2x}{x^2 - 4}\,\mathrm{d}x &= \int_{-3}^{-1.44} \frac{1}{u}\,\mathrm{d}u \\ &= 0.364643 - 1.098612 \\ &= -0.733969.\end{aligned}$$

Problem 15. Determine constants a, b, c, and d that will produce a quadrature formula

$$\int_{-1}^{1} f(x)\,\mathrm{d}x = a \cdot f(-1) + b \cdot f(1) + c \cdot f'(-1) + d \cdot f'(1).$$

that has degree of precision 3.

Solution. Set $f(x) = P_0(x) = 1$. Then

$$2 = a + b.$$

Set $f(x) = P_1(x) = x$. Then

$$0 = -a + b + c + d.$$

Set $f(x) = P_2(x) = x^2$. Then

$$\frac{2}{3} = a + b - 2c + 2d.$$

Set $f(x) = P_3(x) = x^3$. Then

$$0 = -a + b + 3c + 3d.$$

Hence, $(a, b, c, d) = (1, 1, 1/3, -1/3)$. $\square$

Problem 16. The improper integral

$$\int_0^\infty f(x)\,\mathrm{d}x$$

cannot be converted into an integral with finite limits using the substitution $t = \dfrac{1}{x}$ because the limit at zero becomes infinite. The problem is resulved by first writing

$$\int_0^\infty f(x)\,\mathrm{d}x = \int_0^1 f(x)\,\mathrm{d}x + \int_1^\infty f(x)\,\mathrm{d}x.$$

Apply this technique to approximate the following improper integrals to within 10^{-6}.

a. $\displaystyle\int_0^\infty x\frac{1}{1+x^4}\,\mathrm{d}x$; and

b. $\displaystyle\int_0^\infty \frac{1}{(1+x^2)^3}\,\mathrm{d}x$.

Solution.