

Homework 4 of Computational Mathematics

Chang, Yung-Hsuan

111652004

Department of Applied Mathematics

April 29, 2024

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,

$$\begin{aligned}
 f'(3) &= \frac{1}{12 \cdot 1} (f(1) - 8 \cdot f(2) + 8 \cdot f(4) - f(5)) + \frac{h^4}{30} \cdot f^{(5)}(\xi) \\
 &= \frac{1}{12} (2.4142 - 8 \cdot 2.6734 + 8 \cdot 3.0976 - 3.2804) + \frac{(0.1)^4}{30} \cdot f^{(5)}(\xi) \\
 &= 0.8773 + \frac{(0.1)^4}{30} \cdot f^{(5)}(\xi),
 \end{aligned}$$

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,

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

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

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

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

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

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

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

$$M = \int_0^\pi \sin x \, dx.$$

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

Assuming $M = N_1(h) + K_1h^2 + K_2h^4 + K_3h^6 + K_4h^8 + \mathcal{O}(h^{10})$, 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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

$$\int_0^1 f(x) \, dx = \frac{1}{2}f(x_0) + c_1f(x_1)$$

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:

$$\frac{1}{3} = \frac{1}{2}(1 - x_1)^2 + \frac{1}{2}x_1^2$$

$$2 = 3(1 - x_1)^2 + 3x_1^2$$

$$x_1 = \frac{3 \pm \sqrt{3}}{6}.$$

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

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

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

to within 10^{-4} . Use

- a. the composite trapezoidal rule;
- b. composite Simpson's rule; and
- c. the 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. We use composite Simpson's rule to answer. The desired integral is

$$2 \cdot \int_0^\pi \sqrt{(-3 \sin \theta)^2 + (2 \cos \theta)^2} d\theta.$$

The function $f(x)$ can be re-written as $\sqrt{4 + 5(\sin \theta)^2}$. Choose $n = 1000$, so that the error term

$$\begin{aligned} \frac{\pi - 0}{180} \cdot \left(\frac{\pi - 0}{1000}\right)^4 \cdot f^{(4)}(\mu) &\leq \frac{\pi - 0}{180} \cdot \left(\frac{\pi - 0}{1000}\right)^4 \cdot \sup_{x \in \mathbb{R}} |f^{(4)}(x)| \\ &< \frac{\pi}{180} \cdot 0.01^4 \cdot 20 \\ &< 3.5 \times 10^{-9}. \end{aligned}$$

By Python and composite Simpson's rule,

$$\begin{aligned} 2 \cdot \int_0^\pi \sqrt{(-3 \sin \theta)^2 + (2 \cos \theta)^2} d\theta &\approx 2 \cdot \frac{\pi}{1000} \cdot \frac{1}{3} \left[f(0) + 2 \cdot \sum_{j=1}^{499} f(x_{2j}) + 4 \cdot \sum_{j=1}^{500} f(x_{2j-1}) + f(\pi) \right] \\ &= 15.8654393826. \end{aligned}$$

The true value is around $8E\left(-\frac{5}{4}\right) = 15.8654395893$; thus the absolute error is

$$\begin{aligned} |15.8654393826 - 15.8654395893| &= 0.0000002067 \\ &< 3 \times 10^{-7} \\ &< 10^{-6}. \end{aligned}$$

□

```
111652004_CM_HW4.tex M 111652004_CM_HW4_P9.py U x
HW4 > 111652004_CM_HW4_P9.py > ...
1 import math
2
3 a = 0
4 b = math.pi
5 n = 1000
6
7 h = (b - a) / n
8
9 def x(n):
10     return a + n * h
11
12 def f(x):
13     a = math.sqrt(4 + 5 * math.sin(x) ** 2)
14     return a
15
16 sum = f(a) + f(b)
17
18 for i in range(n//2 - 1):
19     sum += 2 * f(x(2 * i))
20
21 for i in range(n//2):
22     sum += 4 * f(x(2 * i-1))
23
24 print(2 * h * sum / 3)
25
```

PROBLEMS OUTPUT DEBUG CONSOLE TERMINAL PORTS GITLENS COMMENTS

```
/usr/bin/python3 "/Users/eiken/Visual Studio/Github_Clone/CM_HW/HW4/111652004_CM_HW4_P9.py"
eiken@Eikens-MacBook-Air CM_HW % /usr/bin/python3 "/Users/eiken/Visual Studio/Github_Clone/CM_HW/HW4/111652004_CM_HW4_P9.py"
15.865439382587326
```

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

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

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

Solution.

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

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

Solution. We use the Romberg extrapolation for higher accuracy.

$$R_{1,1} = 4 \cdot (2.4142 + 3.2804) = 22.7784;$$

$$R_{2,1} = 2 \cdot (2.4142 + 2.8974 + 3.2804) = 17.184;$$

$$R_{3,1} = 1 \cdot (2.4142 + 2.6734 + 2.8974 + 3.0976 + 3.2804) = 14.363;$$

$$R_{2,2} = R_{2,1} + \frac{1}{4^1 - 1} (R_{2,1} - R_{1,1})$$

$$= 15.3192;$$

$$R_{3,2} = R_{3,1} + \frac{1}{4^1 - 1} (R_{3,1} - R_{2,1})$$

$$= 13.4227;$$

$$R_{3,3} = R_{3,2} + \frac{1}{4^2 - 1} (R_{3,2} - R_{2,2})$$

$$= 13.2963.$$

□

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 $n = 4, 6, 8, \dots$, 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 the adaptive quadrature produce any improvement?

a. $\int_0^\pi x \sin(x^2) \, dx$; and

b. $\int_0^\pi x^2 \sin x \, dx$.

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.

$$\int_1^{1.6} \frac{2x}{x^2 - 4} dx.$$

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

$$\int_{-1}^1 \frac{0.6t + 2.6}{\left(\frac{0.6t + 2.6}{2}\right)^2 - 4} \cdot \frac{0.6}{2} dt = \int_{-1}^1 \frac{6t + 26}{3t^2 + 26t - 77} dt.$$

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

$$\begin{aligned} & 1 \cdot \frac{12 \cdot 0.57735 + 26}{(0.57735)^2 + 26 \cdot 0.57735 - 77} + 1 \cdot \frac{12 \cdot (-0.57735) + 26}{(-0.57735)^2 + 26 \cdot (-0.57735) - 77} \\ &= -0.73072. \end{aligned}$$

We now deal with the case $n = 3$. Using Table 4.12, the approximation is

$$\begin{aligned} & 0.55556 \cdot \frac{12 \cdot 0.77460 + 26}{(0.77460)^2 + 26 \cdot 0.77460 - 77} \\ & + 0.88889 \cdot \frac{12 \cdot 0 + 26}{(0)^2 + 26 \cdot 0 - 77} \\ & + 0.55556 \cdot \frac{12 \cdot (-0.77460) + 26}{(-0.77460)^2 + 26 \cdot (-0.77460) - 77} \\ &= -0.73370. \end{aligned}$$

We now deal with the case $n = 4$. Using Table 4.12, the approximation is

$$\begin{aligned} & 0.34785 \cdot \frac{12 \cdot 0.86114 + 26}{(0.86114)^2 + 26 \cdot 0.86114 - 77} \\ & + 0.65215 \cdot \frac{12 \cdot 0.33998 + 26}{(0.33998)^2 + 26 \cdot 0.33998 - 77} \\ & + 0.65215 \cdot \frac{12 \cdot (-0.33998) + 26}{(-0.33998)^2 + 26 \cdot (-0.33998) - 77} \\ & + 0.34785 \cdot \frac{12 \cdot (-0.86114) + 26}{(-0.86114)^2 + 26 \cdot (-0.86114) - 77} \\ &= -0.73396. \end{aligned}$$

The exact value of the integral is

$$\begin{aligned}\int_1^{1.6} \frac{2x}{x^2 - 4} dx &= \int_{-3}^{-1.44} \frac{1}{u} du \\ &= \ln(0.48) \\ &= -0.73397.\end{aligned}$$

The relative errors are 0.0044228, 0.00022582, and 0.000012200, in the order of $n = 2$, $n = 3$, and $n = 4$.

The process of calculation is done by Python. □

```
HW4 > 111652004_CM_HW4_P14.py > ...
1  import math
2
3  def f(t):
4      return (6 * t + 26) / (3 * t ** 2 + 26 * t - 77)
5
6  n_values = []
7
8  node_data = {
9      2: ([0.57735, -0.57735], [1, 1]),
10     3: ([0.77460, 0, -0.77460], [0.55556, 0.88889, 0.55556]),
11     4: ([0.86114, 0.33998, -0.33998, -0.86114], [0.34785, 0.
12         65215, 0.65215, 0.34785])
13 }
14
15 for num_nodes in range(2, 5):
16     sum = 0
17     roots, coeffs = node_data[num_nodes]
18     for i in range(num_nodes):
19         sum += coeffs[i] * f(roots[i])
20     n_values.append(sum)
21
22 rel_error = []
23
24 for i in range(3):
25     rel_error.append(abs(n_values[i] - math.log(0.48)) / abs(math.
26         log(0.48)))
27
28 print(n_values)
29 print(rel_error)
```

PROBLEMS OUTPUT DEBUG CONSOLE TERMINAL PORTS GITLENS COMMENTS

```
/usr/bin/python3 "/Users/eiken/Visual Studio/Github_Clone/CM_HW/HW4/111652004_CM_HW4_P14.py"
eiken@Eikens-MacBook-Air CM_HW % /usr/bin/python3 "/Users/eiken/Visual Studio/Github_Clone/CM_HW/HW4/111652
[-0.7307229812146365, -0.7338034323569402, -0.7339602207957825]
[0.0044227931850260565, 0.00022581700824436885, 1.2199809912944473e-05]
```

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

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

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

□

Problem 16. The improper integral

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

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

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

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

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

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

Solution.