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

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

$\square$

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:

$$f'(x) = 3e^x + 3xe^x + \sin x$$

$$\implies f''(x) = 6e^x + 3xe^x + \cos x$$

$$\implies f''(1.3) = 6e^{1.3} + 3\cdot 1.3\cdot e^{1.3} + \cos(1.3)$$

$$= 36.59354.$$

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

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

and calculator, 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	1.999991	1.999999

□

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. $\square$

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. the composite trapezoidal rule;

b. composite Simpson's rule; and

c. the composite midpoint rule.

Solution. The real value of the integral is

$$\begin{aligned}\int_0^2 e^{2x} \sin 3x \, \mathrm{d}x &= \left[\frac{1}{13} e^{2x} (2 \sin 3x - 3 \cos 3x)\right]_0^2 \\ &= -14.21397712986\end{aligned}$$

a. It is clear that $f \in C^2[0, 2]$. Choose $n = 20000$. Then $h = 0.0001$. Using the composite trapezoidal rule,

$$\begin{aligned}\int_0^2 e^{2x} \sin 3x \, \mathrm{d}x &\approx \frac{0.0001}{2} \left[0 + 2 \cdot \sum_{j=1}^{19999} e^{2x_j} \sin(3x_j) + e^4 \sin(6)\right] \\ &= -14.213977026729639,\end{aligned}$$

where $x_j = 0.0001 \cdot j$.

b. It is clear that $f \in C^4[0, 2]$. Choose $n = 20000$. Then $h = 0.0001$. Using composite Simpson's rule,

$$\begin{aligned}\int_0^2 e^{2x} \sin 3x \, \mathrm{d}x &\approx \frac{0.0001}{3} \left[0 + 2 \cdot \sum_{j=1}^{9999} e^{2x_{2j}} \sin(3x_{2j}) + 4 \cdot \sum_{j=1}^{10000} e^{2x_{2j-1}} \sin(3x_{2j-1}) + e^2 \sin(6)\right] \\ &= - - 14.213977129862458,\end{aligned}$$

where $x_j = 0.0001 \cdot j$.

c. It is clear that $f \in C^2[0, 2]$. Choose $n = 19998$. Then $h = 0.0001$. Using the composite midpoint rule,

$$\int_0^2 e^{2x} \sin 3x \, \mathrm{d}x \approx 2 \cdot 0.0001 \cdot \sum_{j=0}^{9999} f(x_{2j})$$

$$= -14.213977336128231,$$

where $x_j = 0.0001 \cdot (j+1)$.

It can be seen that all of the three methods are accurate within 10^{-4} (even more precise). $\square$

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HW4 > 111652004_CH_MW4_P8.py > ...

```python
import math

a = 0
b = 2
n = 20000

h = (b-a)/n

def x(i):
    return a + h*i

def f(x):
    return math.e ** (2 * x) * math.sin(3 * x)

ctSum = f(a)+f(b)
for i in range(n-1):
    ctSum += 2 * f(x(i+1))
print("Composite trapezoidal rule:", h * ctSum / 2)

cSSum = f(a)+f(b)
for i in range(n//2-1):
    cSSum += 2 * f(x(2*(i+1)))
for i in range(n//2):
    cSSum += 4 * f(x(2*(i+1)-1))
print("Composite Simpson's rule:", h * cSSum / 3)


def x_cm(i):
    return a + h*(i+1)
n = 19998
h = (b-a)/(n+2)
cmSum = 0
for i in range(n//2+1):
    cmSum += f(x_cm(2*i))
print("Composite midpoint rule:", 2 * h * cmSum)
```

PROBLEMS   OUTPUT   DEBUG CONSOLE   TERMINAL   PORTS   GITLENS   COMMENTS

```
thub_Clone/CM_HW/HW4/111652004_CH_MW4_P8.py"
Composite trapezoidal rule: -14.213977026729639
Composite Simpson's rule: -14.213977129862458
Composite midpoint rule: -14.213977336128231
```

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

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

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

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

By Python and composite Simpson's rule,

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

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

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

$\square$

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HW4 > 111652004_CM_HW4_P9.py > ...

```python
import math

a = 0
b = math.pi
n = 1000

h = (b - a) / n

def x(n):
    return a + n * h

def f(x):
    a = math.sqrt(4 + 5 * math.sin(x) ** 2)
    return a

sum = f(a) + f(b)

for i in range(n//2 - 1):
    sum += 2 * f(x(2 * i))

for i in range(n//2):
    sum += 4 * f(x(2 * i-1))

print(2 * h * sum / 3)
```

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/HW4/111652
15.865439382587326
```

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. We use the Romberg extrapolation for higher accuracy.

$$
\begin{aligned}
R_{1,1} &= 4 \cdot (2.4142 + 3.2804) = 22.7784;\\
R_{2,1} &= 2 \cdot (2.4142 + 2.8974 + 3.2804) = 17.184;\\
R_{3,1} &= 1 \cdot (2.4142 + 2.6734 + 2.8974 + 3.0976 + 3.2804) = 14.363;\\
R_{2,2} &= R_{2,1} + \frac{1}{4^1 - 1}\left(R_{2,1} - R_{1,1}\right)\\
&= 15.3192;\\
R_{3,2} &= R_{3,1} + \frac{1}{4^1 - 1}\left(R_{3,1} - R_{2,1}\right)\\
&= 13.4227;\\
R_{3,3} &= R_{3,2} + \frac{1}{4^2 - 1}\left(R_{3,2} - R_{2,2}\right)\\
&= 13.2963.
\end{aligned}
$$

□

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 the 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

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

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

$$\int_{1}^{1.6} \frac{2x}{x^2-4}\,\mathrm{d}x = \int_{-3}^{-1.44} \frac{1}{u}\,\mathrm{d}u$$

$$= \ln(0.48)$$

$$= -0.73397.$$

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. $\square$

HW4 > 111652004_CM_HW4_P14.py > ...

```python
import math

def f(t):
    return (6 * t + 26) / (3 * t ** 2 + 26 * t - 77)

n_values = []

node_data = {
    2: ([0.57735, -0.57735], [1, 1]),
    3: ([0.77460, 0, -0.77460], [0.55556, 0.88889, 0.55556]),
    4: ([0.86114, 0.33998, -0.33998, -0.86114], [0.34785, 0.65215, 0.65215, 0.34785])
}

for num_nodes in range(2, 5):
    sum = 0
    roots, coeffs = node_data[num_nodes]
    for i in range(num_nodes):
        sum += coeffs[i] * f(roots[i])
    n_values.append(sum)

rel_error = []

for i in range(3):
    rel_error.append(abs(n_values[i] - math.log(0.48)) / abs(math.log(0.48)))

print(n_values)
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/HW4/11165
[-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

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

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

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

Solution.