MATH 3940 Numerical Analysis for Computer Scientists

Problem Set 6 Solutions

1. Consider the data

x	0.9	0.97	1.04
$f(x)$	-0.17101	-0.05733	0.08486

Find the approximations to $f'(0.9)$, $f'(0.97)$, $f'(1.04)$, and $f''(0.97)$ of order $\mathbf{O}(h^2)$.

Solution. Looking at the table, we should take $h = 0.07$. For $f'(0.9)$, we will use forward-difference formula.

$$\begin{aligned}
f'(x) &= \frac{-3f(x) + 4f(x+h) - f(x+2h)}{2h} \\
f'(0.9) &= \frac{-3f(0.9) + 4f(0.9+0.07) - f(0.9+0.14)}{2(0.07)} \\
&= \frac{-3f(0.9) + 4f(0.97) - f(1.04)}{0.14} \\
&= \frac{-3(-0.17101) + 4(-0.05733) - (0.08486)}{0.14} \\
&= \frac{0.19885}{0.14} = 1.420357
\end{aligned}$$

For $f'(0.97)$, we will use central-difference formula.

$$\begin{aligned}
f'(x) &= \frac{f(x+h) - f(x-h)}{2h} \\
f'(0.97) &= \frac{f(0.97+0.07) - f(0.97-0.07)}{2(0.07)} \\
&= \frac{f(1.04) - f(0.9)}{0.14} \\
&= \frac{0.08486 - (-0.17101)}{0.14} \\
&= \frac{0.25587}{0.14} = 1.82764
\end{aligned}$$

For $f'(1.04)$, we will use backward-difference formula.

$$\begin{aligned}
f'(x) &= \frac{3f(x) - 4f(x-h) + f(x-2h)}{2h} \\
f'(1.04) &= \frac{3f(1.04) - 4f(1.04-0.07) + f(1.04-0.14)}{2(0.0.07)} \\
&= \frac{3f(1.04) - 4f(0.97) + f(0.9)}{0.14} \\
&= \frac{3(0.08486) - 4(-0.05733) + (-0.17101)}{0.14} \\
&= \frac{0.32189}{0.14} = 2.2349
\end{aligned}$$

For $f''(0.97)$, we have

$$\begin{aligned}
f''(x) &= \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} \\
f''(0.97) &= \frac{f(0.97+0.07) - 2f(0.97) + f(0.97-.07)}{(0.07)^2} \\
&= \frac{f(1.04) - 2f(0.97) + f(0.90)}{0.0049} \\
&= \frac{0.08486 - 2(-0.05733) - 0.17101}{0.0049} \\
&= \frac{0.02851}{0.0049} = 5.81837
\end{aligned}$$

$\square$

2. Let $f(x) = xe^x$ and $h = 0.06$.

(a) Find $f'(2)$ using the formula $f'(x) = \dfrac{f(x+h) - f(x)}{h}$

(b) Find $f''(2)$ using the formula $f''(x) = \dfrac{f(x+h) - 2f(x) + f(x-h)}{h^2}$

(c) Find the exact error for the approximation obtained in part (b).

Solution. (a) For $h = 0.06$ we have

$$\begin{aligned}
f'(x) &= \frac{f(x+h) - f(x)}{h} \\
f'(2) &= \frac{f(2+0.06) - f(2)}{0.06} = \frac{f(2.06) - f(2)}{0.06} \\
&= \frac{2.06e^{2.06} - 2e^2}{0.06} = \frac{1.3846}{0.06} = 23.0767
\end{aligned}$$

(b) For $h = 0.06$ we have

$$\begin{aligned}
f''(x) &= \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} \\
f''(2) &= \frac{f(2+0.06) - 2f(2) + f(2-0.06)}{(0.06)^2} \\
&= \frac{f(2.06) - 2f(2) + f(1.94)}{0.0036} \\
&= \frac{2.06e^{2.06} - 2(2e^2) - 1.94e^{1.94}}{0.0036} = \frac{0.10645}{0.0036} = 29.5694
\end{aligned}$$

(c) $f(x) = xe^x$

$f'(x) = e^x + xe^x = (1+x)e^x$ and $f''(x) = e^x + (1+x)e^x = (2+x)e^x$.

The exact value is $f''(2) = (2+2)e^2 = 29.5562$.

For the approximation in part (b), the exact error is $|29.5694 - 29.5562| = 0.0132$.

$\square$

3. Find the order of error in the following approximation (show your steps)

$$f''(x) = \frac{2f(x) - 5f(x-h) + 4f(x-2h) - f(x-3h)}{h^2}$$

Solution. We use Taylor polynomial expansion for the functions and obtain

$$f(x-h) = f(x) - h\frac{f'(x)}{1!}h + \frac{f''(x)}{2!}h^2 - \frac{f'''(x)}{3!}h^3 + \frac{f^{(4)}(c_1)}{4!}h^4$$

$$\begin{aligned} f(x-2h) &= f(x) - 2\frac{f'(x)}{1!}h + 4\frac{f''(x)}{2!}h^2 - 8\frac{f'''(x)}{3!}h^3 + 16\frac{f^{(4)}(c_2)}{4!}h^4 \\ f(x-3h) &= f(x) - 3\frac{f'(x)}{1!}h + 9\frac{f''(x)}{2!}h^2 - 27\frac{f'''(x)}{3!}h^3 + 81\frac{f^{(4)}(c_3)}{4!}h^4 \end{aligned}$$

Multiplying first equation by -5, second equation by 4 and the third equation by -1 and adding them

$$\begin{array}{c} -5f(x-h) = -5f(x) + 5\frac{f'(x)}{1!}h - 5\frac{f''(x)}{2!}h^2 + 5\frac{f'''(x)}{3!}h^3 - 5\frac{f^{(4)}(c_1)}{4!}h^4 \\ 4f(x-2h) = 4f(x) - 8\frac{f'(x)}{1!}h + 16\frac{f''(x)}{2!}h^2 - 32\frac{f'''(x)}{3!}h^3 + 64\frac{f^{(4)}(c_2)}{4!}h^4 \\ -f(x-3h) = -f(x) + 3\frac{f'(x)}{1!}h - 9\frac{f''(x)}{2!}h^2 + 27\frac{f'''(x)}{3!}h^3 - 81\frac{f^{(4)}(c_3)}{4!}h^4 \\ \hline -5f(x-h) + 4f(x-2h) - f(x-3h) = -2f(x) + 2\frac{f''(x)}{2!}h^2 + O(h^4) \end{array}$$

Thus we obtain

$$\begin{aligned} h^2 f''(x) &= 2f(x) - 5f(x-h) + 4f(x-2h) - f(x-3h) + O(h^4) \\ \Rightarrow \; f''(x) &= \frac{2f(x) - 5f(x-h) + 4f(x-2h) - f(x-3h)}{h^2} + O(h^2) \end{aligned}$$

Thus the order of error in the given approximation is $O(h^2)$. $\square$

4. Consider the integral $\displaystyle\int_0^1 \sin \pi x \, dx$

(a) Approximate the above integral using trapezoidal rule.

(b) Approximate the above integral using Simpson's rule.

(c) Approximate the above integral by Simpson's $\frac{3}{8}$ rule.

(d) Using the error formula find a bound for the error of Trapezoidal rule and compare this to the actual error.

Solution. (a) For trapezoidal rule: $h = 1 - 0 = 1$.

The nodes are $x_0 = 0$ and $x_1 = 1$.

Here $f(x) = \sin \pi x$, so we have $f_0 = \sin 0 = 0$ and $f_1 = \sin \pi = 0$.

$$\int_0^1 \sin \pi x \, dx = \frac{h}{2}[f_0 + f_1] = \frac{1}{2}[\sin 0 + \sin \pi] = \frac{1}{2}(0+0) = 0$$

(b) For Simpson's rule: $h = \frac{1-0}{2} = \frac{1}{2}$.

The nodes are $x_0 = 0$, $x_1 = 1/2$, and $x_2 = 1$.

Here $f(x) = \sin \pi x$, so we have

$f_0 = \sin 0 = 0$, $f_1 = \sin(\pi/2) = 1$ and $f_2 = \sin \pi = 0$.

$$\int_0^1 \sin \pi x \, dx = \frac{h}{3}[f_0+4f_1+f_2] = \frac{1/2}{3}[\sin 0+4\sin\frac{\pi}{2}+\sin\pi] = \frac{1}{6}(0+4+0) = \frac{4}{6} = \frac{2}{3}$$

(c) For Simpson's $\frac{3}{8}$ rule: $h = \frac{1-0}{3} = \frac{1}{3}$.

The nodes are $x_0 = 0$, $x_1 = 1/3$, $x_2 = 2/3$, and $x_3 = 1$.

Here $f(x) = \sin \pi x$, so we have

$$\begin{aligned}\int_0^1 \sin \pi x \, dx &= \frac{3h}{8}[f_0 + 3f_1 + 3f_2 + f_3] \\ &= \frac{3(1/3)}{8}[\sin 0 + 3\sin\frac{\pi}{3} + 3\sin\frac{2\pi}{3} + \sin\pi] \\ &= \frac{1}{8}[0 + 3(0.866) + 3(0.866) + 0] = \frac{5.196}{8} = 0.6495\end{aligned}$$

(d) The error for Trapezoidal rule is $\left|-\frac{h^3}{12}f''(c)\right|$ for $c \in [0,2]$.

$f(x) = \sin \pi x \Rightarrow f'(x) = \pi \cos \pi x \Rightarrow f''(x) = -\pi^2 \sin \pi x$.

For critical numbers of $f''(x)$, we need $f'''(x) = 0 \Rightarrow -\pi^3 \cos \pi x = 0 \Rightarrow x = \frac{1}{2}$.

Now we will find values of $|f''|$ at the critical number and the end points.

$|f''(1/2)| = |-\pi^2 \sin(\pi/2)| = \pi^2$,

$|f''(0)| = |-\pi^2 \sin 0| = 0$, and $|f''(1)| = |-\pi^2 \sin \pi| = 0$.

So the maximum value is π^2.

The error bound is $|E| = \left|-\frac{h^3}{12}f''(c)\right| \leq \left|\frac{(1^3)}{12}(\pi^2)\right| = 3.28987$.

The exact value of the integral is

$$\int_0^1 \sin \pi x \, dx = \frac{-\cos \pi x}{\pi}\Bigg|_0^1 \frac{-\cos\pi - (-\cos 0)}{\pi} = \frac{2}{\pi} = 0.63662$$

The actual error is $|0.63662 - 0| = 0.63662$ which is smaller than the error bound.

$\square$

5. Consider the integral $\displaystyle\int_0^4 x^2 e^{-x} \, dx$

(a) Approximate the above integral using composite Trapezoidal rule with $n = 8$.

(b) Approximate the above integral using composite Simpson's rule with $n = 8$.

Solution. (a) Using composite Trapezoidal rule we have $h = \dfrac{b-a}{8} = \dfrac{4-0}{8} = \dfrac{1}{2}$.
The nodes are $x_0 = 0$, $x_1 = 1/2$, $x_2 = 1$, $x_3 = 3/2$, $x_4 = 2$, $x_5 = 5/2$, $x_6 = 3$, $x_7 = 7/2$, and $x_8 = 4$.
Here $f(x) = x^2 e^{-x}$, so we have

$$f_0 = 0, \quad f_1 = \frac{1}{4}e^{-1/2} = 0.1516, \quad f_2 = e^{-1} = 0.3679, \quad f_3 = \frac{9}{4}e^{-3/2} = 0.5020,$$

$$f_4 = 4e^{-2} = 0.5413, \quad f_5 = \frac{25}{4}e^{-5/2} = 0.5130, \quad f_6 = 9e^{-3} = 0.4481,$$

$$f_7 = \frac{49}{4}e^{-7/2} = 0.3699, \quad f_8 = 16e^{-4} = 0.2931$$

Using composite trapezoidal rule, we have

$$\begin{aligned}\int_0^4 x^2 e^{-x}\,dx &= \frac{h}{2}[f_0 + 2(f_1 + f_2 + f_3 + f_4 + f_5 + f_6 + f_7) + f_8] \\ &= \frac{1/2}{2}[0 + 2(0.1516 + 0.3679 + 0.502 + 0.5413 + 0.513 + 0.4481 + 0.3699) + 0.2931] \\ &= \frac{6.0807}{4} = 1.520175\end{aligned}$$

(b) Using composite Simpson's rule with $n = 8$, we have $h = \frac{4-0}{8} = \frac{1}{2}$.
The nodes are same as in part (a). Using the values of f from part(a) and composite Simpson's rule, we have

$$\begin{aligned}\int_0^4 x^2 e^{-x}\,dx &= \frac{h}{3}[f_0 + 4(f_1 + f_3 + f_5 + f_7) + 2(f_2 + f_4 + f_6) + f_8] \\ &= \frac{1}{6}[4(0.1516 + 0.502 + 0.513 + 0.3699) + 2(0.3679 + 0.5413 + 0.4481) + 0.2931] \\ &= \frac{9.1537}{6} = 1.5256\end{aligned}$$

$\square$