MAE 384 Homework 5 Discussion

Prob. 1 The result for (b) is much more accurate than those for (a) and (c), because the scheme in (b) is "4th order" with a truncation error of $O(h^4)$, while the other two are of $O(h^2)$ accuracy. This shows that the truncation error ($O(h)$, $O(h^2)$, etc.) is a critical part of the numerical scheme and should be treated seriously. Note that if the numerical scheme used in (c) is replaced by a 4th order scheme taken from Table 6-1, one will also obtain a much better result for $f''(x)$ that is comparable in accuracy to the result of (b).

Prob. 2 The key idea for this problem is to combine the Taylor series expansions at $x = x_{i-1}$ and $x = x_{i+1}$ to eliminate the terms with $f'(x_i)\,h$. This ensures that in the finite-difference approximation $f''(x_i)$ can be written as a function of $f(x_{i-1})$, $f(x_i)$ and $f(x_{i+1})$ only. See sample solution. Also, in this process, the terms with $f'''(x_i)\,h^3$ cannot be eliminated entirely (this is different from the case when $(x_i - x_{i-1}) = (x_{i+1} - x_i) = h$), therefore the resulted truncation error is of order $O(h)$ instead of $O(h^2)$.

Prob. 3 To obtain a formula for $f'(x_i)$ with $O(h^3)$ accuracy, we need to eliminate the terms with $f''(x_i)\,h^2$ and $f'''(x_i)\,h^3$ in the Taylor series. This requires the combination of 3 Taylor series at 3 neighboring points of x_i. The sample solution is for the case when the Taylor series at $x = x_{i-1}$, x_{i+1}, and x_{i+2} are used. Note that there is a systematic way to solve this type of problems. Using the notation in the sample solution, the 3 Taylor series are (L1), (L2), and (L4). Our goal is to combine the three to form the finite difference formula with vanishing $f''(x_i)\,h^2$ and $f'''(x_i)\,h^3$ terms. Let's assume that the desirable formula is

$$1 \times (L1) + A \times (L2) + B \times (L4) \quad . \qquad (1)$$

(The coefficient for (L1) can be set to 1 because only the ratios among the 3 coefficients are relevant.) The requirement for the h^2 and h^3 terms to vanish leads to $1 + A + 4B = 0$ and $1 - A + 8B = 0$, or

$$\begin{pmatrix} 1 & 4 \\ -1 & 8 \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} -1 \\ -1 \end{pmatrix} \quad .$$

Plugging the solution, $(A, B) = (-1/3\ , -1/6)$ back to Eq. (1) one obtains the desirable formula. (Make sure you understand the argument.)

Prob. 4 With the designated value of $h = 0.5$, the interval [0,6] contains 12 sub-intervals. Clearly, the numerical integration needs to be performed with the composite Trapezoidal method (Eq. 7.13) and composite Simpson's 1/3 method (Eq. 7.19). See first sample solution. This problem can be efficiently solved with a computer code since the summation is tedious but routine. See second sample solution using Matlab.

Sample solution, Prob 1 (Thanks to Chelsea Dickkut)

$f(x) = e^{-x}\sin(x)$ $\quad h = 0.5$

1) Evaluate $f'(x)$ at $x = 1$, using
a) three-point backward scheme
b) four-point central difference scheme
Evaluate $f''(x)$ at $x = 1$, using
c) four-point backward scheme
d) Compare results a–c with exact values obtained from analytic expressions $f'(x)$ and $f''(x)$ – evaluate the true relative errors.

a)
$$f'(x_i) = \frac{f(x_{i-2}) - 4f(x_{i-1}) + 3f(x_i)}{2h}$$
$$f'(x=1) = \frac{f(0) - 4f(0.5) + 3f(1)}{2(0.5)}$$
$$= \frac{e^0\sin(0) - 4e^{-0.5}\sin(0.5) + 3e^{-1}\sin(1)}{1} = \boxed{-0.2344655259}$$

b)
$$f'(x_i) = \frac{f(x_{i-2}) - 8f(x_{i-1}) + 8f(x_{i+1}) - f(x_{i+2})}{12h}$$
$$f'(x=1) = \frac{f(0) - 8f(0.5) + 8f(1.5) - f(2)}{12(0.5)}$$
$$= \frac{e^0\sin(0) - 8e^{-0.5}\sin(0.5) + 8e^{-1.5}\sin(1.5) - e^{-2}\sin(2)}{6}$$
$$= \boxed{-0.1114634336}$$

c)
$$f''(x_i) = \frac{-f(x_{i-3}) + 4f(x_{i-2}) - 5f(x_{i-1}) + 2f(x_i)}{h^2}$$
$$f''(x=1) = \frac{-f(-0.5) + 4f(0) - 5f(0.5) + 2f(1)}{(0.5)^2}$$
$$= \frac{-e^{0.5}\sin(-0.5) + 4e^0\sin(0) - 5e^{-0.5}\sin(0.5) + 2e^{-1}\sin(1)}{0.25}$$
$$= \boxed{-0.1774904262}$$

d) analytic expressions:
$$f'(x) = e^{-x}\cos(x) - e^{-x}\sin(x)$$
$$f'(1) = e^{-1}\cos(1) - e^{-1}\sin(1) = -0.1107937653$$
$$f''(x) = -e^{-x}\sin(x) - e^{-x}\cos(x) - e^{-x}\cos(x) + e^{-x}\sin(x)$$
$$f''(x) = -2e^{-x}\cos(x)$$
$$f''(1) = -2e^{-1}\cos(1) = -0.3975322207$$

error for a) $\left|\frac{-0.1107937653 - (-0.2344655259)}{-0.1107937653}\right| = \boxed{\begin{array}{c}1.116233935\\ 111.62\%\end{array}}$

error for b) $\left|\frac{-0.1107937653 - (-0.1114634336)}{-0.1107937653}\right| = \boxed{\begin{array}{c}0.0060442778\\ 0.604\%\end{array}}$

error for c) $\left|\frac{-0.3975322207 - (-0.1774904262)}{-0.3975322207}\right| = \boxed{\begin{array}{c}0.5535193955\\ 55.35\%\end{array}}$

The four-point central difference scheme proved to provide the best answer with the least amount of error.

Sample solution, Prob. 2 (Thanks to Elie Chmouni)

The objective of this problem is to Derive a finite difference formula for the second derivative, f "(xi), that depends on the values of f(xi) at three points x_{i-1} , x_i , and x_{i+1} , where the spacing is

$x_i - x_{i-1} = h$ and $x_{i+1} - x_i = 2h$.

Thus using Eq (6.26) with modification to the spacing between x_i and x_{i+1} gives;

$$f(x_{i+1}) = f(x_i) + f'(x_i)(2h) + \frac{f''(x_i)}{2!}(2h)^2 + \frac{f^{(3)}(\zeta_1)}{3!}(2h)^3 + \ldots \qquad \ldots\ldots (1)$$

Also using Eq (6.27) the spacing between x_i and x_{i+1} is h and gives;

$$f(x_{i-1}) = f(x_i) - f'(x_i)(h) + \frac{f''(x_i)}{2!}(h)^2 - \frac{f^{(3)}(\zeta_2)}{3!}(h)^3 + \ldots \qquad \ldots\ldots (2)$$

thus we need to get rid of f '(x) by performing the following algebraic manipulation:

Result= Eq(1)+2*Eq(2)

$$f(x_{i+1}) + 2f(x_{i-1}) = \underline{\underline{f(x_i)}} + \cancel{f'(x_i)(2h)} + \frac{f''(x_i)}{2!}(2h)^2 + \frac{f^{(3)}(\zeta_1)}{3!}(2h)^3 + \underline{\underline{2f(x_i)}} \cancel{-2f'(x_i)(h)} + \cancel{2}\frac{f''(x_i)}{\cancel{2}!}(h)^2 - 2\frac{f^{(3)}(\zeta_2)}{3!}(h)^3$$

$$f(x_{i+1}) + 2f(x_{i-1}) = \underline{\underline{3f(x_i)}} + 3f''(x_i)(h)^2 + \underline{\underline{\frac{f^{(3)}(\zeta_1)}{3!}(2h)^3 - 2\frac{f^{(3)}(\zeta_2)}{3!}(h)^3}}$$

$$f(x_{i+1}) + 2f(x_{i-1}) = \underline{\underline{3f(x_i)}} + 3f''(x_i)(h)^2 + \underline{\underline{O(h)^3}}$$

$$f''(x_i) = \frac{f(x_{i+1}) + 2f(x_{i-1}) - 3f(x_i) - O(h)^3}{3h^2} \Rightarrow$$

$$f''(x_i) = \frac{f(x_{i+1}) + 2f(x_{i-1}) - 3f(x_i)}{3h^2} + O(h)$$

thus the order of the truncation error is O(h)

Sample solution, Prob. 3 (Thanks to Elie Chmouni)

Choose $x_{i-1}, x_{i+1}, x_{i+2}$

STEP #1

$$\text{(L1) } F(x_{i+1}) = F(x_i) + F'(x_i)h + \frac{F''(x_i)}{2}h^2 + \frac{F'''(x_i)}{6}h^3 + \frac{F^{(4)}(x_i)}{24}h^4 + \ldots$$

$$\text{(L2) } F(x_{i-1}) = F(x_i) - F'(x_i)h + \frac{F''(x_i)}{2}h^2 - \frac{F'''(x_i)}{6}h^3 + \frac{F^{(4)}(x_i)}{24}h^4 + \ldots$$

L3=L1-L2

$$\text{(L3) } F(x_{i+1}) - F(x_{i-1}) = 2F'(x_i)h + \frac{F'''(x_i)}{3}h^3 + O(h^5)$$

Step #2

$$(L2)\ F(x_{i-1}) = F(x_i) - F'(x_i)h + \cancel{\frac{F''(x_i)}{2}h^2} - \frac{F'''(x_i)}{6}h^3 + \frac{F^{(4)}(x_i)}{24}h^4 + \ldots$$

$$(L4)\ F(x_{i+2}) = F(x_i) + F'(x_i)(2h) + \cancel{\frac{F''(x_i)}{2}(2h)^2} + \frac{F'''(x_i)}{6}(2h)^3 + \frac{F^{(4)}(x_i)}{24}(2h)^4 + \ldots$$

(L5)=(L4)-4(L2)

$$\text{(L5) } F(x_{i+2}) - 4F(x_{i-1}) = -3F(x_i) + 6F'(x_i)h + 2F'''(x_i)h^3 + 0.5F^{(4)}(x_i)h^4$$

Step #3

(L6)=6(L3)-(L5)

$$6F(x_{i+1}) - 6F(x_{i-1}) = 12F'(x_i)h + \cancel{2F'''(x_i)h^3} + O(h^5)$$

$$-F(x_{i+2}) + 4F(x_{i-1}) = 3F(x_i) - 6F'(x_i)h\ \cancel{-2F'''(x_i)h^3} - 0.5F^{(4)}(x_i)h^4$$

$$\text{(L6) } 6F(x_{i+1}) - 2F(x_{i-1}) - F(x_{i+2}) = 3F(x_i) + 6F'(x_i)h - 0.5F^{(4)}(x_i)h^4$$

Thus solving for the first derivative $F'(x_i)$

$$F'(x_i) = \frac{6F(x_{i+1}) - 2F(x_{i-1}) - F(x_{i+2}) - 3F(x_i)}{6h} + O(h^3)$$

Sample solution, Prob. 4 (version 1, solved by hand) (Thanks to Chelsea Dickkut)

Evaluate the integral $I = \int_0^6 \sin(4x)\,dx$ using

(i) Trapezoidal method
(ii) Simpson's 1/3 method

Assume $h = 0.5$. Compare the numerical results with the exact value obtained from the analytic expression of I. Determine which numerical method provides the better answer.

Eqn. (7.12) $\qquad h = \frac{b-a}{N} \quad N = 12$

(i) $I(f) = \int_a^b f(x)\,dx \doteq \frac{h}{2}\left[f(a) + f(b)\right] + h\sum_{i=2}^{N-1} f(x_i)$

$$I(f) = \frac{0.5}{2}\left[\sin(4\cdot 0) + \sin(4\cdot 6)\right] + 0.5\sum_{i=2}^{11} f(x_i)$$

$$\sum_{i=2}^{11} f(x_i) = \sin(4) + \sin(6) + \sin(8) + \sin(10) + \sin(12) + \sin(14) + \sin(16) + \sin(18) + \sin(20) + \sin(22) + \sin(2)$$

$$= 0.6376543847$$

$$I(f) = -0.2263945905 + 0.5(0.6376543847) = \boxed{0.0924326019 = I}$$

Eqn. (7.19)

(ii) $I(f) = \int_a^b f(x)\,dx = \frac{h}{3}\left[f(a) + 4\sum_{i=2,4,6}^{12} f(x_i) + 2\sum_{j=3,5,7}^{11} f(x_j) + f(b)\right]$

$$\sum_{i=2,4,6}^{12} f(x_i) = \sin(2) + \sin(6) + \sin(10) + \sin(14) + \sin(18) + \sin(22)$$
$$= 0.3166296174$$
$$\sum_{j=3,5,7}^{11} f(x_j) = \sin(4) + \sin(8) + \sin(12) + \sin(16) + \sin(20)$$
$$= 0.3210247674$$

$$I(f) = \frac{0.5}{3}\left[0 + 4(0.3166296174) + 2(0.3210247674) + \sin(6\cdot 4)\right]$$

$$\boxed{I = 0.1671649404}$$

Exact value: $I = \int_0^6 \sin(4x)\,dx = -\frac{1}{4}\cos(4x)\Big|_0^6 = \boxed{0.143955248166 = I}$

error for trapezoidal : $\left|\frac{0.143955248166 - 0.0924326019}{0.143955248166}\right| = 35.79\%$

error for Simpson's 1/3 : $\left|\frac{0.143955248166 - 0.1671649404}{0.143955248166}\right| = 16.12\%$

$\boxed{\text{The Simpson's 1/3 method provides the better answer.}}$

Sample solution, Prob. 4 (version 2, using Matlab)   (Thanks to Shane Mello)

```
(i)Trapezoidal Method
h = 0.5;                              %define h
x = h;                                %initialize x
I = h/2*(sin(4*0) + sin(4*6));        %initialize I
while x < 6
    I = I + h*sin(4*x);
    x = x + h;
end
I

(ii)Simpson's 1/3 Method
h = 0.5;                              %define h
I = h/3*(sin(4*0)+sin(4*6));          %initialize I
x = h;                                %initialize x
while x < 6                           %perform even subintervals
    I = I+h/3*4*sin(4*x);
    x = x+2*h;
end
x = 2*h;                              %reset x
while x < 6                           %perfom odd subintervals
    I = I+h/3*2*sin(4*x);
    x = x+2*h;
end
I
```