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APPM 4650

Homework 3: Numerical Differentiation and Integration

1. *Use the most accurate three-point formula to determine each missing entry in the following table.*

x	$f(x)$	$f'(x)$
1.1	9.025013	17.7697
1.2	11.02318	22.1936
1.3	13.46374	27.1073
1.4	16.44465	32.5109

Explanation:

To determine the estimated values for $f'(x)$ at each $x=1.1, 1.2, 1.3, 1.4$, two different formulas, one for the end points $x=1.1, 1.4$ and for middle points $x=1.2, 1.3$. Although the same general formula was used for each endpoint, the sign associated with the coefficients was actually the opposite of each other.

Thus for $x=1.1$,

$$f'(x_0)=\frac{1}{2h}[-3f(x_0)+4f(x_0+h)-f(x_0+2h)]+error$$

$$f'(1.1)\approx\frac{1}{0.2}[-3f(1.1)+4f(1.2)-f(1.3)]$$

$$f'(1.1)\approx\frac{1}{0.2}[-3(9.025013)+4(11.02318)-(13.46374)]$$

$$f'(1.1)\approx 17.7697$$

Similarly for $x=1.4$,

$$f'(x_0)=\frac{1}{2h}[f(x_0-2h)-4f(x_0-h)+3f(x_0)]+error$$

$$f'(1.4)\approx\frac{1}{0.2}[f(1.2)-4f(1.3)+3f(1.4)]$$

$$f'(1.4)\approx\frac{1}{0.2}[f(11.02318)-4f(13.46374)+3(16.44465)]$$

$$f'(1.4)\approx 32.5109$$

Then for the two middle points, I used the following formulas

$$f'(x_0)=\frac{1}{2h}[-f(x_0-h)_f(x_0+h)]+error$$

Note that the error bound for both end points is $\frac{h^2}{3}f^{(3)}(z)$ and at the mid points is $\frac{h^2}{6}f^{(3)}(z)$ for some unknown value of z between x_0-2h and x_0+2h .

2. *Derive a five-point method for approximating* $f'''(x_0)$ *by expanding the function* $f(x)$ *in a fourth-order Taylor polynomial about* x_0. *The result should be written in terms of* f *evaluated at* $x_0, x_0 \pm h$, *and* $x_0 \pm 2h$. show that the error is $O(h^2)$.

Three Point Midpoint Formula

$$f'(x_0) = \frac{1}{2h}\left[f(x_0+h) - f(x_0-h)\right] - \frac{h^2}{6} f^{(3)}(\xi)$$

$$f'''(x_0) = c_1 f(x_0-2h) + c_2 f(x_0-h) + c_3 f(x_0) + c_4 f(x_0+h) + c_5 f(x_0+2h)$$

Note that

$$f(x_0-2h) = f(x_0) + f'(x_0)(-2h) + \frac{f''(x_0)}{2!}(-2h)^2 + \frac{f'''(x_0)}{3!}(-2h)^3 + \frac{f''''(x_0)}{4!}(-2h)^4 + \frac{f^{(5)}(x_0)}{5!}(-2h)^5$$

$$f(x_0-h) = f(x_0) + f'(x_0)(-h) + \frac{f''(x_0)}{2!}(-h)^2 + \frac{f'''(x_0)}{3!}(-h)^3 + \frac{f''''(x_0)}{4!}(-h)^4 + \frac{f^{(5)}(x_0)}{5!}(-h)^5$$

$$f(x_0) = f(x_0)$$

$$f(x_0+h) = f(x_0) + f'(x_0)(h) + \frac{f''(x_0)}{2!}(h)^2 + \frac{f'''(x_0)}{3!}(h)^3 + \frac{f''''(x_0)}{4!}(h)^4 + \frac{f^{(5)}(x_0)}{5!}(h)^5$$

$$f(x_0+2h) = f(x_0) + f'(x_0)(2h) + \frac{f''(x_0)}{2!}(2h)^2 + \frac{f'''(x_0)}{3!}(2h)^3 + \frac{f''''(x_0)}{4!}(2h)^4 + \frac{f^{(5)}(x_0)}{5!}(2h)^5$$

Now counting

	LHS		RHS
$f(x_0)$	0	=	$c_1 + c_2 + c_3 + c_4 + c_5$
$f'(x_0)$	0	=	$(-2h)c_1 + (-h)c_2 + (h)c_4 + (2h)c_5$
$f''(x_0)$	0	=	$\frac{(-2h)^2}{2}c_1 + \frac{(-h)^2}{2}c_2 + \frac{(h)^2}{2}c_4 + \frac{(2h)^2}{2}c_5$
$f'''(x_0)$	1	=	$\frac{(-2h)^3}{3!}c_1 + \frac{(-h)^3}{3!}c_2 + \frac{(h)^3}{3!}c_4 + \frac{(2h)^3}{3!}c_5$
$f''''(x_0)$	0	=	$\frac{(-2h)^4}{4!}c_1 + \frac{(-h)^4}{4!}c_2 + \frac{(h)^4}{4!}c_4 + \frac{(2h)^4}{4!}c_5$

$$\Rightarrow 0 = c_1 h^4 + c_2 h^4 + c_3 h^4 + c_4 h^4 + c_5 h^4$$

$$0 = -2h^4 c_1 - h^4 c_2 + h^4 c_4 + 2h^4 c_5$$

$$0 = 2h^4 c_1 + \frac{1}{2}h^4 c_2 + \frac{1}{2}h^4 c_4 + 2h^4 c_5$$

$$h = -\frac{4}{3}h^4 c_1 - \frac{1}{6}h^4 c_2 + \frac{1}{6}h^4 c_4 + \frac{4}{3}h^4 c_5$$

$$0 = \frac{2}{3}h^4 c_1 + \frac{1}{24}h^4 c_2 + \frac{1}{24}h^4 c_4 + \frac{2}{3}h^4 c_5$$

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ -2 & -1 & 0 & 1 & 2 \\ 2 & \frac{1}{2} & 0 & \frac{1}{2} & 2 \\ -\frac{4}{3} & -\frac{1}{6} & 0 & \frac{1}{6} & \frac{4}{3} \\ \frac{2}{3} & \frac{1}{24} & 0 & \frac{1}{24} & \frac{2}{3} \end{pmatrix} \begin{bmatrix} c_1 h^4 \\ c_2 h^4 \\ c_3 h^4 \\ c_4 h^4 \\ c_5 h^4 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \\ h \\ 0 \end{bmatrix}$$

$$\left[\begin{array}{ccccc|c} 1 & 1 & 1 & 1 & 1 & 0 \\ 0 & 1 & 2 & 3 & 4 & 0 \\ 0 & -3/2 & -2 & -3/2 & -2 & 0 \\ 0 & 7/6 & 4/3 & 3/2 & 8/3 & h \\ 0 & -5/8 & -2/3 & -5/8 & 0 & 0 \end{array}\right]$$

$$\left[\begin{array}{ccccc|c} 1 & 1 & 1 & 1 & 1 & 0 \\ 0 & 1 & 2 & 3 & 4 & 0 \\ 0 & 0 & 1 & 3 & 4 & 0 \\ 0 & 0 & -1 & -2 & -2 & h \\ 0 & 0 & 7/12 & 5/4 & 5/2 & 0 \end{array}\right]$$

$$\left[\begin{array}{ccccc|c} 1 & 1 & 1 & 1 & 1 & 0 \\ 0 & 1 & 2 & 3 & 4 & 0 \\ 0 & 0 & 1 & 3 & 4 & 0 \\ 0 & 0 & 0 & -1/2 & 1/6 & 0 \\ 0 & 0 & 0 & 1 & 13/2 & h \end{array}\right]$$

$$\left[\begin{array}{ccccc|c} 1 & 1 & 1 & 1 & 1 & 0 \\ 0 & 1 & 2 & 3 & 4 & 0 \\ 0 & 0 & 1 & 3 & 4 & 0 \\ 0 & 0 & 0 & -1/2 & 1/6 & 0 \\ 0 & 0 & 0 & 0 & 41/6 & h \end{array}\right]$$

$$\left[\begin{array}{ccccc|c} 1 & 1 & 1 & 1 & 1 & 0 \\ 0 & 1 & 2 & 3 & 4 & 0 \\ 0 & 0 & 1 & 3 & 4 & 0 \\ 0 & 0 & 0 & 1 & -1/3 & 0 \\ 0 & 0 & 0 & 0 & 1 & \frac{6}{41} h \end{array}\right]$$

$$\left[\begin{array}{ccccc|c} 1 & 1 & 1 & 1 & 0 & \frac{-6}{41} h \\ 0 & 1 & 2 & 3 & 0 & (-24/41) h \\ 0 & 0 & 1 & 3 & 0 & (-24/41) h \\ 0 & 0 & 0 & 1 & 0 & \frac{2}{41} h \\ 0 & 0 & 0 & 0 & 1 & \frac{6}{41} h \end{array}\right]$$

$$\left[\begin{array}{ccccc|c} 1 & 1 & 1 & 0 & 0 & (-8/41) h \\ 0 & 1 & 2 & 0 & 0 & (-30/41) h \\ 0 & 0 & 1 & 0 & 0 & (-30/41) h \\ 0 & 0 & 0 & 1 & 0 & (2/41) h \\ 0 & 0 & 0 & 0 & 1 & \frac{6}{41} h \end{array}\right]$$

$$\left[\begin{array}{ccccc|c} 1 & 1 & 0 & 0 & 0 & (22/41) h \\ 0 & 1 & 0 & 0 & 0 & (30/41) h \\ 0 & 0 & 1 & 0 & 0 & (-30/41) h \\ 0 & 0 & 0 & 1 & 0 & (2/41) h \\ 0 & 0 & 0 & 0 & 1 & (6/41) h \end{array}\right]$$

$$\left[\begin{array}{ccccc|c} 1 & 0 & 0 & 0 & 0 & (-8/41)h \\ 0 & 1 & 0 & 0 & 0 & (30/41)h \\ 0 & 0 & 1 & 0 & 0 & (-30/41)h \\ 0 & 0 & 0 & 1 & 0 & \left(\frac{2}{41}\right)h \\ 0 & 0 & 0 & 0 & 1 & \left(\frac{6}{41}\right)h \end{array}\right]$$

$\therefore c_1 h^4 = \left(\frac{-8}{41}\right)h \quad c_2 h^4 = \left(\frac{30}{41}\right)h \quad c_3 h^4 = \left(\frac{-30}{41}\right)h \quad c_4 h^4 = \left(\frac{2}{41}\right)h \quad c_5 h^4 = \left(\frac{6}{41}\right)h$

$c_1 = \left(\frac{-8}{41}\right)\left(\frac{1}{h^3}\right) \quad c_2 = \left(\frac{30}{41}\right)\left(\frac{1}{h^3}\right) \quad c_3 = \left(\frac{-30}{41}\right)\left(\frac{1}{h^3}\right) \quad c_4 = \left(\frac{2}{41}\right)\left(\frac{1}{h^3}\right) \quad c_5 = \left(\frac{6}{41}\right)\left(\frac{1}{h^3}\right)$

$\Rightarrow f'''(x_0) = \left(\frac{-8}{41}\right)\left(\frac{1}{h^3}\right)f(x_0-2h) + \left(\frac{30}{41}\right)\left(\frac{1}{h^3}\right)f(x_0-h) + \left(\frac{-30}{41}\right)\left(\frac{1}{h^3}\right)f(x_0) + \left(\frac{2}{41}\right)\left(\frac{1}{h^3}\right)f(x_0+h) + \left(\frac{6}{41}\right)\left(\frac{1}{h^3}\right)f(x_0+2h)$

$f^{(5)}(x_0) \quad 0 = \frac{(-2h)^5}{5!}c_1 + \frac{(-h)^5}{5!}c_2 + \frac{(h)^5}{5!}c_4 + \frac{(2h)^5}{5!}c_5 + \varepsilon$

$0 = \frac{(-2h)^5}{5!}\left(\frac{-2}{41h^3}\right) + \frac{(-h)^5}{5!}\left(\frac{30}{41h^3}\right) + \frac{h^5}{5!}\left(\frac{2}{41h^3}\right) + \frac{(2h)^5}{5!}\left(\frac{6}{41h^3}\right) + \varepsilon$

$0 = h^2\left(\frac{64-30+2+384}{(5!)(41)}\right) + \varepsilon$

$0 = h^2\left(\frac{420}{120(41)}\right) + \varepsilon$

$\therefore$ The error must be of order h^2.

Final answer: $f'''(x_0) \approx \frac{1}{41h^3}[-8f(x_0-2h)+30f(x_0-h)-30f(x_0)+2f(x_0+h)+6f(x_0+2h)]$

3. *Use Taylor series expansions to find three-point forward and backward expressions for* $f''(x)$ *. (Note: also attached in back if print-out is not legible)*

$F''(x_0) = c_1 f(x_0) + c_2 f(x_0+h) + c_3 f(x_0+2h)$ forward

$f''(x_0) = d_1 f(x_0-2h) + d_2 f(x_0-h) + d_3 f(x_0)$ backward

$f(x_0) = f(x_0)$

$f(x_0+h) = f(x_0) + h f'(x_0) + \frac{h^2}{2} f''(x_0) + \frac{h^3}{6} f'''(x_0)$

$f(x_0+2h) = f(x_0) + 2h f'(x_0) + 2h^2 f''(x_0) + \frac{4}{3} h^3 f'''(x_0)$

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

$f(x_0-2h) = f(x_0) - 2h f'(x_0) + 2h^2 f''(x_0) - \frac{4}{3} h^3 f'''(x_0)$

counting forward

	left	Right
$f(x_0)$	0	$= c_1 + c_2 + c_3$
$f'(x_0)$	0	$= h c_2 + 2h c_3$
$f''(x_0)$	1	$= \frac{h^2}{2} c_2 + 2h^2 c_3$

counting backward

	left	right
$f(x_0)$	0	$= d_1 + d_2 + d_3$
$f'(x_0)$	0	$= -2hd_1 - hd_2$
$f''(x_0)$	1	$= 2h^2 d_1 + \frac{h^2}{2} d_2$

$1 = \frac{h^2}{2} c_2 + 2h^2 c_3 \quad 0 = h^2 c_2 + 2h^2 c_3 \quad 0 = h^2(c_1+c_2+c_3)$

$$\left[\begin{array}{ccc|c} 1 & 1 & 1 & 0 \\ 0 & 1 & 2 & 0 \\ 0 & \frac{1}{2} & 2 & 1 \end{array}\right] \downarrow \left[\begin{array}{ccc|c} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & -2 \\ 0 & 0 & 1 & 1 \end{array}\right]$$

$\therefore h^2 c_1 = 1 \quad h^2 c_2 = -2 \quad h^2 c_3 = 1$

$c_1 = \frac{1}{h^2} \quad c_2 = \frac{-2}{h^2} \quad c_3 = \frac{1}{h^2}$

$F''(x_0) = \frac{1}{h^2} f(x_0) - \frac{2}{h^2} f(x_0+h) + \frac{1}{h^2} f(x_0+2h)$

$0 = (d_1 + d_2 + d_3)h^2 \quad 0 = -2h^2 d_1 - h^2 d_2 \quad 1 = 2h^2 d_1 + \frac{h^2}{2} d_2$

$$\left[\begin{array}{ccc|c} 1 & 1 & 1 & 0 \\ -2 & -1 & 0 & 0 \\ 2 & \frac{1}{2} & 0 & 1 \end{array}\right] \downarrow \left[\begin{array}{ccc|c} 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & -2 \\ 0 & 0 & 1 & 1 \end{array}\right]$$

$\therefore h^2 d_1 = 1 \quad h^2 d_2 = -2 \quad h^2 d_3 = 1$

$d_1 = \frac{1}{h^2} \quad d_2 = \frac{-2}{h^2} \quad d_3 = \frac{1}{h^2}$

$\therefore F(x_0) = \frac{1}{h^2} f(x_0-2h) - \frac{2}{h^2} f(x_0-h) + \frac{1}{h^2}(x_0)$

4. *Use Taylor series expansions to arrive at the expression*

$$f'(x) \approx \frac{1}{h}\left(\frac{-3}{2}f(x) + 2f(x+h) - \frac{1}{2}f(x+2h)\right)$$

which we found in class using Lagrange polynomials.

(4) $f'(x) \approx \frac{1}{h}\left(\frac{-3}{2}f(x) + 2f(x+h) - \frac{1}{2}f(x+2h)\right)$

$f'(x) = a f(x) + b f(x+h) + c f(x+2h)$

$f(x) = f(x)$

$f(x+h) = f(x) + h f'(x) + \frac{h^2}{2} f''(x)$

$f(x+2h) = f(x) + 2h f'(x) + \frac{(2h)^2}{2} f''(x)$

Counting

	LHS		RHS
$f(x)$	0	$=$	$a+b+c$
$f'(x)$	1	$=$	$bh + 2ch$
$f''(x)$	0	$=$	$\frac{h^2}{2}b + \frac{(2h)^2}{2}c$

$$0 = ah^2 + bh^2 + ch^2$$
$$\Rightarrow h = bh^2 + 2ch^2$$
$$0 = \tfrac{1}{2}bh^2 + 2ch^2$$

$$\left[\begin{array}{ccc|c} 1 & 1 & 1 & 0 \\ 0 & 1 & 2 & h \\ 0 & \frac{1}{2} & 2 & 0 \end{array}\right] = \left[\begin{array}{ccc|c} 1 & 1 & 1 & 0 \\ 0 & 1 & 4 & 0 \\ 0 & 0 & -2 & h \end{array}\right]$$

$$= \left[\begin{array}{ccc|c} 1 & 1 & 0 & h/2 \\ 0 & 1 & 0 & 2h \\ 0 & 0 & 1 & -h/2 \end{array}\right]$$

$$= \left[\begin{array}{ccc|c} 1 & 0 & 0 & -\frac{3h}{2} \\ 0 & 1 & 0 & 2h \\ 0 & 0 & 1 & -\frac{h}{2} \end{array}\right]$$

$\therefore\ ah^2 = \frac{-3h}{2} \quad bh^2 = 2h \quad ch^2 = \frac{-h}{2}$

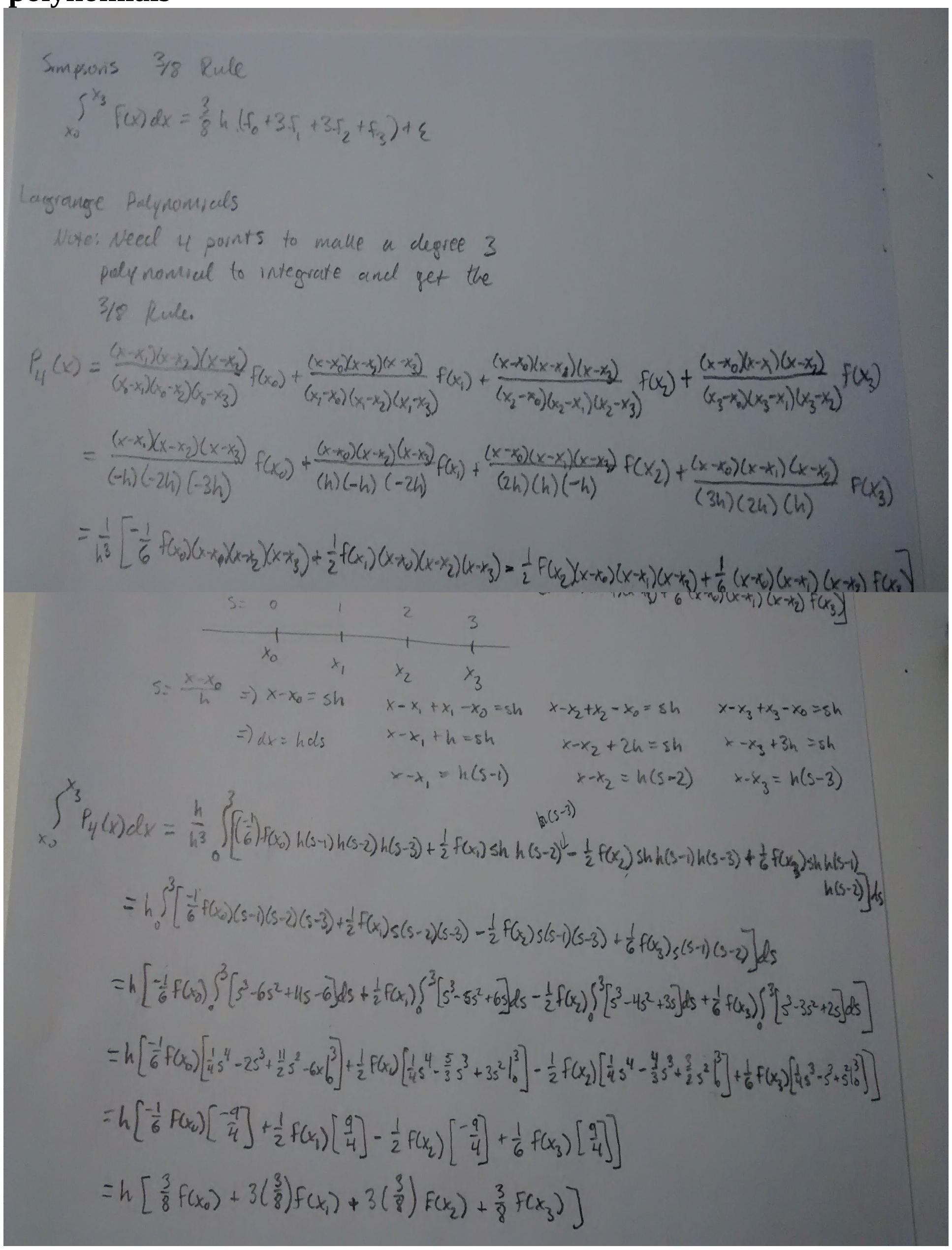
$a = \frac{-3}{2h} \quad b = \frac{2}{h} \quad c = \frac{-1}{2h}$

$\Rightarrow f'(x) \approx \frac{-3}{2h} f(x) + \frac{2}{h} f(x+h) - \frac{1}{2h} f(x+2h)$

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

5. *Derive Simpson's* $\frac{3}{8}$ *Rule using*
   (a) *Lagrange polynomials*
   (b) *Taylor comparison*

(a) Lagrange polynomials



Simpsons 3/8 Rule

$$\int_{x_0}^{x_3} f(x)\,dx = \frac{3}{8}h\,(f_0 + 3f_1 + 3f_2 + f_3) + \varepsilon$$

Lagrange Polynomials

Note: Need 4 points to make a degree 3 polynomial to integrate and get the 3/8 Rule.

$$P_4(x) = \frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)}f(x_0) + \frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)}f(x_1) + \frac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)}f(x_2) + \frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)}f(x_3)$$

$$= \frac{(x-x_1)(x-x_2)(x-x_3)}{(-h)(-2h)(-3h)}f(x_0) + \frac{(x-x_0)(x-x_2)(x-x_3)}{(h)(-h)(-2h)}f(x_1) + \frac{(x-x_0)(x-x_1)(x-x_3)}{(2h)(h)(-h)}f(x_2) + \frac{(x-x_0)(x-x_1)(x-x_2)}{(3h)(2h)(h)}f(x_3)$$

$$= \frac{1}{h^3}\left[-\frac{1}{6}f(x_0)(x-x_1)(x-x_2)(x-x_3) + \frac{1}{2}f(x_1)(x-x_0)(x-x_2)(x-x_3) - \frac{1}{2}f(x_2)(x-x_0)(x-x_1)(x-x_3) + \frac{1}{6}(x-x_0)(x-x_1)(x-x_2)f(x_3)\right]$$

s: 0 1 2 3

x_0 x_1 x_2 x_3

$s = \frac{x-x_0}{h} \Rightarrow x - x_0 = sh$

$\Rightarrow dx = h\,ds$

$x - x_1 + x_1 - x_0 = sh$ $\quad$ $x - x_2 + x_2 - x_0 = sh$ $\quad$ $x - x_3 + x_3 - x_0 = sh$

$x - x_1 + h = sh$ $\quad$ $x - x_2 + 2h = sh$ $\quad$ $x - x_3 + 3h = sh$

$x - x_1 = h(s-1)$ $\quad$ $x - x_2 = h(s-2)$ $\quad$ $x - x_3 = h(s-3)$

$$\int_{x_0}^{x_3} P_4(x)\,dx = \frac{h}{h^3}\int_0^3\left[\left(-\frac{1}{6}\right)f(x_0)\,h(s-1)\,h(s-2)\,h(s-3) + \frac{1}{2}f(x_1)\,sh\,h(s-2)\,h(s-3) - \frac{1}{2}f(x_2)\,sh\,h(s-1)\,h(s-3) + \frac{1}{6}f(x_3)\,sh\,h(s-1)\,h(s-2)\right]ds$$

$$= h\int_0^3\left[-\frac{1}{6}f(x_0)(s-1)(s-2)(s-3) + \frac{1}{2}f(x_1)s(s-2)(s-3) - \frac{1}{2}f(x_2)s(s-1)(s-3) + \frac{1}{6}f(x_3)s(s-1)(s-2)\right]ds$$

$$= h\left[-\frac{1}{6}f(x_0)\int_0^3[s^3-6s^2+11s-6]\,ds + \frac{1}{2}f(x_1)\int_0^3[s^3-5s^2+6s]\,ds - \frac{1}{2}f(x_2)\int_0^3[s^3-4s^2+3s]\,ds + \frac{1}{6}f(x_3)\int_0^3[s^3-3s^2+2s]\,ds\right]$$

$$= h\left[-\frac{1}{6}f(x_0)\left[\frac{1}{4}s^4 - 2s^3 + \frac{11}{2}s^2 - 6x\right]_0^3 + \frac{1}{2}f(x_1)\left[\frac{1}{4}s^4 - \frac{5}{3}s^3 + 3s^2\right]_0^3 - \frac{1}{2}f(x_2)\left[\frac{1}{4}s^4 - \frac{4}{3}s^3 + \frac{3}{2}s^2\right]_0^3 + \frac{1}{6}f(x_3)\left[\frac{1}{4}s^4 - s^3 + s^2\right]_0^3\right]$$

$$= h\left[-\frac{1}{6}f(x_0)\left[-\frac{9}{4}\right] + \frac{1}{2}f(x_1)\left[\frac{9}{4}\right] - \frac{1}{2}f(x_2)\left[-\frac{9}{4}\right] + \frac{1}{6}f(x_3)\left[\frac{9}{4}\right]\right]$$

$$= h\left[\frac{3}{8}f(x_0) + 3\left(\frac{3}{8}\right)f(x_1) + 3\left(\frac{3}{8}\right)f(x_2) + \frac{3}{8}f(x_3)\right]$$

Finally,

$$\int_{x_0}^{x_3} f(x)\,dx \approx \frac{3}{8}h\big(f(x_0)+3f(x_1)+3f(x_2)+f(x_3)\big)$$

6. *Approximate the value of* $\int_0^2 x^2 e^{-x^2}\,dx$ *using the following methods with* $h=0.25$.

(a) *Composite Midpoint rule.*
(b) *Composite Trapezoidal rule.*
(c) *Composite Simpson's* $1/3$ *rule.*

(a) Recall that the Composite Midpoint Rule is for $i=a,a+h,a+2h,\ldots,b$. Using this expression, I found

$$\int_0^2 x^2 e^{-x^2}\,dx \approx 0.423296$$

(b) Recall that the Composite Trapezoidal Rule is $\int_a^b f(x)\,dx \approx \frac{h}{2}\left(f(a)+f(b)+\sum_{i=a+h}^{b-h} f(i)\right)$ for $i=a+h,a+2h,\ldots,b-h$. Using this expression, I found

$$\int_0^2 x^2 e^{-x^2}\,dx \approx 0.421582$$

(c) Recall that the Simpson's Composite Rule is

$$\int_a^b f(x)\,dx \approx \frac{h}{3}\left(f(a)+2\sum_{j=1,\,j\,odd}^{n-2} f(x_j)+4\sum_{j=1,\,j\,even}^{j=n-1} f(x_j)+f(b)\right)$$

Using this expression, I found

$$\int_0^2 x^2 e^{-x^2}\,dx \approx 0.422716$$

7. *Approximate the integral* $\int_0^1 x^2 e^{-x} dx$ *using Gaussian quadrature and compare your results to the exact values of the integral.*
(a) *Use* $n=2$ (b) *Use* $n=3$

Solution
Note that, before performing the computer-based calculation, first consider the true value of the given integral.

$$\begin{aligned}\int_0^1 x^2 e^{-x} dx &= -x^2 e^{-x} + 2\int x e^{-x} dx \\ &= -x^2 e^{-x} + 2[-xe^{-x} + \int e^{-x} dx] \\ &= -x^2 e^{-x} + 2[-xe^{-x} - e^{-x}] \Big|_0^1 \\ &= 2 - \frac{5}{e} \approx 0.16060\end{aligned}$$

With the known answer in mind, now consider the Gaussian quadrature. Recall that for Gaussian quadrature to work, the bounds on the integral must be between -1 and 1. To do this, we first apply the transformation $t = \frac{2x-a-b}{b-a}$ which implies $\int_a^b f(x) dx = \int_{-1}^1 f\left(\frac{(b-a)t+a+b}{2}\right)\left(\frac{b-a}{2}\right) dt$.

After simplifying, for our equation, we get $\int_0^1 x^2 e^{-x} dx = \frac{1}{2}\int_{-1}^1 \left(\frac{t+1}{2}\right)^2 e^{-\frac{t+1}{2}} dt$.

(a) Using this, we can now find the Gaussian Quadrature for $n=2$. Recall that the optimal values for t are $t = \frac{\pm 1}{\sqrt{3}}$. Now we apply the algorithm:

$$\begin{aligned}\frac{1}{2}\int_{-1}^1 \left(\frac{t+1}{2}\right)^2 e^{-\frac{t+1}{2}} dt &= \frac{1}{2}\left(f\left(\frac{-1}{2\sqrt{(3)}} + \frac{1}{2}\right) + f\left(\frac{1}{2\sqrt{(3)}} + \frac{1}{2}\right)\right) \\ &\approx \frac{1}{2}(0.318821) \\ &\approx 0.15941\end{aligned}$$

Note that this result is off by $0.16060 - 0.15941 = 0.00119$ from the exact answer, or $\approx 10^{-3}$.

(b) Now consider for $n=3$. Recall that the optimal values for t are $0, \pm\sqrt{\frac{3}{5}}$ with coefficients of $\frac{8}{9,}\frac{5}{9}$ as in the following:

$$\begin{aligned}\frac{1}{2}\int_{-1}^1 \left(\frac{t+1}{2}\right)^2 e^{-\frac{t+1}{2}} dt &= \frac{1}{2}\left(\frac{5}{9} f\left(\frac{-1}{2}\sqrt{\frac{3}{5}} + \frac{1}{2}\right) + \frac{8}{9} f\left(0 + \frac{1}{2}\right)\right) + \frac{5}{9} f\left(\frac{1}{2}\sqrt{(3/5)} + \frac{1}{2}\right) \\ &\approx \frac{1}{2}(0.321191) \\ &\approx 0.160595\end{aligned}$$

Note that this result is off by $0.16060 - 0.160595 = 5 * 10^{-6}$