

Numerical Differentiation and Integration

1] Numerical Differentiation:

$f''(x)$	Method	Numerical approximation	Function Error (T.E.)
1 st derivative	1] Forward	$f'(x) = \frac{1}{h} [f(x+h) - f(x)] + O(h)$	$T.E \leq \frac{h}{2} M_2, \quad x \leq c \leq x+h$
	2] backward	$f'(x) = \frac{1}{h} [f(x) - f(x-h)] + O(h)$	$T.E \leq \frac{h}{2} M_2, \quad x-h \leq c \leq x$
	3] Central	$f'(x) = \frac{1}{2h} [f(x+h) - f(x-h)] + O(h^2)$	$T.E \leq \frac{h^2}{6} M_3, \quad x-h \leq c \leq x+h$
	4] Richardson's Extrapolation	$f'(x) = [\frac{4}{3} \phi(\frac{h}{2}) - \frac{1}{3} \phi(h)] + O(h^4)$ $\phi(h) = \frac{1}{2h} [f(x+h) - f(x-h)]$	$T.E \leq \frac{h^4}{480} M_5, \quad x-h \leq c \leq x+h$
2 nd derivative	1] Forward	$f''(x) = \frac{1}{h^2} [f(x) - 2f(x+h) + f(x+2h)] + O(h)$	$T.E \leq h M_3, \quad x \leq c \leq x+2h$
	2] backward	$f''(x) = \frac{1}{h^2} [f(x) - 2f(x-h) + f(x-2h)] + O(h)$	$T.E \leq h M_3, \quad x-2h \leq c \leq x$
	3] Central	$f''(x) = \frac{1}{h^2} [f(x+h) - 2f(x) + f(x-h)] + O(h^2)$	$T.E \leq \frac{h^2}{12} M_4, \quad x-h \leq c \leq x+h$

2] Numerical Integration:

$$M_n = \max_{a \leq c \leq b} |f^{(n)}(c)|$$

Method	Numerical approximation	Function Error (T.E.)
1] Trapezoidal Rule	$\int_a^b f(x) dx = \frac{h}{2} [f_0 + f_n + 2(f_1 + f_2 + \dots + f_{n-1})]$ $b = x_n, a = x_0$	$T.E \leq \frac{nh^3}{12} M_2, \quad a \leq c \leq b$
2] Simpson's Rule	$\int_a^b f(x) dx = \frac{h}{3} [f_0 + f_n + 4(f_1 + f_3 + \dots + f_{n-2}) + 2(f_2 + f_4 + \dots + f_{n-1})]$ n is even	$T.E \leq \frac{nh^5}{180} M_4, \quad a \leq c \leq b$
3] Gaussian Quadrature	$\int_a^b f(x) dx = \int_{-1}^1 g(t) dt = \sum_{i=1}^n w_i \cdot g(t_i), \quad \frac{x-a}{b-a} = \frac{t+1}{2}, \quad dx = \frac{b-a}{2} dt$ 1] one-point (mid point) $n=1$ [$w_1=2, t_1=0$] $I = \int_{-1}^1 g(t) dt = 2g(0)$ 2] Two-point $n=2$ [$w_1=w_2=1, t_1=-\frac{1}{\sqrt{3}}, t_2=\frac{1}{\sqrt{3}}$] $I = \int_{-1}^1 g(t) dt = g(-\frac{1}{\sqrt{3}}) + g(\frac{1}{\sqrt{3}})$ 3] Three-point $n=3$ [$w_1=w_3=\frac{5}{9}, w_2=\frac{8}{9}, t_1=-\sqrt{\frac{3}{5}}, t_2=0, t_3=\sqrt{\frac{3}{5}}$] $I = \int_{-1}^1 g(t) dt = \frac{5}{9} \cdot g(-\sqrt{\frac{3}{5}}) + \frac{8}{9} \cdot g(0) + \frac{5}{9} \cdot g(\sqrt{\frac{3}{5}})$	

1] For the following data, find $f'(6)$ with error $O(h)$ and $f'(6.3)$ with error $O(h^2)$

Sol.

x	6	6.1	6.2	6.3	6.4
f(x)	-0.175	-0.1998	-0.2223	-0.2422	-0.2596

① $f'(6) \rightarrow$ using forward difference formula

$$f'(6) = \frac{f(6.1) - f(6)}{0.1} = \frac{-0.1998 + 0.175}{0.1} = -0.248$$

② $f'(6.3) \rightarrow$ using central difference formula

$$f'(6.3) = \frac{f(6.4) - f(6.2)}{2 \times 0.1} = \frac{-0.2596 + 0.2223}{0.2} = -0.183$$

2] Find $f'(1.4)$ using backward difference formula, central difference formula and Richardson's extrapolation where $F(x) = x \cos x - 3x$ with $h = 0.2$. Then find the absolute and truncation error

Sol.

1] backward difference formula:

$$f'(x) = \frac{1}{h} [f(x) - f(x-h)] \Rightarrow f'(1.4) = \frac{1}{0.2} [f(1.4) - f(1.2)] = -3.984376527$$

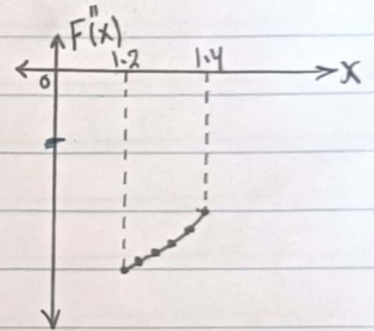
$$\therefore F'(x) = -x \sin x + \cos x - 3 \Rightarrow F'(1.4) = -4.209662479$$

$$EY(1.4) = |F'(1.4) - f'(1.4)| = 2.252859 \times 10^{-1}$$

$$T.E \leq \frac{h}{2} |F''(c)|, \quad 1.2 \leq c \leq 1.4, \quad F''(x) = -x \cos x - 2 \sin x$$

$$\leq \frac{0.2}{2} |F''(1.2)|, \quad F''(1.2) = -2.2989074$$

$$\leq 2.298989 \times 10^{-1}, \quad F''(1.4) = -2.208853$$



2] Central difference formula:

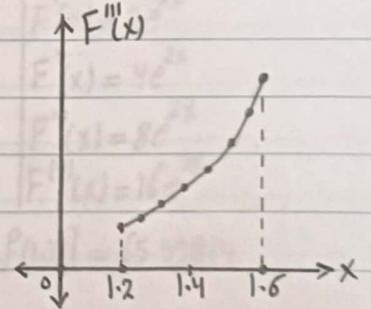
$$f'(x) = \frac{1}{2h} [f(x+h) - f(x-h)] \Rightarrow f'(1.4) = \frac{1}{0.4} [f(1.6) - f(1.2)] = -4.203871353$$

$$EY(1.4) = |F'(1.4) - f'(1.4)| = 5.7911265 \times 10^{-3}$$

$$T.E \leq \frac{h^2}{6} |F'''(c)|, \quad 1.2 \leq c \leq 1.6, \quad F'''(x) = x \sin x - 3 \cos x$$

$$\leq \frac{(0.2)^2}{6} |F'''(1.6)|, \quad F'''(1.2) = 0.0313736$$

$$\leq 1.12461 \times 10^{-2}, \quad F'''(1.6) = 1.6869163$$



3] Richardson's extrapolation:

$$f'(x) = \frac{4}{3} \phi\left(\frac{h}{2}\right) - \frac{1}{3} \phi(h), \quad \phi(h) = \frac{1}{2h} [f(x+h) - f(x-h)]$$

$$f'(1.4) = \frac{4}{3} \phi(0.1) - \frac{1}{3} \phi(0.2), \quad \phi(0.2) = \frac{1}{2 \times 0.2} [f(1.4+0.2) - f(1.4-0.2)] = -4.203871353$$

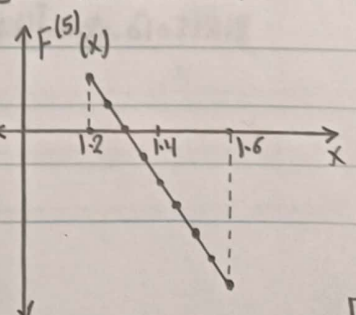
$$= -4.209660709, \quad \phi(0.1) = \frac{1}{2 \times 0.1} [f(1.4+0.1) - f(1.4-0.1)] = -4.20821337$$

$$EY(1.4) = |F'(1.4) - f'(1.4)| = 1.77 \times 10^{-6}$$

$$T.E \leq \frac{h^4}{480} |F^{(5)}(c)|, \quad 1.2 \leq c \leq 1.6, \quad F^{(5)}(x) = x \cos x + 4 \sin x$$

$$\leq \frac{(0.2)^4}{480} |F^{(5)}(1.6)|, \quad F^{(5)}(x) = -x \sin x + 5 \cos x$$

$$\leq 5.8177 \times 10^{-6}$$



[3] Find $f'(2.3)$ with $h=0.2$ where $f(x) = xe^x - x^2$ using Richardson's extrapolation, link 1.e

sol

$$f'(2.3) = \frac{4}{3} \phi\left(\frac{0.2}{2}\right) - \frac{1}{3} \phi(0.2) \quad \phi(0.2) = \frac{1}{2 \times 0.2} [f(2.3+0.2) - f(2.3-0.2)] = 28.66819521$$

$$= \frac{4}{3} \phi(0.1) - \frac{1}{3} \phi(0.2) \quad \phi(0.1) = \frac{1}{2 \times 0.1} [f(2.3+0.1) - f(2.3-0.1)] = 28.40296807$$

$$f'(2.3) = \frac{4}{3} \times 28.40296807 - \frac{1}{3} \times 28.66819521 = 28.31455903$$

$$F'(x) = xe^x + e^x - 2x = (x+1)e^x - 2x \Rightarrow F'(2.3) = 28.3148021$$

$$ER(2.3) = |F'(2.3) - f'(2.3)| = 2.430708 \times 10^{-4}$$

$$T.E \leq \frac{h^4}{180} |F^{(5)}(c)|, \quad 2.1 \leq c \leq 2.5$$

$$\leq \frac{(0.2)^4}{180} |F^{(5)}(2.5)|$$

$$\leq 8.12166 \times 10^{-4}$$

$$F(x) = xe^x - x^2$$

$$F'(x) = (x+1)e^x - 2x$$

$$F''(x) = (x+2)e^x - 2$$

$$F'''(x) = (x+3)e^x$$

$$F^{(4)}(x) = (x+4)e^x$$

$$F^{(5)}(x) = (x+5)e^x$$

[4] Given $f(x) = e^{2x}$ and $h=0.1$. Estimate $f''(1.5)$ using

1) Forward difference formula.

2) Backward difference formula.

3) Central difference formula.

Then find the absolute error and truncation error.

sol

[1] Forward difference formula:

$$f''(x) = \frac{1}{h^2} [f(x) - 2f(x+h) + f(x+2h)] \Rightarrow f''(1.5) = \frac{1}{0.1^2} [f(1.5) - 2f(1.6) + f(1.7)] = 98.45765764$$

$$ER(1.5) = |F''(1.5) - f''(1.5)| = 18.1155099$$

$$T.E \leq h |F'''(c)|, \quad 1.5 \leq c \leq 1.7$$

$$\leq 0.1 |F'''(1.7)| \leq 23.97128$$

$$F''(1.5) = 80.34214769$$

$$F(x) = e^{2x}$$

$$F'(x) = 2e^{2x}$$

$$F''(x) = 4e^{2x}$$

$$F'''(x) = 8e^{2x}$$

$$F^{(4)}(x) = 16e^{2x}$$

[2] Backward difference formula:

$$f''(x) = \frac{1}{h^2} [f(x) - 2f(x-h) + f(x-2h)] \Rightarrow f''(1.5) = \frac{1}{0.1^2} [f(1.5) - 2f(1.4) + f(1.3)] = 65.99814$$

$$ER(1.5) = |F''(1.5) - f''(1.5)| = 14.344$$

$$T.E \leq h |F'''(c)|, \quad 1.3 \leq c \leq 1.5$$

$$\leq 0.1 |F'''(1.5)| \leq 16.068429$$

[3] Central difference formula:

$$f''(x) = \frac{1}{h^2} [f(x-h) - 2f(x) + f(x+h)] \Rightarrow f''(1.5) = \frac{1}{0.1^2} [f(1.4) - 2f(1.5) + f(1.6)] = 80.61031218$$

$$ER(1.5) = |F''(1.5) - f''(1.5)| = 2.6816 \times 10^{-1}$$

$$T.E \leq \frac{h^2}{12} |F^{(4)}(c)|, \quad 1.4 \leq c \leq 1.6$$

$$\leq \frac{0.1^2}{12} |F^{(4)}(1.6)| \leq 3.271 \times 10^{-1}$$

5] Using Taylor's series, deduce a forward difference formula for the first derivative such that the truncation error is of order $O(h^2)$

Sol

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) + \frac{h^4}{4!} f^{(4)}(x) + \dots$$

$$f(x+2h) = f(x) + 2hf'(x) + \frac{4h^2}{2!} f''(x) + \frac{8h^3}{3!} f'''(x) + \frac{16h^4}{4!} f^{(4)}(x) + \dots$$

$$4f(x+h) = 4f(x) + 4hf'(x) + \frac{4h^2}{2!} f''(x) + \frac{4h^3}{3!} f'''(x) + \frac{4h^4}{4!} f^{(4)}(x) + \dots$$

$$4f(x+h) - f(x+2h) = 3f(x) + 2hf'(x) - \frac{4h^3}{3!} f'''(x) - \frac{12h^4}{4!} f^{(4)}(x) - \dots$$

$$f'(x) = \frac{1}{2h} [-3f(x) + 4f(x+h) - f(x+2h)] + \frac{h^2}{3} f'''(x) + \frac{h^3}{4} f^{(4)}(x) + \dots$$

$$\therefore f'(x) = \frac{1}{2h} [-3f(x) + 4f(x+h) - f(x+2h)] + O(h^2) \quad , \quad T.E \leq \frac{h^2}{3} |f'''(c)| \quad , \quad x \leq c \leq x+2h$$

6] Using Taylor's series, deduce a central difference formula for the 3rd derivative such that the truncation error is of order $O(h^2)$

Sol

$$a \quad f(x+2h) = f(x) + 2hf'(x) + \frac{4h^2}{2!} f''(x) + \frac{8h^3}{3!} f'''(x) + \frac{16h^4}{4!} f^{(4)}(x) + \frac{32h^5}{5!} f^{(5)}(x) + \frac{64h^6}{6!} f^{(6)}(x) + \dots \quad * a$$

$$b \quad f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!} f''(x) + \frac{h^3}{3!} f'''(x) + \frac{h^4}{4!} f^{(4)}(x) + \frac{h^5}{5!} f^{(5)}(x) + \frac{h^6}{6!} f^{(6)}(x) + \dots \quad * b$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!} f''(x) - \frac{h^3}{3!} f'''(x) + \frac{h^4}{4!} f^{(4)}(x) - \frac{h^5}{5!} f^{(5)}(x) + \frac{h^6}{6!} f^{(6)}(x) + \dots$$

$$c \quad f(x-2h) = f(x) - 2hf'(x) + \frac{4h^2}{2!} f''(x) - \frac{8h^3}{3!} f'''(x) + \frac{16h^4}{4!} f^{(4)}(x) - \frac{32h^5}{5!} f^{(5)}(x) + \frac{64h^6}{6!} f^{(6)}(x) + \dots \quad * c$$

$$\therefore a f(x+2h) + b f(x+h) + f(x-h) + c f(x-2h) = (a+b+1+c) f(x) + h(2a+b-1-2c) f'(x) + \frac{h^2}{2} (4a+b+1+4c) f''(x) + \frac{h^3}{3!} (8a+b-1-8c) f'''(x) + \frac{h^4}{4!} (16a+b+1+16c) f^{(4)}(x) + \frac{h^5}{5!} (32a+b-1-32c) f^{(5)}(x) + \dots$$

$$\therefore \begin{cases} 2a+b-1-2c=0 \rightarrow 2a+b-2c=1 \\ 4a+b+1+4c=0 \rightarrow 4a+b+4c=-1 \\ 16a+b+1+16c=0 \rightarrow 16a+b+16c=-1 \end{cases} \quad \left. \vphantom{\begin{matrix} 2a+b-1-2c=0 \\ 4a+b+1+4c=0 \\ 16a+b+1+16c=0 \end{matrix}} \right\} a = \frac{1}{2}, \quad b = -1, \quad c = -\frac{1}{2}$$

$$\frac{1}{2} f(x+2h) - f(x+h) + f(x-h) - \frac{1}{2} f(x-2h) = h^3 f'''(x) + \frac{h^5}{4} f^{(5)}(x) + \dots$$

$$f'''(x) = \frac{1}{2h^3} [f(x+2h) - 2f(x+h) + 2f(x-h) - f(x-2h)] - \frac{h^2}{4} f^{(5)}(x) - \dots$$

$$T.E \leq \frac{h^2}{4} M_5$$

18] Use Composite Trapezoidal rule and Simpson's rule to get $\int_1^2 \frac{2}{\sqrt{x}} dx$ with $n=8$ then find the absolute and function error.

Sol.

$$h = \frac{b-a}{n} = \frac{2-1}{8} = 0.125 \quad , \quad f(x) = \frac{2}{\sqrt{x}}$$

[1] Trapezoidal Rule:

$$I = \frac{h}{2} [f_0 + f_8 + 2[f_1 + f_2 + \dots + f_7]]$$

$$= \frac{0.125}{2} \left[\frac{2}{\sqrt{1}} + \frac{2}{\sqrt{2}} + 2 \left[\frac{2}{\sqrt{1.125}} + \frac{2}{\sqrt{1.25}} + \frac{2}{\sqrt{1.375}} + \frac{2}{\sqrt{1.5}} + \frac{2}{\sqrt{1.625}} + \frac{2}{\sqrt{1.75}} + \frac{2}{\sqrt{1.875}} \right] \right] = 1.657694825$$

$$I_{\text{exact}} = \int_1^2 \frac{2}{\sqrt{x}} dx = 4\sqrt{x} \Big|_1^2 = 4[\sqrt{2} - 1] = 1.656854249$$

$$E_T = |I_{\text{exact}} - I_{\text{app}}| = 8.40575 \times 10^{-4}$$

$$T.E \leq \frac{\pi h^3}{12} M_2 \quad , \quad M_2 = \max_{a \leq c \leq b} |f''(c)|$$

$$\leq \frac{8 \times (0.125)^3}{12} \cdot \max_{1 \leq c \leq 2} \left| \frac{1.5}{c^{2.5}} \right|$$

$$\leq \frac{8 \times (0.125)^3}{12} \times \frac{1.5}{1^{2.5}} = 1.953125 \times 10^{-3}$$

$$f = \frac{2}{\sqrt{x}} = 2x^{-\frac{1}{2}}$$

$$f' = -x^{-\frac{3}{2}}$$

$$f'' = \frac{3}{2}x^{-\frac{5}{2}} = \frac{1.5}{x^{2.5}}$$

[2] Simpson's Rule ($O(h^4)$)

$$I = \frac{h}{3} [f_0 + f_8 + 4(f_1 + f_3 + f_5 + f_7) + 2(f_2 + f_4 + f_6)]$$

$$= \frac{0.125}{3} \left[\frac{2}{\sqrt{1}} + \frac{2}{\sqrt{2}} + 4 \left(\frac{2}{\sqrt{1.125}} + \frac{2}{\sqrt{1.375}} + \frac{2}{\sqrt{1.625}} + \frac{2}{\sqrt{1.875}} \right) + 2 \left(\frac{2}{\sqrt{1.25}} + \frac{2}{\sqrt{1.5}} + \frac{2}{\sqrt{1.75}} \right) \right] = 1.656858748$$

$$E_T = 4.499389 \times 10^{-6}$$

$$T.E \leq \frac{\pi h^5}{180} M_4 \quad , \quad M_4 = \max_{a \leq c \leq b} |f^{(4)}(c)|$$

$$\leq \frac{8 \times (0.125)^5}{180} \cdot \max_{1 \leq c \leq 2} \left| \frac{105}{8c^{4.5}} \right|$$

$$\leq \frac{8 \times (0.125)^5}{180} \times \frac{105}{8 \cdot (1)^{4.5}} = 1.780192 \times 10^{-5}$$

$$f''' = -\frac{15}{4}x^{-\frac{7}{2}}$$

$$f^{(4)} = \frac{105}{8}x^{-\frac{9}{2}} = \frac{105}{8x^{4.5}}$$

Using Simpson's Rule ($O(h^7)$)

$$I = \frac{2h}{45} [7(f_0 + f_8) + 32(f_1 + f_3 + f_5 + f_7) + 12(f_2 + f_6) + 14(f_4)]$$

$$= \frac{2 \times 0.125}{45} \left[7 \left(\frac{2}{\sqrt{1}} + \frac{2}{\sqrt{2}} \right) + 32 \left(\frac{2}{\sqrt{1.125}} + \frac{2}{\sqrt{1.375}} + \frac{2}{\sqrt{1.625}} + \frac{2}{\sqrt{1.875}} \right) + 12 \left(\frac{2}{\sqrt{1.25}} + \frac{2}{\sqrt{1.75}} \right) + 14 \left(\frac{2}{\sqrt{1.5}} \right) \right] = 1.656854615$$

$$E_T = 3.6604 \times 10^{-7}$$

$$T.E \leq \frac{2\pi h^7}{945} M_6 = \frac{2 \times 8 \times (0.125)^7}{945} \times \frac{10395}{32 \times (1)^{6.5}} = 2.6226 \times 10^{-6}$$

$$f^{(5)} = -\frac{945}{16}x^{-\frac{11}{2}}$$

$$f^{(6)} = \frac{10395}{32}x^{-\frac{13}{2}} = \frac{10395}{32x^{6.5}}$$

9] Use Simpson's Rule to get $\int_1^2 (2x+1) dx$ with $n=5$

$h = \frac{b-a}{n} = \frac{2-1}{5} = 0.2$, $f(x) = 2x+1$

Sol

	P_0	P_1	P_2	P_3	P_4	P_5
x	1	1.2	1.4	1.6	1.8	2
$f(x)$	3	3.4	3.8	4.2	4.6	5

$\xleftarrow{\quad} \xrightarrow{\quad}$
 Trapezoidal Simpson

$I = I_T + I_S$

$= \frac{h}{2} [f_0 + f_1] + \frac{h}{3} [f_1 + f_5 + 2f_3 + 4(f_2 + f_4)]$

$= \frac{0.2}{2} [3 + 3.4] + \frac{0.2}{3} [3.4 + 5 + 4[3.8 + 4.6] + 2[4.2]]$

$= 4$

$I_{\text{exact}} = \int_1^2 2x+1 dx = x^2 + x \Big|_1^2 = 4$

$Er = 0$

10] Find the number of subintervals to approximate $\int_0^1 \frac{1}{x^2+6} dx$ with error less than 10^{-4} by Trapezoidal Rule.

Sol

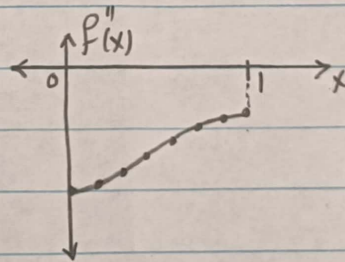
$T.E \leq \frac{n h^3}{12} M_2$, $h = \frac{b-a}{n} = \frac{1}{n}$, $M_2 = \max_{0 \leq c \leq 1} |f''(c)|$

$f = \frac{1}{(x^2+6)} = (x^2+6)^{-1}$
 $f' = -2x(x^2+6)^{-2}$
 $f'' = \frac{6x^2-12}{(x^2+6)^3}$

$\leq \frac{1}{12n^2} \cdot \max_{0 \leq c \leq 1} \left| \frac{6c^2-12}{(c^2+6)^3} \right|$

$\leq \frac{1}{12n^2} \left| \frac{0-12}{(0+6)^3} \right|$

$\leq \frac{1}{216n^2} = 10^{-4}$



$\therefore n^2 = \frac{10^4}{216} \rightarrow n \approx 6.8 \approx 7$

11] Use 3-point and 7-point Gaussian Quadrature method to get $\int_{-2}^2 x e^x dx$