

# Cauvery College for Women (Autonomous)

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Department : Mathematics  
Programme : Msc Mathematics  
Batch : 2018 Onwards  
Semester : IV  
Course : Advanced numerical analysis  
Course Code : P16MA43  
Unit : IV  
Topics Covered : Differentiation and integration- numerical differentiation,gauss legendre integration method and lobatto integration method.

1. Given the following values of  $f(x) = \ln x$ , find the approximate value of  $f(2.0)$  using linear and quadratic interpolation and  $f''(2.0)$  using quadratic interpolation. Also obtain an upper bound on the error.

$i$	0	1	2
$x_i$	2.0	2.2	2.6
$f_i$	0.69315	0.78846	0.95551

Soln:

Quadratic interpolation:

$$f'(x_0) = \frac{2x_0 - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} f_0 + \frac{x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} f_1 + \frac{x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)} f_2$$

$$f'(2.0) = \frac{2(2) - 2.2 - 2.6}{(2 - 2.2)(2 - 2.6)} (0.69315) + \frac{2 - 2.6}{(2.2 - 2)(2.2 - 2.6)} (0.78846) + \frac{2 - 2.2}{(2.6 - 2)(2.6 - 2.2)} (0.95551)$$

$$= 0.49619$$

$$f(x) = \ln x$$

$$f'(x) = \frac{1}{x}$$

The exact value of  $f'(2.0) = \frac{1}{2} = 0.5$

Error bound.

$$f''(x_0) = 2 \left[ \frac{f_0}{(x_0 - x_1)(x_0 - x_2)} + \frac{f_1}{(x_1 - x_0)(x_1 - x_2)} + \frac{f_2}{(x_2 - x_0)(x_2 - x_1)} \right]$$

$$f''(2.0) = 2 \left[ \frac{0.69315}{(2 - 2.2)(2 - 2.6)} + \frac{0.78846}{(2.2 - 2)(2.2 - 2.6)} + \frac{0.95551}{(2.6 - 2)(2.6 - 2.2)} \right]$$

2. The following data for the function  $f(x) = x^4$  is given

$x$	0.4	0.6	0.8
$f(x)$	0.0256	0.1296	0.4096

Find  $f'(0.8)$  and  $f''(0.8)$  using quadratic interpolation. Compare with the exact solution, obtain the bound on the truncation errors.

Soln:

$$\text{Given } f(x) = x^4$$

$$f'(x) = \frac{1}{2h} (f_0 - 4f_1 + 3f_2)$$

$$f'(0.8) = \frac{1}{2(0.2)} [0.0256 - 4(0.1296) + 3(0.4096)]$$

$$= 1.84$$

$$f''(0.8) = \frac{1}{h^2} [f_0 - 2f_1 + f_2]$$

$$= \frac{1}{(0.2)^2} [0.0256 - 2(0.1296) + 0.4096]$$

$$= 4.4$$

$$f(x) = x^4$$

$$f'(x) = 4x^3, \quad f''(x) = 12x^2$$

$$= 4(0.8)^3 \quad = 12(0.8)^2$$

$$= 2.048 \quad = 7.68$$

$$M_3 = \text{Max}_{0.4 \leq x \leq 0.8} |24x|$$

$$= 19.2$$

$$|E_2'(0.8)| \leq \frac{h^2}{3} M_3 = \frac{0.04}{3} (19.2) = 0.256$$

$$|E_2''(0.8)| \leq h M_3 = (0.2) (19.2) = 3.84$$



of  $y = f(x)$  of  $O(h^2)$  using derivative

- (i) Forward difference approximations.
- (ii) backward difference approximations.
- (iii) central difference approximations.

when  $f(x) = \sin x$ , estimate  $f'(\pi/4)$  with  $h = \frac{\pi}{12}$  using the above formula obtain the bounds on the truncation error and compare with the exact solution.

(i) Newton's Forward difference formula is given by

$$f(x) \approx f_0 + u \Delta f_0 + \frac{1}{2} u(u-1) \Delta^2 f_0$$

where  $u = \frac{x-x_0}{h}$  and

$$E = \frac{1}{6} u(u-1)(u-2) h^3 f'''(\xi)$$

we have  $f'(x) = \frac{df}{du} \cdot \frac{du}{dx}$

$$= \frac{1}{h} \left[ \Delta f_0 + \frac{1}{2} (2u-1) \Delta^2 f_0 \right]$$

and  $|E'(x_0)| = |E'(u=0)|$

$$\leq \frac{h^2}{3} M_3$$

where  $M_3 = \max_{x_0 \leq x \leq x_2} |f'''(x)|$

(ii) Newton's backward difference approximation is

given by

$$f(x) = f_2 + u \nabla f_2 + \frac{1}{2} u(u+1) \nabla^2 f_2$$

where  $u = \frac{x-x_2}{h}$  and

$$E = \frac{1}{6} u(u+1)(u+2) h^3 f'''(\xi)$$

we have  $f'(x) = \frac{1}{h} \left[ \nabla f_2 + \frac{1}{2} (2u+1) \nabla^2 f_2 \right]$

$$\text{and } |E'(x_2)| = |E'(u=0)| \leq \frac{h^2}{3} M_3$$

iii) The central difference approximation is given by

$$f(x) = f_0 + \frac{u}{2} [\delta f_{1/2} + \delta f_{-1/2}]$$

where  $u = \frac{(x-x_0)}{h}$  we have

$$\begin{aligned} f'(x) &= \frac{1}{2h} [\delta f_{1/2} + \delta f_{-1/2}] \\ &= \frac{1}{2h} [(f_1 - f_0) + (f_0 - f_{-1})] \\ &= \frac{1}{2h} [(f_1 - f_0) + (f_0 - f_{-1})] \\ &= \frac{1}{2h} [f_1 - f_{-1}] \end{aligned}$$

$$\text{and } |E'(x)| \leq \frac{h^2}{6} M_3$$

We have  $f(x) = \sin x$ ,  $x_0 = \frac{\pi}{4}$ ,  $x_1 = \frac{\pi}{3}$ ,  $x_2 = \frac{5\pi}{12}$ ,  $h=0$

$$f'(\frac{\pi}{4}) = \frac{12}{\pi} [\Delta f_0 - \frac{1}{2} \Delta^2 f_0]$$

$$\begin{aligned} \Delta f_0 &= f(x_1) - f(x_0) \\ &= f(\frac{\pi}{3}) - f(\frac{\pi}{4}) \\ &= \sin(\frac{\pi}{3}) - \sin(\frac{\pi}{4}) \\ &= 0.1589 \end{aligned}$$

$$\begin{aligned} \Delta^2 f_0 &= f(x_2) - 2f(x_1) + f(x_0) \\ &= f(\frac{5\pi}{12}) - 2f(\frac{\pi}{3}) + f(\frac{\pi}{4}) \\ &= \sin(\frac{5\pi}{12}) - 2\sin(\frac{\pi}{3}) + \sin(\frac{\pi}{4}) \\ &= -0.0590 \end{aligned}$$

$$\begin{aligned} \text{and } f'(\frac{\pi}{4}) &= \frac{12}{\pi} [0.1589 + \frac{1}{2}(0.0590)] \\ &= 0.7196 \end{aligned}$$

we take  $x_2 = \pi/4$ ,  $x_1 = \pi/6$ ,  $x_0 = \pi/12$ ,  $u=0$

$$f'(\pi/4) = \frac{12}{\pi} \left( \nabla f_2 + \frac{1}{2} \nabla^2 f_2 \right)$$

$$\nabla f_2 = f(x_2) - f(x_1)$$

$$= f(\pi/4) - f(\pi/6)$$

$$= \sin(\pi/4) - \sin(\pi/6)$$

$$= 0.2071$$

$$\nabla^2 f_2 = f(x_2) - 2f(x_1) + f(x_0)$$

$$= \sin\left(\frac{\pi}{4}\right) - 2\sin\left(\frac{\pi}{6}\right) + \sin\left(\frac{\pi}{12}\right)$$

$$= 0.0341$$

$$f'(\pi/4) = \frac{12}{\pi} \left[ 0.2071 + \frac{1}{2}(-0.0341) \right]$$

$$= 0.7259$$

Using central difference we get,

$$f'(\pi/4) = \frac{6}{\pi} \left[ f(\pi/3) - f(\pi/6) \right]$$

$$= 0.6991$$

Exact soln is,  $f'(\pi/4) = \cos(\pi/4)$

$$= 0.7071$$

$$\text{Let } c = \frac{(\pi/12)}{3} \quad [ \because h^2/3 ]$$

The errors in forwards, backwards, & central difference approximations are respectively, bounded by,

$$|E'| \leq CM_3 = 0.0162$$

$$\therefore M_3 = \text{Max}_{\pi/4 \leq x \leq \frac{5\pi}{12}} |-\cos x| = \cos(\pi/4)$$

$$|E'| \leq CM_3 = 0.0221$$

$$\therefore M_3 = \max_{\frac{\pi}{12} \leq x \leq \frac{\pi}{4}} |-\cos x| = \cos\left(\frac{\pi}{12}\right)$$

$$|E'| \leq \left(\frac{c}{2}\right) M_3 = 0.0099$$

$$M_3 = \max_{\frac{\pi}{6} \leq x \leq \frac{\pi}{3}} |-\cos x| = \cos\frac{\pi}{6}$$

4. A differentiation rule of the form  $h f'(x_2) = d_0 f(x_0) + d_1 f(x_1) + d_2 f(x_3) + d_3 f(x_4)$  where  $x_j = x_0 + jh$ ,  $j = 0, 1, 2, 3, 4$  is given determine the values of  $d_0, d_1, d_2$  &  $d_3$  so that the rule is exact for a poly of degree 4.

(i) Find the error term

(ii) Obtain an expression for the round-off error in calculating  $f'(x_2)$ .

(iii) Calculating  $f'(0.3)$  using 5 place values of  $f(x) = \sin x$  with  $h = 0.1$  compare the result with the exact value  $\cos(0.3)$ .

Soln:

$$h f'(x_2) = d_0 f(x_2 - 2h) + d_1 f(x_2 - h) + d_2 f(x_2 + h) + d_3 f(x_2 + 2h)$$

expanding the terms on the right side in Taylor series & comparing the powers of  $h$  we get,

Taylor's expansion,

$$f(x) = \sum_{h=0}^{\infty} \frac{f^{(h)}(a)}{h!} (x-a)^h$$

$$= f(a) + f'(a)(x-a) + \frac{f''(a)}{2!} (x-a)^2 + \dots$$

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

$$d_0 + d_1 + d_2 + d_3 = 0 \rightarrow \textcircled{1}$$

$$-2d_0 - d_1 + d_2 + 2d_3 = 0 \rightarrow \textcircled{2}$$

$$4d_0 + d_1 + d_2 + 4d_3 = 0 \rightarrow \textcircled{3}$$

$$-8d_0 - d_1 + d_2 + 8d_3 = 0 \rightarrow \textcircled{4}$$

$$\textcircled{1} + \textcircled{2} \quad -d_0 + 2d_2 + 3d_3 = 1 \rightarrow \textcircled{5}$$

$$\textcircled{2} + \textcircled{3} \quad -2d_0 + 2d_2 + 6d_3 = 1 \rightarrow \textcircled{6}$$

$$\textcircled{1} + \textcircled{4} \quad -7d_0 + 2d_2 + 9d_3 = 0 \rightarrow \textcircled{7}$$

$$\textcircled{5} - \textcircled{6} \quad -d_0 + 3d_3 = 0 \rightarrow \textcircled{8}$$

$$\textcircled{5} - \textcircled{7} \quad 6d_0 - 6d_3 = 1 \rightarrow \textcircled{9}$$

$$\textcircled{8} + \textcircled{9} \quad -8d_3 = 2$$

$$d_3 = -2/8$$

$$d_2 = 2/3$$

$$\textcircled{8} \times 6 \quad -6d_0 - 18d_3 = 0$$

$$d_1 = -2/3$$

$$6d_0 + 6d_3 = 1$$

$$d_0 = 1/2$$

$$\boxed{d_3 = -1/12}$$

$$hf'(x_2) = \frac{1}{12} [f(x_0) - 8f(x_1) + 8f(x_3) - f(x_4)]$$

i) The leading term in the expression for error vanishes, Hence the error term becomes,

$$E = \frac{h^5}{120} [-32d_0 - d_1 + d_2 + 32d_3] f^{(5)}(\xi)$$

$$= \frac{-1}{30} h^5 f^{(5)}(\xi), \quad x_2 - 2h < \xi < x_2 + 2h$$

ii) Let  $\epsilon_0, \epsilon_1, \epsilon_2, \epsilon_3$  be the round off errors in

$$f(x_2 - 2h), f(x_2 - h), f(x_2 + h) \text{ and } f(x_2 + 2h)$$

respectively then,

$$|RE| = \frac{1}{12h} |\epsilon_0 - 8\epsilon_1 + 8\epsilon_2 - \epsilon_3|$$

$$\leq \frac{3\epsilon}{2h}$$

Where  $\epsilon = \max[|\epsilon_0|, |\epsilon_1|, |\epsilon_2|, |\epsilon_3|]$

iii) we have,

$$\sin(0.1) = 0.09983$$

$$\sin(0.2) = 0.19867$$

$$\sin(0.4) = 0.38942$$

$$\sin(0.5) = 0.47943$$

$$f'(0.3) = \frac{1}{1.2} [0.09983 - 8(0.19867) + 8(0.38942) - 0.47943]$$

$$= 0.95534$$

The exact value is

$$f'(0.3) = \cos(0.3)$$

$$= 0.95534.$$

5. Assume that  $f(x)$  has a minimum in the interval  $x_{n-1} \leq x \leq x_{n+1}$  where  $x_k = x_0 + kh$ . Show that the interpolation of  $f(x)$  by a polynomial of second degree yields the approximation

$$f_n - \frac{1}{8} \left[ \frac{(f_{n+1} - f_{n-1})^2}{f_{n+1} - 2f_n + f_{n-1}} \right], \quad (f_k = f(x_k))$$

for this minimum value of  $f(x)$ .

Soln:

The interpolating polynomial through the points  $(x_{n-1}, f_{n-1})$ ,  $(x_n, f_n)$  and  $(x_{n+1}, f_{n+1})$  can be written as,



$$f(x) = f_{n-1} + \frac{1}{h} (x - x_{n-1}) \Delta f_{n-1} + \frac{1}{2!h^2} (x - x_{n-1})$$

$$(x - x_n) \Delta^2 f_{n-1} \rightarrow 0$$

For minimum value of  $f(x)$ ,  $f'(x) = 0$  which gives,

$$\frac{1}{h} (x - x_{n-1}) \Delta f_{n-1} + \frac{1}{2h^2} [2x - (x_{n-1} + x_n)] \Delta^2 f_{n-1} = 0$$

(or)

$$x_{\min} = \frac{1}{2} (x_n - x_{n-1}) - h \frac{\Delta f_{n-1}}{\Delta^2 f_{n-1}}$$

Sub this value of  $x$  in (1) we obtain the minimum value of  $f(x)$  as,

$$f_{\min} = f_{n-1} + \frac{1}{h} \left[ \frac{1}{2} (x_n - x_{n-1}) - h \frac{\Delta f_{n-1}}{\Delta^2 f_{n-1}} \right] \Delta f_{n-1}$$

$$+ \frac{1}{2h^2} \left[ \frac{1}{2} (x_n - x_{n-1}) - h \frac{\Delta f_{n-1}}{\Delta^2 f_{n-1}} \right]^2 \Delta^2 f_{n-1}$$

$$+ \frac{1}{6h^3} \left[ \frac{1}{2} (x_n - x_{n-1}) - h \frac{\Delta f_{n-1}}{\Delta^2 f_{n-1}} \right]^3 \Delta^3 f_{n-1}$$

6. Determine the optimal value of  $h$ , using the criteria

(i)  $|RE| = |TE|$

(ii)  $|RE| + |TE| = \text{minimum}$

Using this method and value of  $h$  obtained from the criterion  $|RE| = |TE|$  determine an approximate value of  $f'(2.0)$  from the following tabulated values of  $f(x) = \ln x$

$x$	2.0	2.01	2.02	2.06	2.12
$f(x)$	0.69315	0.69813	0.70310	0.72271	0.75142

Soln:

If  $\epsilon_0, \epsilon_1, \epsilon_2$  are the round off error in function evaluation  $f_0, f_1, f_2$  respectively then we have



$$f'(x_0) = \frac{-3f_0 + 4f_1 - f_2}{2h} + \frac{-3\epsilon_0 + 4\epsilon_1 - \epsilon_2}{2h} + \frac{h^2}{3} f'''(x)$$

$$= \frac{-3f_0 + 4f_1 - f_2}{2h} + RE + TE$$

Using  $\epsilon = \max(|\epsilon_0|, |\epsilon_1|, |\epsilon_2|)$

$$M_3 = \max_{x_0 \leq x \leq x_2} |f'''(x)|$$

We obtain  $|RE| \leq \frac{8\epsilon}{2h}$  and  $M_3 = \max_{x_0 \leq x \leq x_2} (f'''(x))$

We obtain

$$|RE| \leq \frac{8\epsilon}{2h}, \quad |TE| \leq \frac{h^2 M_3}{3}$$

If we use  $|RE| = |TE|$  we get

$$\frac{8\epsilon}{2h} = \frac{h^2 M_3}{3}$$

Which gives

$$h^3 = \frac{12\epsilon}{M_3}$$

$$\text{(or) } h_{opt} = \left( \frac{12\epsilon}{M_3} \right)^{1/3}$$

$$\text{and } |RE| = |TE| = \frac{8\epsilon}{2 \left( \frac{12\epsilon}{M_3} \right)^{1/3}}$$

$$= \frac{8\epsilon}{2(12)^{1/3} \epsilon^{1/3}} M_3^{1/3}$$

$$= \frac{4 \epsilon^{2/3} M_3^{1/3}}{(12)^{1/3}}$$

If we use,

$|RE| + |TE| = \text{minimum}$ , we get

$$\frac{8\epsilon}{2h} + \frac{M_3 h^2}{3} = \text{minimum}$$

$$\frac{4\epsilon}{h} + \frac{M_3 h^2}{3} = 0$$

which gives,

$$-\frac{4\epsilon}{h^2} + \frac{2M_3 h}{3} = 0 \quad [\text{Diff w.r to } h]$$

$$-4\epsilon \times 3 + 2M_3 h^3 = 0$$

$$2M_3 h^3 = 12\epsilon$$

$$h^3 = \frac{6\epsilon}{M_3}$$

$$h_{\text{opt}} = \left(\frac{6\epsilon}{M_3}\right)^{1/3}$$

Minimum Total error

$$= M_3 \left(\frac{6\epsilon}{M_3}\right)^{2/3} \Rightarrow \frac{M_3 b^{2/3} \epsilon^{2/3}}{M_3^{2/3}}$$

$$= b^{2/3} \epsilon^{2/3} M^{1/3}$$

When  $f(x) = \ln(x)$  we have

$$M_3 = \max_{2.0 \leq x \leq 2.12} |f'''(x)| = 1/4$$

Using the criterion.

$|RE| = |TE|$  and  $\epsilon = 5 \times 10^{-6}$  we get,

$$h_{\text{opt}} = \left(\frac{12 \times 5 \times 10^{-6}}{1/4}\right)^{1/3} \approx 0.06$$

For  $h=0.06$  we get

$$f'(2.0) = \frac{-3(0.69315) + 4(0.72271)}{0.12} = 0.75142$$

$$= 0.49975$$

If we take  $h=0.01$  we get

$$f'(2.0) = \frac{-3(0.69315) + 4(0.69813)}{0.02} = 0.70310$$

$$= 0.49850$$

The exact value is  $f'(2.0) = 0.5$ .

This verifies that for  $h < h_{opt}$ , the results deteriorate.

7. Consider the 4 point formula,

$$f'(x_2) = \frac{1}{6h} [-2f(x_1) - 3f(x_2) + 6f(x_3) - f(x_4)] + TE + RE$$

where  $x_j = x_0 + jh$ ,  $j = 0, 1, 2, 3, 4$  and TE, RE are respectively the truncation error and round off error.

i) Determine the form of TE and RE.

ii) Obtain the optimum step length  $h$  satisfying the criterion  $|TE| = |RE|$ .

iii) Determine the total error.

Soln:

$$TE = f'(x_2) - \frac{1}{6h} [-2f(x_1) - 3f(x_2) + 6f(x_3) - f(x_4)]$$

$$= f'(x_2) - \frac{1}{6h} [-2f(x_2 - h) - 3f(x_2) + 6f(x_2 + h) - f(x_2 + 2h)]$$

$$= f'(x_2) - \frac{1}{6h} \left[ -2f \left\{ (x_2) - hf'(x_2) - \frac{h^2}{2} f''(x_2) - \frac{h^3}{6} f'''(x_2) + \frac{h^4}{24} f^{(4)}(x_2) + \dots \right\} \right]$$

$$= f'(x_2) + \frac{1}{3h} f(x_2) + \frac{f'(x_2)}{6} - \frac{h}{12} f''(x_2) +$$

$$\frac{h^2}{36} f'''(x_2) - \frac{h^3}{24(6)} f^{(4)}(x_2) - \frac{1}{6h} [-3f(x_2)$$

$$+ 6f(x_2) + 6hf'(x_2) + 3h^2 f''(x_2) + h^3 f'''(x_2) +$$

$$3h^4 f^{(4)}(x_2) - f(x_2) - 2hf'(x_2) - \frac{4h^2}{2}$$

$$f''(x_2) - \frac{8h^3}{6} f'''(x_2) - \frac{2}{3} h^4 f^{(4)}(x_2)]$$

$$\begin{aligned}
&= f'(x_2) + \frac{1}{3h} f(x_2) + \frac{f''(x_2)}{6} - \frac{1}{12} f''(x_2) + \frac{h^2}{36} f'''(x_2) \\
&\quad - \frac{h^3}{24(6)} f^{(4)}(x_2) + \frac{1}{2h} f(x_2) - \frac{f(x_2)}{h} - f'(x_2) - \\
&\quad \frac{1}{2} h f''(x_2) - \frac{h^2}{6} f'''(x_2) - \frac{1}{2} h^4 f^{(4)}(x_2) + \\
&\quad f(x_2) \frac{1}{6h} + \frac{1}{3} f'(x_2) + \frac{1}{3} h^2 f''(x_2) + \frac{2}{9} f'''(x_2) \\
&\quad + \frac{2}{18} h^4 f^{(4)}(x_2) \\
&= \frac{h^3}{12} f^{(4)}(x_2) + \dots \\
&\approx \frac{h^3}{12} f^{(4)}(\xi), \text{ where } x_1 < \xi < x_4.
\end{aligned}$$

$$\text{(i) } |TE| \leq \frac{h^2}{12} M_4, \quad M_4 = \max_{x_1 \leq x \leq x_4} |f^{(4)}(x)|$$

$$\text{Now } f(x_i) = f_i + \epsilon_i, \quad i = 1, 2, 3, 4$$

$$|RE| \leq \frac{1}{6h} [2|\epsilon_1| + 3|\epsilon_2| + 6|\epsilon_3| + |\epsilon_4|]$$

$$\leq \frac{2\epsilon}{h}$$

$$\text{where } \epsilon = \max [|\epsilon_1|, |\epsilon_2|, |\epsilon_3|, |\epsilon_4|]$$

$$\text{(ii) } |TE| = |RE|$$

$$\frac{h^3}{12} M_4 = \frac{2\epsilon}{h}$$

$$h^4 = \frac{24\epsilon}{M_4}$$

$$h = \left( \frac{24\epsilon}{M_4} \right)^{1/4}$$

$$\text{(iii) } |TE| + |RE| = 2|RE|$$

$$\leq \frac{4\epsilon}{h}$$

$$\leq \frac{4\epsilon}{\left( \frac{24\epsilon}{M_4} \right)^{1/4}}$$

$$\leq 4 \epsilon \left( \frac{M_4}{24 \epsilon} \right)^{1/4}$$

8. The following table of values is given,

$x$ :	-1	1	2	3	4	5	7
$f(x)$ :	1	1	16	81	256	625	2401

Using the formula  $f'(x_1) = \frac{f(x_2) - f(x_0)}{2h}$  and the Richardson extrapolation find  $f'(3)$ .

Soln:

$$\frac{f(x_2) - f(x_0)}{2h} = \frac{1}{2h} [f(x_1+h) - f(x_1-h)] \rightarrow \textcircled{1}$$

Expanding RHS of  $\textcircled{1}$  in Taylor series,

$$= \frac{1}{2h} \left[ f(x_1) + \frac{h}{1!} f'(x_1) + \frac{h^2}{2!} f''(x_1) + \dots \right] -$$

$$f(x_1) + \frac{h}{1!} f'(x_1) - \frac{h^2}{2!} f''(x_1) - \frac{h^3}{3!} f'''(x_1) - \frac{h^4}{4!} f^{IV}(x_1) + \dots$$

$$= \frac{1}{2h} \left[ 2h f'(x_1) + \frac{2h^3}{3!} f'''(x_1) + \frac{2h^5}{5!} f^{IV}(x_1) + \dots \right]$$

$$= f'(x_1) + \frac{h^2}{6} f'''(x_1) + \frac{h^4}{120} f^{IV}(x_1) + \dots$$

$$= g(h) + c_2 h^2 + c_3 h^4 + \dots \quad (\text{say})$$

Take  $h=4, x=3$

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

$$= \frac{f(7) - f(-1)}{2h} = \frac{2401 - 1}{8} = 300$$

$$g\left(\frac{h}{2}\right) = \frac{f\left(x_1 + \frac{h}{2}\right) - f\left(x_1 - \frac{h}{2}\right)}{\frac{2h}{2}}$$

$$= \frac{f(4.4) - f(4.2)}{0.2}$$

$$y'(0.398) \approx \frac{-y(0.400) + 4y(0.399) - y(0.398)}{-2(0.001)}$$

$$= 1.0795$$

The error in the formula is given by,

$$\text{Error} = \frac{h^2}{3} y'''(x_0) \approx \frac{1}{3h} \Delta^3 y_0$$

$$= \frac{1}{3h} (y_3 - 3y_2 + 3y_1 - y_0)$$

$$= \frac{1}{3(0.001)} [y(0.401) - 3y(0.400) + 3y(0.399) - y(0.398)]$$

Taking the error in the error formula,  
we have

$$\text{Error} = \frac{h^3}{4} y^{IV}(x_0) \approx \frac{1}{4h} \Delta^4 y_0$$

$$= \frac{1}{4h} (y_4 - 4y_3 + 6y_2 - 4y_1 + y_0)$$

$$= \frac{1}{0.004} [y(0.402) - 4y(0.401) + 6y(0.400) - 4y(0.399) + y(0.398)]$$

$$= \frac{1}{0.004} [0.410915 - 4(0.411834) + 6(0.41075) - 4(0.409671) + 0.40859]$$

10. Find the Jacobian matrix for the system of eqns

$$f_1(x, y) = x^2 + y^2 - x = 0$$

$$f_2(x, y) = x^2 - y^2 - y = 0$$

at the point (1, 1) using the methods

$$\left(\frac{\partial f}{\partial x}\right)(x_i, y_j) = \frac{f_{i+1, j} - f_{i-1, j}}{2h}$$



$$\left(\frac{\partial f}{\partial y}\right)(x_i, y_j) = \frac{f(x_i, y_{j+1}) - f(x_i, y_{j-1})}{2k}$$

with  $h=k=1$ .

Soln: The Jacobian matrix is given by

$$J = \begin{bmatrix} \frac{\partial f_1}{\partial x} & \frac{\partial f_1}{\partial y} \\ \frac{\partial f_2}{\partial x} & \frac{\partial f_2}{\partial y} \end{bmatrix}$$

$$\frac{\partial f_1}{\partial x} = 2x-1, \quad \frac{\partial f_1}{\partial y} = 2y$$

$$\frac{\partial f_2}{\partial x} = 2x, \quad \frac{\partial f_2}{\partial y} = -2y-1$$

we have  $x_i = 1, y_j = 1$

$$\left(\frac{\partial f_1}{\partial x}\right)_{(1,1)} = \frac{f_1(1+h, 1) - f_1(1-h, 1)}{2h}$$

$$= \frac{f_1(2, 1) - f_1(0, 1)}{2}$$

$$= \frac{3-1}{2} = \frac{2}{2} = 1$$

$$\left(\frac{\partial f_1}{\partial y}\right)_{(1,1)} = \frac{f_1(1, 1+k) - f_1(1, 1-k)}{2k}$$

$$= \frac{f_1(1, 2) - f_1(1, 0)}{2}$$

$$= \frac{4-0}{2} = 2$$

$$\left(\frac{\partial f_2}{\partial x}\right)_{(1,1)} = \frac{f_2(1+h, 1) - f_2(1-h, 1)}{2h}$$

$$= \frac{f_2(2, 1) - f_2(0, 1)}{2}$$

$$= \frac{4-0}{2} = 2$$



$$\begin{aligned} \left(\frac{\partial f_2}{\partial y}\right)_{(1,1)} &= \frac{f_2(1,1+k) - f_2(1,1-k)}{2k} \\ &= \frac{f_2(1,2) - f_2(1,0)}{2} \\ &= -\frac{5-1}{2} = -3 \end{aligned}$$

Hence we get

$$J = \begin{bmatrix} 1 & 2 \\ 2 & -3 \end{bmatrix}$$

11. Gauss - Legendre.

Evaluate  $I = \int_0^1 \frac{dx}{1+x}$  using Gauss Legendre 3 point formula.

Soln:  $\int_{-1}^1 f(x) dx = \frac{1}{9} \left[ 5f\left(-\sqrt{\frac{3}{5}}\right) + 8f(0) + 5f\left(\sqrt{\frac{3}{5}}\right) \right] \Delta x$

To solve the Legendre formula, we have to change  $[0,1]$  to  $[-1,1]$

The transformation is,

$$x = \left(\frac{b-a}{2}\right)t + \left(\frac{b+a}{2}\right)$$

$$x = \left(\frac{1-0}{2}\right)t + \left(\frac{1+0}{2}\right) = \frac{t}{2} + \frac{1}{2} = \frac{t+1}{2}$$

$$1+x = 1 + \frac{1+t}{2} = \frac{t+3}{2}$$

$$\frac{dx}{dt} = \frac{dt}{2}$$

$$I = \int_0^1 \frac{dx}{1+x} = \int_{-1}^1 \frac{(dt/2)}{\left(\frac{t+3}{2}\right)}$$

$$= \int_{-1}^1 \frac{dt}{t+3}$$

$$I = \int_{-1}^1 f(x) dx \text{ where } f(x) = \frac{1}{x+3}$$

$$f\left(-\sqrt{\frac{3}{5}}\right) = \frac{1}{-\sqrt{\frac{3}{5}} + 3} = 0.4494$$

$$f(0) = \frac{1}{0+3} = 0.3333$$

$$f\left(\sqrt{\frac{3}{5}}\right) = \frac{1}{\sqrt{\frac{3}{5}} + 3} = 0.2649$$

From ①

$$\int_{-1}^1 f(x) dx = \frac{1}{9} [5(0.4494) + 8(0.3333) + 5(0.2649)]$$

$$= 0.693122$$

The exact solution is

$$\int_{-1}^1 \frac{dt}{t+3} = (\log(t+3))_{-1}^1$$

$$= 0.693149$$

12. Evaluate the integral  $I = \int_1^2 \frac{2x}{1+x^4} dx$  using

the Gauss-Legendre 1-pt, 2-pt & 3-pt quadrature rules. Compare with the exact solution:

Soln:

The exact solution is

$$I = \int_1^2 \frac{2x}{1+(x^2)^2} dx = \int_1^4 \frac{dt}{1+t^2}$$

$$= (\tan^{-1}(t))_1^4$$

$$= \tan^{-1}(4) - \tan^{-1}(1)$$

$$= \tan^{-1}(4) - \pi/4$$

$$= 0.5404$$

$$x^2 = t$$

$$2x dx = dt$$

$$x=1$$

$$t=1$$

$$x=2$$

$$t=4$$

To use the Gauss-Legendre rule, the interval  $[1, 2]$  is to be reduced to  $[-1, 1]$ .

$$\begin{aligned}
 x &= \left( \frac{b-a}{2} \right) t + \left( \frac{b+a}{2} \right) \\
 &= \left( \frac{2-1}{2} \right) t + \left( \frac{2+1}{2} \right) \\
 &= \frac{t}{2} + \frac{3}{2} = \frac{t+3}{2}
 \end{aligned}$$

$$dx = \frac{dt}{2}$$

$$I = \int_{-1}^1 2 \frac{\left[ \frac{t+3}{2} \right]}{1 + \left( \frac{t+3}{2} \right)^4} \cdot \frac{dt}{2}$$

$$= \int_{-1}^1 \frac{t+3}{\frac{16 + (t+3)^4}{16}} \cdot \frac{dt}{2}$$

$$= \int_{-1}^1 \frac{16(t+3)}{[16 + (t+3)^4]} \cdot \frac{dt}{2}$$

$$= \int_{-1}^1 \frac{8(t+3)}{16 + (t+3)^4} dt$$

$$= \int_{-1}^1 f(t) dt \quad \text{where } f(t) = \frac{8(t+3)}{16 + (t+3)^4}$$

Using 1-pt rule we get

$$I = 2f(0) = 2 \left[ \frac{8(3)}{16 + (3)^4} \right] = 0.4948$$

Using 2-pt rule we get

$$I = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

$$f\left(-\frac{1}{\sqrt{3}}\right) = \frac{8\left(-\frac{1}{\sqrt{3}} + 3\right)}{16 + \left(-\frac{1}{\sqrt{3}} + 3\right)^4} = 0.3842$$

$$f\left(\frac{1}{\sqrt{3}}\right) = \frac{8\left(\frac{1}{\sqrt{3}} + 3\right)}{16 + \left(\frac{1}{\sqrt{3}} + 3\right)^4} = 0.1592$$

$$I = 0.3842 + 0.1592$$

$$= 0.5434$$

Using 3-pt rule we get:

$$I = \frac{1}{9} \left[ 5f\left(-\sqrt{3/5}\right) + 8f(0) + 5f\left(\sqrt{3/5}\right) \right]$$

$$= \frac{1}{9} \left[ 5(0.4393) + 8(0.2474) + 5(0.1379) \right]$$

$$I = 0.5406.$$

13. Evaluate the integral

$$I = \int_0^1 \frac{dx}{2x^2 + 2x + 1}$$

Using the Lobatto 3-pt formulas  
Compare with the exact solution.

Soln:

$$x = \left(\frac{b-a}{2}\right)t + \left(\frac{b+a}{2}\right)$$

$$= \left(\frac{1-0}{2}\right)t + \left(\frac{1+0}{2}\right)$$

$$= \frac{t}{2} + \frac{1}{2} = \frac{t+1}{2}$$

$$dx = \frac{dt}{2}$$

$$I = \int_{-1}^1 \frac{dt/2}{2 \left( \left(\frac{1+t}{2}\right)^2 + 2 \left(\frac{1+t}{2}\right) + 1 \right)}$$

$$= \frac{1}{2} \int_{-1}^1 \frac{dt}{\left(\frac{1+t}{2}\right)^2 + (1+t) + 1}$$

$$= \frac{1}{2} \int_{-1}^1 \frac{dt(2)}{(1+t)^2 + 2 + 2t + 2}$$

$$= \int_{-1}^1 \frac{dt}{(1+t)^2 + 2t + 4} = \int_{-1}^1 f(t) dt$$

Lobatto 3-pt formula is,

$$f(-1) = \frac{1}{(-1+1)^2 + 2(-1) + 4} = \frac{1}{2}$$

$$f(0) = \frac{1}{4}$$

$$f(1) = \frac{1}{(1+1)^2 + 2(1) + 4} = \frac{1}{10}$$

$$I = \frac{1}{3} \left[ \frac{1}{2} + \frac{1}{4} + \frac{1}{10} \right]$$

$$= 0.46667$$

The exact soln is given by,

$$I = \int_0^1 \frac{dx}{2x^2 + 2x + 1}$$

Methods Based on interpolation:

Given the values of  $f(x)$  at a set of points  $x_0, x_1, \dots, x_n$ , the general approach for deriving the numerical differentiation method is to obtain the interpolating polynomial  $P_n(x)$  and then differentiate this polynomial  $r$  times ( $n \geq r$ ) to get  $P_n^{(r)}(x)$ . The value of  $P_n^{(r)}(x_k)$  gives the approximate value of  $f^{(r)}(x)$  at the nodal point  $x_k$ . It may be noted that though  $P_n(x) \neq f(x)$  have same values at the nodal points, yet the derivatives may differ considerably at these points.

The approximation may further, deteriorate as the order of derivative increases. The quantity

$$E^{(r)}(x) = f^{(r)}(x) - P_n^{(r)}(x).$$

is called the error of approximation in the  $n^{\text{th}}$  order derivative at any point  $x$ .

⇒ Non-uniform Nodal points:

If  $(x_i, f_i)$   $i=0, 1, \dots, n$  are  $n+1$  distinct tabular points, then the Lagrange interpolating polynomial fitting this data is given by,

$$P_n(x) = \sum_{k=0}^n L_k(x) f_k \rightarrow \textcircled{1}$$

where  $L_k(x)$  is the Lagrange fundamental polynomial

$$L_k(x) = \frac{\pi(x)}{(x-x_k) \pi'(x_k)}$$

and  $f_k = f(x_k)$ ,  $\pi(x) = (x-x_0)(x-x_1)\dots(x-x_n)$

The error of approximation is given by,

$$E_n(x) = f(x) - P_n(x)$$

$$= \frac{\pi(x)}{(n+1)!} f^{(n+1)}(\xi); \quad x_0 < \xi < x_n \rightarrow \textcircled{2}$$

for any point  $x$  Diff the eqn  $P_n(x)$  w.r. to  $x$  we obtain

$$P_n'(x) = \sum_{k=0}^n L_k'(x) f_k \rightarrow \textcircled{3}$$

$$\text{and } E_n'(x) = \frac{\pi'(x)}{(n+1)!} f^{(n+1)}(\xi) + \frac{\pi(x)}{(n+1)!} \frac{d}{dx} (f^{(n+1)}(\xi))$$



The function  $\xi(x)$  is the 2<sup>nd</sup> term on the RHS is unknown we cannot directly evaluate  $E_n'(x)$ . However, at a nodal point  $x_k$ ,  $\pi(x_k) = 0$  and we get,

$$E_n'(x_k) = \frac{\pi'(x_k)}{(n+1)!} f^{(n+1)}(\xi), \quad x_0 < \xi < x_n$$

provided

$\frac{d}{dx} (f^{(n+1)}(\xi))$  remains bounded for any  $r$ ,  $1 \leq r \leq n$ , we obtain from (1).

$$f^{(r)}(x) \approx P_n^{(r)}(x) = \sum_{k=0}^n L_k^{(r)}(x) f_k \rightarrow (6)$$

at any point  $x$ . The error term may be obtained by using the relation.

$$\frac{1}{(n+1)!} \frac{d^j}{dx^j} (f^{(n+1)}(\xi)) = \frac{j!}{(n+j+1)!} f^{(j+n+1)}(\eta_j), \quad j=1, 2, \dots, 7 \quad (7)$$

where  $\min(x_0, x_1, x_2, \dots, x_n, x) < \eta_j < \max(x_0, x_1, \dots, x_n, x)$

i) Linear Interpolation:

If we use linear interpolation, we have

$$L_0(x) = \frac{x-x_1}{x_0-x_1}, \quad L_1(x) = \frac{x-x_0}{x_1-x_0}$$

$$P_1(x) = \frac{x-x_1}{x_0-x_1} f_0 + \frac{x-x_0}{x_1-x_0} f_1 \rightarrow (8)$$

$$P_1'(x) = \frac{f_1 - f_0}{x_1 - x_0} \rightarrow (9)$$

which is constant for all  $x \in [x_0, x_1]$  we also have.

$$E_1'(x_0) = \frac{x_0 - x_1}{2} f''(\xi) \rightarrow (10)$$

$$E_1'(x_1) = \frac{x_1 - x_0}{2} f''(\xi), \quad x_0 < \xi < x_1 \rightarrow (11)$$



ii) Quadratic Interpolation:

For quadratic interpolation, we have

$$L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}, \quad L_0'(x) = \frac{2x-x_1-x_2}{(x_0-x_1)(x_0-x_2)}$$

$$L_1(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}, \quad L_1'(x) = \frac{2x-x_0-x_2}{(x_1-x_0)(x_1-x_2)}$$

$$L_2(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}, \quad L_2'(x) = \frac{2x-x_0-x_1}{(x_2-x_0)(x_2-x_1)}$$

$$P_2(x) = L_0(x)f_0 + L_1(x)f_1 + L_2(x)f_2 \rightarrow (12)$$

$$P_2'(x) = L_0'(x)f_0 + L_1'(x)f_1 + L_2'(x)f_2 \rightarrow (13)$$

which gives

$$P_2'(x) = \frac{2x_0-x_1-x_2}{(x_0-x_1)(x_0-x_2)} f_0 + \frac{x_0-x_2}{(x_1-x_0)(x_1-x_2)} f_1 +$$

$$\frac{x_0-x_1}{(x_2-x_0)(x_2-x_1)} f_2 \rightarrow (14)$$

and

$$E_2'(x_0) = \frac{1}{6} (x_0-x_1)(x_0-x_2) f'''(\xi), \quad x_0 < \xi < x_2 \quad \downarrow (15)$$

By we obtain

$$P_2''(x) = 2 \left[ \frac{f_0}{(x_0-x_1)(x_0-x_2)} + \frac{f_1}{(x_1-x_0)(x_1-x_2)} + \frac{f_2}{(x_2-x_0)(x_2-x_1)} \right] \quad \downarrow (16)$$

which is constant for all  $x \in [x_0, x_2]$ . The error at the tabular point  $x_0$  is written as,

$$E''(x_0) = \frac{1}{3} (2x_0-x_1-x_2) f'''(\xi) + \frac{1}{24} (x_0-x_1)(x_0-x_2) [f^{IV}(\eta_1) + f^{IV}(\eta_2)] \quad \downarrow (17)$$

where  $x_1, \eta_1, \eta_2 \in (x_0, x_2)$   
 Similar relations can be obtained at  $x = x_1$   
 and  $x = x_2$ .

Uniform Node points:

When the distinct points  $x_0, x_1, \dots, x_n$  are  
 equispaced with step length  $h$ , we have

$$x_i = x_0 + ih, \quad i = 1, 2, \dots, n$$

$$f_i = f(x_i)$$

i) Linear interpolation:

Using linear interpolation we have

$$f'(x_0) \approx P_1'(x_0) = \frac{f_1 - f_0}{h} \rightarrow (1)$$

$$f'(x_1) \approx P_1'(x_1) = \frac{f_1 - f_0}{h} \rightarrow (2)$$

and  $E_1'(x_0) = f'(x_0) - \frac{f_1 - f_0}{h} \rightarrow (3)$

$$E_1'(x_1) = f'(x_1) - \frac{f_1 - f_0}{h} \rightarrow (4)$$

$E_1'$  is the error of approximation or the local  
 truncation error, Expanding the terms in (4)  
 in Taylor's series about the point  $x_0$ , we get.

$$\begin{aligned} E_1'(x_0) &= f'(x_0) - \frac{1}{h} \left[ \left\{ f(x_0) + hf'(x_0) + \frac{h^2}{2} f''(\xi) \right\} - f(x_0) \right] \\ &= -\frac{h}{2} f''(\xi), \quad x_0 < \xi < x_1 \end{aligned}$$

$$\begin{aligned} \text{By } E_1'(x_1) &= f'(x_1) - \frac{1}{h} [f(x_1) - f(x_1-h)] \\ &= f'(x_1) - \frac{1}{h} \left[ f(x_1) - \left\{ f(x_1) - hf'(x_1) + \frac{h^2}{2} f''(\eta) \right\} \right] \\ &= \frac{h}{2} f''(\eta), \quad x_0 < \eta < x_1 \end{aligned} \quad \sqrt{(5)}$$

(ii) Quadratic interpolation:

Using quadratic interpolation, we have

$$f(x) \approx p_2(x) = \frac{1}{2h^2} \left[ (x-x_1)(x-x_2) f_0 - 2(x-x_0)(x-x_2) f_1 + (x-x_0)(x-x_1) f_2 \right]$$

$$f'(x) \approx p_2'(x) = \frac{1}{2h^2} \left[ (2x-x_1-x_2) f_0 - 2(2x-x_0-x_2) f_1 + (2x-x_0-x_1) f_2 \right]$$

With  $x_1 = x_0 + h$  and  $x_2 = x_0 + 2h$  therefore

$$f'(x_0) \approx p_2'(x_0) = \frac{1}{2h^2} \left[ (2x_0 - x_1 - x_2) f_0 - 2(2x_0 - x_0 - x_2) f_1 + (2x_0 - x_0 - x_1) f_2 \right]$$

$$= \frac{1}{2h} \left[ -3f_0 + 4f_1 - f_2 \right] \rightarrow \textcircled{6}$$

$$f'(x_1) \approx p_2'(x_1) = \frac{1}{2h^2} \left[ (2x_1 - x_1 - x_2) f_0 - 2(2x_1 - x_0 - x_2) f_1 + (2x_1 - x_0 - x_1) f_2 \right]$$

$$= \frac{1}{2h} \left[ f_2 - f_0 \right] \rightarrow \textcircled{7}$$

and

$$f'(x_2) \approx p_2'(x_2) = \frac{1}{2h^2} \left[ (2x_2 - x_1 - x_0) f_0 - 2(2x_2 - x_0 - x_0) f_1 + (2x_2 - x_0 - x_1) f_2 \right]$$

$$= \frac{1}{2h} \left[ f_0 - 4f_1 + 3f_2 \right] \rightarrow \textcircled{8}$$

The local truncation error is given by

$$E_2'(x_0) = f'(x_0) - \frac{1}{2h} \left[ -3f(x_0) + 4f(x_0+h) - f(x_0+2h) \right]$$

$$= f'(x_0) - \frac{1}{2h} \left[ -3f(x_0) + 4 \left\{ f(x_0) + hf'(x_0) + \right. \right.$$

$$\left. \frac{h^2}{2!} f''(x_0) \right.$$

$$\left. + \frac{h^3}{3!} f'''(x_0) + \dots \right] - \left\{ f(x_0) + 2hf'(x_0) + \right.$$

$$\left. \frac{4h^2}{2!} f''(x_0) + \frac{8h^3}{3!} f'''(x_0) + \dots \right]$$

$$= -\frac{h^2}{3} f'''(\xi_0) + \dots$$

$$= -\frac{h^2}{3} f'''(\xi), \quad x_0 < \xi < x_2 \rightarrow \textcircled{9}$$

By, we get

$$E_2'(x_1) = f'(x_1) - \frac{1}{2h} [f(x_2) - f(x_0)]$$

$$= f'(x_1) - \frac{1}{2h} [f(x_1+h) - f(x_1-h)]$$

$$= -\frac{h^2}{6} f'''(\eta_1) + \dots$$

$$\approx -\frac{h^2}{6} f'''(\eta_1), \quad x_0 < \eta_1 < x_2 \rightarrow \textcircled{10}$$

$$E_2'(x) = f'(x_2) - \frac{1}{2h} [f(x_0) - 4f(x_1) + 3f(x_2)]$$

$$= f'(x_2) - \frac{1}{2h} [f(x_2-2h) - 4f(x_2-h) + 3f(x_2)]$$

$$= -\frac{h^2}{3} f'''(\eta_2) + \dots$$

$$\approx -\frac{h^2}{3} f'''(\eta_2), \quad x_2 < \eta_2 < x_2 \rightarrow \textcircled{11}$$

$\therefore$  The interpolating polynomial is a quadratic its 2nd derivative is a constant. Hence

$$f''(x_0) \approx P_2''(x_0) = \frac{1}{h^2} [f_0 - 2f_1 + f_2] \rightarrow \textcircled{12}$$

$$f''(x_1) \approx P_2''(x_1) = \frac{1}{h^2} [f_0 - 2f_1 + f_2] \rightarrow \textcircled{13}$$

$$f''(x_2) \approx P_2''(x_2) = \frac{1}{h^2} [f_0 - 2f_1 + f_2] \rightarrow \textcircled{14}$$

The local truncation error is given by

$$E_2''(x_0) = f''(x_0) - \frac{1}{h^2} [f(x_0) - 2f_1 + f_2] \rightarrow \textcircled{15}$$

$$= -h f''(\xi_1), \quad x_0 < \xi_1 < x_2$$

$$E_2''(x_1) = f''(x_1) - \frac{1}{h^2} [f(x_0) - 2f(x_1) + f(x_2)]$$

$$= -\frac{h^2}{12} f''''(\xi_2), \quad x_0 < \xi_2 < x_2 \rightarrow \textcircled{16}$$

Where the Taylor expansions are written about  $x_0, x_1$  and  $x_2$  respectively. We now define the order of a numerical differentiation method.

Definition:

(\*) A numerical differentiation method is said to be order p if,

$$|f^{(r)}(x) - p^{(r)}(x)| \leq ch^p \rightarrow (*)$$

where  $c$  is a constant independent of  $h$ .

Thus, the methods  $f'(x_0) \approx P_1'(x_0) = \frac{f_1 - f_0}{h}$

$$f''(x_2) \approx P_2'(x_2) = \frac{1}{h^2} [f_0 - 2f_1 + f_2]$$

are of 1<sup>st</sup> order, where as methods.

$$f'(x_0) = \frac{1}{2h} [-3f_0 + 4f_1 - f_2]$$

$$f'(x_1) = \frac{1}{2h} [f_2 - f_0]$$

$$f'(x_2) = \frac{1}{2h} [f_0 - 4f_1 + 3f_2]$$

and  $f''(x_1) \approx P_2''(x_1) = \frac{1}{h^2} [f_0 - 2f_1 + f_2]$  are of 2<sup>nd</sup> order.

Methods based on finite Differences:

We consider the relation,

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

$$= \left(1 + hD + \frac{h^2 D^2}{2!} + \dots\right) f(x)$$

$$= e^{hD} f(x) \rightarrow (1)$$

in which  $D = \frac{d}{dx}$  is called the differential operator.

Symbolically, we get from (1)

$$e^{hD} = E \quad (\text{or}) \quad hD = \log E$$



Also,

$$\delta = (E^{1/2} - E^{-1/2}) = (e^{hD/2} - e^{-hD/2}) \\ = 2 \sinh(hD/2) \rightarrow \textcircled{2}$$

Thus, we have

$$AD = \log E$$

$$= \begin{cases} \log(1+\Delta) = \Delta - \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 - \dots \\ -\log(1-\nabla) = \nabla + \frac{1}{2}\nabla^2 + \frac{1}{3}\nabla^3 + \dots \end{cases} \rightarrow \textcircled{3}$$

Also from  $\textcircled{2}$ , we have

$$hD = 2 \sinh^{-1}(\delta/2) = \delta - \frac{1^2}{2^2 \cdot 3!} \delta^3 + \dots \rightarrow \textcircled{4}$$

We can write

$$hf'(x_k) = hD f(x_k)$$

$$= \begin{cases} \Delta f_k - \frac{1}{2}\Delta^2 f_k + \frac{1}{3}\Delta^3 f_k - \dots \\ \nabla f_k + \frac{1}{2}\nabla^2 f_k + \frac{1}{3}\nabla^3 f_k + \dots \\ \delta f_k - \frac{1^2}{2^2 \cdot 3!} \delta^3 f_k + \dots \end{cases}$$

$$\therefore \mu = \sqrt{\left\{1 + \frac{\delta^2}{4}\right\}}$$

We can also write,

$$hD = \frac{\mu}{\sqrt{\left\{1 + \left(\frac{\delta^2}{4}\right)\right\}}} \left[ 2 \sinh^{-1}(\delta/2) \right]$$

$$= \mu \left\{ 1 + \frac{\delta^2}{4} \right\}^{-1/2} \left[ 2 \sinh^{-1}(\delta/2) \right]$$

$$= \mu \left[ 1 - \frac{\delta^2}{8} + \frac{3\delta^4}{128} - \dots \right] \left[ \delta - \frac{1^2}{2^2 \cdot 3!} \delta^3 \right]$$

$$= \mu \left[ \delta - \frac{1^2}{3!} \delta^3 + \frac{1^2 \cdot 2^2}{5!} \delta^5 - \dots \right]$$

Thus we get,

$$hf'(x_k) = \mu \delta f_k - \frac{1^2}{3!} \mu \delta^3 f_k + \frac{1^2 \cdot 2^2}{5!} \mu \delta^5 f_k - \dots \quad \textcircled{5}$$

11<sup>th</sup> we obtain

$$h^r D^r = \begin{cases} \Delta^r - \frac{1}{2} r \Delta^{r+1} + \frac{r(3r+5)}{24} \Delta^{r+2} - \dots \\ \nabla^r + \frac{1}{2} r \nabla^{r+1} + \frac{r(3r+5)}{24} \nabla^{r+2} + \dots \\ \mu \delta^r - \frac{r+3}{24} \mu \delta^{r+2} + \frac{5r^2+52r+135}{5760} \mu \delta^{r+4} - \dots \\ \delta^r - \frac{r}{24} \delta^{r+2} + \frac{r(5r+22)}{5760} \delta^{r+4} - \dots \end{cases}$$

r odd  
r even  $\downarrow$  ⑥

In particular, differentiation method for  $r=1$  and  $r=2$  at  $x=x_k$  become

$$h f'(x_k) = \begin{cases} \Delta f_k - \frac{1}{2} \Delta^2 f_k + \frac{1}{3} \Delta^3 f_k - \dots \\ \nabla f_k + \frac{1}{2} \nabla^2 f_k + \frac{1}{3} \nabla^3 f_k + \dots \\ \mu \delta f_k - \frac{1}{6} \mu \delta^3 f_k + \frac{1}{30} \mu \delta^5 f_k - \dots \end{cases} \quad \downarrow \text{⑦}$$

$$h^2 f''(x_k) = \begin{cases} \Delta^2 f_k - \Delta^3 f_k + \frac{11}{12} \Delta^4 f_k - \dots \\ \nabla^2 f_k + \nabla^3 f_k + \frac{11}{12} \nabla^4 f_k + \dots \\ \delta^2 f_k - \frac{1}{12} \delta^4 f_k + \frac{1}{90} \delta^6 f_k - \dots \end{cases} \rightarrow \text{⑧}$$

Keeping only the 1<sup>st</sup> term in each of the methods in ⑦ we get

$$f'(x_k) = \begin{cases} (f_{k+1} - f_k) / h & \rightarrow \text{⑨} \\ (f_k - f_{k-1}) / h & \rightarrow \text{⑩} \\ (f_{k+1} - f_{k-1}) / (2h) & \rightarrow \text{⑪} \end{cases}$$

It can be verified that the methods ⑨ & ⑩ are of 1<sup>st</sup> order where as the method ⑪ is of 2<sup>nd</sup> order.

11<sup>th</sup>, if we retain only one term in each of the methods in ⑧ then we get,

$$f''(x_k) = \begin{cases} (f_{k+2} - 2f_{k+1} + f_k) / h^2 & \rightarrow \text{⑫} \\ (f_k - 2f_{k-1} + f_{k-2}) / h^2 & \rightarrow \text{⑬} \\ (f_{k-1} - 2f_k + f_{k+1}) / h^2 & \rightarrow \text{⑭} \end{cases}$$



It can be verified that the methods (1) & (2) are of 1<sup>st</sup> order where as the method (4) is of 2<sup>nd</sup> order.

Methods based on undetermined co-efficients

Numerical differentiation methods based on interpolating polynomials express  $f^{(r)}(x)$  as a linear combination of the values of  $f(x)$  at a set of pre-chosen tabular points. In the method of undetermined co-efficients we express  $f^{(r)}(x)$  as a linear combination of the values of  $f(x)$  at an arbitrarily chosen set of tabular points. For eg, if we assume that the tabular points are equispaced with step length  $h$ , we write,

$$h^r f^{(r)}(x_k) = \sum_{v=-p}^p a_v f_{k+v} \rightarrow (1)$$

for symmetric arrangement of tabular points,

$$(or) \quad h^r f^{(r)}(x_k) = \sum_{v=\pm\lambda}^p a_v f_{k+v} \rightarrow (2)$$

for non-symmetric arrangement of tabular points.

The local truncation error is defined by,

$$E^{(r)}(x_k) = \frac{1}{h^r} \left[ h^r f^{(r)}(x_k) - \sum_{v=-p}^p a_v f_{k+v} \right] \rightarrow (3)$$

$$(or) \quad E^{(r)}(x_k) = \frac{1}{h^r} \left[ h^r f^{(r)}(x_k) - \sum_{v=\pm\lambda}^p a_v f_{k+v} \right] \rightarrow (4)$$

The co-efficients  $a_v$ 's in (1) or (2) are determined by requiring the method to be of a particular order. we expand the RHS in (1) or (2) in Taylor's series about the point  $x_k$  and on equating the co-efficients of various order derivative on both sides, we obtain the required number of

equations to determine these co-efficients. The 1<sup>st</sup> non-zero term in (3) (or) (4) gives the error of approximations. As an eg, consid the values  $r=2$  and  $p=2$  in (1) and get,

$$\begin{aligned}
 h^2 f''(x_k) &= a_{-2} f_{k-2} + a_{-1} f_{k-1} + a_0 f_k + a_1 f_{k+1} + a_2 f_{k+2} \\
 &= [a_{-2} + a_{-1} + a_0 + a_1 + a_2] f_{k+h} (-2a_{-2} - a_{-1} + a_1 + 2a_2) f_k' + \\
 &\quad \frac{h^2}{2} (4a_{-2} + a_{-1} + a_1 + 4a_2) f_k'' \\
 &\quad + \frac{h^3}{6} (-8a_{-2} - a_{-1} + 8a_2) f_k''' + \frac{h^4}{24} (16a_{-2} + a_{-1} + 16a_2) f_k^{(4)} + \frac{h^5}{120} (-32a_{-2} - a_{-1} + a_1 + 32a_2) f_k^{(5)} + \frac{h^6}{720} (64a_{-2} + a_{-1} + a_1 + 64a_2) f_k^{(6)} + \dots
 \end{aligned}$$

Comparing the co-efficients of  $f_k^{(i)}$ ,  $i=0,1,2,3,4$  or both sides we get the system of equations.

$$a_{-2} + a_{-1} + a_0 + a_2 = 0$$

$$-2a_{-2} - a_{-1} + a_1 + 2a_2 = 0$$

$$4a_{-2} + a_{-1} + a_1 + 4a_2 = 2$$

$$-8a_{-2} + a_{-1} + a_1 + 8a_2 = 0$$

$$16a_{-2} + a_{-1} + a_1 + 16a_2 = 0$$

Solving the above system of eqns, we get

$$a_{-2} = a_2 = -\frac{1}{12}, \quad a_{-1} = a_1 = \frac{16}{2}, \quad a_0 = -\frac{30}{12}$$

and the method becomes,

$$f''(x_k) = \frac{-f_{k-2} + 16f_{k-1} - 30f_k + 16f_{k+1} - f_{k+2}}{12h^2} \quad \checkmark$$

The 1<sup>st</sup> non-zero term in (3) gives the error of approximation as,

$$\text{Error} = \frac{h^4}{90} f^{(4)}(\xi), \quad x_{k-1} < \xi < x_{k+1}$$

Thus, the method (5) is of 4<sup>th</sup> order.

Optimum Choice of step length:

In numerical differentiation methods, error of approximation or the truncation error is of the form  $ch^p$  which tends to zero as  $h \rightarrow 0$ . However, the method which approximates  $f^{(r)}(x) h^r$  in the denominator. As  $h$  is successively decreased to smaller values, the truncation error decreases, but the round off error in the method may increase as we are dividing by a small number. It may happen that after a certain critical value of  $h$ , the round error may become more dominant than the truncation error and the numerical results obtained may start to increase as  $h$  is further reduced. When  $f(x)$  is given in tabular form these values may not themselves be exact. These values contain the round off errors, that is  $f(x_i) = f_i + \epsilon_i$ , where  $f(x_i)$  is the exact value and  $f_i$  is the tabulated value. To see the effect of this round off error in numerical differentiation method, we consider the method.

$$f'(x_0) = \frac{f(x_1) - f(x_0)}{h} - \frac{h}{2} f''(\xi), \quad x_0 < \xi < x_1 \rightarrow (1)$$

If the round off errors in  $f(x_0)$  and  $f(x_1)$  are  $\epsilon_0$  and  $\epsilon_1$  respectively, then we have

$$f'(x_0) = \frac{f_1 - f_0}{h} + \frac{\epsilon_1 - \epsilon_0}{h} - \frac{h}{2} f''(\xi) \rightarrow (2)$$

(or)

$$f'(x_0) = \frac{f_1 - f_0}{h} + RE + TE \rightarrow (3)$$

Where RE and TE denote the round off errors and truncation error respectively.

If we take,

$$E = \max(|E_1|, |E_2|)$$

$$\text{and } M_2 = \max_{x_0 \leq x \leq x_1} |f''(x)|$$

then, we get

$$|RE| \leq \frac{2E}{h}, \quad |TE| \leq \frac{h}{2} M_2.$$

We may call that value of  $h$  as an optimal value for which one of the following criteria is satisfied,

$$i) |RE| = |TE|$$

$$ii) |RE| + |TE| = \text{minimum} \quad \left. \vphantom{ii)} \right\} \rightarrow (4)$$

If we use the criterion (4) (i) then we have

$$\frac{2E}{h} + \frac{h}{2} M_2 = \text{minimum}$$

$$-\frac{2E}{h^2} + \frac{1}{2} M_2 = 0$$

(or)

$$h_{opt} = 2 \sqrt{E/M_2}$$

The minimum total error is  $2(E M_2)^{1/2}$

This means that if the round off error is of the order  $10^{-k}$  (say) and  $M_2 = O(1)$  then the accuracy given by the method may be approximately of the order  $10^{-k/2}$ . Since in any numerical differentiation method,



The local truncation error is always proportional to some power of  $h$ , the same technique can be used to determine an optimal value of  $h$  for any numerical method which approximates  $f^{(r)}(x_k)$ ,  $r \geq 1$ .

Extrapolation Methods:

Let  $g(h)$  denote the approximate value of  $g$ , obtained by using a method of order  $P$ , with step length  $h$  and  $g(qh)$  denote the value of  $g$  obtained by using the same method of order  $P$ , with step length  $qh$ . we have,

$$g(h) = g + ch^P + o(h^{P+1})$$

$$g(qh) = g + cq^P h^P + o(h^{P+1})$$

Eliminating  $c$  from the above equations, we get

$$g = \frac{q^P g(h) - g(qh)}{q^P - 1} + o(h^{P+1})$$

Thus, we obtain

$$g^{(1)}(h) = \frac{q^P g(h) - g(qh)}{q^P - 1} = g + o(h^{P+1}) \rightarrow \infty$$

which is of order  $P+1$ . This technique of combining two computed values obtained by using the same method with two different step sizes, to obtain a higher order method is called the extrapolation method (or) Richardson's extrapolation.

If the local truncation error associated with the method is known as a power series in  $h$ , then by repeating the extrapolation procedure a number of times, we can obtain the methods

of any arbitrary order. The application of this procedure becomes when the step lengths form a geometric sequence. For simplicity, we generally take  $q = \frac{1}{2}$ . To illustrate the procedure we consider the method.

$$f'(x_0) = \frac{f_1 - f_{-1}}{2h} \rightarrow (2)$$

where  $f_1 = f(x_0 + h)$  and  $f_{-1} = f(x_0 - h)$ . The local truncation error associated with the method (2) is obtained as,

$$E'(x_0) = c_1 h^2 + c_2 h^4 + c_3 h^6 + \dots \rightarrow (3)$$

where  $c_1, c_2, c_3, \dots$  are constants independent of  $h$ . Let  $g(x) = f'(x)$  be the quantity which is to be obtained and  $g(h/2^r)$  denote the approximate value of  $g(x)$  obtained by using the method (2) with step length  $\frac{h}{2^r}$ ,  $r = 0, 1, 2, \dots$

Thus we have

$$g(h) = g(x) + c_1 h^2 + c_2 h^4 + c_3 h^6 + \dots$$

$$g\left(\frac{h}{2}\right) = g(x) + \frac{c_1 h^2}{4} + \frac{c_2 h^4}{16} + \frac{c_3 h^6}{64} + \dots \rightarrow (4)$$

$$g\left(\frac{h}{2^2}\right) = g(x) + \frac{c_1 h^2}{16} + \frac{c_2 h^4}{256} + \frac{c_3 h^6}{4096} + \dots$$

Eliminating  $c_1$  from the above eqns we obtain

$$g^{(1)}(h) = \frac{4g\left(\frac{h}{2}\right) - g(h)}{3}$$

$$= g(x) - \frac{1}{2} c_2 h^4 - \frac{5}{16} c_3 h^6 \dots$$

$$g^{(1)}\left(\frac{h}{2}\right) = \frac{4g\left(\frac{h}{2^2}\right) - g\left(\frac{h}{2}\right)}{3}$$

$$= g(x) - \frac{1}{64} c_2 h^4 - \frac{5}{1024} c_3 h^6 \dots \rightarrow (5)$$

Thus,  $g^{(1)}(h), g^{(1)}\left(\frac{h}{2}\right), \dots$  given by (5) are  $o(h^4)$  approximations to  $g(x)$ . Eliminating  $c_2$  from (5) we obtain,



$$g^{(2)}(h) = \frac{4^2 g^{(1)}\left(\frac{h}{2}\right) - g^{(1)}(h)}{4^2 - 1} + \frac{1}{64} c_3 h^6 + \dots \rightarrow (D)$$

which gives an  $O(h^6)$  approximation. Thus, the successive, higher order results can be obtained from the formula

$$g^{(m)}(h) = \frac{4^m g^{(m-1)}\left(\frac{h}{2}\right) - g^{(m-1)}(h)}{4^m - 1}, \quad m=1, 2, \dots \rightarrow (E)$$

where  $g^{(0)}(h) = g(h)$

This procedure is called repeated extrapolation to the limit. The successive values of  $g^{(m)}(h)$  for various values of  $m$  can be evaluated as given in below table.

It may be noted in table the successive entries in a particular column give better approximation than the preceding entries. Similarly these successive columns give better approximations than the preceding column. The best results can be obtained from the lower diagonal terms. The extrapolation can be stopped then,

$$|g^{(k)}(h) - g^{(k-1)}\left(\frac{h}{2}\right)| < \epsilon \rightarrow (F)$$

for a given error tolerance  $\epsilon$

Extrapolation table

Order	second	Fourth	Sixth	Eighth
$h$	$g(h)$	$g'(h)$	$g^{(2)}(h)$	
$h/2$	$g(h/2)$	$g'(h/2)$		$g^{(3)}(h)$
$h/2^2$	$g(h/2^2)$	$g'(h/2)$	$g^{(2)}(h/2)$	
$h/2^3$	$g(h/2^3)$			

## Partial Differentiation:

We can use any of the three techniques discussed in the previous sections to obtain numerical partial differentiation methods. We consider only one variable at a time and treat the remaining variables as constants. We consider here a function  $f(x, y)$  of two variables only. Let the values of the function  $f(x, y)$  be given at a set of points  $(x_i, y_j)$  in the  $(x, y)$  plane with spacing  $h$  and  $k$  in  $x$  and  $y$  direction respectively we have,

$$x_i = x_0 + ih, \quad y_j = y_0 + jk, \quad i, j = 1, 2, \dots$$

We can now write,

$$\left(\frac{\partial f}{\partial x}\right)_{(x_i, y_j)} = \begin{cases} [f_{i+1, j} - f_{i, j}] / h + o(h) \\ [f_{i, j} - f_{i-1, j}] / h + o(h) \rightarrow \textcircled{1} \\ [f_{i+1, j} - f_{i-1, j}] / (2h) + o(h^2) \end{cases}$$

where  $f_{i, j} = f(x_i, y_j)$

Similarly we can write

$$\left(\frac{\partial f}{\partial y}\right)_{(x_i, y_j)} = \begin{cases} [f_{i, j+1} - f_{i, j}] / k + o(k) \\ [f_{i, j} - f_{i, j-1}] / k + o(k) \rightarrow \textcircled{2} \\ [f_{i, j+1} - f_{i, j-1}] / (2k) + o(k^2) \end{cases}$$

$$\left(\frac{\partial^2 f}{\partial x^2}\right)_{(x_i, y_j)} = \frac{1}{h^2} (f_{i-1, j} - 2f_{i, j} + f_{i+1, j}) + o(h^2) \rightarrow \textcircled{3}$$

$$\left(\frac{\partial^2 f}{\partial y^2}\right)_{(x_i, y_j)} = \frac{1}{k^2} (f_{i, j-1} - 2f_{i, j} + f_{i, j+1}) + o(k^2) \rightarrow \textcircled{4}$$

$$\therefore \frac{\partial^2 f}{\partial x \partial y} = \frac{\partial}{\partial x} \left(\frac{\partial f}{\partial y}\right) = \frac{\partial}{\partial y} \left(\frac{\partial f}{\partial x}\right)$$

We can write,

$$\left(\frac{\partial^2 f}{\partial x \partial y}\right)_{(x_i, y_j)} = \frac{\partial}{\partial x} \left(\frac{\partial f}{\partial y}\right)_{(x_i, y_j)}$$

$$\begin{aligned}
 &= \frac{\partial}{\partial x} \left( \frac{f_{i,j+1} - f_{i,j-1}}{2k} \right) \\
 &= \frac{1}{2k} \left[ \frac{f_{i+1,j+1} - f_{i-1,j+1}}{2h} - \frac{f_{i+1,j-1} - f_{i-1,j-1}}{2h} \right] \\
 &= \frac{f_{i+1,j+1} - f_{i-1,j+1} - f_{i+1,j-1} + f_{i-1,j-1}}{4hk} \rightarrow \textcircled{5}
 \end{aligned}$$

The method  $\textcircled{5}$  is of  $O(h^2+k^2)$  we can also write,

$$\begin{aligned}
 \left( \frac{\partial^2 f}{\partial x \partial y} \right) (x_i, y_j) &= \frac{\partial}{\partial y} \left( \frac{\partial f}{\partial x} \right) (x_i, y_j) \\
 &= \frac{\partial}{\partial y} \left( \frac{f_{i+1,j} - f_{i-1,j}}{2h} \right) \\
 &= \frac{1}{2h} \left[ \frac{f_{i+1,j+1} - f_{i+1,j-1}}{2k} - \frac{f_{i-1,j+1} - f_{i-1,j-1}}{2k} \right] \\
 &= \frac{f_{i+1,j+1} - f_{i+1,j-1} - f_{i-1,j+1} + f_{i-1,j-1}}{4hk}
 \end{aligned}$$

which is same as eqn  $\textcircled{5}$

Methods based on undetermined co-efficients:-

The Newton-Cotes methods derived in the previous section can also be obtained using the approach of methods of undetermined co-efficients.

The Newton-Cotes methods are given by,

$$\int_a^b f(x) dx = \sum_{k=0}^n \lambda_k f_k$$

We shall derive the trapezoidal and Simpson methods the methods undetermined co-efficients.

Newton-Cotes methods:-

Trapezoidal method:

We have  $n=1$ ,  $x_0=a$ ,  $x_1=b$  and  $h=x_1-x_0$  we

write,

$$\int_{x_0}^{x_1} f(x) dx = \lambda_0 f(x_0) + \lambda_1 f(x_1)$$

Using the eqn,

$$R_n = \int_a^b w(x) f(x) dx - \sum_{k=0}^n \lambda_k f(x_k)$$

and the defn, the rule can be made exact for polynomials of degree upto one.

For  $f(x)=1$  and  $x_1$  we get the system of eqns

$$f(x)=1, \quad x_1 - x_0 = \lambda_0 + \lambda_1 \quad (\text{or}) \quad h = \lambda_0 + \lambda_1$$

$$f(x)=x, \quad \frac{1}{2}(x_1^2 - x_0^2) = \lambda_0 x_0 + \lambda_1 x_1$$

We have

$$\frac{1}{2}(x_1 - x_0)(x_1 + x_0) = \lambda_0 x_0 + \lambda_1 x_1$$

$$(\text{or}) \quad \frac{1}{2}h(2x_0 + h) = \lambda_0 x_0 + \lambda_1(x_0 + h)$$

$$(\text{or}) \quad \frac{1}{2}h(2x_0 + h) = (\lambda_0 + \lambda_1)x_0 + \lambda_1 h = hx_0 + \lambda_1 h$$

$$(\text{or}) \quad \lambda_1 h = \frac{h^2}{2} \quad (\text{or}) \quad \lambda_1 = \frac{h}{2}$$

From the first equation, we get  $\lambda_0 = h - \lambda_1 = \frac{h}{2}$

The method becomes,

$$\int_{x_0}^{x_1} f(x) dx = \frac{h}{2} [f(x_0) + f(x_1)]$$

From the eqn,  $c = \int_a^b w(x) x^{n+1} dx - \sum_{k=0}^n \lambda_k x_k^{n+1}$

The error constant is given by,

$$\begin{aligned} c &= \int_{x_0}^{x_1} x^2 dx - \frac{h}{2} [x_0^2 + x_1^2] = \frac{1}{3}(x_1^3 - x_0^3) - \frac{h}{2}(x_0^2 + x_1^2) \\ &= \frac{1}{6} [2(x_0^3 + 3x_0^2h + 3x_0h^2 + h^3) - 2x_0^3 - 3x_0^2h \\ &\quad - 3h(x_0^2 + 2x_0h + h^2)] \\ &= \frac{-h^3}{6} \end{aligned}$$

The truncation error becomes,

$$R_1 = \frac{c}{2} f''(\xi) = -\frac{h^3}{12} f''(\xi), \quad x_0 < \xi < x_1$$

**Simpson's Method:**

We have  $n=2$ ,  $x_0=a$ ,  $x_1=x_0+h$ ,  $x_2=x_0+2h$

$h = (b-a)/2$  we write,



$$\int_{x_0}^{x_2} f(x) dx = \lambda_0 f(x_0) + \lambda_1 f(x_1) + \lambda_2 f(x_2)$$

The rule can be made exact for polynomials of degree upto two. For  $f(x) = 1, x, x^2$  we get the following system of equations.

$$f(x) = 1; \quad x_2 - x_0 = \lambda_0 + \lambda_1 + \lambda_2 \quad (\text{or}) \quad 2h = \lambda_0 + \lambda_1 + \lambda_2 \rightarrow \textcircled{1}$$

$$f(x) = x; \quad \frac{1}{2} (x_2^2 - x_0^2) = \lambda_0 x_0 + \lambda_1 x_1 + \lambda_2 x_2 \rightarrow \textcircled{2}$$

$$f(x) = x^2; \quad \frac{1}{3} (x_2^3 - x_0^3) = \lambda_0 x_0^2 + \lambda_1 x_1^2 + \lambda_2 x_2^2 \rightarrow \textcircled{3}$$

From  $\textcircled{1}$ , we get

$$\frac{1}{2} (x_2 - x_0) (x_2 + x_0) = \lambda_0 x_0 + \lambda_1 (x_0 + 2h)$$

$$\begin{aligned} (\text{or}) \quad \frac{1}{2} (2h) (2x_0 + 2h) &= (\lambda_0 + \lambda_1 + \lambda_2) x_0 + (\lambda_1 + 2\lambda_2) h \\ &= 2hx_0 + (\lambda_1 + 0\lambda_2) h \quad [\text{using } \textcircled{1}] \end{aligned}$$

$$(\text{or}) \quad 2h = 2\lambda_2 + \lambda_1$$

From  $\textcircled{3}$ , we get,

$$\frac{1}{3} [(x_0^3 + 6x_0^2 h + 12x_0 h^2 + 8h^3) - x_0^3] = \lambda_0 x_0^2 +$$

$$\lambda_1 (x_0^2 + 2x_0 h + h^2) + \lambda_2 (x_0^2 + 4x_0 h + 4h^2)$$

(or)

$$2x_0^2 h + 4x_0 h^2 + \frac{8}{3} h^3 = (\lambda_0 + \lambda_1 + \lambda_2) x_0^2 + 2(\lambda_1 + 2\lambda_2) x_0 h + (\lambda_1 + 4\lambda_2) h^2$$

$$= 2hx_0^2 + 4x_0 h^2 + (\lambda_1 + 4\lambda_2) h^2$$

$$(\text{or}) \quad \frac{8}{3} h = \lambda_1 + 4\lambda_2 \rightarrow \textcircled{5}$$

Solving  $\textcircled{4}$  and  $\textcircled{5}$  and using  $\textcircled{1}$  we obtain

$$\lambda_0 = \frac{h}{3}, \quad \lambda_1 = \frac{4h}{3}, \quad \lambda_2 = \frac{h}{3}$$

The method is given by,

$$\int_{x_0}^{x_2} f(x) dx = \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)]$$

From the eqn  $c = -\frac{(b-a)^5}{120}$  the error constant is

$$\text{given by } c = -\frac{4}{15} h^5$$

$$\text{and } R_2 = \frac{c}{4!} f^{(4)}(\eta)$$

$$= -\frac{h^5}{90} f^{(4)}(\eta), \quad x_0 < \eta < x_2$$

The method of undetermined co-efficients can be used to derive quadrature formulas of a given type. We illustrate such derivations through the following problem.

14. Determine  $a, b$  and  $c$  such that the formula

$$\int_0^h f(x) dx = h \{ a f(0) + b f(h/3) + c f(h) \}$$

is exact for polynomials of as high order as possible and determine the order of the truncation error.

Soln:

Making the method exact for polynomials of degree upto 2, we obtain for  $f(x)=1$ ;

$$h = h(a+b+c) \quad (\text{or}) \quad a+b+c=1$$

$$\text{For } f(x)=x; \quad \frac{h^2}{2} = h \left( \frac{bh}{3} + ch \right) \quad (\text{or}) \quad \frac{1}{3}b+c = \frac{1}{2}$$

$$\text{for } f(x)=x^2; \quad \frac{h^3}{3} = h \left( \frac{bh^2}{9} + ch^2 \right) \quad (\text{or}) \quad \frac{1}{9}b+c = \frac{1}{3}$$

Solving the above eqns, we get

$$a=0, \quad b=3/4, \quad c=1/4.$$

The truncation error of the formula is given by,

$$T-E = \frac{c}{3!} f'''(\xi), \quad 0 < \xi < h.$$

$$\text{and } c = \int_0^h x^3 dx - h \left[ \frac{bh^3}{27} + ch^3 \right] = -\frac{h^4}{36}$$

Hence we have

$$T-E = -\frac{h^4}{216} f'''(\xi) = o(h^4)$$



Find the quadrature formula

$$\int_0^1 f(x) \frac{dx}{\sqrt{x(1-x)}} = a_1 f(0) + a_2 f(1/2) + a_3 f(1)$$

which is exact for polynomials of highest possible degree. Then use the formula on  $\int_0^1 \frac{dx}{\sqrt{x-x^3}}$  and compare with the exact value.

Soln

Making the method exact for polynomials of degree upto two we obtain,

$$\text{for } f(x) = 1; \quad I_1 = \int_0^1 \frac{dx}{\sqrt{x(1-x)}} = a_1 + a_2 + a_3$$

$$\text{for } f(x) = x; \quad I_2 = \int_0^1 \frac{x dx}{\sqrt{x(1-x)}} = \frac{1}{2} a_2 + a_3$$

$$\text{for } f(x) = x^2; \quad I_3 = \int_0^1 \frac{x^2 dx}{\sqrt{x(1-x)}} = \frac{1}{4} a_2 + a_3$$

where,

$$I_1 = \int_0^1 \frac{dx}{\sqrt{x(1-x)}} = 2 \int_0^1 \frac{dx}{\sqrt{1-(2x-1)^2}} = \int_{-1}^1 \frac{dt}{\sqrt{1-t^2}} = [\sin^{-1}t]_{-1}^1 = \pi$$

$$I_2 = \int_0^1 \frac{x dx}{\sqrt{x(1-x)}} = 2 \int_0^1 \frac{x dx}{\sqrt{1-(2x-1)^2}} = \int_{-1}^1 \frac{t+1}{2\sqrt{1-t^2}} dt$$

$$= \frac{1}{2} \int_{-1}^1 \frac{t dt}{\sqrt{1-t^2}} + \frac{1}{2} \int_{-1}^1 \frac{dt}{\sqrt{1-t^2}} = \frac{\pi}{2}$$

$$I_3 = \int_0^1 \frac{x^2 dx}{\sqrt{x(1-x)}} = 2 \int_0^1 \frac{x^2 dx}{\sqrt{1-(2x-1)^2}} = \frac{1}{4} \int_{-1}^1 \frac{(t+1)^2}{\sqrt{1-t^2}} dt$$

$$= \frac{1}{4} \int_{-1}^1 \frac{t^2 dt}{\sqrt{1-t^2}} + \frac{1}{2} \int_{-1}^1 \frac{t}{\sqrt{1-t^2}} dt + \frac{1}{4} \int_{-1}^1 \frac{dt}{\sqrt{1-t^2}} = \frac{3\pi}{8}$$

$$a_1 + a_2 + a_3 = \pi$$

$$\frac{1}{2} \alpha_2 + \alpha_3 = \frac{\pi}{2}$$

$$\frac{1}{4} \alpha_2 + \alpha_3 = \frac{3\pi}{8}$$

Which gives  $\alpha_1 = \frac{\pi}{4}$ ,  $\alpha_2 = \pi/2$ ,  $\alpha_3 = \pi/4$

The quadrature formula is given by,

$$\int_0^1 \frac{f(x)}{\sqrt{x(1-x)}} dx = \frac{\pi}{4} [f(0) + 2f(1/2) + f(1)]$$

We now use this formula to evaluate

$$I = \int_0^1 \frac{dx}{\sqrt{x-x^3}} = \int_0^1 \frac{dx}{\sqrt{1+x} \sqrt{x(1-x)}} = \int_0^1 \frac{f(x)}{\sqrt{x(1-x)}} dx$$

Where  $f(x) = \frac{1}{\sqrt{1+x}}$

We obtain

$$I = \frac{\pi}{4} \left[ 1 + \frac{2\sqrt{2}}{\sqrt{3}} + \frac{\sqrt{2}}{2} \right] \approx 2.62331$$

The exact value is

$$I = 2.62205755$$

Gauss - Legendre Integration methods:-

Let the weight function  $w(x) = 1$ . Then, the method,

$$\int_{-1}^1 w(x) f(x) dx = \sum_{k=0}^n \lambda_k f_k \rightarrow \textcircled{1}$$

Then, reduces to

$$\int_{-1}^1 f(x) dx = \sum_{k=0}^n \lambda_k f(x_k) \rightarrow \textcircled{2}$$

In this case all the nodes  $x_k$  and weights  $\lambda_k$  are unknown. Consider the following cases,

One point formula  $n=0$ . The formula is given by

$$\int_{-1}^1 f(x) dx = \lambda_0 f(x_0) \rightarrow \textcircled{3}$$

The method has two unknowns  $\lambda_0, x_0$ .

Making the method exact for  $f(x) = 1$ ,  
we get

$$f(x) = 1, \quad 2 = \lambda_0$$

$$f(x) = x; \quad 0 = \lambda_0 x_0 \quad (\text{or}) \quad x_0 = 0$$

Hence the method is given by,

$$\int f(x) dx = 2 f(0) \rightarrow \textcircled{3}$$

which is same as the mid-point formula.

The error constant is given by,

$$C = \int_{-1}^1 x^3 dx - 2[0] = \frac{2}{3}$$

$$\text{Hence, } R_1 = \frac{C}{2!} f''(\xi)$$

$$= \frac{1}{3} f''(\xi), \quad -1 < \xi < 1$$

Two point formula  $n=1$ , the formula is given by

$$\int f(x) dx = \lambda_0 f(x_0) + \lambda_1 f(x_1) \rightarrow \textcircled{4}$$

The method has 4 unknowns,  $x_0, x_1, \lambda_0$  and  $\lambda_1$ , making the method exact for  $f(x) = 1, x, x^2, x^3$  we get,

$$f(x) = 1, \quad 2 = \lambda_0 + \lambda_1 \rightarrow \textcircled{5}$$

$$f(x) = x, \quad 0 = \lambda_0 x_0 + \lambda_1 x_1 \rightarrow \textcircled{6}$$

$$f(x) = x^2, \quad \frac{2}{3} = \lambda_0 x_0^2 + \lambda_1 x_1^2 \rightarrow \textcircled{7}$$

$$f(x) = x^3, \quad 0 = \lambda_0 x_0^3 + \lambda_1 x_1^3 \rightarrow \textcircled{8}$$

Eliminating  $\lambda_0$  from  $\textcircled{6}, \textcircled{7}$  we get

$$\lambda_1 x_1^3 - \lambda_1 x_1 x_0^2 = 0 \quad (\text{or}) \quad \lambda_1 x_1 (x_1 - x_0) (x_1 + x_0) = 0$$

$\therefore \lambda_1 \neq 0, x_0 \neq x_1$  we get  $x_1 + x_0 = 0$  (or)  $x_1 = -x_0$

Note that if  $x_1 = 0$ , then from  $\textcircled{6}$ , we get  $x_0 = 0$ .

Since  $\lambda_0 \neq 0$  therefore  $x_1 \neq 0$ .

Sub in (5), we get  $\lambda_0 - \lambda_1 = 0$  (or)  $\lambda_0 = \lambda_1$

Sub in (5), we get  $\lambda_0 = \lambda_1 = 1$

Using (4) we get,

$$x_0^2 = \frac{1}{3} \text{ (or) } x_0 = \pm \frac{1}{\sqrt{3}} \text{ and } x_1 = \mp \frac{1}{\sqrt{3}}$$

$\therefore$  The two point Gauss Legendre method is given by,

$$\int_{-1}^1 f(x) dx = f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) \rightarrow (7)$$

The error constant is given by

$$C = \int_{-1}^1 x^4 dx - \left[\frac{1}{9} + \frac{1}{9}\right]$$

$$= \frac{2}{5} - \frac{2}{9} = \frac{8}{45}$$

The error term  $R_4$  becomes,

$$R_4 = \frac{C}{4!} f^{(4)}(\xi) = \frac{1}{135} f^{(4)}(\xi), \quad -1 < \xi < 1 \rightarrow (8)$$

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2m Three point formula  $n=2$ . The method is given by

$$\int_{-1}^1 f(x) dx = \lambda_0 f(x_0) + \lambda_1 f(x_1) + \lambda_2 f(x_2)$$

There are six unknowns in the method and it can be made exact for polynomials of degree upto 5, For  $f(x) = x^i$ ,  $i = 0(1)5$ , we get the system of equations.

$$f(x) = 1; \quad \lambda_0 + \lambda_1 + \lambda_2 = 2 \rightarrow (11)$$

$$f(x) = x; \quad \lambda_0 x_0 + \lambda_1 x_1 + \lambda_2 x_2 = 0 \rightarrow (12)$$

$$f(x) = x^2; \quad \lambda_0 x_0^2 + \lambda_1 x_1^2 + \lambda_2 x_2^2 = \frac{2}{3} \rightarrow (13)$$

$$f(x) = x^3; \quad \lambda_0 x_0^3 + \lambda_1 x_1^3 + \lambda_2 x_2^3 = 0 \rightarrow (14)$$

$$f(x) = x^4; \quad \lambda_0 x_0^4 + \lambda_1 x_1^4 + \lambda_2 x_2^4 = \frac{2}{5} \rightarrow (15)$$

$$f(x) = x^5; \quad \lambda_0 x_0^5 + \lambda_1 x_1^5 + \lambda_2 x_2^5 = 0 \rightarrow (16)$$

Eliminating  $\lambda_0$  from (13), (14) and (14), (15) we get,

$$\lambda_1 x_1 (x_1^2 - x_0^2) + \lambda_2 x_2 (x_2^2 - x_0^2) = 0$$

$$\lambda_1 x_1^3 (x_1^2 - x_0^2) + \lambda_2 x_2^3 (x_2^2 - x_0^2) = 0$$

Eliminating the first term from these two eqns, we get

$$\lambda_2 x_2^3 (x_2^2 - x_0^2) - \lambda_2 x_2 x_1^2 (x_2^2 - x_0^2) = 0$$

$$\text{or) } \lambda_2 x_2 (x_2^2 - x_0^2) (x_2^2 - x_1^2) = 0$$

$\therefore x_0, x_1, x_2$  are distinct, we get on cancelling the terms  $(x_2 - x_0)$  and  $(x_2 - x_1)$ .

$$\lambda_2 x_2 (x_2 + x_0) (x_2 + x_1) = 0$$

We have  $\lambda_2 \neq 0$  and let  $x_2 \neq 0$ . Then we have either  $x_2 = -x_0$  (or)  $x_2 = -x_1$ .

Let  $x_2 = -x_0$ . Then from (13), (14) we get

$$(\lambda_0 - \lambda_2) x_0 + \lambda_1 x_1 = 0$$

$$(\lambda_0 - \lambda_2) x_0^3 + \lambda_1 x_1^3 = 0$$

Eliminating the first term, we get,

$$\lambda_1 x_1 (x_1^2 - x_0^2) = 0$$

$\therefore \lambda_1 \neq 0, x_1 \neq x_0, x_1 \neq -x_0$  (otherwise  $x_1 = x_2$ ),

we get  $x_1 = 0$ . Hence,  $(\lambda_0 - \lambda_2) x_0 = 0$  (or)  $\lambda_0 = \lambda_2$

$$\therefore x_0 \neq 0.$$

Now (13), (15) give,

$$2\lambda_0 x_0^2 = \frac{2}{3}, \quad 2\lambda_0 x_0^4 = \frac{2}{5}$$

Dividing we get  $x_0^2 = 3/5$  (or)  $x_0 = \pm \sqrt{\frac{3}{5}}$ . Then

$x_2 = \mp \sqrt{\frac{3}{5}}$ , Now  $\lambda_0 x_0^2 = \frac{1}{3}$  gives  $\lambda_0 = \frac{5}{9}$  and  $\lambda_2 = \lambda_0 = \frac{5}{9}$

From (10), we get

$$\lambda_1 = 2 - 2\lambda_2 = \frac{8}{9}$$



∴ The 3-point Gauss Legendre method is given by,

$$\int_{-1}^1 f(x) dx = \frac{1}{9} \left[ 5f\left(-\sqrt{\frac{3}{5}}\right) + 8f(0) + 5f\left(\sqrt{\frac{3}{5}}\right) \right] \rightarrow (17)$$

If we take  $x_2 = -x_1$ . Then we get  $x_0 = 0$  and  $x_2 = \pm\sqrt{\frac{3}{5}}$  giving the same method. The nodes are symmetrically placed about  $x=0$ , The error constant is given by,

$$C = \int_{-1}^1 x^6 dx - \frac{1}{9} \left[ 5\left(-\sqrt{\frac{3}{5}}\right)^6 + 0 + 5\left(\sqrt{\frac{3}{5}}\right)^6 \right]$$

$$= \frac{2}{7} - \frac{6}{25}$$

$$C = \frac{8}{175}$$

The error in the method becomes,

$$R_b = \frac{C}{6!} f^{(6)}(\xi) = \frac{8}{(6!) \cdot 175} f^{(6)}(\xi)$$

$$= \frac{1}{15750} f^{(6)}(\xi), \quad -1 < \xi < 1$$

We shall prove that the abscissas of the above formulas are the zeros of the Legendre polynomials of the corresponding order. Hence they are called the Gauss-Legendre quadrature methods.

The nodes and the corresponding weights for the Gauss Legendre integration method for  $n = 1(1)5$  are given in Table

Table

Nodes and weights for Gauss Legendre Integration

n	nodes $x_k$	weights $\lambda_k$
1	$\pm 0.5773502692$	1.00000000
	0.0000000000	0.888888889



2	$\pm 0.7745966692$	$0.5555555556$
	$\pm 0.3399810436$	$0.6521451549$
3	$\pm 0.8611363116$	$0.3473548451$
	$0.0000000000$	$0.5688888889$
4	$\pm 0.5384693101$	$0.4786286705$
	$\pm 0.9061798459$	$0.2369268851$
	$\pm 0.2386191861$	$0.4679139346$
5	$\pm 0.6612093865$	$0.3607615730$
	$\pm 0.9324695142$	$0.1713244924$

b. Evaluate the integral  $I = \int_0^1 \frac{dx}{1+x}$ . Using Gauss-Legendre 3 point formula.

Soln:

First we transform the interval  $[0, 1]$  to the interval  $[-1, 1]$ . Let  $t = ax + b$  we have,

$$-1 = b, \quad 1 = a + b$$

(or)  $a = 2, \quad b = -1$  and  $t = 2x - 1$

$$I = \int_0^1 \frac{dx}{1+x} = \int_{-1}^1 \frac{dt}{1+t}$$

Using Gauss-Legendre 3 point rule corresponding to  $n = 2$ , we get

$$I = \frac{1}{9} \left[ 8 \left( \frac{1}{0+t_3} \right) + 5 \left( \frac{1}{3+\sqrt{3/5}} \right) + 5 \left( \frac{1}{3-\sqrt{3/5}} \right) \right]$$

$$= \frac{131}{189} = 0.693122$$

The exact soln is

$$I = I_{n2} = 0.693147.$$

17. Evaluate the integral  $I = \int_1^2 \frac{2x}{1+x^4} dx$ , Using the Gauss-Legendre 1-point, 2-point and 3-point Quadrature rules. Compare with the exact solution  $I = \tan^{-1}(4) - (\pi/4) \rightarrow \frac{\pi}{4}$

Soln:

To use the Gauss-Legendre rules the interval  $[1, 2]$  is to be reduced to  $[-1, 1]$ . Writing  $x = at + b$ , we get

$$1 = -a + b, \quad 2 = a + b$$

whose soln is  $b = 3/2, a = 1/2$ . Therefore,

$$x = \frac{(t+3)}{2}, \quad dx = \frac{dt}{2} \text{ and}$$

$$I = \int_{-1}^1 \frac{3(t+3)}{[16+(t+3)^4]} dt$$

$$= \int_{-1}^1 f(t) dt$$

Using the 1-point, we get

$$I = 2f(0) = 2 \left[ \frac{24}{16+81} \right] = 0.4948$$

Using the 3-point rule, we get,

$$I = \frac{1}{9} \left[ 5f\left(-\frac{\sqrt{3}}{5}\right) + 8f(0) + 5f\left(\frac{\sqrt{3}}{5}\right) \right]$$

$$= \frac{1}{9} \left[ 5(0.4393) + 8(0.2474) + 5(0.1379) \right]$$

$$= 0.5406$$

The exact soln is

$$I = 0.5404$$

### Lobatto Integration Methods:-

10m

In this case,  $w(x) = 1$  and the end points  $-1$  and  $1$  are always taken as nodes. There making  $n-1$  nodes are to be determined.

The integration formula can be written as,

$$\int_{-1}^1 f(x) dx = \lambda_0 f(-1) + \lambda_n f(1) + \sum_{k=1}^{n-1} \lambda_k f(x_k) \rightarrow \textcircled{1}$$

$\therefore$  There are  $n$  unknowns ( $(n-1)$  nodes and  $n$  weights), this method can be made exact for polynomials of degree upto  $2n-1$ .

For  $n=2$ , we have the method as,

$$\int_{-1}^1 f(x) dx = \lambda_0 f(-1) + \lambda_1 f(x_1) + \lambda_2 f(1) \rightarrow \textcircled{2}$$

Making the formula exact for  $f(x)=1, x, x^2+x^3$  we get,

$$f(x)=1; \lambda_0 + \lambda_1 + \lambda_2 = 2 \rightarrow \textcircled{3}$$

$$f(x)=x; -\lambda_0 + \lambda_1 x_1 + \lambda_2 = 0 \rightarrow \textcircled{4}$$

$$f(x)=x^2; \lambda_0 + \lambda_1 x_1^2 + \lambda_2 = \frac{2}{3} \rightarrow \textcircled{5}$$

$$f(x)=x^3; -\lambda_0 + \lambda_1 x_1^3 + \lambda_2 = 0 \rightarrow \textcircled{6}$$

$\therefore x_1 \neq \pm 1$  we get  $x_1=0$  substitute  $x_1=0$  in  $\textcircled{4}$  +  $\textcircled{5}$  and solving, we get  $\lambda_0 = \lambda_2 = \frac{1}{3}$  from  $\textcircled{5}$  we get

$$\lambda_1 = \frac{4}{3}$$

$$\int_{-1}^1 f(x) dx = \frac{1}{3} [f(-1) + 4f(0) + f(1)] \rightarrow \textcircled{7}$$

The error constant is given by

$$C = \int_{-1}^1 x^4 dx - \frac{1}{3} (1+0+1)$$

$$= \frac{2}{5} - \frac{2}{3} = -\frac{4}{15}$$

$\therefore$  The error in the method is,

$$R_4 = \frac{C}{4!} f^{(4)}(\xi) = \frac{1}{90} f^{(4)}(\xi) \rightarrow \textcircled{8}$$

It can be noted that (7) is the Simpson's rule, with step length  $h=1$ . For  $n=3$  we have the method as

$$\int_{-1}^1 f(x) dx = \lambda_0 f(-1) + \lambda_1 f(x_1) + \lambda_2 f(x_2) + \lambda_3 f(1) \rightarrow (9)$$

The method has 6 unknowns and it can be made exact for polynomials of degree upto 5 for  $f(x) = x^i$ ,  $i = 0, 1, 2, 3, 4, 5$  we get the system of eqns,

$$f(x) = 1; \quad \lambda_0 + \lambda_1 + \lambda_2 + \lambda_3 = 2 \rightarrow (10)$$

$$f(x) = x; \quad -\lambda_0 + \lambda_1 x_1 + \lambda_2 x_2 + \lambda_3 = 0 \rightarrow (11)$$

$$f(x) = x^2; \quad \lambda_0 + \lambda_1 x_1^2 + \lambda_2 x_2^2 + \lambda_3 = \frac{2}{3} \rightarrow (12)$$

$$f(x) = x^3; \quad -\lambda_0 + \lambda_1 x_1^3 + \lambda_2 x_2^3 + \lambda_3 = 0 \rightarrow (13)$$

$$f(x) = x^4; \quad \lambda_0 + \lambda_1 x_1^4 + \lambda_2 x_2^4 + \lambda_3 = \frac{0}{5} \rightarrow (14)$$

$$f(x) = x^5; \quad -\lambda_0 + \lambda_1 x_1^5 + \lambda_2 x_2^5 + \lambda_3 = 0 \rightarrow (15)$$

Subtract (11) from (13) we obtain,

$$\lambda_1 x_1^3 (x_1^2 - 1) + \lambda_2 x_2^3 (x_2^2 - 1) = 0 \rightarrow (16)$$

Taking the second terms of (16), (17) to the RHS and dividing the two eqns, we get  $x_1^2 = x_2^2$

$$\therefore x_1 \neq x_2, \text{ we get } x_2 = -x_1$$

sub in (16) we get

$$(\lambda_1 - \lambda_2) x_1 (x_1^2 - 1) = 0$$

$$\therefore x_1 \neq \pm 1 \text{ and } x_1 \neq 0 \text{ (otherwise } x_0 = 0, x_1 = 0)$$

we get  $\lambda_1 = \lambda_2$

Using (11), we get

$$-\lambda_0 + \lambda_3 = 0 \text{ (or) } \lambda_0 = \lambda_3$$

Using (10), we get

$$\lambda_0 + \lambda_1 = 1 \rightarrow (18)$$

Substituting  $x_1 = -1$  and  $x_2 = 1$  in (10), we get

$$\lambda_1 (1-x_1^2) + \lambda_2 (1-x_2^2) = \frac{4}{3}$$

(or)  $\lambda_1 (1-x_1^2) = \frac{2}{3} \rightarrow (17)$

Subtract (17) from (16) we get,

$$\lambda_1 x_1^2 (1-x_1^2) + \lambda_2 x_2^2 (1-x_2^2) = \frac{2}{3} - \frac{2}{3} = \frac{4}{15}$$

(or)  $\lambda_1 x_1^2 (1-x_1^2) = \frac{2}{15}$

Dividing the last two eqns, we get  $x_1^2 = 1/5$ ,  
Hence we have,

$$x_1 = \frac{-1}{\sqrt{5}} \text{ and } x_2 = -x_1 = \frac{1}{\sqrt{5}}$$

From (19), we get

$$\lambda_1 = \left(\frac{2}{3}\right) \left(\frac{5}{4}\right) = \frac{5}{6}$$

and  $\lambda_2 = \lambda_1 = \frac{5}{6}$

from (18) we get

$$\lambda_0 - 1/6 = \lambda_3$$

$\therefore$  The method is given by,

$$\int_{-1}^1 f(x) dx = \frac{1}{6} \left[ f(-1) + 5f\left(-\frac{\sqrt{5}}{5}\right) + 5f\left(\frac{\sqrt{5}}{5}\right) + f(1) \right] \rightarrow (20)$$

The error constant is given by,

$$C = \int_{-1}^1 x^6 dx - \frac{1}{6} \left[ 1 + 5\left(\frac{1}{125}\right) + 5\left(\frac{1}{125}\right) + 1 \right]$$

$$= \frac{2}{7} - \frac{26}{75} = \frac{-32}{525}$$

The error in the method becomes,

$$R_b = \frac{C}{6!} f^{(6)}(\xi) = \frac{-32}{525(6!)} f^{(6)}(\xi), \quad -1 < \xi < 1 \rightarrow (21)$$

The nodes and corresponding weights the Lobatto integration method for  $h=2(1)5$  are given in table.



# Nodes and weights for Lobatto integration method.

n	Nodes $x_k$	weight $\lambda_k$
2	$\pm 1.000000000$ $0.000000000$	$0.333333333$ $1.333333333$
3	$\pm 1.000000000$ $\pm 0.44721360$	$0.144444444$ $0.833333333$
4	$\pm 0.65465367$ $0.000000000$	$0.666666667$ $0.711111111$
5	$\pm 1.000000000$ $\pm 0.76505532$ $\pm 0.28523152$	$0.666666667$ $0.37847496$ $0.55485837$