Chapter 8 Numerical Differentiation & Integration

8.1 Introduction

Differentiation and integration are basic mathematical operations with a wide range of applications in various fields of science and engineering. Simple continuous algebraic or transcendental functions can be easily differentiated or integrated directly. However at times there are complicated continuous functions which are tedious to differentiate or integrate directly or in the case of experimental data, where tabulated values of variables are given in discrete form, direct methods of calculus are not applicable.

In this chapter, we develop ways to approximate the derivatives of function y = f(x), when only data points are given and also to integrate definite integrals by splitting the area under the curve in specified ways.

8.2 Numerical Differentiation

Numerical differentiation is the process of computing the value of the derivative of an explicitly unknown function, with given discrete set of points (x_i, y_i) , i = 0,1,2,3,...,n. To differentiate a function numerically, we first determine an interpolating polynomial and then compute the approximate derivative at the given point.

If x_i 's are equispaced

- i. Newton's forward interpolation formula is used to find the derivative near the beginning of the table.
- ii. Newton's backward interpolation formula is used to compute the derivation near the end of the table.
- iii. Stirling's formula is used to estimate the derivative near the centre of the table.

If x_i 's are not equispaced, we may find f(x) using Newton's divided difference method or Lagrange's interpolation formula and then differentiate it as many times as required.

8.2.1 Derivatives Using Newton's Forward Interpolation Formula

Newton's forward interpolation formula for the function y = f(x) is given by

$$y \equiv y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \frac{p(p-1)(p-2)(p-3)}{4!}\Delta^4 y_0 + \cdots,$$
$$p = \frac{x - x_0}{h} \qquad \dots \square$$

Differentiating ① with respect to p

$$\frac{dy}{dp} = \Delta y_0 + \frac{2p-1}{2!} \Delta^2 y_0 + \frac{3p^2 - 6p + 2}{3!} \Delta^3 y_0 + \frac{4p^3 - 18p^2 + 22p - 6}{4!} \Delta^4 y_0 + \cdots \qquad \dots @$$

Also
$$\frac{dp}{dx} = \frac{1}{h}$$
 ... (3)

Again
$$\frac{dy}{dx} = \frac{dy}{dp}\frac{dp}{dx}$$
 ... (4)

Using (2) and (3) in (4), we get

$$\frac{dy}{dx} = \frac{1}{h} \left[\Delta y_0 + \frac{2p-1}{2!} \Delta^2 y_0 + \frac{3p^2 - 6p + 2}{3!} \Delta^3 y_0 + \frac{4p^3 - 18p^2 + 22p - 6}{4!} \Delta^4 y_0 + \cdots \right]$$

Now at $x = x_0, p = 0$

$$\therefore \frac{dy}{dx}\Big|_{x = x_0} = \frac{1}{h} \Big[\Delta y_0 - \frac{\Delta^2 y_0}{2} + \frac{\Delta^3 y_0}{3} - \frac{\Delta^4 y_0}{4} + \cdots \Big]$$
Now $\frac{d^2 y}{dx^2} = \frac{1}{dx} \left(\frac{dy}{dx}\right) = \frac{d}{dp} \left(\frac{dy}{dx}\right) \cdot \frac{dp}{dx}$
Or $\frac{d^2 y}{dx^2} = \frac{1}{h^2} \frac{d}{dp} \Big[\Delta y_0 + \frac{2p-1}{2!} \Delta^2 y_0 + \frac{3p^2 - 6p + 2}{3!} \Delta^3 y_0 + \frac{4p^3 - 18p^2 + 22p - 6}{4!} \Delta^4 y_0 + \cdots \Big]$

$$\therefore \frac{d^2 y}{dx^2} = \frac{1}{h^2} \Big[\Delta^2 y_0 + \frac{6p - 6}{6} \Delta^3 y_0 + \frac{12p^2 - 36p + 22}{24} \Delta^4 y_0 + \cdots \Big]$$

$$\frac{d^2 y}{dx^2} \Big]_{x = x_0} = \frac{1}{h^2} \Big[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12} \Delta^4 y_0 - \frac{5}{6} \Delta^5 y_0 + \cdots \Big]$$

8.2.2 Derivatives Using Newton's Backward Interpolation Formula

Newton's backward interpolation formula for the function y = f(x) is given by

$$y \equiv y_n + p \nabla y_n + \frac{p(p+1)}{2!} \nabla^2 y_n + \frac{p(p+1)(p+2)}{3!} \nabla^3 y_n + \frac{p(p+1)(p+2)(p+3)}{4!} \nabla^4 y_n + \cdots,$$

$$p = \frac{x - x_n}{h} \qquad \dots \text{(1)}$$

Differentiating (1) with respect to p

$$\frac{dy}{dp} = \nabla y_n + \frac{2p+1}{2!} \nabla^2 y_n + \frac{3p^2 + 6p + 2}{3!} \nabla^3 y_n + \frac{4p^3 + 18p^2 + 22p + 6}{4!} \nabla^4 y_n + \cdots \qquad \dots$$

Also
$$\frac{dp}{dx} = \frac{1}{h}$$
 ... (3)

Again
$$\frac{dy}{dx} = \frac{dy}{dp}\frac{dp}{dx}$$
 ... (4)

Using (2) and (3) in (4), we get

$$\frac{dy}{dx} = \frac{1}{h} \left[\nabla y_n + \frac{2p+1}{2!} \nabla^2 y_n + \frac{3p^2 + 6p + 2}{3!} \nabla^3 y_n + \frac{4p^3 + 18p^2 + 22p + 6}{4!} \nabla^4 y_n + \cdots \right]$$

Now at $x = x_n, p = 0$

$$\therefore \frac{dy}{dx}\Big]_{x=x_n} = \frac{1}{h} \Big[\nabla y_n + \frac{\nabla^2 y_n}{2} + \frac{\nabla^3 y_n}{3} + \frac{\nabla^4 y_n}{4} + \cdots \Big]$$

Similarly $\frac{d^2 y}{dx^2}\Big]_{x=x_n} = \frac{1}{h^2} \Big[\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12} \nabla^4 y_n + \frac{5}{6} \nabla^5 y_n + \cdots \Big]$

8.2.3 Derivatives Using Stirling's Interpolation Formula

Stirling's central difference interpolation formula (taking x_0 as the middle value of the table) is given by:

$$y \equiv y_0 + p\left(\frac{\Delta y_0 + \Delta y_{-1}}{2}\right) + \frac{p^2}{2!}\Delta^2 y_{-1} + \frac{p(p^2 - 1)}{3!}\left(\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2}\right) + \frac{p^2(p^2 - 1)}{4!}\Delta^4 y_{-2} + \cdots \qquad p = \frac{x - x_0}{h} \qquad \dots$$

Differentiating (1) with respect to p

$$\frac{dy}{dp} = \left(\frac{\Delta y_0 + \Delta y_{-1}}{2}\right) + p\Delta^2 y_{-1} + \frac{3p^2 - 1}{3!} \left(\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2}\right) + \frac{4p^3 - 2p}{4!} \Delta^4 y_{-2} + \cdots \quad \dots \textcircled{2}$$

Also
$$\frac{dy}{dx} = \frac{dy}{h}$$
 ... (3)
Again $\frac{dy}{dx} = \frac{dy}{dx} \frac{dp}{dx}$... (4)

$$dx = dp dx$$

Using (2) and (3) in (4), we get

$$\frac{dy}{dx} = \frac{1}{h} \left[\left(\frac{\Delta y_0 + \Delta y_{-1}}{2} \right) + p \Delta^2 y_{-1} + \frac{3p^2 - 1}{3!} \left(\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2} \right) + \frac{4p^3 - 2p}{4!} \Delta^4 y_{-2} + \cdots \right]$$

Now at $x = x_0, p = 0$

$$\therefore \frac{dy}{dx}\Big|_{x = x_0} = \frac{1}{h} \left[\left(\frac{\Delta y_0 + \Delta y_{-1}}{2} \right) - \frac{1}{6} \left(\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2} \right) + \frac{1}{30} \left(\frac{\Delta^5 y_{-2} + \Delta^5 y_{-3}}{2} \right) - \cdots \right]$$

Similarly $\left. \frac{d^2 y}{dx^2} \right|_{x = x_0} = \frac{1}{h^2} \left[\Delta^2 y_{-1} - \frac{1}{12} \Delta^4 y_{-2} + \frac{1}{90} \Delta^6 y_{-3} - \cdots \right]$

8.2.4 Derivatives of Polynomial with Unequispaced x_i 's

In case where x_i 's are not equispaced in a given data, the polynomial y = f(x) may be found using Newton's divided difference method or Lagrange's interpolation formula and then direct differentiation may be applied.

Remark:

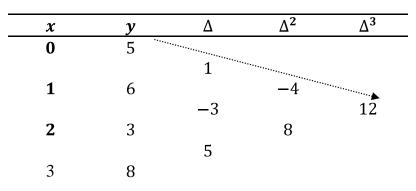
- In case derivative has to be found at a point, whose value needs to be interpolated, then first apply applicable interpolation technique and then differentiate the function.
- > In all the cases irrespective of data points being equispaced or not, the polynomial y = f(x) may be found using the applicable interpolation formulae and then direct differentiation can be done using usual calculus techniques.

Example 1 Given a cubic polynomial with following data points

$$\begin{array}{ccccc} x & 0 & 1 & 2 & 3\\ f(x) & 5 & 6 & 3 & 8 \end{array}$$

Find $\frac{dy}{dx}$ and $\frac{d^2y}{dx^2}$ at $x = 0$

Solution: Derivative has to be evaluated near the starting of the table, thereby constructing forward difference table for the function y = f(x)



To find the derivative at x = 0, taking $x_0 = 0$ and applying the relation: $\frac{dy}{dx}\Big|_{x = x_0} = \frac{1}{h} \Big[\Delta y_0 - \frac{\Delta^2 y_0}{2} + \frac{\Delta^3 y_0}{3} - \frac{\Delta^4 y_0}{4} + \cdots \Big] \qquad \dots \square$ From table h = 1, $\Delta y_0 = 1$, $\Delta^2 y_0 = -4$, $\Delta^3 y_0 = 12$, $\Delta^4 y_0 = 0$ Substituting these values in (1), we get

$$\frac{dy}{dx}\Big|_{x=0} = \frac{1}{1} \left[1 - \frac{(-4)}{2} + \frac{12}{3} + 0 \right] = 7$$

Also $\frac{d^2y}{dx^2}\Big|_{x=x_0} = \frac{1}{h^2} \left[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12} \Delta^4 y_0 - \cdots \right]$
 $\therefore \frac{d^2y}{dx^2}\Big|_{x=0} = \frac{1}{1^2} \left[-4 - 12 + 0 \right] = -16$

Aliter

Newton's forward interpolation formula given by:

$$y = y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \dots, \ p = \frac{x-x_0}{h} \quad \dots \text{(1)}$$
$$x_0 = 0, \ y_0 = 5, \ h = 1 \therefore p = \frac{x-0}{1} = x$$
Also from table $\Delta y_0 = 1, \ \Delta^2 y_0 = -4, \ \Delta^3 y_0 = 12$

Substituting these values in (1), we get

$$y = 5 + x(1) + \frac{x(x-1)}{2}(-4) + \frac{x(x-1)(x-2)}{6}(12)$$

$$\Rightarrow y = 2x^3 - 8x^2 + 7x + 5$$

$$\therefore \frac{dy}{dx} = 6x^2 - 16x + 7$$

$$\Rightarrow \frac{dy}{dx}\Big|_{x=0} = 7$$
Also $\frac{d^2y}{dx^2} = 12x - 16$

$$\therefore \frac{d^2y}{dx^2}\Big|_{x=0} = -16$$

Example 2 Given a polynomial with following data points:

Solution: Derivatives has to be evaluated near the starting as well as towards the end of the table, thereby constructing difference table for the function y = f(x)

x	y = f(x)	1 st diff	2 nd diff	3 rd diff	4 th diff	5 th diff	6 th diff
1.0	7.989						
		0.414					
<u>1.1</u>	8.403		-0.036				
		0.378	·····	0.006			
1.2	8.781		-0.030	••••••	-0.002		
		0.348		0.004	•••••	0.001	
1.3	9.129		-0.026		-0.001		0.002
		0.322		0.003		0.003	
1.4	9.451		-0.023		0.002		
		0.299		0.005			
<u>1.5</u>	9.750		-0.018				
		0.281					
1.6	10.031						

To find the derivative at x = 1.1, taking $x_0 = 1.1$ and applying the relation: $\frac{dy}{dx}\Big|_{x=x_0} = \frac{1}{h} \Big[\Delta y_0 - \frac{\Delta^2 y_0}{2} + \frac{\Delta^3 y_0}{3} - \frac{\Delta^4 y_0}{4} + \frac{\Delta^5 y_0}{5} - \cdots \Big] \qquad \dots \square$ From table h = 0.1, $\Delta y_0 = 0.378$, $\Delta^2 y_0 = -0.03$, $\Delta^3 y_0 = 0.004$, $\Delta^4 y_0 = -0.001$, $\Delta^5 y_0 = 0.003$ Substituting these values in \square , we get $dy\Big|_{x=x_0} = 1 \begin{bmatrix} -0.03 \\ -0.004 \end{bmatrix} = 0.004$

$$\frac{dy}{dx}\Big|_{x=1.1} = \frac{1}{0.1} \Big[0.378 - \frac{(-0.03)}{2} + \frac{0.004}{3} - \frac{(-0.031)}{4} + \frac{0.003}{5} \Big] = 3.952$$

Also $\frac{d^2y}{dx^2}\Big|_{x=x_0} = \frac{1}{h^2} \Big[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12} \Delta^4 y_0 - \frac{5}{6} \Delta^5 y_0 + \cdots \Big]$
 $\therefore \frac{d^2y}{dx^2}\Big|_{x=0} = \frac{1}{(0.1)^2} \Big[-0.03 - 0.004 + \frac{11}{12} (-0.001) - \frac{5}{6} (0.003) \Big] = -3.74$

To find the derivative at x = 1.5, taking $x_n = 1.5$ and applying the relation:

$$\frac{dy}{dx}\Big|_{x=x_n} = \frac{1}{h} \Big[\nabla y_n + \frac{\nabla^2 y_n}{2} + \frac{\nabla^3 y_n}{3} + \frac{\nabla^4 y_n}{4} + \frac{\nabla^4 y_n}{4} + \cdots \Big] \qquad \dots @$$

From table $h = 0.1, \ \nabla y_n = 0.299, \ \nabla^2 y_n = -0.023, \ \nabla^3 y_n = 0.003, \ \nabla^4 y_n = -0.001, \ \nabla^5 y_n = 0.001$
Substituting these values in @, we get
$$\frac{dy}{dx}\Big|_{x=1.5} = \frac{1}{0.1} \Big[0.299 + \frac{(-0.023)}{2} + \frac{0.003}{3} + \frac{(-0.001)}{4} + \frac{0.001}{5} \Big] = 2.8845$$

Also
$$\frac{d^2 y}{dx^2}\Big|_{x=x_n} = \frac{1}{h^2} \Big[\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12} \nabla^4 y_n + \frac{5}{6} \nabla^5 y_n + \cdots \Big] \\ \therefore \frac{d^2 y}{dx^2}\Big|_{x=n} = \frac{1}{(0.1)^2} \Big[-0.023 + 0.003 + \frac{11}{12} (-0.001) + \frac{5}{6} (0.001) \Big] = -2.0083$$

Example3 Following table gives the census population of a state for the years 1961 to 2001.

Year	1961	1971	1981	1991	2001
Population (Million)	19.96	36.65	58.81	77.21	94.61

Find the rate of growth of the population in the year 2001

Solution: Derivative has to be evaluated near the end of the table, thereby constructing backward difference table for the function y = f(x)

Year x	Population $f(x)$	∇	∇^2	∇^3	∇^4
1961	19.96				
		16.69			
1971	36.65		5.47		
		22.16		-9.23	
1981	58.81		-3.76		11.99
		18.40		2.76	
1991	77.21		-1.00		
		17.40			
2001	94.61				

To find rate of growth (derivative) in the year 2001, taking $x_n = 2001$ and applying the relation:

 $\frac{dy}{dx}\Big]_{x=x_n} = \frac{1}{h} \Big[\nabla y_n + \frac{\nabla^2 y_n}{2} + \frac{\nabla^3 y_n}{3} + \frac{\nabla^4 y_n}{4} + \cdots \Big] \qquad \dots \square$ From table h = 10, $\nabla y_n = 17.40$, $\nabla^2 y_n = -1$, $\nabla^3 y_n = 2.76$, $\nabla^4 y_n = 11.99$ Substituting these values in (1), we get

$$\frac{dy}{dx}\Big|_{x=2011} = \frac{1}{10} \Big[17.40 + \frac{(-1)}{2} + \frac{2.76}{3} + \frac{(11.99)}{4} \Big] = 2.08175$$

Example4 A slider in a machine moves along a fixed straight rod. Its distance x cm along the rod is given below for various values of the time. Find the velocity and acceleration of the slider when t = 0.3 seconds.

$$t(seconds) = 0 \quad 0.1 \quad 0.2 \quad 0.3 \quad 0.4 \quad 0.5 \quad 0.6$$

 $x(cm) \quad 30.13 \quad 31.62 \quad 32.87 \quad 33.64 \quad 33.95 \quad 33.81 \quad 33.24$

Solution: Derivatives has to be evaluated towards the centre of the table, thereby constructing central difference table for the function x = f(t). Also $\Delta^n x_0$, n = 1, 2, 3, 3, 4, 5, 6 lie along the dotted line as shown.

t	x = f(t)	1 st diff	2 nd diff	3 rd diff	4 th diff	5 th diff	6 th diff
0	30.13						
		1.49					
0.1	31.62		-0.24				
		1.25		-0.24			
0.2	32.87		-0.48		0.26		
		0.77		0.02		-0.27	
<u>0.3</u>	33.64		-0.46		-0.01		0.29
		0.31	•••••	0.01		0.02	
0.4	33.95		-0.45	·····	0.01		
		-0.14		0.02			
0.5	33.81		-0.43				
		-0.57					
0.6	33.24						

To find the velocity (derivative) at t = 0.3, taking $t_0 = 0.3$ and applying the relation:

$$\frac{dx}{dt}\Big|_{t=t_0} = \frac{1}{h} \left[\left(\frac{\Delta x_0 + \Delta x_{-1}}{2} \right) - \frac{1}{6} \left(\frac{\Delta^3 x_{-1} + \Delta^3 x_{-2}}{2} \right) + \frac{1}{30} \left(\frac{\Delta^5 x_{-2} + \Delta^5 x_{-3}}{2} \right) - \cdots \right] \quad \dots \text{(1)}$$

From table h = 0.1, $\Delta x_0 = 0.31$, $\Delta x_{-1} = 0.77$, $\Delta^3 x_{-1} = 0.01$, $\Delta^3 x_{-2} = 0.02$, $\Delta^5 x_{-2} = 0.02$., $\Delta^5 x_{-3} = -0.27$ All the positions have been shown, enclosed in boxes.

Substituting these values in (1), we get

$$\frac{dx}{dt}\Big|_{t=0.3} = \frac{1}{0.1} \left[\left(\frac{0.31 + 0.77}{2} \right) - \frac{1}{6} \left(\frac{0.01 + 0.02}{2} \right) + \frac{1}{30} \left(\frac{0.02 - 0.27}{2} \right) \right] = 5.33 \text{ cm/seconds}$$

To find the acceleration (second derivative) at t = 0.3 and applying the relation

$$\frac{d^2x}{dt^2}\Big]_{t=t_0} = \frac{1}{h^2} \Big[\Delta^2 x_{-1} - \frac{1}{12} \Delta^4 x_{-2} + \frac{1}{90} \Delta^6 x_{-3} - \cdots \Big] \qquad \dots 2$$

Also from table, $\Delta^2 x_{-1} = -0.46$, $\Delta^4 x_{-2} = -0.01$, $\Delta^6 x_{-3} = 0.29$

Substituting these values in (2), we get

$$\frac{d^2x}{dt^2}\Big]_{t=0.3} = \frac{1}{(0.1)^2} \Big[(-0.46) - \frac{1}{12} (-0.01) + \frac{1}{90} (0.29) \Big] = -45.60 \text{ cm/seconds}^2$$

Example5 The following data gives corresponding values of pressure 'P' and specific volume 'V' of a super heated expandable system

Find the rate of change of volume with respect to pressure, when P = 105 units.

Solution: Values of *P* are not equispaced, thereby constructing divided difference table for the function V = f(P)

Р	V = f(P)	1 st diff	2 nd diff	3 rd diff	4 th diff
105	2	-0.032			
		-0.032	•••••••••••••••••••••••••		
42.7	4		0.001	••••••	
		-0.115		-0.00005	•••••••••••••••••••••••••••••••••••••••
25.3	6		0.005		0.000007
		-0.233		-0.0007	
16.7	8		0.025		
		-0.541			
13	10				

Newton's divided difference formula is given by

$$\begin{split} V &= f(P) \equiv f(P_0) + (P - P_0)f(P_0, P_1) + (P - P_o)(P - P_1)f(P_0, P_1, P_2) + \\ (P - P_0)(P - P_1)(P - P_2)f(P_0, P_1, P_2, P_3) + \cdots & \dots \end{split}$$

 Here $P_0 = 105$, $P_1 = 42.7$, $P_2 = 25.3$, $P_3 = 16.7$ $f(P_0) = 2$, $f(P_0, P_1) = -0.032$, $f(P_0, P_1, P_2) = 0.001$, $f(P_0, P_1, P_2, P_3) = -0.00005$, $f(P_0, P_1, P_2, P_3, P_4) = 0000007$
 Substituting these values in ①, we get $V = f(P) \equiv 2 + (P - 105)(-0.032) + (P - 105)(P - 42.7)(0.001) + (P - 105)(P - 42.7)(P - 25.3)(-0.00005) + (P - 105)(P - 42.7)(P - 25.3)(P - 16.7)(0.00007) \\ \therefore \frac{dV}{dP} = -0.032 + (2P - 147.7)(.001) + (3P^2 - 505.4P + 1992)(-.000005) + [(3P^2 - 505.4P + 1992)(P - 16.7) + (P - 105)(P - 42.7)(P - 25.3(1)](0.00007) \\ \frac{dV}{dP}\Big|_{P=105} = -0.032 + 0.0623 + 0.9 - 11.1258 = -10.1955$
 It is evident that volume decreases with increase in pressure.

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

Example6 Find y'(1) for the following the following data points of a polynomial y = f(x).

Solution: To find y'(1) or $\frac{dy}{dx}\Big|_{x=1}$, constructing forward difference table for the function y = f(x).

x	y = f(x)	Δ	Δ^2	Δ^3	Δ^4
0	4		••.		
		4	•••••		
2	8		3	•••••	
		7		-18	•••••••
4	15		-15		40
		-8		22	
6	7		7		
		-1			
8	6				

Newton's forward interpolation formula given by:

$$y \equiv y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \frac{p(p-1)(p-2)(p-3)}{4!}\Delta^4 y_0 + \cdots$$

$$p = \frac{x - x_0}{h} \qquad \dots \text{(1)}$$

$$\Rightarrow \frac{dy}{dp} = \Delta y_0 + \frac{2p-1}{2!}\Delta^2 y_0 + \frac{3p^2 - 6p + 2}{3!}\Delta^3 y_0 + \frac{4p^3 - 18p^2 + 22p - 6}{4!}\Delta^4 y_0 + \cdots \text{(2)}$$
Also $\frac{dp}{dx} = \frac{1}{h} \qquad \dots \text{(3)}$

Again
$$\frac{dy}{dx} = \frac{dy}{dp}\frac{dp}{dx}$$
 ... (4)

Using (2) and (3) in (4), we get

$$\frac{dy}{dx} = \frac{1}{h} \left[\Delta y_0 + \frac{2p-1}{2!} \Delta^2 y_0 + \frac{3p^2 - 6p + 2}{3!} \Delta^3 y_0 + \frac{4p^3 - 18p^2 + 22p - 6}{4!} \Delta^4 y_0 + \cdots \right] \quad \dots \quad (5)$$

Now for x = 1, $x_0 = 0$, h = 2, $\therefore p = \frac{1-0}{2} = 0.5$ Also from table $\Delta y_0 = 4$, $\Delta^2 y_0 = 3$, $\Delta^3 y_0 = -18$, $\Delta^4 y_0 = 40$ Substituting these values in (5), we get

$$\frac{dy}{dx}\Big|_{x=1} = \frac{1}{2} \Big[4 + \frac{1-1}{2} (3) + \frac{3(0.5)^2 - 6(0.5) + 2}{6} (-18) + \frac{4(0.5)^3 - 18(0.5)^2 + 22(0.5) - 6}{24} (40) \Big]$$

$$\Rightarrow y'(1) = \frac{dy}{dx}\Big|_{x=1} = \frac{1}{2} \Big[4 + 0 + 0.75 + 1.667 \Big] = \frac{1}{2} \Big[6.417 \Big] = 3.2085$$

Note: Here formula for computing derivatives can not be applied directly as $p \neq 0$ at x = 1 *i.e.* point at which derivative has to be computed does not exist in the table and has to be interpolated first.

8.2.5 Maxima and Minima of a Tabulated Function:

Newton's forward interpolation formula for the function y = f(x) is given by

$$y \equiv y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \frac{p(p-1)(p-2)(p-3)}{4!}\Delta^4 y_0 + \cdots,$$
$$p = \frac{x - x_0}{h} \qquad \dots \text{(1)}$$

Differentiating (1) with respect to p

$$\frac{dy}{dp} = \Delta y_0 + \frac{2p-1}{2!} \Delta^2 y_0 + \frac{3p^2 - 6p + 2}{3!} \Delta^3 y_0 + \frac{4p^3 - 18p^2 + 22p - 6}{4!} \Delta^4 y_0 + \cdots \qquad \dots \textcircled{2}$$

For finding maxima/minima of a function y = f(x), $\frac{dy}{dx} = \frac{dy}{dp} \frac{dp}{dx} = 0$ $\frac{dp}{dx} = \frac{1}{h} \neq 0$, $\therefore \frac{dy}{dp} = 0$... (3)

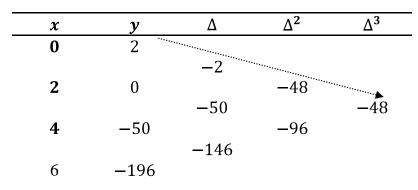
Neglecting 4^{th} and higher order differences in equation (2) and substituting in (3),

we get a quadratic equation of the form $A + Bp + Cp^2 = 0$, where A, B, C are constants. Solving for p and substituting in $x = x_0 + ph$, we get points of maxima/minima for the function y = f(x).

Newton's forward method is apt for finding extreme values of a tabulated data, wherever their location may be, by index p assuming values |p| ≥ 1, if the extreme value is not in vicinity of the point (x₀, y₀). Yet we may also use Newton's backward or Stirling's central differences formulae to locate extreme values, if desired.

Example 7 From the following data, find maximum and minimum values of *y*.

Solution: Constructing forward difference table for the function y = f(x)



Newton's forward interpolation formula for the function y = f(x) is given by $y \equiv y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \cdots, \quad p = \frac{x-x_0}{h} \qquad \dots$ (1) Taking $x_0 = 0$, $y_0 = 2$, $\Delta y_0 = -2$, $\Delta^2 y_0 = -48$, $\Delta^3 y_0 = -48$ Substituting these values in (1), we get $y \equiv 2 + p(-2) + \frac{p(p-1)}{2}(-48) + \frac{p(p-1)(p-2)}{6}(-48)$

$$\Rightarrow y \equiv 2 - 2p - 24(p^{2} - p) - 8(p^{3} - 3p^{2} + 2p)$$

$$\Rightarrow y \equiv -8p^{3} + 6p + 2 \qquad \dots 2$$

Differentiating 2 with respect to p, we get

$$\frac{dy}{dp} = -24p^{2} + 6$$

For y to be maximum, $\frac{dy}{dp} = 0$

$$\Rightarrow -24p^{2} + 6 = 0$$

$$\Rightarrow p = 0.5, -0.5$$

Substituting in 2, maximum and minimum values of y are 4 and 0 respectively. **Example 8** From the following table, find x for which y is maximum.

Also find maximum value of *y*.

Solution: Constructing forward difference table for the function y = f(x), upto third differences

x	y = f(x)	Δ	Δ^2	Δ^3
3	0.205	•••••		
		0.035	••••••	
4	0.240		-0.016	•••••••
		0.019		0
5	0.259		-0.016	
		0.003		0.001
6	0.262		-0.015	
		-0.012		0.001
7	0.250		-0.014	
		-0.026		
8	0 2 2 4			

Newton's forward interpolation formula for the function y = f(x) is given by $y \equiv y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \cdots, p = \frac{x-x_0}{h} \qquad ... 1$ Taking $x_0 = 3$, $y_0 = 0.205$, $\Delta y_0 = 0.035$, $\Delta^2 y_0 = -0.016$, $\Delta^3 y_0 = 0$ Substituting these values in 1, we get $y \equiv (0.205) + p(0.035) + \frac{p(p-1)}{2}(-0.016) + 0 \qquad ... 2$ Differentiating with respect to p, we get $\frac{dy}{dp} = 0.035 + \frac{2p-1}{2}(-0.016) = 0.035 - (0.008)(2p-1)$ For y to be maximum, $\frac{dy}{dp} = 0$ $\Rightarrow 0.035 - (0.008)(2p-1) = 0$

$$\Rightarrow p = 2.6875$$
Also $p = \frac{x - x_0}{h}$ or $x = x_0 + ph$

$$\Rightarrow x = 3 + 2.6875(1) = 5.6875$$

$$\therefore y \text{ is maximum when } x = 5.6875 \text{ or } p = 2.6875$$
Substituting in 2, maximum value of y is given by
$$y \equiv (0.205) + (2.6875)(0.035) + \frac{(2.6875)(2.6875 - 1)}{2}(-0.016) = 0.2628$$

8.3 Numerical Integration

Numerical Integration is the process of computing the value of definite integral $\int_{a}^{b} y dx$, when the integrand function y = f(x) is given as discrete set of points (x_i, y_i) , i = 0, 1, 2, 3, ..., n. As in case of numerical differentiation, here also the integrand y = f(x) is first replaced with an interpolating polynomial, and then it is integrated to compute the value of the definite integral. This gives us 'quadrature formula' for numerical integration.

Newton Cotes Quadrature Formula

For an explicitly known function y = f(x), let y take values y_0 , y_1 , y_2 , ..., y_n for x taking values x_0 , x_1 , x_2 , ..., x_n , where x_i 's are equispaced.

To evaluate $I = \int_{a}^{b} f(x)dx$, divide the interval (a, b) into *n* equal parts, each of width *h*, such that $a = x_0 < x_1 < x_2 < \dots < x_n = b$ Clearly $x_n = x_0 + nh$ Then $I = \int_{a}^{b} f(x)dx = \int_{x_0}^{x_0+nh} f(x)dx$, nh = b - a

By Newton's forward interpolation formula:

$$\begin{split} f(x) &\equiv y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \cdots, \quad x = x_0 + ph \\ &\therefore I = \int_{x_0}^{x_0 + nh} f(x)dx = h\int_0^n f(x_0 + ph)dp \\ &\because x = x_0 + ph \Rightarrow dx = hdp, \text{ also when } x = x_0, = 0, x = x_0 + nh, p = n \\ &\Rightarrow I \equiv h\int_0^n \left[y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \cdots \right] dp \\ &\equiv h \left[py_0 + \frac{p^2}{2}\Delta y_0 + \frac{1}{2!} \left(\frac{p^3}{3} - \frac{p^2}{2} \right)\Delta^2 y_0 + \frac{1}{3!} \left(\frac{p^4}{4} - p^3 + p^2 \right)\Delta^3 y_0 + \cdots \right]_0^n \\ &\Rightarrow I \equiv nh \left[y_0 + \frac{n}{2}\Delta y_0 + \left(\frac{n^2}{3} - \frac{n}{2} \right) \frac{\Delta^2 y_0}{2!} + \left(\frac{n^3}{4} - n^2 + n \right) \frac{\Delta^3 y_0}{3!} + \cdots \right] \quad \dots \end{split}$$

This is known as Newton's Cote's quadrature formula. Different quadrature formulae are derived by taking n = 1, 2, 3, ... in equation ①.

8.3.1Numerical Integration Using Trapezoidal Rule

If we put n = 1 in Newton's Cote's quadrature formula given by ①, we get the curve through (x_0, y_0) and (x_1, y_1) as a straight line and being linear equation in x, 2^{nd} and higher order differences are zero.

$$\therefore (1) \Rightarrow I = \int_{x_0}^{x_0+h} f(x) dx = h \left[y_0 + \frac{1}{2} \Delta y_0 \right] = h \left[y_0 + \frac{1}{2} (y_1 - y_0) \right] = \frac{h}{2} (y_0 + y_1)$$

Similarly $\int_{x_0+h}^{x_0+2h} f(x) dx = \frac{h}{2} (y_1 + y_2)$
$$\vdots$$

 $\int_{x_0+(n-1)h}^{x_0+nh} f(x) dx = \frac{h}{2} (y_{n-1} + y_n)$

Adding areas of all these intervals, we get:

$$\int_{x_0}^{x_0+nh} f(x)dx = \frac{h}{2}(y_0 + y_1) + \frac{h}{2}(y_1 + y_2) + \dots + \frac{h}{2}(y_{n-1} + y_n)$$

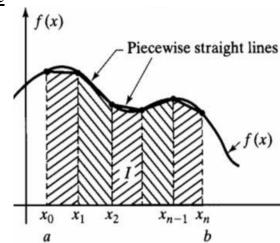
$$\Rightarrow \int_a^b f(x)dx = \frac{h}{2}[y_0 + 2(y_1 + y_2 + \dots + y_{n-1}) + y_n]$$

This is known as trapezoidal rule to evaluate $\int_a^b f(x)dx$, where the function y = f(x) is given as discrete set of points (x_i, y_i) , i = 0, 1, 2, 3, ..., n.

Geometrical Significance of Trapezoidal Rule

In trapezoidal rule, the curve y = f(x) is replaced by *n* piecewise straight lines joining the points (x_0, y_0) and (x_1, y_1) ; (x_1, y_1) and (x_2, y_2) ; ...; (x_{n-1}, y_{n-1}) and (x_n, y_n) .

The area under the curve y = f(x), between the ordinates $x = x_0$; $x = x_n$ and above x axis is approximately equal to the sum of areas of *n* trapezoids obtained within the enclosed region, shown by shaded portion of adjoining figure.



Error in Trapezoidal Rule

Area of first trapezoid in the interval $[x_0, x_1]$ is given by

$$A_1 = \frac{n}{2}(y_0 + y_1) \qquad ... (1)$$

Also expanding y = f(x) by Taylor's series about $x = x_0$

$$y = f(x) = y_0 + (x - x_0)y'_0 + \frac{1}{2!}(x - x_0)^2 y''_0 + \dots$$
 ... 2

Putting
$$x = x_1 = x_0 + h$$
, we get
 $\Rightarrow y_1 = y_0 + hy'_0 + \frac{h^2}{2!}y''_0 + \cdots$... ③
 $\therefore at \ x = x_1, y = y_1$

Substituting (3) in (1), we get

$$A_{1} = \frac{h}{2} \Big(y_{0} + y_{0} + hy_{0}' + \frac{h^{2}}{2!} y_{0}'' + \cdots \Big)$$

$$\Rightarrow A_{1} = \frac{h}{2} \Big(2y_{0} + hy_{0}' + \frac{h^{2}}{2!} y_{0}'' + \cdots \Big) = hy_{0} + \frac{h^{2}}{2} y_{0}' + \frac{h^{3}}{2.2!} y_{0}'' + \cdots$$

Again taking area of single strip, under the curve y = f(x), between the ordinates $x = x_0$ and $x = x_1$ and above x - axis

$$A_{1}' = \int_{x_{0}}^{x_{0}+h} y dx = \int_{x_{0}}^{x_{0}+h} \left[y_{0} + (x - x_{0})y_{0}' + \frac{1}{2!}(x - x_{0})^{2}y_{0}'' + \cdots \right] dx \quad \text{using } @$$

= $\left[y_{0}x + \frac{(x - x_{0})^{2}}{2!}y_{0}' + \frac{(x - x_{0})^{3}}{3}\frac{y_{0}''}{2!} + \cdots \right]_{x_{0}}^{x_{0}+h}$
= $hy_{0} + \frac{h^{2}}{2!}y_{0}' + \frac{h^{3}}{3!}y_{0}'' + \cdots$

 \therefore Error in the interval $[x_0, x_1]$ is given by

$$A_{1}^{'} - A_{1} = \left[hy_{0} + \frac{h^{2}}{2!}y_{0}^{'} + \frac{h^{3}}{3!}y_{0}^{''} + \cdots \right] - \left[hy_{0} + \frac{h^{2}}{2}y_{0}^{'} + \frac{h^{3}}{2.2!}y_{0}^{''} + \cdots \right]$$
$$= \left(\frac{1}{6} - \frac{1}{4}\right)h^{3}y_{0}^{''} + \cdots = -\frac{h^{3}}{12}y_{0}^{''} + \cdots$$

Thus lowest order error in interval $[x_0, x_1] \approx -\frac{h^3}{12}y_0''$ Similarly lowest error in interval $[x_1, x_2] \approx -\frac{h^3}{12}y_1''$

:

$$\therefore \text{ Lowest error in interval } [x_{n-1}, x_n] \approx -\frac{h^3}{12} y_{n-1}''$$

Total error $E = -\frac{h^3}{12} [y_0'' + y_1'' + \dots + y_{n-1}'']$
If $y_x'' = \text{Maximum}[y_0'', y_1'', \dots, y_{n-1}'']$
Then Maximum $E \le -\frac{nh^3}{12} y_x''$
 $= -\frac{nhh^2}{12} y_x'' = -\frac{(b-a)h^2}{12} y_x''$ $\therefore nh = (b-a)$
 $\therefore E \le kh^2$, where $k = -\frac{(b-a)}{12} y_x''$

Hence the error in trapezoidal rule is of $orderh^2$, where *h* is the height of the interval.

8.3.2Numerical Integration Using Simpson's One-Third Rule

If we put n = 2 in Newton's Cote's quadrature formula given by (1), we get the curve through the points (x_0, y_0) , (x_1, y_1) , (x_2, y_2) as a parabolic figure and being quadratic equation in x, 3^{rd} and higher order differences are zero.

 $\therefore (1) \Rightarrow I = \int_{x_0}^{x_0 + 2h} f(x) dx = 2h \left[y_0 + \frac{2}{2} \Delta y_0 + \left(\frac{4}{3} - \frac{2}{2}\right) \frac{\Delta^2 y_0}{2!} \right]$ $= 2h \left[y_0 + (y_1 - y_0) + \frac{1}{6} (y_2 - 2y_1 + y_0) \right]$ $= \frac{h}{3} (y_0 + 4y_1 + y_2)$ Similarly $\int_{x_0 + 2h}^{x_0 + 4h} f(x) dx = \frac{h}{3} (y_2 + 4y_3 + y_4)$ \vdots

$$\int_{x_0+(n-2)h}^{x_0+nh} f(x)dx = \frac{h}{3}(y_{n-2} + 4y_{n-1} + y_n)$$

Adding areas of all these intervals, we get:

$$\int_{x_0}^{x_0+nh} f(x)dx = \frac{h}{3}(y_0 + 4y_1 + y_2) + \frac{h}{3}(y_2 + 4y_3 + y_4) + \dots + \frac{h}{3}(y_{n-2} + 4y_{n-1} + y_n)$$

$$\therefore \int_a^b f(x)dx = \frac{h}{3}[(y_0 + y_n) + 4(y_1 + y_3 + \dots + y_{n-1}) + 2(y_2 + y_4 + \dots + y_{n-2})]$$

This is known as Simpson's one-third rule to evaluate $\int_a^b f(x)dx$, where the function y = f(x) is given as discrete set of points (x_i, y_i) , i = 0, 1, 2, 3, ..., n.

Geometrical Significance of Simpson's One-Third Rule

In Simpson's one-third rule, the curve y = f(x) is replaced by arcs of 2^{nd} degree parabolas with vertical axis as shown in given figure.

Simpson's one-third rule requires the given interval to be divided into even number of sub-intervals, since we are finding areas of two strips at a time.

Error in Simpson's One-Third Rule

Area of first two strips in the interval $[x_0, x_2]$ is given by

$$A_2 = \frac{n}{3}(y_0 + 4y_1 + y_2)$$

Also expanding y = f(x) by Taylor's series about $x = x_0$

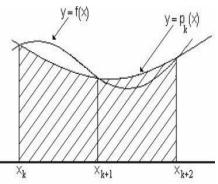
$$y = f(x) = y_0 + (x - x_0)y'_0 + \frac{1}{2!}(x - x_0)^2 y''_0 + \frac{1}{3!}(x - x_0)^3 y''_0 \dots \dots \square$$

Putting
$$x = x_1 = x_0 + h$$
 in (2), we get

$$\Rightarrow y_1 = y_0 + hy'_0 + \frac{h^2}{2!}y''_0 + \frac{h^3}{3!}y'''_0 + \cdots \qquad \dots ③$$

$$\therefore at \ x = x_1, y = y_1$$

Putting
$$x = x_2 = x_0 + 2h$$
 in (2) , we get
 $\Rightarrow y_2 = y_0 + 2hy'_0 + \frac{4h^2}{2!}y''_0 + \frac{8h^2}{3!}y''_0 + \cdots$... (4)
 $\therefore at \ x = x_2, y = y_2$



...(1)

Substituting (3) and (4) in (1), A_2 may be written as

$$\frac{h}{3} \left(y_0 + 4 \left(y_0 + h y_0' + \frac{h^2}{2!} y_0'' + \frac{h^3}{3!} y_0''' \right) + \left(y_0 + 2h y_0' + \frac{4h^2}{2!} y_0'' + \frac{8h^2}{3!} y_0''' \right) + \cdots \right)$$

$$\Rightarrow A_2 = \frac{h}{3} \left(6y_0 + 6h y_0' + \frac{8h^2}{2!} y_0'' + \frac{12h^3}{3!} y_0''' + \cdots \right)$$

$$= 2h y_0 + 2h^2 y_0' + \frac{4h^3}{3} y_0'' + \frac{2h^4}{3} y_0''' + \frac{5h^5}{18} y_0^{i\nu} + \cdots$$

Again taking actual area of two strip, under the curve y = f(x), between the ordinates $x = x_0$ and $x = x_2$ and above x - axis

$$A'_{2} = \int_{x_{0}}^{x_{0}+2h} y dx = \int_{x_{0}}^{x_{0}+2h} \left[y_{0} + (x - x_{0})y'_{0} + \frac{1}{2!}(x - x_{0})^{2}y''_{0} + \cdots \right] dx \text{ using } (2)$$

$$= \left[y_{0}x + \frac{(x - x_{0})^{2}}{2!}y'_{0} + \frac{(x - x_{0})^{3}}{3}\frac{y''_{0}}{2!} + \cdots \right]_{x_{0}}^{x_{0}+2h}$$

$$= 2hy_{0} + \frac{4h^{2}}{2!}y'_{0} + \frac{8h^{3}}{3!}y''_{0} + \frac{16h^{4}}{4!}y''_{0} + \frac{32h^{5}}{5!}y_{0}^{i\nu} + \cdots$$

$$= 2hy_{0} + 2h^{2}y'_{0} + \frac{4h^{3}}{3}y''_{0} + \frac{2h^{4}}{3}y''_{0} + \frac{4h^{5}}{15}y_{0}^{i\nu} + \cdots$$

 \therefore Error in the interval $[x_0, x_2]$ is given by

$$A'_{2} - A_{2} = \left[2hy_{0} + 2h^{2}y'_{0} + \frac{4h^{3}}{3}y''_{0} + \frac{2h^{4}}{3}y''_{0} + \frac{4h^{5}}{15}y''_{0} + \cdots\right] - \left[2hy_{0} + 2h^{2}y'_{0} + \frac{4h^{3}}{3}y''_{0} + \frac{2h^{4}}{3}y''_{0} + \frac{5h^{5}}{18}y''_{0} + \cdots\right] = \left(\frac{4}{15} - \frac{5}{18}\right)h^{5}y''_{0} + \cdots = -\frac{h^{5}}{90}y''_{0} + \cdots$$

Thus lowest order error in interval $[x_0, x_2] \approx -\frac{h^5}{90} y_0^{i\nu}$ Similarly lowest order error in interval $[x_1, x_2] \approx -\frac{h^5}{90} y_1^{i\nu}$

 \vdots Thus lowest order error in interval $[x_{n-1}, x_n] \approx -\frac{h^5}{90} y_{n-1}^{iv}$ Total error $E = -\frac{h^5}{90} [y_0^{iv} + y_1^{iv} + \dots + y_{n-1}^{iv}]$ If $y_x^{iv} = \text{Maximum} [y_0^{iv}, y_1^{iv}, \dots, y_{n-1}^{iv}]$ Then Maximum $E \leq -\frac{nh^5}{180} y_x^{iv} \qquad \because \text{ number of intervals is } \frac{n}{2}$ $= -\frac{nhh^4}{180} y_x^{iv} = -\frac{(b-a)h^4}{180} y_x^{iv} \qquad \because nh = (b-a)$ $\therefore E \leq ph^4 \text{ , where } p = -\frac{(b-a)}{180} y_x^{iv}$

Hence the error in Simpson's one-third rule is of order h^4 , where h is the height of the interval.

8.3.3 Numerical Integration Using Simpson's Three-Eighth Rule

If we put n = 3 in Newton's Cote's quadrature formula given by (1), we get the curve through the points (x_0, y_0) , (x_1, y_1) , (x_2, y_2) , (x_3, y_3) as a cubic polynomial and hence 4th and higher order differences are zero.

∴Newton's Cote's quadrature formula reduces to:

$$I = \int_{x_0}^{x_0+3h} f(x)dx = 3h \left[y_0 + \frac{3}{2}\Delta y_0 + \left(\frac{9}{3} - \frac{3}{2}\right)\frac{\Delta^2 y_0}{2!} + \left(\frac{27}{4} - 9 + 3\right)\frac{\Delta^3 y_0}{3!} \right]$$

= $3h \left[y_0 + \frac{3}{2}(y_1 - y_0) + \frac{3}{4}(y_2 - 2y_1 + y_0) + \frac{1}{8}(y_3 - 3y_2 + 3y_1 - y_0) \right]$
= $\frac{3h}{8} \left[8y_0 + 12(y_1 - y_0) + 6(y_2 - 2y_1 + y_0) + (y_3 - 3y_2 + 3y_1 - y_0) \right]$
= $\frac{3h}{8} \left[(8 - 12 + 6 - 1)y_0 + (12 - 12 + 3)y_1 + (6 - 3)y_2 + y_3 \right]$
= $\frac{3h}{8} \left[y_0 + 3y_1 + 3y_2 + y_3 \right]$
Similarly $\int_{x_0+3h}^{x_0+6h} f(x)dx = \frac{3h}{8} \left[y_3 + 3y_4 + 3y_5 + y_6 \right]$
:
 $\int_{x_0+(n-3)h}^{x_0+nh} f(x)dx = \frac{3h}{8} \left[y_{n-3} + 3y_{n-2} + 3y_{n-1} + y_n \right]$

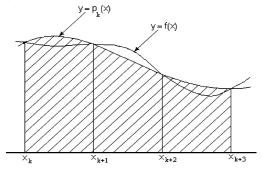
Adding areas of all these intervals, we get:

$$\int_{x_0}^{x_0+nh} f(x)dx = \frac{3h}{8} \left[y_0 + 3y_1 + 3y_2 + y_3 \right] + \frac{3h}{8} \left[y_3 + 3y_4 + 3y_5 + y_6 \right]$$
$$+ \dots + \frac{3h}{8} \left[y_{n-3} + 3y_{n-2} + 3y_{n-1} + y_n \right]$$
$$\therefore \int_a^b f(x)dx = \frac{3h}{8} \left[(y_0 + y_n) + 3(y_1 + y_2 + y_4 + y_5 + \dots + y_{n-2} + y_{n-1}) + 2(y_3 + y_6 + \dots + y_{n-3}) \right]$$

This is known as Simpson's three-eighths rule to evaluate $\int_a^b f(x)dx$, where the function y = f(x) is given as discrete set of points (x_i, y_i) , i = 0, 1, 2, 3, ..., n.

Geometrical Significance of Simpson's Three-Eighth Rule

The Simpson's 3/8 rule is similar to the 1/3 rule except that curve y = f(x) is replaced by arcs of 3^{rd} degree polynomial curve, as shown in given figure. It is used when it is required to take 3 segments at a time. Thus number of intervals must be a multiple of 3.



It can be derived that the lowest order error in interval $[x_0, x_3] \approx -\frac{3h^5}{80} y_0^{iv}$

Maximum $E \le -\frac{nh^5}{80} y_x^{iv}$ \therefore number of intervals is $\frac{n}{3}$ $= -\frac{nhh^4}{80} y_x^{iv} = -\frac{(b-a)h^4}{80} y_x^{iv} \qquad \therefore nh = (b-a)$ $\therefore E \le qh^4 \text{ , where } q = -\frac{(b-a)}{80} y_x^{iv}$

Hence error in Simpson's 3/8 rule is of order h^4 , where h is the height of the interval.

8.3.4 Applications of Numerical Integration

Numerical integration has numerous practical applications in the field of calculus. Simpson's $\frac{1}{3}$ rule due to its ease in application and higher accuracy is a preferred method in various application areas as given below:

- Area bounded by a curve y = f(x) between the ordinates x = a and x = b, above x - axis is given by $A = \int_a^b y dx$.
- Volume of solid formed by revolving the curve y = f(x) between the ordinates x = a and x = b along x axis is given by $V = \int_a^b \pi y^2 dx$.
- Length of an arc of the curve y = f(x) between the ordinates x = a and x = b and x axis is given by $\int_{a}^{b} \sqrt{1 + \left(\frac{dy}{dx}\right)^{2} dx}$
- To find velocity when acceleration at different times is given in tabular form.
- To find displacement when velocity is given as a function of time in discrete form.

Remarks:

- Simpson's rules ideally returns more accurate results compared to trapezoidal rule provided h is small, less than one essentially.
- Simpson's $\frac{1}{3}$ rule requires odd number of points (even number of subintervals) for application.
- Simpson's $\frac{3}{8}$ rule requires number of sub-intervals to be multiple of 3.

Example9 Evaluate $\int_0^1 \frac{1}{1+x^2} dx$ using

- *i*. Trapezoidal rule taking $h = \frac{1}{5}$
- *ii.* Simpson's $\frac{1}{3}$ rule taking $h = \frac{1}{4}$
- *iii.* Simpson's $\frac{3}{8}$ rule taking $h = \frac{1}{6}$

Solution: *i*. To solve
$$\int_0^1 \frac{1}{1+x^2} dx$$
 using trapezoidal rule
Taking $h = \frac{1}{5} = 0.2$, $n = \frac{b-a}{h} = \frac{1-0}{0.2} = 5$

: Dividing the interval (0,1) into 5 equal parts for the function $f(x) = \frac{1}{1+x^2}$

$$x$$
00.20.40.60.81 $y = f(x)$ 10.960.860.740.610.5

By trapezoidal rule $\int_0^1 \frac{1}{1+x^2} dx = \frac{h}{2} [y_0 + 2(y_1 + y_2 + y_3 + y_4) + y_5]$ = $\frac{0.2}{2} [1 + 2(0.96 + 0.86 + 0.74 + 0.61) + 0.5]$

 $\therefore \int_{0}^{1} \frac{1}{1+x^{2}} dx = 0.784 \text{ using trapezoidal rule.}$ *ii.* To solve $\int_{0}^{1} \frac{1}{1+x^{2}} dx$ using Simpson's $\frac{1}{3}$ rule Taking $h = \frac{1}{4} = 0.25, n = \frac{b-a}{h} = \frac{1-0}{0.25} = 4$ \therefore Dividing the interval (0,1) into 4 equal parts for the function $f(x) = \frac{1}{1+x^{2}}$ $x = 0 \quad 0.25 \quad 0.5 \quad 0.75 \quad 1$ $y = f(x) \quad 1 \quad 0.94 \quad 0.8 \quad 0.64 \quad 0.5$ By Simpson's $\frac{1}{3}$ rule $\int_{0}^{1} \frac{1}{1+x^{2}} dx = \frac{h}{3} [(y_{0} + y_{4}) + 4(y_{1} + y_{3}) + 2(y_{2})]$ $= \frac{0.25}{3} [(1 + 0.5) + 4(0.94 + 0.64) + 2(0.8)]$

 $\therefore \int_0^1 \frac{1}{1+x^2} dx = 0.7850 \text{ using Simpson's } \frac{1}{3} \text{ rule}$ *iii.* To solve $\int_0^1 \frac{1}{1+x^2} dx$ using Simpson's $\frac{3}{8}$ rule Taking $h = \frac{1}{6}, n = \frac{b-a}{h} = \frac{1-0}{\frac{1}{6}} = 6$

: Dividing the interval (0,1) into 6 equal parts for the function $f(x) = \frac{1}{1+x^2}$

$$x = 0 \quad \frac{1}{6} \quad \frac{2}{6} \quad \frac{3}{6} \quad \frac{4}{6} \quad \frac{5}{6} \quad 1$$

$$y = f(x) \quad 1 \quad 0.97 \quad 0.9 \quad 0.8 \quad 0.69 \quad 0.59 \quad 0.5$$

By Simpson's $\frac{3}{8}$ rule $\int_0^1 \frac{1}{1+x^2} dx = \frac{3h}{8} [(y_0 + y_6) + 3(y_1 + y_2 + y_4 + y_5) + 2(y_3)]$

$$= \frac{3}{8} \cdot \frac{1}{6} [(1 + 0.5) + 3(0.97 + 0.9 + 0.69 + 0.59) + 2(0.8)]$$

 $\therefore \int_0^1 \frac{1}{1+x^2} dx = 0.7844$ using Simpson's $\frac{3}{8}$ rule

Example10 Evaluate $\int_0^{\frac{\pi}{2}} \sin x \, dx$ using

i. Trapezoidal rule *ii*. Simpson's $\frac{1}{3}$ rule *iii*. Simpson's $\frac{3}{8}$ rule, taking n = 6Solution: Taking n = 6, $h = \frac{b-a}{n} = \frac{\frac{\pi}{2}-0}{6} = \frac{\pi}{12}$

: Dividing the interval $\left(0, \frac{\pi}{2}\right)$ into 6 equal parts for the function $f(x) = \sin x$

x	0	π	2π	3π	4π	5π	π
			12	12	12	12	2

$$\begin{aligned} \boxed{y = f(x) \mid 0 \mid 0.2588 \mid 0.5 \mid 0.7071 \mid 0.866 \mid 0.9659 \mid 1} \\ i. To solve $\int_{0}^{\frac{\pi}{2}} \sin x \, dx$ using trapezoidal rule
 $\int_{0}^{\frac{\pi}{2}} \sin x \, dx = \frac{h}{2} [y_0 + 2(y_1 + y_2 + y_3 + y_4 + y_5) + y_6] \\ = \frac{\pi}{12} \cdot \frac{1}{2} [0 + 2(0.2588 + 0.5 + 0.7071 + 0.866 + 0.9659) + 1] \\ \therefore \int_{0}^{\frac{\pi}{2}} \sin x \, dx = 0.9943$ using trapezoidal rule.
ii. To solve $\int_{0}^{\frac{\pi}{2}} \sin x \, dx$ using Simpson's $\frac{1}{3}$ rule
 $\int_{0}^{\frac{\pi}{2}} \sin x \, dx = \frac{h}{3} [(y_0 + y_6) + 4(y_1 + y_3 + y_5) + 2(y_2 + y_4)] \\ = \frac{\pi}{12} \cdot \frac{1}{3} [(0 + 1) + 4(.2588 + .7071 + .9659) + 2(0.5 + .866)] \\ \therefore \int_{0}^{\frac{\pi}{2}} \sin x \, dx = 1.000004$ using Simpson's $\frac{1}{3}$ rule
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Example11 Evaluate $\int_{0.5}^{1.3} \frac{1}{1+\log x} \, dx$ using
i. Trapezoidal rule *ii*. Simpson's $\frac{1}{3}$ rule *iii*. Simpson's $\frac{3}{8}$ rule, taking $n = 8$
Solution: Taking $n = 8$, $h = \frac{1.3 - .05}{8} = 0.1$
 \therefore Dividing the interval (0.5.1.3) into 8 equal parts for $f(x) = \frac{1}{1+\log x}$
 $\frac{\frac{x \mid 0.5 \quad 0.6 \quad 0.7 \quad 0.8 \quad 0.9 \quad 1 \quad 1.1 \quad 1.2 \quad 1.3 \quad 1.1 \quad 1.5 \quad 1.29 \quad 1.12 \quad 1 \quad 0.91 \quad 0.89 \quad 0.79}$
i. To solve $\int_{0.5}^{1.3} \frac{1}{1+\log x} \, dx$ using trapezoidal rule
 $\int_{0.5}^{1.3} \frac{1}{1+\log x} \, dx = \frac{h}{2} [y_0 + 2(y_1 + y_2 + \dots + y_7) + y_8] = \frac{0.1}{2} [3.26 + 2(2.04 + 1.55 + 1.29 + 1.12 + 1 + .91 + .89) + .79] = 0.05[21.65] = 1.0825$
 $\therefore \int_{0.5}^{1.3} \frac{1}{1+\log x} \, dx$ using trapezoidal rule.
ii. To solve $\int_{0.5}^{1.3} \frac{1}{1+\log x} \, dx$ using trapezoidal rule.
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 $\int_{0.5}^{1.3} \frac{1}{1+\log x} dx = \frac{h}{3} [(y_0 + y_8) + 4(y_1 + y_3 + y_5 + y_7) + 2(y_2 + y_4 + y_6)]$ = $\frac{0.1}{3} [(3.26 + .79) + 4(2.04 + 1.29 + 1 + .89) + 2(1.55 + 1.12 + .91)]$ = $\frac{0.1}{3} [32.09] = 1.070$ $\therefore \int_{0.5}^{1.3} \frac{1}{1+\log x} dx = 1.070$ using Simpson's $\frac{1}{3}$ rule *iii*. Simpson's $\frac{3}{8}$ rule is not applicable, as n is not a multiple of 3 Example12 Evaluate $\int_{0}^{\frac{\pi}{2}} e^{\cos x} dx$ up to 4 decimal places, using trapezoidal rule. Solution: Taking n = 3, i.e. $h = \frac{\frac{\pi}{2} - 0}{3} = \frac{\pi}{6}$ x = 0 $\frac{\pi}{6}$ $\frac{\pi}{3}$ $\frac{\pi}{2}$

$$x = 6$$
 3 2
 $y = f(x)$ 2.71828 2.37744 1.64872 1

By trapezoidal rule

$$\int_{0}^{\frac{\pi}{2}} e^{\cos x} dx = \frac{h}{2} [y_0 + 2(y_1 + y_2) + y_3]$$

= $\frac{\pi}{6} \cdot \frac{1}{2} [2.71828 + 2(2.37744 + 1.64872) + 1]$
= $\frac{\pi}{12} [11.7706] = 3.0815$
 $\therefore \int_{0}^{\frac{\pi}{2}} e^{\cos x} dx = 3.0815$ using trapezoidal rule

Example13 From the following table, find the area bounded by the curve and x - axis, between the ordinates x = 7.47 to x = 7.52.

			7.49			
y = f(x)	1.93	1.95	1.98	2.01	2.03	2.06

Solution: As n = 5, Simpson's $\frac{1}{3}$ rule Simpson's $\frac{3}{8}$ rules are not applicable. Applying trapezoidal rule with h = 0.01

$$\int_{7.47}^{7.52} f(x)dx = \frac{.01}{2} [1.93 + 2(1.95 + 1.98 + 2.01 + 2.03) + 2.06]$$

= 0.005[19.93] = 0.09965 square units

Example14 The velocity v of an airplane which starts from rest is given at fixed intervals of time t as shown:

t (minutes)	2	4	6	8	10	12	14	16	18	20
v = f(t) (km/minutes)	8	17	24	28	30	20	12	6	2	0

Estimate the approximate distance covered in 20 minutes.

Solution: Since the airplane starts from rest, its initial velocity is zero. So the time/velocity relationship may be tabulated as:

t (minutes) 0 2 4 6 8 10 12 14 16 18 20

v = f(t)(km/minutes) 0 8 17 24 28 30 20 12 6 2 0

Let *S* be the distance covered at any instant of time *t*, Then $v = \frac{dS}{dt}$ or dS = v dt

: Distance covered in 20 minutes is given by: r^{20} r^{20} h

$$S = \int_0^{20} dS = \int_0^{20} v \, dt = \frac{n}{3} [(v_0 + v_{10}) + 4(v_1 + v_3 + v_5 + v_7 + v_9)$$
$$2(v_2 + v_4 + v_6 + v_8)]$$

Applying Simpson's $\frac{1}{3}$ rule with h = 2, as n = 10 $\Rightarrow S = \frac{2}{3} [(0+0) + 4(8+24+30+12+2) + 2(17+28+20+6)]$ $\therefore S = 297.33 \text{ km}$

Example15 A solid of revolution is formed by rotating about x – axis, the area between x – axis, the line x = 0 and a curve through the points with the following coordinates:

Estimate the volume of solid formed, giving the answer upto 3 decimal places.

Solution: Volume of solid formed by revolving the curve y = f(x) between the ordinates x = a and y = b along x - axis is given by $V = \int_{a}^{b} \pi y^{2} dx$

By Simpson's $\frac{1}{3}$ rule with h = 0.25, as n = 4

$$\therefore V = \pi \int_0^1 y^2 dx = \frac{\pi h}{3} [y_0^2 + y_4^2] + 4(y_1^2 + y_3^2) + 2(y_2^2)]$$

$$\Rightarrow V = \frac{\pi}{12} \{ [1^2 + (0.7328)^2] + 4[(0.5846)^2 + (0.5085)^2] + 2[(0.5586)^2] \}$$

$$= \frac{\pi}{12} [1.5370 + 4(0.60033) + 2(0.31203)] = 1.944$$