CHAPTER SIX

Numerical Differentiation

6.1- Introduction:

In the previous chapters we have seen finding the polynomial curve y=f(x), passing through the ordered pairs (x_i, y_i), i=0, 1, 2, ...n. Now we try to find the derivative value of such curve at a given value of x. **Numerical differentiation** is the process of calculating the derivative of a function at some particular value of the independent variable by means of a set of given values of that function.

Before we study this subject, we need to learn (Taylor Series).

6.2-Taylor Series: It is of great value in the study of numerical method, since it provides a means to **predict** a function value at one point in terms of the function value and its derivatives at another points. In chapter (5) we studied interpolation i.e. missing data within a certain interval. Prediction means we extrapolate the value of a function i.e. outside the given data interval or range.

For example, the first-order approximation is developed by:

$$f(x) \approx f(x_i) + f'(x_i)(x_{i+1} - x_i) \ldots .(1)$$

For better approximation, second-order can be used:

$$f(x) \approx f(x_i) + f'(x_i)(x_{i+1} - x_i) + \frac{f''(x_i)}{2!}(x_{i+1} - x_i)^2 \ldots \ldots (2)$$

For more accurate we take four or more terms.

If we define step size: $h = (x_{i+1} - x_i)$, then,

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

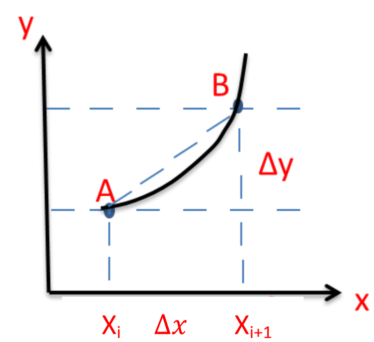
Equation (3) is Taylor series and (R)is the remainder error if we take limited number of terms.

6.3-Numerical Differentiation:

Let y = f(x) , then $\frac{\Delta y}{\Delta x} = slope\ of\ the\ function$

Using finite difference method: $\frac{\Delta y}{\Delta x} = \frac{f(x+\Delta x) - f(x)}{\Delta x}$

Or $\frac{dy}{dx} = \frac{\Delta y}{\Delta x}$ (*as* Δx *approaches zero*).



Then $\frac{dy}{dx} = \lim_{\Delta x \to 0} \left[\frac{f(x+\Delta x)-f(x)}{\Delta x}\right]$

If $h = \Delta x$

$$x_{i+1} = (x_i + \Delta x) \equiv (x_i + h)$$

Using Taylor series expansion for the functions f(x_i+h) and f(x_i-h) we get:

$$f(x_{i+1}) = f(x_i + h) = f(x_i) + hf'(x_i) + \frac{h^2}{2!}f''(x_i) + \ldots + \cdots .(4)$$

$$f(x_{i-1}) = f(x_i - h) = f(x_i) - hf'(x_i) + \frac{h^2}{2!}f''(x_i) - \ldots + \cdots ..(5)$$

If equation(5) subtracted from equation(4) we get:

$$f(x_{i+1}) - f(x_{i-1}) = 2hf'(xi) + \frac{h^3 f'''(x_i)}{3} \ldots .(6)$$

From equation(6) we get that

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} - \frac{h^2 f'''(x_i)}{6} \ldots .(7)$$

Equation(7)is the **central first derivative** of (y)with respect of (x) at point (x_i), or (**the two-point central difference formula**)this can be approximated to:

$$\boldsymbol{f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h}} + R(h^2) \ldots .(8)$$

Where (R) is the remainder or (error) which is a function of (h^2). For more accurate first derivative, equation(7) is used i.e. f'''(x_i) is taken into consideration we get:

$$\boldsymbol{f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h}} + R(h^4)..(9)$$

This is called **the four-point central difference formula.**

6.3.2-Derivation of 2nd derivative:

To find a formula for the second derivative, then by adding equations (4 and 5) we get:

$$f(x_{i+1}) + f(x_{i-1}) = 2f\big(x(i)\big) + h^2 f''(x_i) + \frac{h^4 f''''(x_i)}{12}$$

$$f''(x_i) = \frac{f(x_{i+1}) + f(x_{i-1}) - 2f(x_i)}{h^2} - \frac{h^2 f''''(x_i)}{12}$$

This can be approximated to:

$$\boldsymbol{f''(x_i) = \frac{f(x_{i+1}) + f(x_{i-1}) - 2f(x_i)}{h^2}} + R(h^2) \ldots (\mathbf{10})$$

This is the **second derivative approximation.**

In the same way 3rd derivative is:

$$f'''(x(i)) = \frac{-f(x_{i+3}) + 8f(x_{i+2}) - 13f(x_{i+1}) + 13f(x_{i-1}) - 8f(x_{i-2}) + f(x_{i-3})}{8h^3}$$

Example 6.1: Consider the function [y=f(x) = x^3 +2x]. Find, f '(x) and f ''(x) by low and high accuracy formula at (x=1.5), use step size h=0.25.

Solution: x_i =1.5 , f(1.5) =6.375
x_{i+1}= 1.75 , f(1.75)=8.859
x_{i+2}= 2.0 , f(2) =12.0
x_{i-1}= 1.25, f(1.25)=4.453
x_{i-2}= 1.0 , f(1.0) =3.0

Applying equation(8):

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} = \frac{8.859 - 4.453}{2 * 0.25} = 8.813$$

Applying equation(9):

$$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h}$$
$$= \frac{-12 + 8 * 859 - 8 * 4.453 + 3}{12 * 0.25} = 8.75$$

Exact value:

$$f'(x) = 3x^2 + 2 \ , \quad then \ \ f'(1.5) = 3 * 1.5^2 + 2 = 8.75$$

To find f''(x_i) we use equation (10):

$$f''(x_i) = \frac{f(x_{i+1}) + f(x_{i-1}) - 2f(x_i)}{h^2} = \frac{8.859 - 2 * 6.375 + 4.453}{(0.25)^2} = 9$$

Exact value of $f''(x) = 6x \ , \quad then \ \ f''(1.5) = 9$

6. 4-Numerical Differentiation Based on Interpolation:
6.4.1- Non-uniform nodal points:

If $(x_i,f(x_i))$, i=0,1,…,n are (n+1) points, then the lagrange interpolating polynomial fitting this data is given by:

$$P_n(x) = \sum_{k=0}^{n} L_k(x) * \quad f(x) \ldots\ldots (11)$$

1. Linear interpolation:

In this case we have only two points (x_0 and x_1), then we must find L_0 and L_1 and their derivatives:

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

$$\text{Then, } P1(x) = \frac{(x-x_1)}{(x_0-x_1)} f(x_0) + \frac{(x-x_0)}{(x_1-x_0)} f(x_1)$$

$$\text{Then, } P'1(x) = \frac{f(x_0)}{(x_0-x_1)} + \frac{f(x_1)}{(x_1-x_0)}$$

$$\text{Or, } P'1(x) = \frac{f(x_1)-f(x_0)}{(x_1-x_0)} \ldots\ldots\ldots\ldots. (12)$$

2. Quadratic Interpolation:

In this case we have only three points (x_0, x_1 and x_2), then we must find L_0, L_1 and L_2 and their derivatives:

$$L_0 = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}, \qquad L'_0 = \frac{2x-x_1-x_2}{(x_0-x_1)(x_0-x_2)}$$

$$L_1 = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} \qquad L'_1 = \frac{2x-x_0-x_2}{(x_1-x_0)(x_1-x_2)}$$

$$L_2 = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} \qquad L'_2 = \frac{2x-x_0-x1}{(x_2-x_0)(x_2-x_1)}$$

Then the 2nd degree polynomial will be:

$P2(x) = L_0(x)\, f(x_0) + L_1(x) f(x_1) + L_2(x) f(x_2)$

And its 1st derivative is:

$P'2(x) = L'_0(x)\, f(x_0) + L'_1(x) f(x_1) + L'_2(x) f(x_2)$

Or

$$P'2(x) = \frac{2x-x_1-x_2}{(x_0-x_1)(x_0-x2)} f(x_0) + \frac{2x-x_0-x_2}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{2x-x_0-x_1}{(x_2-x_0)(x_2-x_1)} f(x_2) \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (\mathbf{13})$$

Similarly, the 2nd derivative of the quadratic polynomial will be:

$$P''_2 = 2\left[\frac{f(x_0)}{(x_0 - x_1)(x_0 - x_2)} + \frac{f(x_1)}{(x_1 - x_0)(x_1 - x_2)} + \frac{f(x_2)}{(x_2 - x_0)(x_2 - x_1)}\right] \ldots (14)$$

Q1/ B: Given the following values of f(x)=ln(x). Find the approximate value of f'(2) using linear and quadratic interpolation and f''(2) using quadratic interpolation. Also obtain percentage relative error.

X(i)	**x_0=2.0**	**x_1=2.2**	**x_2=2.6**
F(xi)	F(2)=0.69315	F(2.2)=0.78846	F(2.6)=0.95551

Solution: Since the spacing is not equal, we use the rules of the non-uniform points i.e.:

1. Using linear method (equation 12):

$$P'1(x) = \frac{f(x_1) - f(x_0)}{(x_1 - x_0)} = f'(2) = \frac{0.78846 - 0.69315}{(2.2 - 2.0)} = 0.47655$$

2. Using quadratic method (equation 13):

$$P'2(x_0) = \frac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{2x - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)} f(x2)$$

$$P'2(2) = f'(2) = \frac{4-2.2-2.6}{(2-2.2)(2-2.6)}(0.69315) + \frac{2-2.6}{(2.2-2)(2.2-2.6)}(0.78846) + \frac{(2-2.2)}{(2.6-2)(2.6-2.2)}(0.95551) = 0.49619$$

The exact value is (f'(2)=0.5), then ϵ_r=0.762%

3. The 2nd derivative can be found using equation (14):

$$P''_2 = 2\left[\frac{f(x_0)}{(x_0 - x_1)(x_0 - x_2)} + \frac{f(x_1)}{(x_1 - x_0)(x_1 - x_2)} + \frac{f(x_2)}{(x_2 - x_0)(x_2 - x_1)}\right]$$

$$P''_2(2) = 2\left[\frac{0.69315}{(2 - 2.2)(2 - 2.6)} + \frac{0.78846}{(2.2 - 2)(2.2 - 2.6)} + \frac{0.95551}{(2.6 - 2)(2.6 - 2.2)}\right] = -\ 0.19642$$

The exact value of f''(2)= -0.25, then ϵ_r=21.4%

6.4.2- Uniform nodal points:

When the points $x_0, x_1, \ldots, x_n$ are equispaced with step length (h), we have: $x_i = x_0 + i * h \qquad for\ i = 1, 2, \ldots, n$

For <u>linear interpolation</u> equation (12) can be rewritten as follows: $f'(x_0) = P'1(x_0) = \frac{f(x_1) - f(x_0)}{h}$

And $f'(x_1) = P'1(x_1) = \frac{f(x_2) - f(x1)}{h}$

And for <u>quadratic interpolation</u>, we have :

$$x_1 = x_0 + h \qquad and \qquad x_2 = x_0 + 2h$$

Then equation (13) becomes:

$$f'(x) = p'(x) = \frac{1}{2h^2}[(2x - x_1 - x2)f(x_0) - 2(2x - x_0 - x_2)f(x_1) + (2x - x_0 - x_1)f(x_2)] \ldots\ldots\ldots\ldots (13a)$$

Now to find the 1st dervative at each point is by substituting (x) by the value of that point i.e.

$$f'(x_0) = P'_2(x) = \frac{1}{2h^2}[(2x_0 - x_1 - x_2)f(x_0) - 2(2x_0 - x_0 - x_1)f(x_1) + (2x_0 - x_0 - x_1)f(x_2)]$$
$$= \frac{1}{2h}[-3f(x_0) + 4f(x_1) - f(x_2)]$$

Similarly, we can find that f(x1) and f(x2) are:

$$f'(x_1) = P'_2(x1) = \frac{1}{2h}[f(x_2) - f(x_0)]$$

$$f'(x_2) = P'_2(x_2) = \frac{1}{2h}[f(x_0) - 4f(x_1) + 3f(x_2)]$$

Since the interpolating polynomial is quadratic, its 2nd derivative is a <u>constant</u> i.e.:

$$f''(x_0) = P''_2(x_0) = \frac{1}{h^2}[f(x_0) - 2f(x_1) + f(x_2)] = f''(x_1) = f''(x_2)$$

Example 6.3: Consider the function [$f(x)= e^x$], find f'(1) for:

1. h=0.1,
2. h=0.01,
3. h=0.001.

The exact value =2.718281828

Solution: Applying equation (8):

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

1. for h=0.1,

$$f^{'}(1) = \frac{f(1+0.1) - f(1-0.1)}{2*0.1} = \frac{3.004166024 - 2.45960311}{0.2} = 2.722814$$

2. for h=0.01,

$$f^{'}(1) = \frac{f(1+0.01) - f(1-0.01)}{2*0.01} = 2.718327$$

3. for h=0.001,

$$f^{'}(1) = \frac{f(1+0.001) - f(1-0.001)}{2*0.001} = 2.718282282$$

Problems: From the following table of values of x and y obtain (y') and (y'') for:

X	1.0	1.2	1.4	1.6	1.8	2.0	2.2
y	2.7183	3.3201	4.0552	4.953	6.0496	7.3891	9.025

1. x=1.2 ans.: y'=3.3205, y''=3.318
2. x= 2.2 ans.: y'=9.0228, y''=8.992
3. x= 1.6 ans.: y'=4.9530, y''=4.9525

solution:-

X	1.0	1.2	1.4	1.6	1.8	2.0	2.2
y	2.7183	3.3201	4.0552	4.953	6.0496	7.3891	9.025

$$f'(x_1) = P'_2(x1) = \frac{1}{2h}[f(x_2) - f(x_0)]$$

$$f'(x) = p'(x) = \frac{1}{2h^2}[(2x - x_1 - x2)f(x_0) - 2(2x - x_0 - x_2)f(x_1) + (2x - x_0 - x_1)f(x_2)] \ldots\ldots\ldots\ldots (13a)$$

X=1.2=x1

$$f'(x1) = p'(x1) = \frac{1}{2h^2}[(2*1.2 - 1.2 - 1.4)2.7183 - 2(2*1.2 - 1 - 1.4)3.3201 + (2*1.2 - 1 - 1.2)4.0552]$$

$$f'(x1) = p'(x1) = \frac{1}{2(0.2)^2}[(1.2 - 1.4)2.7183 - 2(2*1.2 - 1 - 1.4)3.3201 + (2*1.2 - 1)4.0552]$$

$$f'(x1) = p'(x1) = \frac{1}{0.08}[(-0.2)2.7183 - 2(0)3.3201 + (0.2)4.0552]$$

$$f'(1.2) = p'(1.2) = \frac{1}{0.08}[(-0.54366) - 0 + (0.811042)]=3.342275$$

$$f''(x_0) = P''_2(x_0) = \frac{1}{h^2}[f(x_0) - 2f(x_1) + f(x_2)] = f''(x_1) = f''(x_2)$$

$$f''(1.2) = P''_2(x1) = \frac{1}{(0.2)^2}[2.7183 - 2*3.3201 + 4.0552] = f''(x_1) = f''(x_2)$$

=3.3325

Numerical Integration

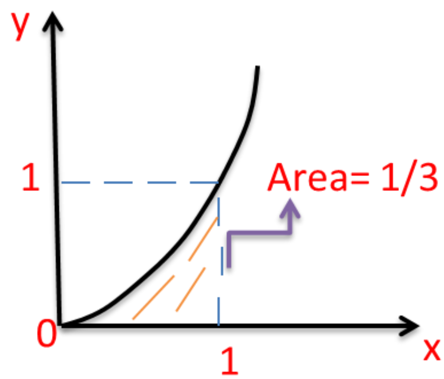
6.5- Introduction: There are two different types of integrals:
- Indefinite
- Definite

A typical indefinite integral is: $\int x^2 dx = \frac{x^3}{3}$, then the answer is a function of (x).

A typical definite integral is: $\int_0^1 x^2\, dx = 1/3,$ then the answer to this integration is a number (in this case =1/3).

Only definite integrals can be solved by computers, using several methods.

Integral can be interpreted as: " The area under the curve $y=x^2$, between the limits x=0 and x=1.



6.6-Trapezoidal method: The basic idea behind most formulas for approximating:

$$I(f) = \int_a^b f(x)dx$$

Is to replace f(x) by an approximating function whose integral can be evaluated. Those functions are based on using linear and quadratic interpolation.

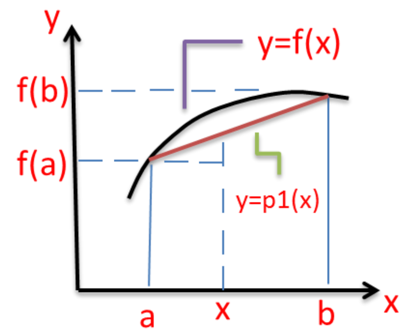
Approximate f(x) by the linear polynomial:

$$P1(x) = \frac{(b-a)*f(a)+(x-a)*f(b)}{(b-a)} \quad \ldots..(1)$$

Which interpolates f(x) at (a) and (b). The integral of P1(x) over [a,b] is the area of the trapezoid, it is given by:

$$T1(f) = (b-a)*\left[\frac{f(a)+f(b)}{2}\right] \ldots\ldots\ldots (2)$$

This approximates the integral [I(f)] if f(x) is almost linear on [a, b] interval.



Example 6.1: Approximate the integral:

$$I = \int_0^1 \frac{dx}{(1+x)} = \ln(2) = 0.693147$$

Solution:

Using equation(2) we obtain:

$$T1 = \frac{1}{2}\left[1 + \frac{1}{2}\right] = \frac{3}{4} = 0.75$$

The error is I – T1 = 0.693147 – 0.75 = -0.0569

To improve the approximation T1(f) in equation (2) , by breaking the interval [a. b] into smaller subintervals and apply equation(2) on **each** subinterval.

Example 6.2: Evaluate the preceding example by using T1(f) on two equal subintervals.

Solution: For two subintervals,

$$T2 = \int_0^{\frac{1}{2}} \frac{dx}{(1+x)} + \int_{\frac{1}{2}}^1 \frac{dx}{(1+x)}$$

$$= \frac{1}{2}\left[\frac{1+\frac{1}{2}}{2}\right] + \frac{1}{2}\left[\frac{\frac{2}{3}+\frac{1}{2}}{2}\right] = \frac{17}{24} \approx 0.70833$$

Thus I – T2 = - 0.0152 which is 25% of previous error

We can derive a general formula to simplify the calculations when using several subintervals of equal length. Let the number of subintervals be denoted by (n), and let (h) be the length of each subinterval. Then

h = (b – a)/n *…….(3)*

Thus, $\boldsymbol{xj} = \boldsymbol{a} + \boldsymbol{j} * \boldsymbol{h}(j = 0,1,2,\ldots.,n)$ ..(4)

Then the integral shall be :

$$I(f) = \int_{x0}^{x1} f(x)dx + \int_{x1}^{x2} f(x)dx + .. + \int_{x(n-1)}^{xn} f(x)dx$$

By approximating each interval using equation(2) we get:

$$I(f) \approx T(f) = h\left[\frac{f(x0)+f(x1)}{2}\right] + h\left[\frac{f(x1)+f(x2)}{2}\right] + .. + h\left[\frac{f(x4)+f(x5)}{2}\right]$$

Or $\quad Tn(f) = h\left[\frac{1}{2}f(x0) + f(x1) + f(x2) + \cdots + \frac{1}{2}f(xn)\right]$

Or $\boldsymbol{Tn(f) = \frac{h}{2}\left[\left(f(x0) + f(xn)\right) + \ 2\left(f(x1) + f(x2) + .. + f\left(x(n-1)\right)\right)\right] \ldots (5)}$

This is called "Trapezoidal Numerical Integration Rule".

Example 6.3: Evaluate $\int_{4}^{5.2} \ln(x)\, dx$ using trapezoidal rule. Take h=0.2

Solution:

Step#1: Use equation (3) to find (n):

$$n = \frac{(b-a)}{h} = \frac{(5.2-4)}{0.2} = 6$$

Step#2: Find the values of (x_j) using equation(4):

$$x0 = x0 + 0 * h = 4 + 0 = 4$$
$$x1 = x0 + 1 * h = 4 + 0.2 = 4.2$$
$$x2 = x0 + 2 * h = 4 + 2 * 0.2 = 4.4$$
$$x3 = x0 + 3 * h = 4 + 3 * 0.2 = 4.6$$
$$x4 == x0 + 4 * h = 4 + 4 * 0.2 = 4.8$$
$$x5 = x0 + 5 * h = 4 + 5 * 0.2 = 5$$
$$x6 = x0 + 6 * h = 4 + 6 * 0.2 = 5.2$$

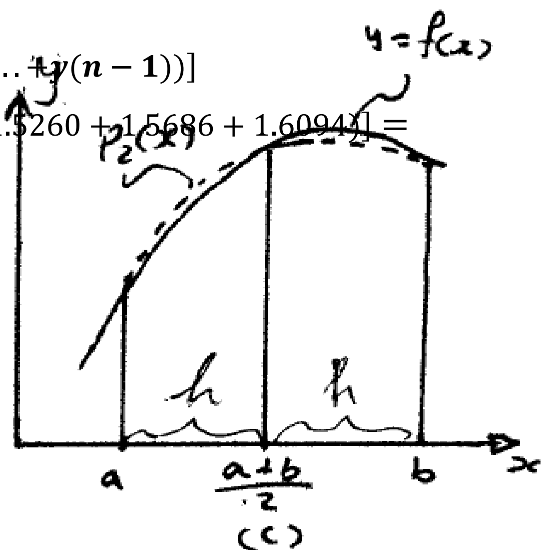
Step#3: Prepare a table for the values of x and y:

X	X0=4	4.2	4.4	4.6	4.8	5.0	5.2
Y	Y0=1.3863	1.4351	1.4816	1.5260	1.5686	1.6094	1.6486

Step#4: Apply trapezoidal rule (i.e. equation (5)):

$$\boldsymbol{Tn(f) = \frac{h}{2}\left[(y0 + yn) + \ 2(y1 + y2 + .. + y(n-1))\right]}$$

$T6(f) = \frac{0.2}{2}\left[(1.3863 + 1.6486) + \ 2(1.4351 + 1.4816 + 1.5260 + 1.5686 + 1.6094)\right] =$ 1.82764



6.7-Simpson's 1/3Rule ($S_{1/3}$):

It is to use quadratic interpolation to approximate f(x) on the range [a,b]. Let P2(x) be the quadratic polynomial that interpolates f(x) at a, b and c (where c = (a+b)/2). We get:

$$I(f) \approx \int_a^b P2(x)dx$$
$$= \int_a^b \left[\frac{(x-c)(x-b)}{(a-c)(a-b)} f(a) + \frac{(x-a)(x-b)}{(c-a)(c-b)} f(c) + \frac{(x-a)(x-c)}{(b-a)(b-c)} f(b)\right] dx \ldots..(6)$$

The complete evaluation of equation(6) is:

$$\boldsymbol{S2(f) = \frac{h}{3}[f(a) + 4f(\frac{(a+b)}{2}) + f(b)]} \quad \ldots.(7)$$

Where h=(b-a)/2 (i.e. n=2 in this case)

If we assume x0=a, x1=c and x2=b then equation(6) can be rewritten as:

$$I(f) \approx \int_a^b P2(x)dx$$
$$= \int_a^b \left[\frac{(x-x1)(x-x2)}{(x0-x1)(x0-x2)} f(x0) + \frac{(x-x0)(x-x2)}{(x1-x0)(x1-x2)} f(x1) + \frac{(x-x0)(x-x1)}{(x2-x0)(x2-x1)} f(x2)\right] dx \ldots..(6')$$

Integrating and simplifying the above equation becomes:

$$\int_{x0}^{x2} ydx = \frac{h}{3}[y0 + 4y1 + y2] \ldots\ldots\ldots\ldots\ldots(7')$$

Example 6.4: Resolve the previous example $[I = \int_0^1 \frac{dx}{(1+x)} = \ln(2)]$ using Simpson's rule for n=2.

Solution: h= (b-a)/2 = (1-0)/2 = 0.5

Then $S2 = \frac{0.5}{3}\left[1 + 4\left(\frac{2}{3}\right) + \frac{1}{2}\right] = \frac{25}{36} \approx 0.69444$

The error: I - S2= ln(2)-0.69444 = -0.0013

By applying equation (7) for (n) intervals the general **Simpson's 1/3rule** will be:

$$\boldsymbol{Sn(f) = \frac{h}{3}[f(x0) + 4f(x1) + 2f(x2) + 4f(x3) + .. + f(xn)]} \ldots(8)$$

The above integration formula can be written as:

$$\int_{x0}^{xn} ydx = \frac{h}{3}[(Sum\ of\ first\ and\ last\ terms) + 4(Sum\ of\ odd\ terms) + 2(sum\ of\ even\ terms)]$$

Note: This formula is used when there are **EVEN** number of segments (i.e. ODD number of points).

Example 6.5: Evaluate $\int_0^{\frac{3\pi}{20}} (1 + 2sinx)dx$ using Simpson's 1/3rule. Take (4) segments.

Solution: Here a=0, and b= $\frac{3\pi}{20}$ or 27^0 .
Step#1: find (h). Since we have 4 segments,
i.e. n=4 , then h=(27-0)/4 = $\frac{3\pi}{80}$ = 6.75^0
Step#2: Calculate values of x (using xj = x0 + j*h):
X0= 0+ 0*6.75 = 0
X1= 0 + 1*6.75 = 6.75..and so on to find
X2=13.5^0, x3=20.25^0 and x4=27^0

Step#3: Make the table:

X	**X0=0**	**X1=6.75**	**X2=13.5**	**X3=20.25**	**X4=27**
Y	Y0=1	Y1=1.2350748	Y2=1.4668907	Y3=1.692234	Y4=1.907981

Step#4: The last step is to apply Simpson's 1/3rule:

$$Sn(f) = \frac{h}{3}[f(x0) + 4f(x1) + 2f(x2) + 4f(x3) + .. + f(xn)]$$

$$\int_0^{\frac{3\pi}{20}} (1 + 2sinx)dx \approx \frac{\frac{3\pi}{80}}{3}[(1 + 1.90798) + 4(1.2350748 + 1.6922341) + 2(1.466890)]$$
$$= 0.689226$$

6.8-Simpson's 3/8Rule ($S_{3/8}$):

In Simpson's 1/3rule, we approximate the three points by a parabola (quadratic). Let us consider that four points are taken and they are interpolated by a polynomial of degree (3). This polynomial is integrated to obtain approximate integration of given function. This method is then called Simpsons' 3/8rule.

6.8.1-Derivation of Simpson's 3/8rule:

Let the four points be (x0,y0), (x1,y1), (x2,y2) and (x3,y3). The given function can be approximated by Lagrange's 3rd degree polynomial. i.e. :

$$f(x)=\frac{(x-x1)(x-x2)(x-x3)}{(x0-x1)(x0-x2)(x0-x3)}*f(x0)+\frac{(x-x0)(x-x2)(x-x3)}{(x1-x0)(x1-x2)(x1-x3)}*f(x1)+\frac{(x-x0)(x-x1)(x-x3)}{(x2-x0)(x2-x1)(x2-x3)}*f(x2)+\frac{(x-x0)(x-x1)(x-x2)}{(x3-x0)(x3-x1)(x3-x2)}*f(x3)$$

Integrating and simplifying the above equation we get:

$$\int_{x0}^{x3} ydx=\frac{(x3-x0)}{8}[f(x0)+3f(x1)+3f(x2)+f(x3)]$$

Or if h=(x3-x2)=(x2-x1)=(x1-x0) ,   hence (x3-x0)=3h

Thus,

$$\int_{x0}^{x3} ydx=\frac{3h}{8}[f(x0)+3f(x1)+3f(x2)+f(x3)]$$

Or can be written :

$$\int_{x0}^{x3} ydx=\frac{3h}{8}[y0+3y1+3y2+y3]$$

The general formula for n>3 segments will be:

$$\int_{x0}^{xn} ydx=\frac{3h}{8}[(y0+yn)+3(y1+y2+y4+y5+..)+2(y3+y6+y9+....)]........(9)$$

This formula can also be written as:

$$\int_{x0}^{x3} ydx=\frac{3h}{8}[(sum\ of\ first\ and\ last\ term)+3(Sum\ of terms\ which\ are\ not\ multiple\ of\ 3)+2(Sum\ of\ terms\ which\ are\ multiple\ of\ 3))]$$

Example 6.6: Evaluate $\int_0^{\pi}\frac{sin^2\theta}{5+4cos\theta}d\theta$ by Simpson's 3/8rule taking (h=$\pi/6$).

Solution: Here   y= $\sin^2\theta/(5+4cos\theta)$

Number of segments = $\frac{(\pi-0)}{\frac{\pi}{6}}=6$,   i.e. n=6

The values of (θ) and (y) are given in the table:

θ	$\theta0$=0	$\theta1=\pi/6$	$\theta2=\pi/3$	$\theta3=\pi/2$	$\theta4=2\pi/3$	$\theta5=5\pi/6$	$\theta6=\pi$
Y	0	0.0295365	0.1071428	0.2	0.25	0.162771	0

Last step is to apply Simpson's 3/8rule:

$$\int_{x0}^{xn} ydx = \frac{3h}{8}[(y0 + yn) + 3(y1 + y2 + y4 + y5+..) + 2(y3 + y6 + y9+....)]$$

$$\int_{x0}^{xn} ydx = \frac{3h}{8}[(0 + 0) + 3(0.0295365 + 0.1071428 + 0.25 + 0.1627711) + 2(0.2)]$$

= 0.4021928

The table below shows the relation between the number of points, segments and the method to be used:

Points	**2**	**3**	**4**	**5**	**6**	**7**	**8**	**9**	**10**
Segments	1	2	3	4	5	6	7	8	9
Trap.Rule	Y	Y	Y	Y	Y	Y	Y	Y	Y
Simpson1/3	N	Y	N	Y	N	Y	N	Y	N
Simpson3/8	N	N	Y	N	N	Y	N	N	Y

Example 6.7: Consider the integral ($I = \int_0^2 \frac{x}{\sqrt{2+x^2}} dx$). Use number of segments (n=5)then integrate using:

1. Simpson's rules
2. Trapezoidal method

Solution: h=(b-a)/n = (2-0)/5 = 0.4

Thus, x0=0, x1=0.4, x2=0.8, x3=1.2, x4=1.6, x5=2.0

Y=f(x)=$\frac{x}{\sqrt{2+x^2}}$ so we must find y0..y_n and put it in a table:

X	**0**	**0.4**	**0.8**	**1.2**	**1.6**	**2.0**
Y=f(x)	0	0.2721	0.4923	0.647	0.7492	0.81649

3. Since n=5, then ($S_{1/3}$, or $S_{3/8}$) cannot be used for the whole interval, so we shall use ($S_{3/8}$) for the first three segments, then we can use ($S_{1/3}$) for the last two segments as follows:

$$\int_{x0}^{xn} ydx = \frac{3h}{8}[(y0 + yn) + 3(y1 + y2 + y4 + y5+..) + 2(y3 + y6 + y9+....)]$$

$S_{3/8}$= $\frac{3*0.4}{8}[(0 + 0.647) + 3(0.2721 + 0.4923)] = 0.44103$

$$\int_{x0}^{xn} ydx = \frac{h}{3}[f(x0) + 4f(x1) + 2f(x2) + 4f(x3)+..+f(xn)]$$

$S_{1/3}$ =$\frac{0.4}{3}[(0.647 + 0.81649) + 4(0.7492)] = 0.5947$

Thus S = $S_{3/8}$ + $S_{1/3}$ = 0.44103+0.5947 = 1.03573

4. Solving using trapezoidal method:

$$Tn(f) = \frac{h}{2}[(f(x0) + f(xn)) + 2(f(x1) + \cdots + f(x(n-1))]$$

$$T5(f) = \frac{0.4}{2}[(0 + 0.81649) + 2(0.2721 + 0.4923 + 0.647 + 0.7492)]$$

= 1.027538

6.9-Integration with unequal segments:

All previous formulas have been for equally spaced data points. In practice there are many situations where this assumption does not hold and we must deal with unequal-sized segments. For example, experimental derived data is often of this type. For these cases we can use two ways:

5. First way, is to apply the trapezoidal rule to each segment (multiple application of trapezoidal method) and sum the results.

$$I(f) \approx h1\frac{f(x1) + f(x0)}{2} + h2\frac{f(x2) + f(x1)}{2} + .. + hn\frac{f(xn) + f(x(n-1))}{2}$$

6. Second way, If some of the data have equi-distance then we can apply Simpson's 1/3rule for even number of segments and Simpson's 3/8rule for number of segments which is multiple of (3).

Example 6.8: Determine the integral for the data in the table.

X	**0**	**0.12**	**0.22**	**0.32**	**0.36**	**0.4**	**0.44**	**0.54**	**0.64**	**0.7**	**0.8**
F(x)	0.2	1.31	1.3	1.74	2.07	2.45	2.84	3.51	3.18	2.36	0.23

Note: Exact answer is (1.6405).

Solution #1:

Make a table for (h) values:

H	**0.12**	**0.1**	**0.1**	**0.04**	**0.04**	**0.04**	**0.1**	**0.1**	**0.06**	**0.1**

Apply trapezoidal rule to the data we get:

$$I(f) = 0.12\left\{\frac{1.31 + 0.2}{2}\right] + 0.1\left[\frac{1.3 + 1.31}{2}\right] + .. + 0.1[\frac{0.23 + 2.36}{2}]$$

=1.5935

$$\epsilon r\% = \frac{(1.5935 - 1.6405)}{1.6405} * 100 = 2.88\%$$

Solution #2: From the (h) table notice that there are some adjacent equal values, so for those equal values we can apply Simpson's rule in the following way:

With (h1) use trapezoidal method
With (h2,h3) use Simpson's 1/3rule
With (h4,h5,h6) use Simpson's 3/8rule
With (h7,h8) use Simpson's 1/3rule
With (h9) use trapezoidal rule
With (h10) use trapezoidal rule
Complete the solution and compare the result with solution#1.

Problems:

7. Evaluate the integral $(I = \int_0^1 \sqrt{x}\,dx = \frac{2}{3})$ using Simpson's rules for n= 2, 3,4,8 and 9, and find the relative error in each case.
8. Use trapezoidal rule to solve $(I = \int_0^2 \frac{x}{\sqrt{2+x^2}}\,dx)$. Take n=4.
9. The velocity of a car at intervals of (2) minutes are given below

Time(min)	**0**	**2**	**4**	**6**	**8**	**10**	**12**
Velocity(km/h)	0	22	30	27	18	7	0

Find the distance covered by the car using Simpson's 1/3rule.
Answer: 3.5555km.