Chapter 3

Numerical Differentiation :-

Numerical differentiation is the process of obtaining the value of derivative of a function from a set of numerical value of that function. There are basically, two situations, where numerical differentiation is required

① Differentiation of continuous function is required when the function to be differentiated is complicated and it is difficult to differentiate.

② Differentiation of discrete function is required when functional value at some discrete points are known but function is unknown.

1. Differentiating ~~continuous~~ function :-

In this, we discuss the process of approximating the derivatives; $f'(x)$ of a function $f(x)$, when the function itself is available. If the function becomes too complex it is sometimes easier to differentiate numerically rather than analytically.

2. Forward Difference Approximation from Taylor's series.

Taylor's Theorem says that

If we know the value of a function $f(x)$ at point a and all its derivatives at that point, provided the derivatives are continuous between x_i and x_{i+1}, then

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

Let us consider that,

$$h = x_{i+1} - x_i$$

then,

$$f(x_i + h) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \cdots$$

$$\Rightarrow f'(x_i) = \frac{f(x_i+h) - f(x_i)}{h} - \frac{f''(x_i)}{2!}h^2 + \cdots$$

$$\therefore f'(x_i) = \frac{f(x_i+h) - f(x_i)}{h} + E$$

$$\boxed{f'(x_i) \simeq \frac{f(x_i+h) - f(x_i)}{h}} \quad \text{(1)}$$

Backward

$$f'(x) = \frac{f(x) - f(x-h)}{h}$$

Here, E is the error term in the approximation. This equation (1) is called Two point forward difference formula.

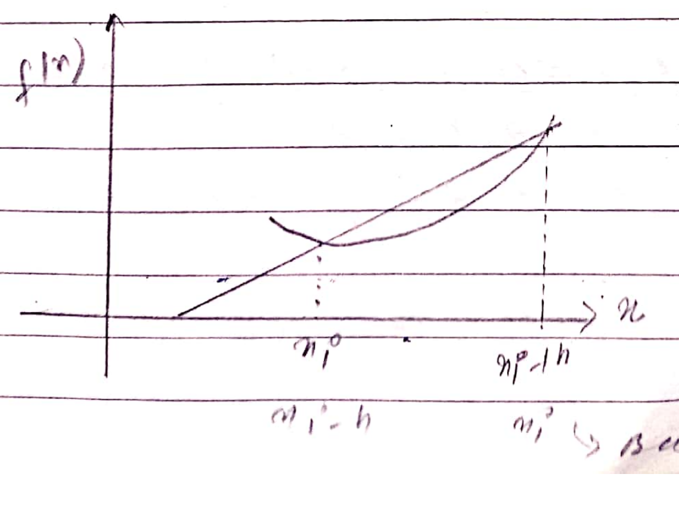


fig: Graphical representation of forward difference approximation of first order derivate.

8. Find value of derivative at $x=1$ for a function $f(x)=x^2$ use $h=0.2$ and 0.5

⇒ **Soln:** for $h=0.2$ ⇒ case I

$f(x)=x^2$

$f(1)=1$

$f(x+h)=(x+h)^2$

$= (1+0.2)^2$

$= 1.44$

$f'(x)=2x$

$f'(1)=2$

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

$$= \frac{1.44-1}{0.2}$$

$= 2.2$

For $h=0.5$ ⇒ Case II

$f(x+h) = (1+0.5)^2 = 1.1025$

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

$$= \frac{1.1025-1}{0.5}$$

$= 2.05$

Now, $f'(x)=2x$ ~~at x=1~~

At $x=1$, $f'(x)=2$ (exact value)

So,

$$\text{Error} = \left|\frac{\text{Exact value} - \text{approx. value}}{\text{Exact value}}\right| \times 100\%$$

For case I, $h=0.2$, $f'(x)=2.2$

$$E = \left|\frac{2-2.2}{2}\right| \times 100\% = 10\%$$

$h=0.5$, $f'(x)=2.05$, $E = \left|\frac{2-2.05}{2}\right| \times 100\%$

$= 2.5\%$

Algorithm:

1. Start
2. Read x, h and f(x)
3. Calculate f(x+h) and f(x)
4. Calculate $f'(x) = \frac{f(x+h) - f(x)}{h}$
5. Display f'(x)
6. Stop

6. <u>Backward Difference Approximation:</u>

Taylor's Theorem says that if we know the value of a function f(x) at point a and all its derivatives at that point, provided the derivatives are continuous between x_i and x_{i-1}, then

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

~~Let us consider that,~~

$$h = x_{i-1} - x_i$$

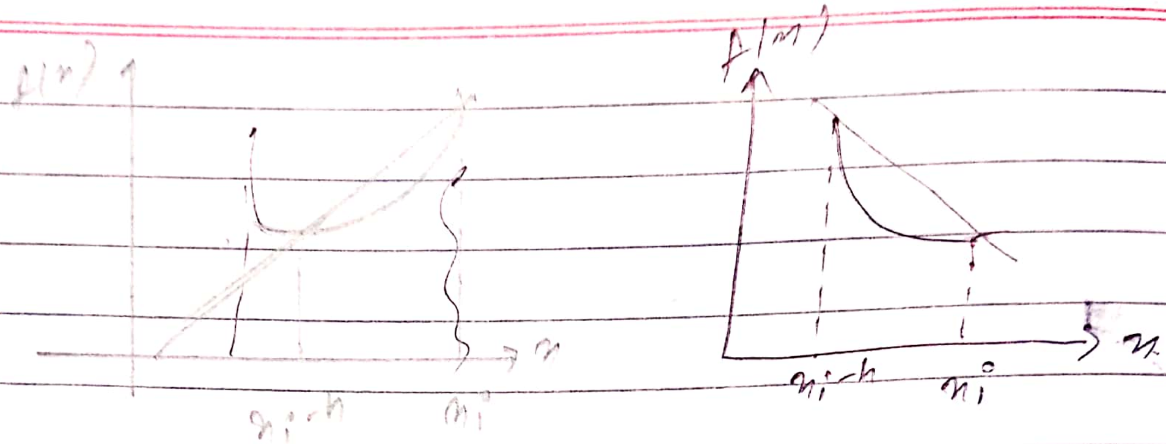
$$f(x_i - h) = f(x_i) - f'(x_i)h + \frac{f''(x_i)h^2}{2!} - \ldots$$

$$f'(x_i) = \frac{f(x_i) - f(x_i - h)}{h} + \frac{f''(x_i)h^2}{2!} - \ldots$$

$$\therefore f'(x_i) = \frac{f(x_i) - f(x_i - h)}{h} + E$$

$$\boxed{f'(x) \approx \frac{f(x_i) - f(x_i - h)}{h}} \leftarrow \text{(II)}$$

Here E is the error term in the approxim.
This eqn is called two point backward difference formula.



fig'n Graphical Representation of backward difference

Algorithm for Backward Difference Approx.

1. Start
2. Read x, h and $f(x)$
3. Compute $f(x)$ and $f(x-h)$
4. Compute $f'(x) = \dfrac{f(x) - f(x-h)}{h}$
5. print $f'(x)$
6. Stop

Q. Find value of derivative at $x=1$ for a function $f(x)=x^2$ use $h=0.2$ & 0.5 {Backward difference}

⇒ Soln:

Case I : for $h=0.2$

$f(x)=x^2$, ~~ft~~

At $x=1$ $f(1)=1$

$f(x-h)=(x-h)^2=(1-0.2)^2=0.64$

$$f'(x)=\frac{f(x)-f(x-h)}{h}=\frac{1-0.64}{0.2}=1.8$$

Case II : for $h=0.5$, $x=1$

$f(x-h)=(x-h)^2=(1-0.5)^2=0.25$

$$f'(x)=\frac{f(x)-f(x-h)}{h}=\frac{1-0.25}{0.5}=1.5$$

Now,

$f'(x)=2x$

At $x=1$, $f'(x)=2$

So,

$$\text{Error}=\left|\frac{\text{Exact value}-\text{approx. value}}{\text{Exact value}}\right|\times 100\,\%$$

For, $h=0.2$, $f'(x)=1.8$

$$E=\left|\frac{2-1.8}{2}\right|\times 100\,\%=10\,\%$$

For $f'(x)=1.5$

$$E=\left|\frac{2-1.5}{2}\right|\times 100\,\%=25\,\%$$

c. **Central Difference Approximation from Taylor Theorem.**

$$f(x_i+h) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{3!}h^3 + \dots \quad \text{--- (I)}$$

$$f(x_i-h) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f'''(x_i)}{3!}h^3 + \dots \quad \text{--- (II)}$$

Now, subtracting eq^n (II) from (I) we get,

$$f(x_i+h) - f(x_i-h) = 2f'(x_i)h + 2\frac{f'''(x_i)}{3!}h^3 + \dots \quad \text{(III)}$$

Thus we have,

$$f'(x_i) = \frac{f(x_i+h) - f(x_i-h)}{2h} + E$$

$$\therefore f'(x_i) = \frac{f(x_i+h) - f(x_i-h)}{2h} \quad \text{--- (iv)}$$

Eq^n (iv) is called the central difference approximation. This is also known as three-point formula.

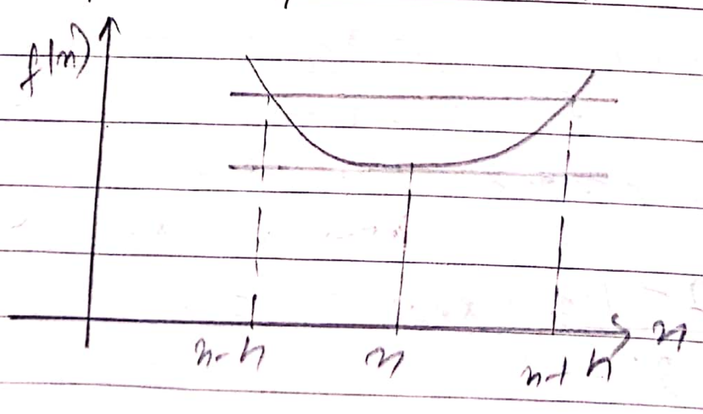


fig: Illustration of Three-point formula

Q. Find the value of derivative at $x=1$ for a function $f(x)=x^2$. Use $h=0.2$ and 0.05 for central difference approximation.

$\Rightarrow$ Soln:

Case I: For $h=0.2$

$f(x)=x^2$

At $x=1$, $f(1)=1$

$f(x+h)=(1+0.2)^2=1.44$

$f(x-h)=(1-0.2)^2=0.64$

$$f'(x)=\frac{f(x+h)-f(x-h)}{2h}=\frac{1.44-0.64}{2\times0.2}=2$$

Case II For $h=0.05$

At $x=1$ $f(1)=1$

$f(x+h)=(1+0.05)^2=1.1025$

$f(x-h)=(1-0.05)^2=0.9025$

$$f'(x)=\frac{f(x+h)-f(x-h)}{2h}=\frac{1.1025-0.9025}{2\times0.05}=2$$

Algorithm:

1. Start
2. Read x, h and $f(x)$
3. Compute $f(x+h)$ and $f(x-h)$
4. Compute $f'(x)=\frac{f(x+h)-f(x-h)}{2h}$
5. Display $f'(x)$
6. Stop

$a_0 + a_1(x - x_0)$

Differentiating Discrete (Tabulated) Functions

Let us consider that we are given a set of data points (x_i, f_i), $i = 0, 1, \ldots n$ which correspond to the values of an unknown function $f(x)$ and we want to estimate the derivatives at these points. Two situations exists here:

a) If the data points are ~~eq~~ unequally spaced then we should use Newton's Divided Difference formula.

b. If the data points are equally spaced, we will use Newton forward formula, if we want to find the derivative of the function at a point near to beginning. If we want to find the derivative of the function at a point near to end we will use Newton backward difference formula.

a. Derivation using Newton's Divided Difference formula:- (Data points are unequally spaced)

We know that, the general form of the Newton's divided difference polynomial for $(x_0, y_0), (x_1, y_1) \ldots (x_n, y_n)$ is given as:-

$$P_n(x) = f(x) = a_0 + a_1(x - x_0) + a_2(x - x_0)(x - x_1) + \ldots + a_n(x - x_0)(x - x_1)\ldots(x - x_{n-1})$$

$$P_n(x) = f[x_0] + f[x_1, x_0](x - x_0) + \ldots + f[x_n, x_{n-1} \ldots x_1, x_0](x - x_0)(x - x_1)\ldots(x - x_{n-1}) \rightarrow (1)$$

$$= f[x_0] + \sum_{i=1}^{n} f[x_0, x_1, \ldots x_n] \prod_{j=0}^{i-1} (x - x_j)$$

where the definitions of the m^{th} divided difference is

$$f[x_m \ldots x_0] = \frac{f[x_m \ldots x_1] - f[x_{m-1} \ldots x_0]}{x_m - x_0}$$

Differentiating eq^n ① w.r.t x we get

(By product rule) $f'(x) = f[x_1, x_0] + f[x_2, x_1, x_0]\{(x - x_1) + (x - x_0)\} + f[x_3, x_2, x_1, x_0]\{(x - x_1)(x - x_2) + (x - x_0)(x - x_2) + (x - x_0)(x - x_1)\} + \ldots$ — ②

By putting $x = a$ in eq^n ② we can get value of first derivative at $x = a$.

Again, differentiating eq^n ② w.r.t x, we get

$f''(x) = 2f[x_2, x_1, x_0] + 2f[x_3, x_2, x_1, x_0]\{(x - x_0) + (x - x_2)\} + \ldots$ — ③

By putting $x = a$ in eq^n ③ we get value of second derivative at $x = a$.

Q. Find $f'(10)$ from the following table:

x	3	5	11	27	34
$f(x)$	-13	23	899	17315	35606

Soln:

⇒ Since data point are unevenly spaced so we use the Newton's divided formula. The Newton's divided difference table is given as:-

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II Find $f'(10)$ from the following table:

x	3	5	11	27	34
$f(x)$	-13	23	899	17315	35606

⇒ ~~Sol~~ⁿ:

Since data values are ~~unequal~~ & unevenly distributed so we use Newton's divided difference table

x	$f(x)$	1st diff	2nd diff	3rd diff	4th diff
3	-13				
		$18 = \frac{23+13}{2}$			
5	23		16		
		146		1	
11	899		40		0
		1026		1	
27	17315		69		
		2613			
34	35606				

$$f'(x) = f[x_1, x_0] + f[x_2, x_1, x_0]\{(x-x_1)+(x-x_0)\} + f[x_3, x_2, x_1, x_0]\{(x-x_1)(x-x_2)+(x-x_0)(x-x_2)+(x-x_0)(x-x_1)\} + f[x_4, x_3, x_2, x_1, x_0]\{(x-x_1)(x-x_2)(x-x_3)+(x-x_0)(x-x_1)(x-x_2)+(x-x_0)(x-x_1)(x-x_3)+(x-x_0)(x-x_2)(x-x_3)\}$$

$$f'(10) = 18 + 16\{(10-5)+(10-3)\} + 1\{(10-5)(10-11) + (10-3)(10-11) + (10-3)(10-5)\} + 0$$

$$= 233$$

$$f''(x) = 2f[x_2, x_1, x_0] + 2f[x_3, x_2, x_1, x_0]\{(x-x_0)+(x-x_2)\}$$

Algorithm for Derivation using Newton's Divided difference

1. Read number of points say n.
2. Read n data points.
3. Read the value at which derivative is needed say x.
4. for i = 0 to n-1
   dd[i] = fx[i]
5. for i = 0 to n-1
   for j = n-1 to i+1
   $$dd[j] = \frac{dd[j] - dd[j-1]}{x[j] - x[j-1-i]}$$
   end for
   end for
6. vod = dd[1]
7. for i = 2 to n-1
8. term = 0
   for j = 0 to i
   for k = 0 to i
   if (j != k)
   factor = factor * (x - x[k])
   end for
   term = term + factor
   end for
   vod = vod + (dd[i] * term)
   end for
9. Print the value of vod

Numerical Differentiation

b. **Equally spaced data:**

1. Derivative Using Newton's forward difference formula.

Let us consider the n+1 data points as $(x_0, f(x_0)), (x_1, f(x_1)), \ldots (x_n, f(x_n))$. Now, Newton's forward difference formula for n+1 data points can be written as:

$$f(x) = f(x_0) + s\Delta f(x_0) + \frac{1}{2!} s(s-1)\Delta^2 f(x_0) +$$

$$\frac{1}{3!} s(s-1)(s-2)\Delta^3 f(x_0) + \ldots \quad \text{— } (1)$$

where, $s = \frac{(x - x_0)}{h}$

Now, differentiating eqn (1) wrt x we get

use product rule

$$f'(x) = \frac{d}{ds}\left[f(x_0) + s\Delta f(x_0) + \frac{1}{2!} s(s-1)\Delta^2 f(x_0) + \right.$$

$s\frac{d(s-1)}{ds} + (s-1)\frac{ds}{ds}$

$$\left.\frac{1}{3!} s(s-1)(s-2)\Delta^3 f(x_0) + \ldots\right] \frac{ds}{dx}$$

$$= \left[\Delta f(x_0) + \frac{1}{2!}(2s-1)\Delta^2 f(x_0) + \frac{1}{3!}(3s^2 - 6s + 2)\Delta^3 f(x_0) + \right.$$

$$\left.\frac{1}{4!}(4s^3 - 18s^2 + 22s - 6)\Delta^4 f(x_0) + \ldots\right] \frac{ds}{dx} \quad \text{— } (2)$$

$$\left\{\text{Since, } \quad s = \frac{x - x_0}{h} \Rightarrow \frac{ds}{dx} = \frac{1}{h}\right\}$$

Now, eqn (2) becomes,

$$f'(x) = \frac{1}{h}\left[\Delta f(x_0) + \frac{1}{2!}(2s-1)\Delta^2 f(x_0) + \frac{1}{3!}(3s^2-6s+2)\Delta^3 f(x_0) + \frac{1}{4!}(4s^3-18s^2+22s-6)\Delta^4 f(x_0) + \cdots \right] \quad \text{--- (3)}$$

By putting $x = a$ eq^n (3) can be used to find the value of first derivative at the point $x = a$.

Again, differentiating eq^n (3) wrt x we get

$$f''(x) = \frac{d}{ds}\left[\frac{1}{h}\left\{ \Delta f(x_0) + \frac{1}{2!}(2s-1)\Delta^2 f(x_0) + \frac{1}{3!}(3s^2-6s+2)\Delta^3 f(x_0) + \frac{1}{4!}(4s^3-18s^2+22s-6)\Delta^4 f(x_0) + \cdots \right\}\right]\frac{ds}{dx}$$

$$\left[\frac{ds}{dx} = \frac{1}{h}\right]$$

$$= \frac{1}{h}\left\{ \Delta^2 f(x_0) + \frac{1}{3!}(6s-6)\Delta^3 f(x_0) + \frac{1}{4!}(12s^2-36s+22)\Delta^4 f(x_0) + \cdots \right\}\frac{ds}{dx}$$

$$= \frac{1}{h^2}\left\{ \Delta^2 f(x_0) + \frac{1}{3!}(6s-6)\Delta^3 f(x_0) + \frac{1}{4!}(12s^2-36s+22)\Delta^4 f(x_0) + \cdots \right\} \quad \text{--- (4)}$$

By putting $x = a$ in eq^n (4) can be used to find the value of second derivative at point $x = a$.

Example :

Find the first and second derivatives of the functions tabulated below at the point 1.1

x	1	1.2	1.4	1.6	1.8	2
$f(x)$	0	0.128	0.544	1.296	2.432	4

⇒ Sol^n:

$$s = \frac{x - x_0}{h} = \frac{1.1 - 1}{0.2} = 0.5$$

x	$f(x)$	$\Delta f(x_0)$	$\Delta^2 f(x_0)$	$\Delta^3 f(x_0)$	$\Delta^4 f(x_0)$	$\Delta^5 f(x_0)$
1	0					
		0.128				
1.2	0.128		0.288			
		0.416		0.048		
1.4	0.544		0.336		0	
		0.752		0.048		0
1.6	1.296		0.384		0	
		1.136		0.048		
1.8	2.432		0.432			
		1.568				
2	4					

1st derivative

$$f'(1.1) = \frac{1}{h}\Big[\Delta f(x_0) + \frac{1}{2!}(2s-1)\Delta^2 f(x_0) + \frac{1}{3!}(3s^2 - 6s + 2)$$

$$\Delta^3 f(x_0) + \frac{1}{4!}(4s^3 - 18s^2 + 22s - 6)\Delta^4 f(x_0) +$$

$$\frac{1}{5!}($$

$$= \frac{1}{0.2}\Big[0.128 + \frac{1}{2}(2\times 0.5 - 1) + \frac{1}{6}(3\times 0.25 - 6\times 0.5 + 2)\times 0.048$$

$$+ 0 + 0$$

$$= 0.63$$

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Second derivative:

$$f''(1.1) = \frac{1}{h^2}\left[\Delta^2 f(x_0) + \frac{1}{3!}(6S-6)\Delta^3 f(x_0) + \frac{1}{4!}(12S^2-36S+\cdot)\right.$$
$$\left.\Delta^4 f(x_0) + 0\right]$$

$$= \frac{1}{(0.2)^2}\left[0.288 + \frac{1}{6}(6\times 0.5-6)\, 0.048 + 0 + 0\right]$$

$$= 6.6$$

Q. Compute from following table the value of the derivatives of $y=f(x)$ at $x = 1.7489$

x	1.73	1.74	1.75	1.76	1.77
y	1.772844100	1.552040006	1.737799435	1.720448638	1.7033293

→ Soln:

x	$f(x)$	$\Delta f(x_0)$	$\Delta^2 f(x_0)$	$\Delta^3 f(x_0)$	$\Delta^4 f(x_0)$
1.73	1.772844100				
		−0.220804094			
1.74	1.55204006		0.406503415		
		0.185699375		−0.609493587	
1.75	1.737739435		−0.202990172		0.8126558
		−0.017290797		0.203162219	
1.76	1.720448638		0.000172047		
		−0.01711875			
1.77	1.703329888				

$$S = \frac{1.7489 - 1.73}{0.01}$$

$$= 1.89$$

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$$f'(1.7489) = \frac{1}{h}\left[\Delta f(x_0) + \frac{1}{2!}(2s-1)\Delta^2 f(x_0) + \frac{1}{3!}(3s^2-6s+2)\Delta^3 f(x_0) + \frac{1}{4!}(4s^3-18s^2+22s-6)\Delta^4 f(x_0)\right]$$

$$= \frac{1}{0.01}\left[-0.22080404 + \frac{1}{2}(2\times0.01-1)\,0.406503415 + \frac{1}{6}(3\times(1.89)^2 - 6\times1.89+2)\times-0.60949358 + \frac{1}{24}\,4\times(1.89)^3 - 18\times(1.89)^2 + 22\times1.89 - 6\times0.812655806\right]$$

$=$

II Derivatives using Newton's Backward Difference formula.

Let us consider the $n+1$ data points are $(x_0, f(x_0)), \ldots (x_n, f(x_n))$. Now, Newton's backward difference formula for $n+1$ data points can be written as,

$$f(x) = f(x_n) + s\nabla f(x_n) + \frac{s(s+1)}{2!}\nabla^2 f(x_n) + \cdots \quad (1)$$

where $s = \frac{x - x_n}{h}$

Now, Differentiating eq^n (1) wrt x we get,

$$f'(x) = \frac{d}{ds}\left[f(x_n) + s\nabla f(x_n) + \frac{s(s+1)}{2!}\nabla^2 f(x_n) + \frac{s(s+1)(s+2)}{3!}\nabla^3 f(x_n) + \frac{s(s+1)(s+2)(s+3)}{4!}\nabla^4 f(x_n)\right] ds/dx \quad (2)$$

$$s = \frac{x - x_n}{h} \Rightarrow \frac{ds}{dx} = 1/h$$

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Now, eq^n 2 becomes,

$$f'(x) = \frac{1}{h}\Big[\nabla f(x_n) + \frac{1}{2!}(2s+1)\nabla^2 f(x_n) + \frac{1}{3!}(3s^2+6s+2)\nabla^3 f(x_n) + \frac{1}{4!}(4s^3+18s^2+22s+6)\nabla^4 f(x_n) + \cdots\Big] \quad \text{--- } (3)$$

By putting $x = a$ eq^n (3) can be used to find the value of first derivative at the point $x = a$.

Again, differentiating eq^n (3) w.r.t x,

$$f''(x) = \frac{d}{ds}\Big[\frac{1}{h}\Big(\nabla f(x_n) + \frac{1}{2!}(2s+1)\nabla^2 f(x_n) + \frac{1}{3!}(3s^2+6s+2)\nabla^3 f(x_n) + \frac{1}{4!}(4s^3+18s^2+22s+6)\nabla^4 f(x_n) + \cdots\Big]\frac{ds}{dx}$$

$$= \frac{1}{h^2}\Big(\nabla^2 f(x_n) + \frac{1}{3!}(6s+6)\nabla^3 f(x_n) + \frac{1}{4!}(12s^2+36s+22)\nabla^4 f(x_n) + \cdots\Big] \quad \text{--- } (4)$$

By putting $x = a$ in eq^n (4) can be used to find the value of second derivative at point $x = a$.

Q. The table below gives the values of distance travelled by a car at various time intervals during the initial running.

x(sec)	5	6	7	8	9
f(x) km	10	14.5	19.5	22.5	32.0

Estimate velocity and acceleration at time $t=5$ and $t=9$.

⇒ Sol^n:

x	$f(x)$	$\Delta f(x_0)$ / $\nabla f(x_n)$	$\Delta^2 f(x_0)$ / $\nabla^2 f(x_n)$	$\Delta^3 f(x_0)$ / $\nabla^3 f(x_n)$	$\Delta^4 f(x_0)$ / $\nabla^4 f(x_n)$
5	10				
		4.5			
6	14.5		0.5		
		5		-2.5	
7	19.5		-2		11
		3		8.5	
8	22.5		6.5		
		9.5			
9	32.0				

For forward,

$$s = \frac{x - x_0}{h} = \frac{5-5}{1} = 0$$

Velocity is given by:

$$f'(5) = \frac{1}{h}\Big[4.5 + \frac{1}{2}(2\times 0-1)\times 0.5 + \frac{1}{6}(3\times 0 - 6\times 0 + 2)\times$$

$$-2.5 + \frac{1}{24}(4\times 0 - 18\times 0 + 22\times 0 - 6)\times 11$$

$= 0.77666$ km/sec

Acceleration is given by:

$$f''(x) = \frac{1}{h^2}\left[\Delta^2 f(x_0) + \frac{1}{3!}(6s-6)\Delta^3 f(x_0) + \frac{1}{4!}(12s^2-36s+22)\Delta^4 f(x_0)\right]$$

$$= \frac{1}{1}\left[0.5 + \frac{1}{6}(6\times 0-6)\times -2.5 + \frac{1}{24}(12\times 0-36\times 0+22)\times 11\right]$$

$$= 13.0833 \text{ km/sec}^2$$

For backward:

$$s = \frac{x-x_n}{h} = \frac{9-9}{1} = 0$$

velocity:

$$f'(9) = \frac{1}{h}\left[\nabla f(x_n) + \frac{1}{2!}(2s+1)\nabla^2 f(x_n) + \frac{1}{3!}(3s^2+6s+2)\nabla^3 f(x_n) + \frac{1}{4!}(4s^2+18s^2+22s+6)\nabla^4 f(x_n)\right]$$

$$= \frac{1}{1}\left[9.5 + \frac{1}{2}(2\times 0+1)\times 6.5 + \frac{1}{6}(3\times 0+6\times 0+2)\times 8.5 + \frac{1}{24}(4\times 0+18\times 0+22\times 0+6)\times 11\right]$$

$$= 18.3333 \text{ km/sec}$$

Acceleration:

$$f''(g) = \frac{1}{h^2}\left[\nabla^2 f(x_n) + \frac{1}{3!}(6s+6)\nabla^3 f(x_n) + \frac{1}{4!}(12s^2+36s+22)\nabla^4 f(x_n)\right]$$

$$= \frac{1}{1}\left[6.5 + \frac{1}{6}(6\times0+6)\times8.5 + \frac{1}{24}(12\times0+36\times0+22)\times11\right]$$

$= 25.0833$ km/sec^2

II Maxima and Minima of Tabulated value:

The maximum and minimum values of a function can be computed by equating first order derivatives of the function to zero and solving for unknown variables. The similar concept can be applied to determine the maxima and minima of tabulated functions.

We know that Newton's ~~formula~~ forward difference formula is given by,

$$f(x) = f(x_0) + s\Delta f(x_0) + \frac{s(s-1)}{2!}\Delta^2 f(x_0) + \frac{s(s-1)(s-2)}{3!}\Delta^3 f(x_0) \quad \text{--- (1)}$$

where, $s = \frac{x-x_0}{h}$

Differentiating eq^n (1) wrt x we get,

$$f'(x) = \frac{1}{h}\left\{\Delta f(x_0) + \frac{1}{2!}(2s-1)\Delta^2 f(x_0) + \frac{1}{3!}(3s^2-6s+2)\Delta^3 f(x_0) \cdots\right\} \quad \text{--- (2)}$$

for maxima or minima $f'(x)$ must be zero.
By retaining the terms after third order difference in RHS and equating it with zero, we get

$$\Delta f(x_0) + \frac{1}{2!}(2s-1)\Delta^2 f(x_0) + \frac{1}{3!}(3s^2-6s+2)\Delta^3 f(x_0) = 0$$

multiply

$$\Rightarrow \{\Delta f(x_0) - \frac{1}{2}\Delta^2 f(x_0) + \frac{1}{3}\cdot\Delta^3 f(x_0)\} + \{\Delta^2 f(x_0) - \Delta^3 f(x_0)\}s + \frac{1}{2}\Delta^3 f(x_0)s^2 = 0$$

$$\Rightarrow as^2 + bs + c = 0 \quad \text{--- (3)}$$

where,

$$a = \frac{1}{2}\Delta^3 f(x_0)$$
$$b = \Delta^2 f(x_0) - \Delta^3 f(x_0)$$
$$c = \Delta f(x_0) - \frac{1}{2}\Delta^2 f(x_0) + \frac{1}{3}\Delta^3 f(x_0)$$

Eqn (3) is quadratic in 's' and can be solved. Then values of x can be computed from the relation,

$$x = x_0 + sh$$

Example:

Data ____
Page ____

Algorithm:

1. Read number of data points say n.
2. Read n data points, say $x[i]$ and $fx[i]$.
3. Calculate $h = x[i] - x[0]$
4. for $i = 0$ to $n-1$

   $fd[i] = fx[i]$
5. for $i=0$ to $n-1$

   for $j = n-1$ to $i+1$

   $fd[j] = fd[j] - fd[j-1]$

   end for

   end for
6. Compute the values

   $a = \frac{1}{2} fd[3]$

   $b = fd[2] - fd[3]$

   $c = fd[1] - \frac{1}{2} fd[2] + \frac{1}{3} fd[3]$
7. Compute $\{ as^2+bs+c=0 ,\ s = (-b \pm \sqrt{b^2-4ac})/2a \}$

   $s_1 = (-b + sqrt(b*b - 4*a*c)) / (2*a)$

   $s_2 = (-b - sqrt(b*b - 4*a*c)) / (2*a)$
8. Compute

   $x_1 = x[0] + s_1 h$

   $x_2 = x[0] + s_2 h$
9. value $= [fd[2] + ((6*s_1 - 6) * fd[3] / 6)] / (h*h)$
10. if (value < 0)

    Display the maxima at x as x_1

    else

    minima at x as x_1
11. value $= [fd[2] + ((6*s_2 - 6) * fd[3] / 6)] / (h*h)$

    if (value < 0)

    Display the maxima as x as x_2

    else minima at x as x_2.

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Numerical Interation:

The process of evaluating a definite integration from a set of tabulated values of the integrand $f(x)$ is called numerical integration. It is the process of measuring the area under a function ploted on a graph. It is represented as:

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

and can be treated as the area under the curve $y = f(x)$, enclosed between the limits $x = a$ and $x = b$. The graphical representation is given as,

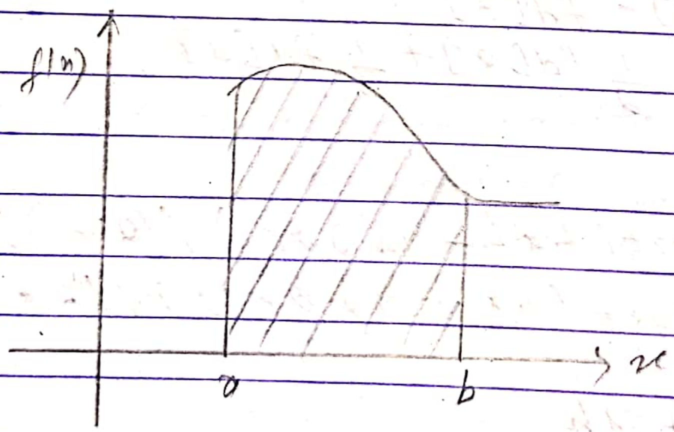

fig:- Graphical representation of integral of a function

The problem of integration is then simply reduced to the problem of finding the shaded area.

Newton-Cote's Quadrature Formula:-

Let $I = \int_{x_0}^{x_n} f(x)\,dx$ ——— (1)

Let us divide the interval (x_0, x_n) into n sub-intervals of equal width, ie

$$h = \frac{x_n - x_0}{n}$$

Thus, $x_1 = x_0 + h$, $x_2 = x_0 + 2h$, $x_3 = x_0 + 3h, \ldots x_n = x_0 + nh$

From, Newton's forward difference formula we know that, $f(x) = f(x_0) + s\Delta f(x_0) + \frac{s(s-1)}{2!}\Delta^2 f(x_0) + \frac{s(s-1)(s-2)}{3!}\Delta^3 f(x_0) + \ldots$ ——— (2)

where, $s = \frac{x - x_0}{h}$

Now,

Eq^n (1) can be written as;

$$\int_{x_0}^{x_n} f(x)\,dx = \int_{x_0}^{x_n} \{ f(x_0) + s\Delta f(x_0) + \frac{s(s-1)}{2!}\Delta^2 f(x_0) + \frac{s(s-1)(s-2)}{3!}\Delta^3 f(x_0) + \ldots \}\,dx$$

Since, $x = x_0 + sh$

$\Rightarrow dx = h \cdot ds$

$\frac{s^{n+1}}{n+1}$

$$\therefore \int_{x_0}^{x_n} f(x)\,dx = h \int_0^{n} \{ f(x_0) + s\Delta f(x_0) + \frac{s(s-1)}{2!}\Delta^2 f(x_0) + \frac{s(s-1)(s-2)}{3!}\Delta^3 f(x_0) + \ldots \}\,ds$$

$s^2 - s$

Integrating,

$s^3 - 3s^2 + 2s$

$\int s^3 - 3s^2 + 2s$

$\frac{s^4}{4} - \frac{3s^3}{3} + \frac{2s^2}{2}$

$$= h\left[s f(x_0) + \frac{s^2}{2}\Delta f(x_0) + \frac{1}{2!}\left(\frac{s^3}{3} - \frac{s^2}{2}\right)\Delta^2 f(x_0) + \frac{1}{3!}\left(\frac{s^4}{4} - s^3 + s^2\right)\Delta^3 f(x_0) + \ldots \right]_0^n$$

$$= nh\left[f(x_0) + \frac{n}{2} \Delta f(x_0) + \frac{1}{2!}\left(\frac{n^2}{3} - \frac{n}{2}\right) \Delta^2 f(x_0) + \frac{1}{3!}\left(\frac{n^3}{4} - n^2 + n\right) \Delta^3 f(x_0) + \cdots \right]$$

$$\therefore \int_{x_0}^{x_n} f(x)\,dx = nh\left[f(x_0) + \frac{n}{2} \Delta f(x_0) + \frac{1}{12}(2n^2 - 3n) \Delta^2 f(x_0) + \frac{1}{24}(n^3 - 4n^2 + 4n) \Delta^3 f(x_0) + \cdots \right] \quad \text{---} \; (3)$$

This eqn (3) is called Newton-Cote's formula. From this formula we can obtain different integration by putting $n = 1, 2, 3, \cdots$ etc.

Trapezoidal Rule:

Trapezoidal rule is based on the Newton-Cote's formula. The trapezoidal rule works by approximating the region under the graph of the function $f(x)$ as trapezoid and calculating its area. The trapezoidal rule assume $n = 1$, ie it approximates the integral by a linear polynomial.

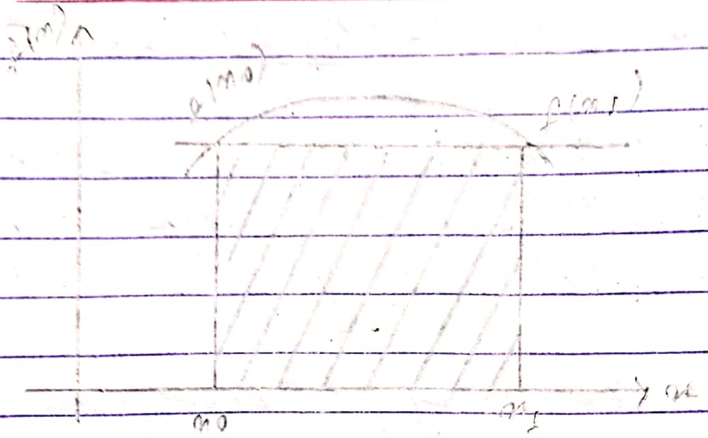

fig: Geometrical representation of trapezoidal rule

The Newton-Cote's Qudrature formula for integration is given by,

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_0+nh=x_n} f(x)\,dx$$

$$= nh\left[f(x_0) + \frac{n}{2}\Delta f(x_0) + \frac{1}{12}(2n^2-3n)\Delta^2 f(x_0) + \frac{1}{24}(n^3-4n^2+4n)\Delta^3 f(x_0) + \cdots\right] \text{ --- } (1)$$

By putting $n=1$ in equation (1) and neglecting the higher order, forward difference can be written as,

$$\int_{x_0}^{x_0+nh} f(x)\,dx = \int_{x_0}^{x_1} f(x)\,dx$$

$$= h\left[f(x_0) + \frac{1}{2}\Delta f(x_0)\right]$$

$h = \frac{x_n - x_0}{n}$ $\quad = h\left[f(x_0) + \frac{1}{2}(f(x_1) - f(x_0))\right]$

i.e. $n = 1$ $\quad = \frac{(x_1 - x_0)}{n}\left(\frac{f(x_0) + f(x_1)}{2}\right)$ $\quad \left[h = \frac{x_1 - x_0}{n}\right]$

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Page

$$\therefore \int_{x_0}^{x_1} f(x)\,dx = (x_1 - x_0)\left[\frac{f(x_0)+f(x_1)}{2}\right] \quad \text{--- (11)}$$

Eq^n (11) is called Trapezoidal Rule it is the area of trapezoid where width is $(x_1 - x_0)$ and height is the average of $f(x_0)$ and $f(x_1)$

Q. Find $\int_2^8 (x^3+2)\,dx$ by using trapezoidal rule.

⇒ Sol^n:

$n = 1$

$h = \frac{x_n - x_0}{n}$

$x_1 - x_0 = 8 - 2 = 6$

$= x_n - x_0 \; [n = 1]$

$f(x_0) = 10$

$f(x_1) = 514$

$\therefore \int_2^8 f(x)\,dx = 6 \times \frac{514+10}{2}$

$= 1572$

Algorithm:

1. Start
2. Read the value of lower and upper limits say x_0 and x_1 respectively.
3. Calculate the value of $f(x_0)$ and $f(x_1)$.
4. Compute $h = x_1 - x_0$
5. Calculate the value of Integration as:
   value $= \int_{x_0}^{x_1} f(x)\,dx$
   $= \frac{h}{2}[f(x_0) + f(x_1)]$
6. Print the value of value
7. Stop.

Composite Trapezoidal Rule / Multiple segment Trapezoidal

In order to improve the accuracy of the trapezoidal rule, the integration interval can be divided into k segments of equal width.

This form of trapezoidal rule is called multiple-segment or composite integration formula. Divide $(x_n - x_0)$ into k equal segments as:

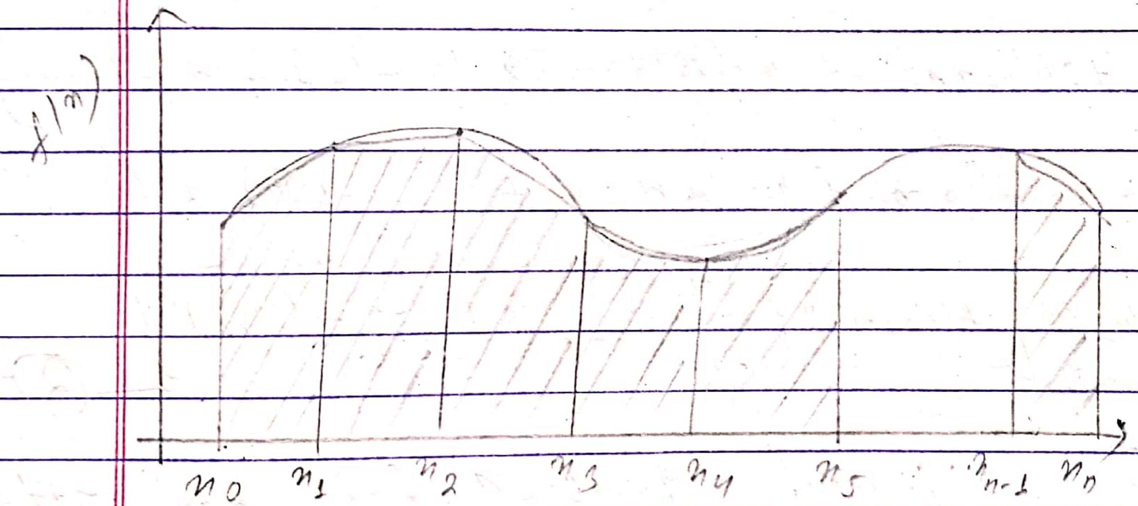

fig:- Multiple segment Trapezoidal Rule

Then, the width of each segment is

$$h = \frac{x_n - x_0}{k}$$

Now, the integral can be broken into k integral as

$$\int_{x_0}^{x_n} f(x)\,dx = \int_{x_0}^{x_0+h} f(x)\,dx + \int_{x_0+h}^{x_0+2h} f(x)\,dx + \dots + \int_{x_0+(k-2)h}^{x_0+(k-1)h} f(x)\,dx + \int_{x_0+kh} f(x)\,dx$$

$$\int_{x_0}^{x_n} f(x)\,dx = \int_{x_0}^{x_0+h} f(x)\,dx + \int_{x_0+h}^{x_0+2h} f(x)\,dx + \cdots + \int_{x_0+(k-2)h}^{x_0+(k-1)h} f(x)\,dx + \int_{x_0+(k-1)h}^{x_0+kh = x_n} f(x)\,dx \quad \text{(1)}$$

Applying trapezoidal rule on each segments of eqn (1) which gives,

$$\int_{x_0}^{x_n} f(x)\,dx = \{(x_0+h)-x_0\}\left\{\frac{f(x_0)+f(x_0+h)}{2}\right\} + \{(x_0+2h)-(x_0+h)\}\left\{\frac{f(x_0+h)+f(x_0+2h)}{2}\right\} + \cdots + \{x_n-(x_0+(k-1)h)\}\left\{\frac{f(x_0+(k-1)h)+f(x_n)}{2}\right\}$$

$$= \frac{h}{2}\left[f(x_0)+f(x_0+h)+f(x_0+h)+f(x_0+2h)+\cdots+f(x_0+(k-1)h)+f(x_n)\right]$$

$$= \frac{h}{2}\left[f(x_0)+2f(x_0+h)+2f(x_0+2h)+\cdots+2f(x_0+(k-1)h)+f(x_n)\right]$$

$$= \frac{h}{2}\left[f(x_0)+2\{f(x_0+h)+f(x_0+2h)+\cdots+f(x_0+(k-1)h)\}+f(x_n)\right]$$

$$\Rightarrow \int_{x_0}^{x_n} f(x)\,dx = \frac{h}{2}\left[f(x_0)+2\left\{\sum_{i=1}^{k-1} f(x_0+ih)\right\}+f(x_n)\right] \quad \text{(2)}$$

Eqn (2) is required equation for composite trapezoidal rule.

$\int_0^2 x^2$, $k = 10$, $h = \frac{2-0}{10} = \frac{1}{5} = 0.2$

$f(x_0) = f(0) = 0$ $f(x_0+ih) =$

$f(2) = 2^2 = 4$ $f(x_0+h) = f(0+0.2) = 0.04$

$f(x_0+2h) = f(0.4)$ 0.16

$f(x_0+8h) = f(1.6)$ 2.56 $f(x_0+3h) = f(0.6)$ 0.36

$f(x_0+9h) = f(1.8)$ 3.24 $f(x_0+4h) = f(0.8)$ 0.64

$f(x_0+10h) = f(2) = 4$ $f(x_0+5h) = f(1)$ 1

$f(x_0+6h) = f(1.2)$ 1.44

$f(x_0+7h) = f(1.4)$

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Algorithm:

1. Read the value of lower and upper limit say x_0 and x_n.
2. Read number of segments k.
3. Calculate $h = \frac{x_n - x_0}{k}$
4. Set $sum = f(x_0) + f(x_n)$
5. for $i = 1$ to $k-1$
6. $sum = sum + 2 * f(x_0 + ih)$
6. Calculate the value of integration by using $value = \frac{h}{2} * sum$
7. Display "value".

8. Compute the integral $\int_{-1}^{1} e^x dx$ for $k=2$ and for $k=4$ by using composite trapezoidal rule.

→ Soln:

For $k=2$

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

$f(x_0) = f(-1) = e^{-1} = 0.3678$

$f(x_n) = f(1) = e^1 = 2.7183$

Now, $f(x_0 + ih) = f(x_0 + h) = f(-1+1) = f(0) = e^0 = 1$

$$\int_{-1}^{1} f(x) dx = \frac{h}{2}\left[\underbrace{f(-1)}_{x_0} + \underbrace{f(1)}_{x_n} + 2\left\{\sum_{i=1} f(x_0 + ih)\right\}\right]$$

$$= \frac{1}{2}\left[0.3678 + 2.7182 + 2 \times 1\right]$$

$$= 2.543$$

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for $k=4$

$h = \frac{1+1}{4} = 0.5$

$f(x_0) = 0.3678$
$f(x_1) = 2.7182$
$f(x_0+h) = f(-1+0.5) = f(-0.5) = 0.6065$
$f(x_0+2h) = f(-1+2\times0.5) = f(0) = 1$
$f(x_0+3h) = f(-1+3\times0.5) = f(0.5) = 1.6487$

$$\int_{-1}^{1} e^x dx = \frac{0.5}{2}\left[0.3678 + 2(0.6065+1+1.6487) + 2.7182\right]$$
$$= 2.3991$$

```
#include <stdio.h>
float f(float x)
{ return x*x;
}
main()
{
  float a,b,h, sum=0, integral, x;
  int k,i;
  printf("Enter the lower limit ");
  scanf("%f", &a);
  printf("Enter upper limit");
  scanf("%f", &b);
  printf("Enter the no. of sub-intervals\n");
  scanf("%d", &k);
```

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Simpson's 1/3 Rule: (three point)

Simpson's 1/3 rule is an extension of trapezoidal rule where the integrand is approximated by a second order polynomial.

The Simpson's 1/3 rule assumes $n=2$. The general quadrature formula for integration is given by,

$$\int_a^b f(x)dx = \int_{x_0}^{x_0+nh} f(x)dx = nh\Big[f(x_0) + \frac{n}{2}\Delta f(x_0) + \frac{1}{12}(2n^2-3n)\Delta^2 f(x_0) + \frac{1}{24}(n^3-4n^2+4n)\Delta^3 f(x_0) + \cdots\Big] \quad \text{--- (1)}$$

where $h = \frac{b-a}{n}$ / $\frac{x_2-x_0}{n=2}$

By putting $n=2$ in eqn (1) and neglecting higher order forward difference, it can be written as:

$$\int_{x_0}^{x_0+2h} f(x)dx = \int_{x_0}^{x_2} f(x)dx = 2h\Big[f(x_0) + \Delta f(x_0) + \frac{1}{6}\Delta^2 f(x_0)\Big]$$

$$= 2h\Big[f(x_0) + \{f(x_1) - f(x_0)\} + \frac{1}{6}(f(x_0) - 2f(x_1) + f(x_2))\Big]$$

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

$$\therefore \int_{x_0}^{x_2} f(x)dx = \frac{h}{3}\Big[f(x_0) + 4f(x_1) + f(x_2)\Big] \quad \text{--- (2)}$$

This eqn (2) is called Simpson's 1/3 rule.

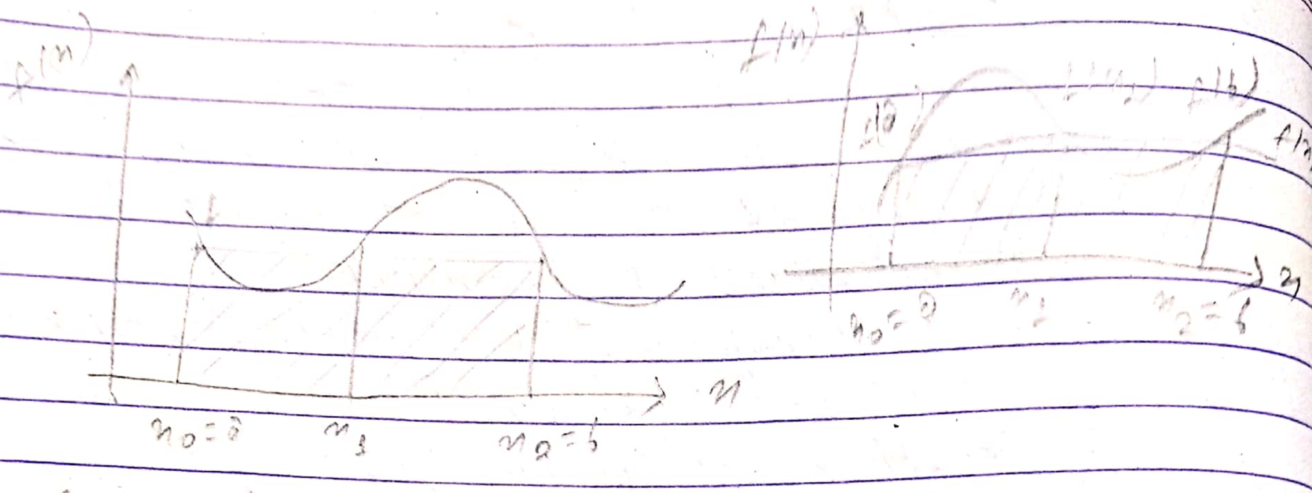


Fig: Geometrical interpretation of Simpson's 1/3 rule.

Example:

Calculate the $\int_0^1 \sqrt{1-x^2}\,dx$ using Simpson's 1/3 rule.

⇒ Soln: $n = 2$ [from Newton cote's]

$$h = \frac{x_2 - x_0}{n} = \frac{1-0}{2} = 0.5$$

$x_1 = x_0 + h = 0+1\times0.5$

Here, $x_0 = 0$, $x_2 = 1$

$x_1 = x_0 + h = 0 + 0.5 = 0.5$

$f(x_0) = f(0) = \sqrt{1-0} = 1$

$f(x_1) = f(0.5) = \sqrt{1-(0.5)^2} = 0.866$

$f(x_2) = f(1) = \sqrt{1-1} = 0$

$$\therefore \int_0^1 \sqrt{1-x^2}\,dx = \frac{0.5}{3}\left[1 + 0.866\times4 + 0\right]$$

$$= 0.744$$

Algorithm:

1. Read the value of lower limit and upper limit say x_0 and x_2 respectively.
2. Calculate the values of $f(x_0)$ and $f(x_2)$
3. compute $h = \frac{x_2 - x_0}{2}$
4. compute $x_1 = x_0 + h$ and $f(x_1)$
5. Calculate the value of integration as
$$value = \int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right]$$
6. Display "value".

Composite Simpson's 1/3 Rule:

Divide the interval [a, b] into k segments and apply Simpson's 1/3 rule repeatedly over every two segments. Note that k needs to be even. The segment width is given by;

$$h = \frac{b-a}{k}$$

Apply Simpson's 1/3 rule over each two interval

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_n} f(x)\,dx$$

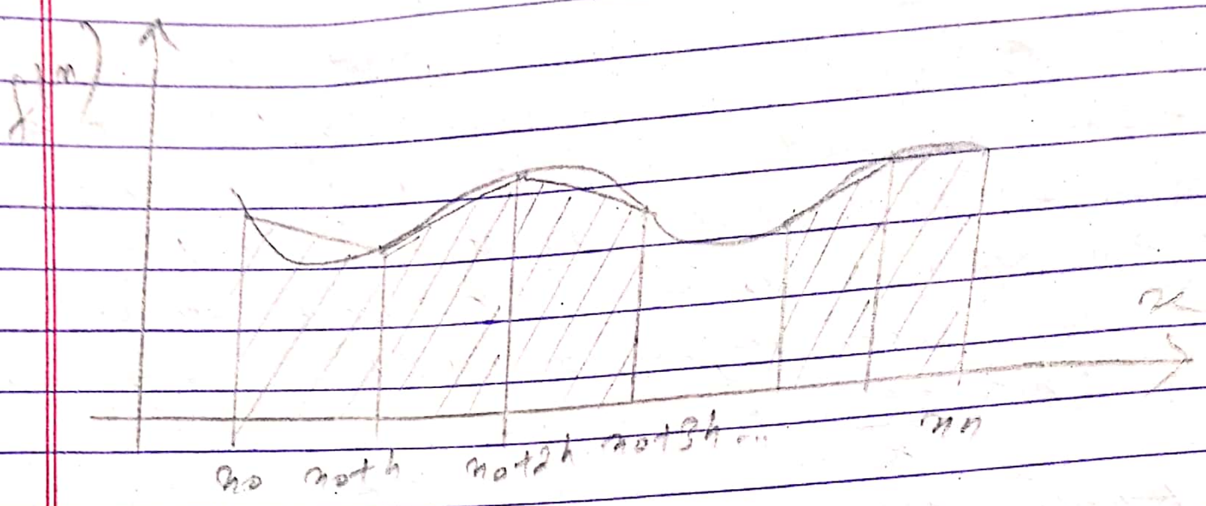
$$= \int_{x_0}^{x_2} f(x)\,dx + \int_{x_2}^{x_4} f(x)\,dx + \int_{x_4}^{x_6} f(x)\,dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)\,dx$$

$$= \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right] + \frac{h}{3}\left[f(x_2) + 4f(x_3) + f(x_4)\right] + \cdots + \frac{h}{3}\left[f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\right]$$

$$= \frac{h}{3}\left[f(x_0) + 4\{f(x_1) + f(x_3) + \cdots + f(x_{n-1})\} + 2\{f(x_2) + f(x_4) + \cdots + f(x_{n-2})\} + f(x_n)\right]$$

$$= \frac{h}{3}\left[f(x_0) + 4\sum_{\substack{i=1 \\ i=\text{odd}}}^{k-1} f(x_i) + 2\sum_{\substack{i=2 \\ i=\text{even}}}^{k-2} f(x_i) + f(x_n)\right] \quad \text{--- (1)}$$

This eqn (1) is called composite Simpson's 1/3 rule.



Algorithm:

1. Read value of lower and upper limit say x_0 and x_n
2. Read number of segments, say k
3. Calculate $h = (x_n - x_0)/k$
4. Set sum = $f(x_0) + f(x_n)$
5. for i=1 to k-1
   sum = sum + 4 * f(x_0 + i*h)
   i = i+2 // i+1
   end for
6. for i=2 to k-2
   sum = sum + 2 * f(x_0 + i*h)
   i = i+2
   end for
7. Calculate the value of integration as,
   value = $\frac{h}{3}$ * sum
8. Display the "value".

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Ex:

Apply Simpson's 1/3 rule to evaluate $\int_0^1 \sqrt{1-x^2}\,dx$ using $k=4$ and $k=8$

$\Rightarrow$ Sol^n: for $k=4$, $x_0=0$, $x_4=1$

$h = \frac{1-0}{4} = \frac{1}{4}$

$f(0) = \sqrt{1-0^2} = 1 = f(x_0)$

$f(1) = \sqrt{1-1^2} = 0 = f(x_4)$

$x_1 = x_0 + h = 0 + \frac{1}{4} = 1/4$

$f(x_1) = 0.968 \Rightarrow f(x_0+h)$

$x_3 = x_0 + 3h = 0 + \frac{3}{4}$, $f(x_3) = 0.661$

$x_2 = x_0 + 2h = \frac{1}{2}$, $f(x_2) = 0.866$

$\therefore \int_0^1 \sqrt{1-x^2} = \frac{h}{3}\left[f(x_0) + 4\{f(x_1) + f(x_3)\} + 2f(x_2) + f(x_4)\right]$

$= \frac{1}{12}\left[1 + 4(0.968 + 0.661) + 2 \times 0.866 + 0\right]$

$= \frac{1}{12} \times 9.248$

$= 0.77$

$\Rightarrow$ for $k=8$, $h = \frac{1-0}{8} = 1/8$, $x_0 = 0$, $x_8 = 1$

$f(x_0) = \sqrt{1-0^2} = 1$

$f(x_8) = \sqrt{1-1^2} = 0$

$x_1 = x_0 + h = 0 + \frac{1}{8} = 1/8$, $f(x_1) = \sqrt{1-(1/8)^2}$

$= 0.992$

$x_2 = x_0 + 2h = \frac{2}{8} = \frac{1}{4}$, $f(x_2) = \sqrt{1-(1/4)^2}$

$= 0.968$

$x_3 = x_0 + 3h = 0 + 3 \times \frac{1}{8} = 3/8$, $f(x_3) = \sqrt{1-(3/8)^2}$

$= 0.927$

$x_4 = x_0 + 4h = 4/8 = 1/2$, $f(x_4) = \sqrt{1-(1/2)^2}$

$= 0.866$

$x_5 = x_0 + 5h = 5/8$, $f(x_5) = \sqrt{1-(5/8)^2}$

$= 0.780$

$x_6 = x_0 + 6h = 6/8$, $f(x_6) = \sqrt{1-(6/8)^2}$

$= 0.661$

$x_7 = x_0 + 7h = 7/8 = f(x_7) = \sqrt{1-(7/8)^2}$

$= 0.484$

$\therefore \int_0^1 \sqrt{1-x^2}\, dx = \frac{1}{8 \times 3}\Big[f(x_0) + 4\{ f(x_1) + f(x_3) + f(x_5) + f(x_7)\} +$

$2\{ f(x_2) + f(x_4) + f(x_6)\} + f(x_8)\Big]$

$= \frac{1}{24}\Big[1 + 4(0.992 + 0.927 + 0.78 + 0.484) +$

$2(0.968 + 0.866 + 0.661) + 0\Big]$

$= \frac{1}{24}\Big[1 + 4 \times 3.183 + 2 \times 2.495\Big]$

$= 0.78$

Simpson's 3/8 Rule:

Simpson's 3/8 rule for Integration can be derived by approximating the given function $f(x)$ with 3rd order polynomial.

General quadrature formula for Integration is given by,

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_0+nh} f(x)\,dx = nh\Big[f(x_0) + \frac{n}{2}\Delta f(x_0) + \frac{1}{12}(2n^2-3n)\Delta^2 f(x_0) + \frac{1}{24}(n^3-4n^2+4n)\Delta^3 f(x_0) + \cdots \quad (1)$$

where,

$$h = \frac{b-a}{n}$$

By putting $n=3$ in eq^n (1) and neglecting the higher order difference it can be written as,

$$\int_{x_0}^{x_0+nh} f(x)\,dx = 3h\left[f(x_0) + \frac{3}{2}\Delta f(x_0) + \frac{3}{4}\Delta^2 f(x_0) + \frac{1}{8}\Delta^3 f(x_0)\right]$$

$$= \frac{3h}{8}\Big[8f(x_0) + 12\{f(x_1) - f(x_0)\} + 6\{f(x_0) - 2f(x_1) + f(x_2)\} + (-f(x_0) + 3f(x_1) - 3f(x_2) + f(x_3))\Big]$$

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

$$\therefore \int_{x_0}^{x_3} f(x)\,dx = \frac{3}{8}h\left[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right] \quad (2)$$

This is called Simpson's 3/8 rule.

Appy Simpson's 3/8 rule to calculate

$$\int_0^1 \sqrt{1-x^2}\,dx.$$

⇒ Sol^n: $n = 3$, $x_0 = 0$, $x_3 = 1$

$$h = \frac{1-0}{3} = \frac{1}{3}$$

$f(x_0) = \sqrt{1-0^2} = 1$

$f(x_3) = \sqrt{1-1^2} = 0.$

$x_1 = x_0 + nh = 0 + 1 \times \frac{1}{3} = \frac{1}{3}$, $f(x_1) = 0.942$

$x_2 = x_0 + nh = 0 + 2 \times \frac{1}{3} = \frac{2}{3}$, $f(x_2) = 0.745$

$$\int_0^1 f(x)\,dx = \frac{3h}{8}\left[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right]$$

$$= \frac{3}{8} \times \frac{1}{3}\left[1 + 3 \times 0.942 + 3 \times 0.745 + 0\right]$$

$$= \frac{1}{8} \times 6.061$$

$$= 0.757$$

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Algorithm:

1. Read the value of lower limit and upper limit say x_0 and x_3 resp.
2. Calculate the values of $f(x_0)$ and $f(x_3)$
3. Compute, $h = \frac{x_3 - x_0}{3}$
4. Compute $x_1 = x_0 + h$ and $f(x_1)$, $x_2 = x_0 + 2h$ and $f(x_2)$
5. Calculate the value of integration as
   $$\text{value} = \int_{x_0}^{x_3} f(x)\,dx$$
   $$= \frac{3h}{8}\left[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right]$$
6. Display "value".

Composite Simpson's 3/8 rule.

Let's subdivide the interval $[x_0, x_n]$ into k segments and apply Simpson's 3/8 rule repeatedly over every three segments. Now the segment width is given by

$$h = \frac{x_n - x_0}{k}$$

Apply Simpson's 3/8 rule over each three interval.

$$\int_{x_0}^{x_n} f(x)\,dx = \frac{3}{8}h\left[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right] +$$

$$\frac{3}{8}h\left[f(x_3) + 3f(x_4) + 3f(x_5) + f(x_6)\right] + \cdots +$$

$$\frac{3}{8}h\left[f(x_{n-6})+3f(x_{n-5})+3f(x_{n-4})+f(x_{n-3})\right]+$$

$$\frac{3}{8}h\left[f(x_{n-3})+3f(x_{n-2})+3f(x_{n-1})+f(x_n)\right]$$

$$\therefore \int_{x_0}^{x_n} f(x)\,dx = \frac{3h}{8}\left[f(x_0)+3\sum_{\substack{i=1 \\ i \bmod k \neq 0}}^{k-1} f(x_i)+2\sum_{\substack{i=2 \\ i \bmod k = 0}}^{k-1} f(x_i)+f(x_n)\right]$$

Algorithm:

1. Read the value of lower and upper limit say x_0 and x_n resp.
2. Read number of segments say k.
3. Calculate,
   $$h = \frac{x_n - x_0}{k}$$
4. Set Sum = $f(x_0) + f(x_n)$
5. for $i = 1$ to $k-1$
   if (i mod k != 0)
   Sum = sum + 3 * f(x_0 + i * h)
6. else
   Sum = sum + 2 * f(x_0 + i * h)
7. Calculate the value of integration as
   Int value = $\frac{3}{8}$ * h * Sum
8. Display the value of integration as "Int Value".

Example:

Q. Calculate the integral value of following tabulated function from $x=0$ to $x=1.6$ using Simpson's $3/8$ rule.

x	0	0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.6
$f(x)$	0	0.24	0.55	0.92	1.13	1.84	2.37	2.95	3.56

⇒ Solⁿ:

$x_0 = 0$, $x_n = 1.6$, $k = 8$

$$h = \frac{x_n - x_0}{k} = \frac{1.6 - 0}{8} = 0.2$$

$$\int_0^{1.6} f(x)\,dx = \frac{3}{8} h \left[f(x_0) + 3 \sum_{\substack{i=1 \\ i \bmod 3 \neq 0}}^{k-1} f(x_i) + 2 \sum_{\substack{i=1 \\ i \bmod 3 = 0}}^{k-1} f(x_i) + f(x_n) \right]$$

$$= \frac{3}{8} h \left[f(x_0) + 3\{ f(x_1) + f(x_2) + f(x_4) + f(x_5) + f(x_7) \} + 2\{ f(x_3) + f(x_6) \} + f(x_8) \right]$$

$$= \frac{3 \times 0.2}{8} \left[0 + 3(0.24 + 0.55 + 1.63 + 1.84 + 2.95) + 2(0.93 + 2.37) + 3.56 \right]$$

$$= 0.075 (3 \times 7.21 + 6.6 + 3.56)$$

$$= 2.38$$

0 1 2

Q. Use Simpson's 3/8 rule to evaluate:

a. $\int_1^2 (x^3+1)\,dx$ b. $\int_0^{\pi/2} \sqrt{\sin(x)}\,dx$

a) ⇒ Soln:

$x_0 = 1, \quad x_3 = 2, \quad n = 3$

$h = \frac{x_n - x_0}{n} = \frac{2-1}{3} = \frac{1}{3}$

$f(x_0) = f(1) = 1^3 + 1 = 2$

$x_1 = x_0 + h = 1 + \frac{1}{3} = 4/3, \quad f(x_1) = 2.77$

$x_2 = x_0 + 2h = 1 + 2/3 = 5/3, \quad f(x_2) = 4.12$

$f(x_3) = 9$

$\therefore \int_1^2 f(x^3+1)\,dx = 3/8 \times 1/3 \left[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3) \right]$

$= 1/8 \left[2 + 3 \times 2.77 + 3 \times 4.12 + 9 \right]$

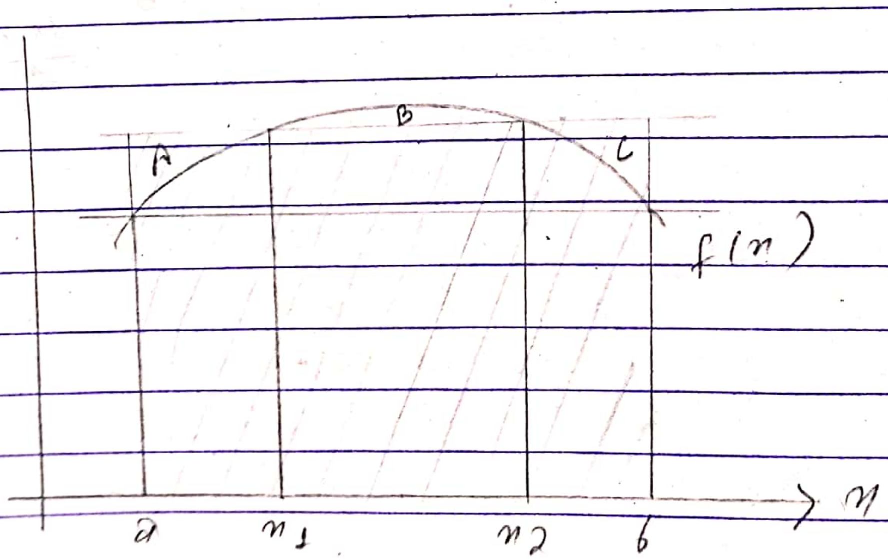
~~= 1/8 [2 + (2×2.77) + 3~~

$= 4.75$

II Gaussian Integration:-

Gaussian integration is based on the concept that accuracy of numerical integration can be improved by choosing the sampling points wisely rather than on the basis of equal spacing. Consider the following figure, if we choose points x_1 and x_2 as in figure below, rather than points a and b, integration error can be minimized. We should choose the points x_1 and x_2 such that,

area B = area A + area C



Thus, the two-point Gaussian integration rule is an extension of the trapezoidal rule, where the arguments of the function are not predetermined as a and b but as unknown x_1 and x_2. So in two points Gauss-quadrature rule, the Integration is approximated as,

$$I = \int_{-1}^{1} f(x)\,dx = c_1 f(x_1) + c_2 f(x_2)$$

There are four unknowns x_1, x_2, c_1 and c_2. These are found by assuming that the formula gives the exact results for integrating a general third order polynomial,

$$f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$$

$$\therefore \int_{-1}^{1} f(x)\,dx = \int_{-1}^{1} (a_0 + a_1 x + a_2 x^2 + a_3 x^3)\,dx$$

$$= \left[a_0 x + \frac{a_1 x^2}{2} + \frac{a_2 x^3}{3} + \frac{a_3 x^4}{4}\right]_{-1}^{1}$$

$$= a_0 + \frac{a_1}{2} + \frac{a_2}{3} + \frac{a_3}{4} - \left\{-a_0 + \frac{a_1}{2} - \frac{a_2}{3} + \frac{a_3}{4}\right\}$$

$$= a_0 + \frac{a_1}{2} + \frac{a_2}{3} + \frac{a_3}{4} + a_0 - \frac{a_1}{2} + \frac{a_2}{3} - \frac{a_3}{4}$$

$$= 2a_0 + \frac{2a_2}{3} \quad \text{---} \quad (1)$$

Thus, $\int_{-1}^{1} f(x)\,dx = c_1 f(x_1) + c_2 f(x_2)$

$$= c_1(a_0 + a_1 x_1 + a_2 x_1^2 + a_3 x_1^3) + c_2(a_0 + a_1 x_2 + a_2 x_2^2 + a_3 x_2^3)$$

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$= a_0(c_1+c_2)+a_1(c_1x_1+c_2x_2)+a_2(c_1x_1^2+c_2x_2^2)+a_3(c_1x_1^3+c_2x_2^3)$ — (2)

So, from equation (1) and (2) we get

$$2a_0+\frac{2}{3}a_2 = a_0(c_1+c_2)+a_1(c_1x_1+c_2x_2)+a_2(c_1x_1^2+c_2x_2^2)+a_3(c_1x_1^3+c_2x_2^3)$$

Equating the term on both sides,

$$c_1+c_2=2$$
$$c_1x_1+c_2x_2=0$$
$$c_1x_1^2+c_2x_2^2=2/3$$
$$c_1x_1^3+c_2x_2^3=0$$

We can find that the above four simultaneous non-linear equations have only one acceptable solution

$$c_1=c_2=1$$

$\therefore x_1=(-1/\sqrt{3})=-0.5773502$

$x_2=(1/\sqrt{3})=0.5773502$

Thus we have Gaussian quadrative formula for $n=2$ as

$$\int_{-1}^{1} f(x)\,dx = f(-1/\sqrt{3})+f(1/\sqrt{3}) \quad \text{— (3)}$$

This eq^n (3) is also known as Gauss-Legendre formula.

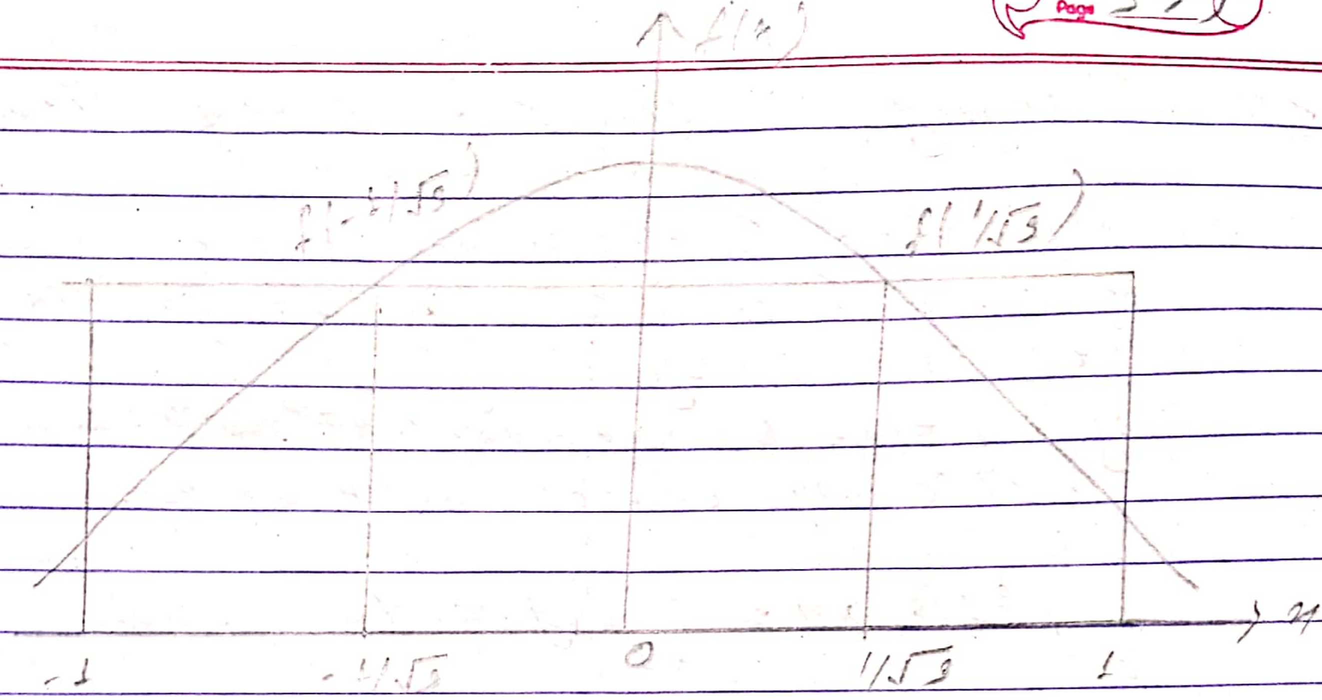

fig:- Illustration of Gauss Integration for two points.

Q. Compute $\int_{-1}^{1} e^{x}\,dx$ using two point Gauss-Legendre formula.

⇒ Soln:

$$f(-1/\sqrt{3}) = e^{-1/\sqrt{3}} = 0.56138$$

$$f(1/\sqrt{3}) = e^{1/\sqrt{3}} = 1.78131$$

$$\therefore \int_{-1}^{1} f(x)\,dx = f(-1/\sqrt{3}) + f(1/\sqrt{3})$$

$$= 0.56138 + 1.78131$$

$$= 2.34269$$

1/3 => 3 points
3/8 => 4

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Changing the limits of Integration:

Gaussian integration imposes the restriction on limits of integration from -1 to 1. By using the concept of "interval transformation" this restriction can be overcome.

Let

$$\int_a^b f(x)\,dx = C\int_{-1}^{1} g(z)\,dz$$

Assume, the following transformation between x and z.

$$x = Az + B$$

This must satisfy the following conditions,

$x = a$, $z = -1$ and $x = b$, $z = 1$

i.e. $B - A = a$

$A + B = b$

Then,

$$A = \frac{b-a}{2} \quad \text{and} \quad B = \frac{a+b}{2}$$

$$\therefore x = \frac{b-a}{2} z + \frac{a+b}{2}$$

$$dx = \frac{b-a}{2} dz$$

$$\Rightarrow C = \frac{b-a}{2}$$

Thus, the integral becomes,

$$\frac{b-a}{2}\int_{-1}^{1} g(z)\,dz$$

The Gaussian formula for this integration is $\frac{b-a}{2}\int_{-1}^{1} g(z)\,dz = \frac{b-a}{2}\sum_{i=1}^{2} w_i\, g(z_i)$

where w_i and z_i are the weights and quadrature points for integration domain $[-1, 1]$

Q. Calculate the integral $\int_{-2}^{2} e^{-x/2}\,dx$ using Gaussian two-point formula.

⇒ Soln:

$a = -2$, $b = 2$

$c = \frac{b-a}{2} = \frac{2+2}{2} = 2$

$x = \frac{b-a}{2} z + \frac{a+b}{2} = \underline{2z}$

$\left[dx = \frac{b-a}{2} dz = 2\,dz\right]$

After changing the limits we get,

$$\int_a^b e^{-x/2}\,dx = \frac{b-a}{2}\int_{-1}^{1} g(z)\,dz$$

$$= 2\int_{-1}^{1} g(z)\,dz$$

$$= 2\int_{-1}^{1} e^{-z}\,dz.$$

Now,

$$\therefore \int_a^b e^{-x/2}\,dx = 2\int_{-1}^{1} e^{-z}\,dz \rightarrow$$

From Gaussian two point formula, we know that

$$\int_{-1}^{1} e^{-z} dz = f(-1/\sqrt{3}) + f(1/\sqrt{3})$$

$$\therefore \int_{-2}^{2} e^{-x/2} dx = 2\int_{-1}^{1} e^{-2z/2} dz$$

$$= 2\int_{-1}^{1} e^{-z} dz$$

$$= 2[f(x_1) + f(x_2)]$$

$$= 2[f(-1/\sqrt{3}) + f(1/\sqrt{3})]$$

$$= 2(1.78131 + 0.56138)$$

$$= 4.68538$$

Algorithm:

1. Read the values of upper and lower limit as b and a respectively.
2. Set $z_1 = -0.5773502$ and $z_2 = 0.5773502$
3. Compute:

$$x_1 = \frac{b-a}{2} z_1 + \frac{b+a}{2}$$

$$x_2 = \frac{b-a}{2} z_2 + \frac{b+a}{2}$$

4. Calculate value $= \frac{b-a}{2}(f(x_1) + f(x_2))$
5. Print the "value".

Alternative

$\Rightarrow$ $z_1 = -1/\sqrt{3}$, $z_2 = 1/\sqrt{3}$

$a = -2$, $b = 2$

$$x_1 = \frac{b-a}{2} z_1 + \frac{b+a}{2}$$

$$= \frac{2+2}{2} \times -\frac{1}{\sqrt{3}} + \frac{2-2}{2}$$

$$= -2/\sqrt{3}$$

$$= -1.1547$$

$$x_2 = \frac{b-a}{2} z_2 + \frac{b+a}{2}$$

$$= 2 \times \frac{1}{\sqrt{3}} + 0$$

$$= 1.1547$$

$f(x_1) = 1.781311$

$f(x_2) = e^{-x/2} = 0.561384$

$$\int_{-2}^{2} e^{-x/2}\, dx = \frac{b-a}{2} \left[f(x_1) + f(x_2) \right]$$

$$= 2 (1.781311 + 0.561384)$$

$$= 4.68539$$

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