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Unit-3

NUMERICAL DIFFERENTIATION & INTEGRATION:

A) Numerical Differentiation:-

① Definition and introduction:- Numerical differentiation is the process of finding the numerical value of a derivative of a given function at a given point. The derivative or differentiation of a function represents the rate of change of a variable with respect to another variable.

For example: The velocity of a body is defined as the rate of change of the location of the body with respect to time. The location is dependent variable while time is independent variable.

Applications: (Used):

- 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 (tabulated) functions is required when function values at some discrete points are known but function is unknown.

Numerical differentiation is used in continuous functions (complicated functions) and discrete functions (tabulated functions).

1) Differentiating continuous functions:

This is the process of approximating the derivatives $f'(x)$ of a function $f(x)$, when the function itself is available.

a) Two Point Forward Difference Formula:

Consider a small increment $\Delta x = h$ in x ,
Now according to Taylor's theorem;

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

$$\text{or, } f'(x) = \frac{f(x+h) - f(x)}{h} - \frac{f''(x).h}{2!} - \dots$$

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

Thus if h is chosen to be sufficiently small, $f'(x)$ can be approximated by;

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

①

with the truncation error of;

$$E = -\frac{f''(x).h}{2!} \quad \text{--- (ii)}$$

The equation ⑦ is called two point forward difference formula.
This equation is also called forward difference quotient.

Eg.1. Find the value of derivative at $x=1$ for the function $f(x)=x^2$ by using $h=0.2$ and 0.05 .

Solution: For $h=0.2$

We know that,

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

$$f'(1) = \frac{f(1+0.2) - f(1)}{0.2} = \frac{1.44 - 1}{0.2} = 2.2$$

True value of derivative at $x=1$ is,

$$f'(x) = 2x = 2$$

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

For $h=0.05$

$$f'(1) = \frac{f(1+0.05) - f(1)}{0.05} = \frac{f(1.05) - f(1)}{0.05} = \frac{1.1025 - 1}{0.05} = 2.05$$

True value of derivative at $x=1$ is,

$$f'(x) = 2x = 2 \times 1 = 2$$

$$\therefore \text{Error} = \left| \frac{2 - 2.05}{2} \right| \times 100\% = 2.5\%$$

From this example it is clear that error decreases as the value of h becomes smaller.

Eg.2. Find the value of derivative at $x=45^\circ$ for the function $f(x)=\sin x + 1$ by using $h=0.1$ and 0.001 .

Solution:

Angle in degree = 45

Angle in radian = $(\pi * 45)/180 = 0.788$

$$\therefore x = 0.788$$

Now we can solve in a same way as we did in

Eg.1 [Note that $f'(x)=\cos x$.]

Similar question is solved after this page in (b).

b) Two Point Backward Difference Formula:-

Consider a small change $\Delta x = h$ in x . Now, According to Taylor's theorem, we have:

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

$$\text{or, } f'(x) = \frac{f(x-h) + f(x)}{h} + \frac{f''(x)h}{2!} \dots$$

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

Thus if h is chosen to be sufficiently small, $f'(x)$ can be approximated as;

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

with a truncation error of,

$$E = \frac{f''(x)h}{2!} \quad \textcircled{P}$$

Eqn \textcircled{P} is called two point backward difference formula. This eqn is also called backward difference quotient.

E.g.1 Find the derivative at $x=45^\circ$ for the function $f(x)=\sin x+1$ by using $h=0.01$ and 0.001 .

Solution: Angle in degree = 45

Angle in radian = $(\pi \times 45)/180 = 0.788$

For $h=0.1$

We know that, $f'(x) \approx \frac{f(x) - f(x-h)}{h}$

$$\text{or, } f'(45^\circ) = f'(0.788) = \frac{f(0.788) - f(0.788-1)}{0.1} = \frac{f(0.788) - f(0.688)}{0.1}$$

$$= \frac{0.709 - 0.635}{0.1}$$

$$= 0.74$$

True value of derivative at $x=0.788$ is;

$$f'(x) = \cos x = 0.705.$$

$$\therefore \text{Error} = \left| \frac{0.705 - 0.74}{0.705} \right| = 0.049 = 4.9\%$$

For $h=0.01$

$$f'(45^\circ) = f(0.788) = \frac{f(0.788) - f(0.788+0.01)}{0.01} = \frac{0.709 - 0.702}{0.01} = 0.70$$

True value of derivative at $x=0.788$ is;

$$f'(x) = \cos x = 0.705$$

$$\therefore \text{Error} = \left| \frac{0.705 - 0.70}{0.705} \right| = 0.007 = 0.7\%$$

c). Three Point Formula:

From Taylor's series;

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

$$f(x-h) = f(x) - f'(x) \cdot h + \frac{f''(x) \cdot h^2}{2!} - \dots \quad (ii)$$

Subtracting eqn (ii) from (i) we get.

$$f(x+h) - f(x-h) = f'(x) \cdot 2h + \dots$$

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

Thus if h is closer to be sufficiently small, $f'(x)$ can be approximated by;

~~\cancel{x}~~ $f'(x) = \frac{f(x+h) - f(x-h)}{2h}$ — (iii)

with a truncation error of.

~~\cancel{x}~~ $E = \frac{f'''(x) \cdot 2h^2}{3!}$ — (iv)

The equation (iv) is called three point formula. This is also known as central difference quotient.

E.g. Find the value of derivative at $x=1$ for the function $f(x) = x^2$ by using $h=0.2$ and 0.05

Solution

For $h=0.2$

we know that, $f'(x) = \frac{f(x+h) - f(x-h)}{2h}$

$$\therefore f'(1) = \frac{f(1+0.2) - f(1-0.2)}{2 \times 0.2} = \frac{1.44 - 0.64}{0.4} = 2.$$

True value of derivative at $x=1$ is;

$$f'(x) = 2x = 2$$

$$\therefore \text{Error} = \left| \frac{2-2}{2} \right| \times 100\% = 0\%.$$

For $h=0.05$

$$\text{We know that, } f'(x) = \frac{f(x+h) - f(x-h)}{2h}$$

$$\text{or, } f'(1) = \frac{f(1+0.05) - f(1-0.05)}{2 \times 0.05} = 2$$

$$\therefore \text{Error} = \left| \frac{2-2}{2} \right| \times 100\% = 0\%.$$

* Algorithms:-

For two-Point Forward difference Formula

1. Start
2. Read the value at which derivative is needed, say x .
3. Read interval gap, say h .
4. Calculate $f(x_p)$ & $f(x_p+h)$.
5. Calculate $d = f'(x_p) = (f(x_p+h) - f(x_p)) / h$
6. Display the value derivative.
7. Terminate.

For two-Point Backward difference formula

Other steps are same as above except these;

4. Calculate $f(x_p)$ & $f(x_p-h)$.
5. Calculate $d = f'(x_p) = (f(x_p) - f(x_p-h)) / h$

For three-Point formula

Other steps are same as above except this;

5. calculate $d = f'(x_p) = (f(x_p+h) - f(x_p-h)) / 2h$.

2) Differentiating discrete (tabulated) functions:-

This is the process of approximating the derivatives $f'(x)$ of a function $f(x)$ when the functional value is known at some points but function is not known. We can still find derivatives of such tabulated functions.

→ To find derivative of the function at a point near to beginning we use Newton-Gregory forward formula.

→ " " at a point near to end we use Newton-Gregory backward formula.

→ " " near the middle we use Central difference formula.

→ In case the arguments are unequally spaced then we should use Newton's divided difference formula.

a) Derivatives Using Newton's Divided Difference Formula:

We know that, the general form of the Newton's divided difference polynomial is given by;

$$P_n(x) = f(x) = f[x_0] + f[x_1, x_0](x-x_0) + f[x_2, x_1, x_0](x-x_0)(x-x_1) \\ + f[x_3, x_2, x_1, x_0](x-x_0)(x-x_1)(x-x_2) + \dots \quad (i)$$

The first derivative of eqn (i) w.r.t. x , we get,

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

→ By putting $x=a$ in eqn (ii) we can get value of first derivative at $x=a$,

→ Again differentiating eqn (i) w.r.t. x we get,

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

→ By putting $x=a$ in eqn (iii) we can get value of second derivative at $x=a$.

Example: Find $f'(10)$ from the following data points:

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

Solution:

Since we have to find value at $x=10$, which lies around center of data points, so we use Newton's divided difference formula.

The divided difference table is given below:

$f(x)$	1 st Divided Differences	2 nd Divided Differences	3 rd Divided Differences	4 th Divided Differences
-13		$f[x_1, x_0]$		
23	$\frac{23 - (-13)}{5 - 3} = 18$		$f[x_2, x_1, x_0]$	
899		$\frac{146 - 18}{11 - 3} = 16$		$f[x_3, x_2, x_1, x_0]$
.			$\frac{40 - 16}{27 - 3} = 1$	$f[x_4, x_3, x_2, x_1, x_0]$
17315	$\frac{17315 - 899}{27 - 11} = 1026$			$\frac{1 - 1}{34 - 3} = 0$
35606		$\frac{2613 - 1026}{34 - 11} = 69$		
	$\frac{35606 - 17315}{34 - 27} = 2613$			

We know that,

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

At $x=10$

$$\begin{aligned} f'(10) &= 18 + 16 \{(10-5) + (10-3)\} + 1 \{(10-5)(10-11) + (10-3)(10-11) + (10-3)(10-5)\} \\ &= 18 + 16 \times 12 + 1 \times \{-5 - 7 + 35\} \\ &= 18 + 192 + 23 \\ &= 233. \end{aligned}$$

b) Derivatives Using Newton's Forward Difference Formula:

Newton's Forward difference formula is given by;

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

1st Derivative:

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

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

2nd Derivative

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

Example: Find the first and second derivatives of the functions tabulated below at 1.1.

x	1.0	1.2	1.4	1.6	1.8	2.0
f(x)	0.0	0.128	0.544	1.296	2.432	4.000

Solution:

Since $x = 1.1$ lies near the beginning of the table therefore in this case we shall use Newton's Gregory forward formula. The difference table is as below:-

x	f(x)	First Divided Differences	Second Divided Differences	Third Divided Differences	4 th Divided Difference	5 th Difference
1.0	0.0					
		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				
2.0	4.0					

We know that,

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

Here,

$h = 0.2$ and $s = \frac{(x-x_0)}{h} = \frac{(1.1-1.0)}{0.2} = 0.5$

n=2
4 data
6 terms
gr
76

Thus 1st Derivative;

$$f'(x) = \frac{1}{0.2} \left\{ 0.128 + \frac{1}{2}(2 \times 0.5 - 1) 0.288 + \frac{1}{6}(3 \times 0.25 - 6 \times 0.5 + 2) 0.048 \right\}$$

$$= \frac{1}{0.2} \{ 0.128 + 0 - 0.002 \}$$

$$= 0.63$$

Again, 2nd Derivative;

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

$$= \frac{1}{0.2^2} \left\{ 0.288 + \frac{1}{6}(6 \times 0.5 - 6) \cdot 0.048 + \frac{1}{24}(12 \times 0.25 - 36 \times 0.5 + 22) \times 0 \right\}$$

$$= \frac{1}{0.04} \{ 0.288 + (-0.024) + 0 \}$$

$$= 6.6$$

C. Derivatives Using Newton's Backward Difference Formula:

Newton's Backward Difference formula is given by;

$$f(x) = f(x_n) + \nabla f(x_n) s + \frac{1}{2} \nabla^2 f(x_n) s(s+1) + \dots + \frac{1}{n!} \nabla^n f(x_n) s(s+1)\dots(s+n-1)$$

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

1st Derivative;

$$f'(x) = \frac{1}{h} \left\{ \nabla f(x_n) + \frac{1}{2!}(2s+1) \nabla^2 f(x_n) + \frac{1}{3!}(3s^2 + 6s + 2) \nabla^3 f(x_n) + \dots \right\}$$

2nd Derivative;

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

Example: Find the first and second derivatives of the functions tabulated below at $x=9$.

x	5	6	7	8	9
$f(x)$	10.0	14.5	19.5	25.5	32.0

Solution:

Since $x=9$ lies at the end of the table therefore we use Newton's Gregory backward formula. The difference table is as below.

x	$f(x)$	1 st Divided Differences	2 nd Divided Differences	3 rd Divided Differences	4 th Divided Differences
5	10				
6	14.5	4.5	0.5		
7	19.5		5.0	0.5	-1.0
8	25.5			0.5	
9	32.0	6.5			

Here,
 Since backward
 so we select
 last values

$$h = 1.0 \text{ and } s = \frac{(x - x_n)}{h} = \frac{(9 - 9)}{1.0} = 0.$$

We know that,

1st Derivative;

$$f'(x) = \frac{1}{h} \left\{ \nabla f(x_n) + \frac{1}{2!} (2s+1) \nabla^2 f(x_n) + \frac{1}{3!} (3s^2+6s+2) \nabla^3 f(x_n) + \dots \right\}$$

Thus,

$$f'(9) = \frac{1}{1.0} \left\{ 6.5 + \frac{1}{2} (2 \times 0 + 1) 0.5 + \frac{1}{6} (3 \times 0 - 6 \times 0 + 2) (-0.5) \right\}$$

$$\text{or, } f'(9) = \frac{1}{1.0} \left\{ 6.5 + 0.25 - 0.166 \right\}$$

$$\text{or, } f'(9) = 6.584.$$

Again 2nd Derivative;

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

$$\text{or, } f''(9) = \frac{1}{1.0} \left\{ 0.5 + \frac{1}{6} (0+6) (-0.5) + \frac{1}{24} (0+0+22) (-1) \dots \right\}$$

$$\text{or, } f''(9) = \frac{1}{1.0} \left\{ 0.5 - 0.5 - 0.9166 \right\}$$

$$\text{or, } f''(9) = -0.9166$$

3) MAXIMA AND MINIMA OF TABULATED FUNCTIONS:

We know that first derivative of Newton's forward difference formula is given by;

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

For maxima or minima $f'(x)$ must be zero. Terminating the terms after third order and equating with zero, we get,

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

Now solving this.

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

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

Arranging terms on the basis of power of s , we get;

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

which can be written as;

$$as^2 + bs + c = 0 \quad \text{--- (1)}$$

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 (1) is quadratic in 's' and can be solved. Then value of x can be computed from the relation $x = x_0 + sh$.

Example. Find maximum and minimum values of the function tabulated below:

x	0	1	2	3
$f(x)$	-5	-7	-3	13

Solution:

The forward difference table is as below:

x	$f(x)$	1 st Divided Differences	2 nd Divided Differences	3 rd Divided Differences
0	-5			
1	-7		<u>6</u>	
2	-3		12	
3	13			

We know that,

$$as^2 + bs + c = 0 \quad \text{--- (1)}$$

where,

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

$$= \frac{1}{2} \times 6 = 3$$

$$b = \Delta^2 f(x_0) - \Delta^3 f(x_0) = 6 - 6 = 0$$

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

$$= -2 - \frac{1}{2} \times 6 + \frac{1}{3} \times 6$$

$$= -2 - 3 + 2$$

$$= -3$$

Thus eqn (1) becomes

$$as^2 + bs + c = 0$$

$$\Rightarrow 3s^2 - 3 = 0$$

$$\Rightarrow s = \pm 1$$

Again, $x = x_0 + sh$

Here, $x_0 = 0$ and $h = 1$

$$\Rightarrow x = 0 + (\pm 1) \times 1 = \pm 1$$

Again putting $s = x$ in Newton's forward difference formula;

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

$$\text{or, } f(x) = (-5) + x(-2) + \frac{1}{2} x(x-1) \times 6 + \frac{1}{6} x(x-1)(x-2) 6$$

$$\text{or, } f(x) = x^3 - 3x - 5$$

$$\Rightarrow f'(x) = 3x^2 - 3 \Rightarrow f''(x) = 6x. \text{ Hence, we have maxima at } x = -1 \text{ & minima at } x = 1.$$

B) NUMERICAL INTEGRATION:

② Definition and Application:-

Numerical integration is the process of computing the approximate value of a definite integral using a set of numerical values of the integrand. Integration is the process of measuring the area under a function plotted on a graph. It is represented by $\int_a^b f(x) \cdot dx$.

where, symbol \int is an integral sign

& a and b are the lower and upper limits of integration.

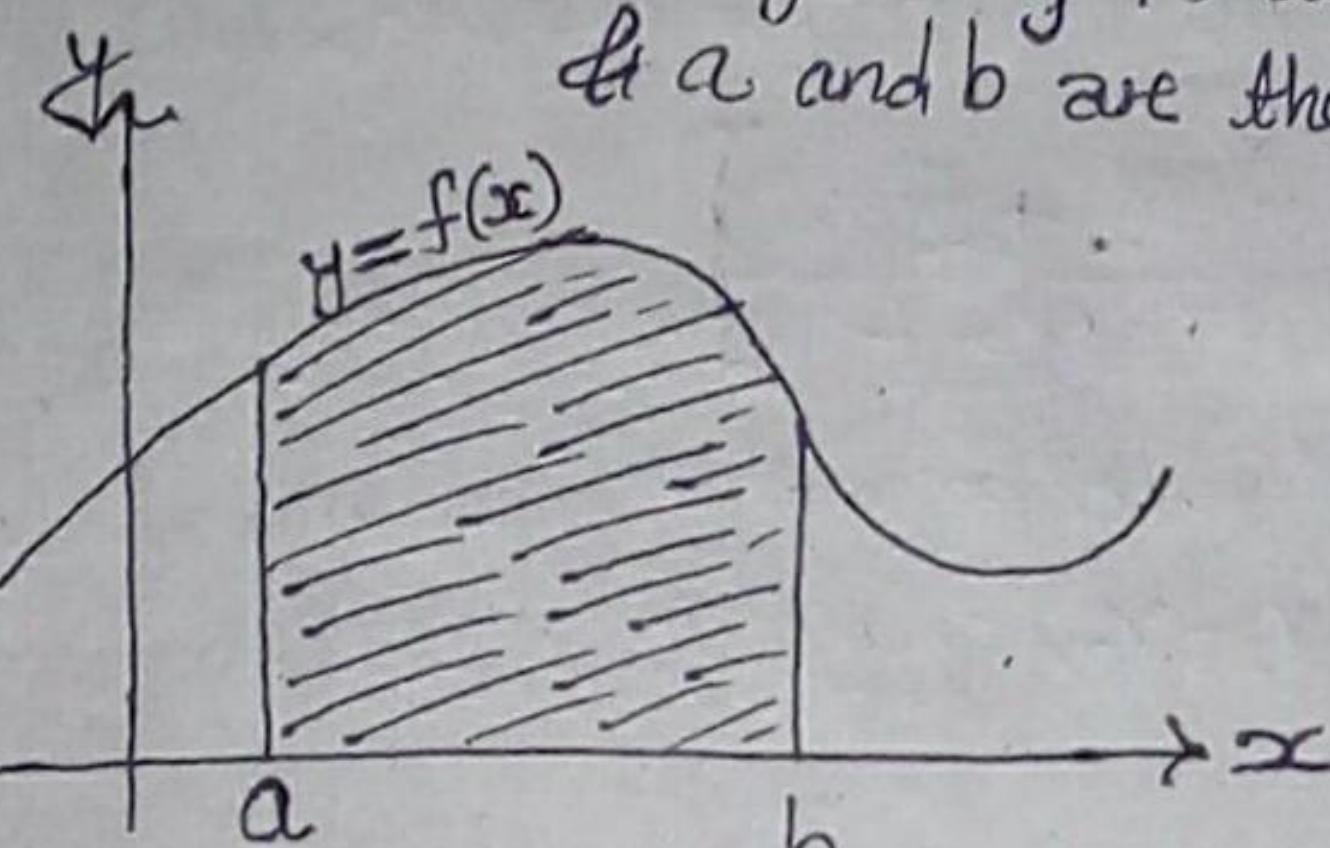


fig. Area of region under curve, $\text{Area} = \int_a^b f(x) \cdot dx$.

Applications:

- ▷ It is used to calculate numerical approximation for the value for the area under defined curve.
- ▷ It is used to evaluate a definite integral when there is no closed form expression for the integral or when the data is available in tabular form only.

Note: Integration is the reverse process of differentiation.

③ NEWTON-COTES INTEGRATION FORMULE:

It is a strategy to replace a complicated function or tabulated data with simpler polynomial for easy integration. Newton-Cotes integration comes in following two forms;

▷ Closed form → If the limits of integration a and b are in the set of interpolating points then the formula is referred to as closed form

▷ Open form → If the limits of integration a and b lie beyond the set of interpolating points then the formula is referred to as open form.

Some of the closed form methods are:-

a) Trapezoidal rule

b) Simpson's 1/3 rule

c) Simpson's 3/8 rule.

* General quadrature formula for equally spaced arguments:-

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

This equation is called general quadrature formula. From this formula we can obtain different integration by putting $n=1, 2, 3, \dots$ etc.

@ Trapezoidal Rule:- (OR Two-point trapezoidal rule)

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

This eqn is called trapezoidal rule and it is the area of the trapezoid whose width is $(x_1 - x_0)$ and height is the average of $f(x_0)$ and $f(x_1)$.

Example 1: Find $\int_2^8 \{x^3 + 2\} dx$ by using trapezoidal rule.

Solution:

$$\text{Here, } x_0 = 2, x_1 = 8$$

From trapezoidal rule we know that,

$$\begin{aligned} \int_{x_0}^{x_1} f(x) dx &= (x_1 - x_0) \left[\frac{f(x_0) + f(x_1)}{2} \right] \\ \Rightarrow \int_2^8 \{x^3 + 2\} dx &= (8 - 2) \left[\frac{10 + 514}{2} \right] \\ &= 1572 \end{aligned}$$

Example 2: Find $\int_0^1 e^{-x^2} dx$ by using trapezoidal rule.

Solution: Here, $x_0 = 0$ and $x_1 = 1$.

Now, from trapezoidal rule, we know that,

$$\begin{aligned} \int_{x_0}^{x_1} f(x) dx &= (x_1 - x_0) \left[\frac{f(x_0) + f(x_1)}{2} \right] \\ \Rightarrow \int_0^1 f(x) dx &= (1 - 0) \left[\frac{1 + 0.368}{2} \right] \\ &= 0.684. \end{aligned}$$

Q. Composite Trapezoidal Rule:- (OR Multiple-segment trapezoidal rule).

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

$$\text{where, } h = \frac{x_n - x_0}{k}$$

This equation is called composite trapezoidal formula.

Example 1: Compute the integral $\int_{-1}^1 e^x dx$ for $k=2$ and for $k=4$ using composite or multiple segment trapezoidal rule.

Solution:

$$\text{Here, } x_0 = -1 \text{ and } x_1 = 1$$

For $k=2$

$$h = \frac{(x_n - x_0)}{k} = \frac{(1+1)}{2} = 1$$

Using Formula,

$$\begin{aligned} \int_{-1}^1 e^x dx &= \frac{h}{2} \left[f(x_0) + 2 \left\{ \sum_{i=1}^{k-1} f(x_0 + ih) \right\} + f(x_2) \right] \\ &= \frac{1}{2} \left[e^{-1} + 2e^0 + e^1 \right] \\ &= \frac{2}{54} \\ &= \frac{1}{27} \end{aligned}$$

$$\begin{aligned} x_0 + ih &= -1 + 1 \times 1 \\ &= 0 \end{aligned}$$

For $k=4$

$$h = \frac{(x_n - x_0)}{k} = \frac{(1+1)}{4} = 0.5$$

$$\begin{aligned} \text{Now, } \int_{-1}^1 e^x dx &= \frac{h}{2} \left[f(x_0) + 2 \left\{ \sum_{i=1}^{k-1} f(x_0 + ih) \right\} + f(x_2) \right] \\ &= \frac{0.5}{2} \left[e^{-1} + 2e^{-0.5} + 2e^0 + 2e^{0.5} + e^1 \right] \\ &= 2.399 \end{aligned}$$

$$\begin{aligned} i &= 1 \text{ to } k-1 \\ i &= 1 \text{ to } 3 \\ x_0 + ih &= -1 + 1 \times 0.5 \\ &= -0.5 \end{aligned}$$

$$\begin{aligned} x_0 + ih &= -1 + 2 \times 0.5 \\ &= -1 + 1 \\ &= 0 \end{aligned}$$

$$\begin{aligned} x_0 + ih &= -1 + 3 \times 0.5 \\ &= -1 + 1.5 \\ &= 0.5 \end{aligned}$$

Example 2: Compute the integral $\int_1^5 \sqrt{1+x^2} dx$ for $k=4$ and $k=8$ by using composite or multiple-segment trapezoidal rule.

Solution:-

Here, $x_0 = 1$ and $x_n = 5$

For $k=4$

$$h = \frac{(x_n - x_0)}{k} = \frac{(5-1)}{4} = 1$$

$$\begin{aligned}\therefore \int_1^5 \sqrt{1+x^2} dx &= \frac{h}{2} \left[f(x_0) + 2 \left\{ \sum_{i=1}^{k-1} f(x_0 + ih) \right\} + f(x_k) \right] \\ &= \frac{1}{2} \left[1.414 + 2 \times \{2.236 + 3.162 + 4.123\} + 5.099 \right] \\ &= 12.78\end{aligned}$$

For $k=8$

$$h = \frac{(x_n - x_0)}{k} = \frac{(5-1)}{8} = 0.5$$

$$\begin{aligned}\therefore \int_1^5 \sqrt{1+x^2} dx &= \frac{h}{2} \left[f(x_0) + 2 \left\{ \sum_{i=1}^{k-1} f(x_0 + ih) \right\} + f(x_k) \right] \\ &= \frac{0.5}{2} \left[1.414 + 2 \times \{1.803 + 2.236 + 2.696 + 3.162 \right. \\ &\quad \left. + 3.64 + 4.123 + 4.609\} + 5.099 \right] \\ &= 12.76\end{aligned}$$

(b) Simpson's $\frac{1}{3}$ Rule:

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

where, $h = \frac{b-a}{n}$ (we take $n=2$ in this rule).

This equation is called Simpson's $\frac{1}{3}$ rule.

Example 1: Apply Simpson's $\frac{1}{3}$ rule to calculate $\int_0^1 \sqrt{1-x^2} dx$.

Solution:

$$\text{Here, } h = \frac{b-a}{n} = \frac{1-0}{2} = 0.5$$

Since,

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

$$\Rightarrow f(x_0) = f(0) = 1$$

$$f(x_1) = f(x_0+h) = f(0.5) = 0.866$$

$$f(x_2) = f(x_0+2h) = f(1) = 0.$$

Thus, Simpson's $\frac{1}{3}$ rule is given by;

$$\begin{aligned} I &= \int_{x_0}^{x_2} f(x) dx = \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)] \\ &= \frac{0.5}{3} [1 + 4 \times 0.866 + 0] \\ &= 0.744 \end{aligned}$$

Example 2: Apply Simpson's $\frac{1}{3}$ rule to calculate $\int_0^\pi \sin x dx$.

Solution:

$$\text{Here, } h = \frac{\pi-0}{2} = \frac{\pi}{2}$$

Simpson's $\frac{1}{3}$ rule is given by,

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

Since, $f(x) = \int_0^\pi \sin x dx$

$$\Rightarrow f(x_0) = f(0) = 0$$

$$\Rightarrow f(x_1) = f(x_0+h) = f\left(\frac{\pi}{2}\right) = 1$$

$$\Rightarrow f(x_2) = f(x_0+2h) = f(\pi) = 0$$

Thus,

$$\begin{aligned} I &= \int_{x_0}^{x_2} f(x) dx = \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)] \\ &= \frac{\pi}{6} [0 + 4 \times 1 + 0] \\ &= 2.101 \end{aligned}$$

$$\begin{array}{c} x_2 \\ \int_{x_0}^{x_2} f(x) dx = \int_0^1 \sqrt{1-x^2} dx \\ \text{so, } x_0=0 \\ x_2=1 \end{array}$$

④ Composite Simpson's $\frac{1}{3}$ Rule:

In this method one can divide the subdivide the interval $[a, b]$ into k segments as $(x_0 + ih)$ where $i=0$ to $i=k-1$ and apply Simpson's $\frac{1}{3}$ rule repeatedly over every two segments. Note that k needs to be even. We divide interval $[a, b]$ into n equal segments, so that segment width is given by;

$$h = \frac{b-a}{k} \quad (\text{OR } h = \frac{x_n - x_0}{k}) \quad (\text{both are same})$$

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

This equation is called composite Simpson's $\frac{1}{3}$ rule.

Example: Apply Simpson's $\frac{1}{3}$ rule to calculate $\int_{-1}^1 1-x^2 dx$ by using 4 segments (i.e., $k=4$) and 8 segments (i.e., $k=8$).

Solution: Here, $x_0 = 0$ and $x_n = 1$.

For $k=4$

$$h = \frac{x_n - x_0}{k} = \frac{1-0}{4} = 0.25$$

From composite Simpson's rule, we know that,

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

$$\text{or, } \int_{x_0}^{x_n} f(x) \cdot dx = \frac{h}{3} \left[f(x_0) + 4 \{f(x_1) + f(x_3)\} + 2 \{f(x_2)\} + f(x_n) \right]$$

Since, $f(x_0) = f(0) = 1$

$$f(x_1) = f(x_0 + h) = f(0.25) = 0.968$$

$$f(x_2) = f(x_0 + 2h) = f(0.5) = 0.866$$

$$f(x_3) = f(x_0 + 3h) = f(0.75) = 0.661$$

$$f(x_4) = f(x_0 + 4h) = f(1) = 0.$$

Thus,

$$\int_{x_0}^{x_n} f(x) \cdot dx = \frac{h}{3} [f(x_0) + 4\{f(x_1) + f(x_3)\} + 2\{f(x_2)\} + f(x_n)]$$

$$= \frac{h}{3} [1 + 4\{0.968 + 0.661\} + 2\{0.866\} + 0]$$

$$= \frac{0.25}{3} \{9.248\}$$

$$= 0.771$$

Similarly we can do for k=8.

③ Simpson's $\frac{3}{8}$ Rule:

$$I = \int_{x_0}^{x_3} f(x) \cdot dx = \frac{3}{8} h [f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)]$$

where, $h = \frac{b-a}{n}$. (In this rule we take $n=3$)

This equation is called Simpson's $\frac{3}{8}$ rule.

Example: Apply Simpson's $\frac{3}{8}$ rule to calculate $\int_0^2 (2 + \cos(2\sqrt{x})) dx$.

Solution: Here, $h = \frac{2-0}{3} = 0.666$

Simpson's $\frac{3}{8}$ rule is given by,

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

Since, $f(x) = 2 + \cos(2\sqrt{x})$

$$\Rightarrow f(x_0) = f(0) = 3$$

$$f(x_1) = f(x_0 + h) = f(0.666) = 1.939$$

$$f(x_2) = f(x_0 + 2h) = f(1.332) = 1.328$$

$$f(x_3) = f(x_0 + 3h) = f(2) = 1.049$$

$$\therefore I = \int_{x_0}^{x_3} f(x) \cdot dx = \frac{3}{8} h [f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)]$$

$$= \frac{3}{8} \times 0.666 [3 + 3 \times 1.939 + 3 \times 1.328 + 1.049]$$

$$= 3.46$$

Q. Composite Simpson's 3/8 Rule:-

This method divides the interval $[x_0, x_n]$ into n segments and apply Simpson's 3/8 rule repeatedly every three segments. Therefore n needs to be multiple of 3. Now, the segment width is given by, $h = \frac{x_n - x_0}{n}$.

$$\int_{x_0}^{x_n} f(x) dx = \frac{3}{8} h \left[f(x_0) + 3 \sum_{q=1}^{\frac{n-1}{3}} f(x_q) + 2 \sum_{q=2}^{\frac{n-1}{3}} f(x_q) + f(x_n) \right]$$

$\begin{matrix} q \bmod 3 \neq 0 \\ q \bmod 3 = 0 \end{matrix}$

This equation is called composite Simpson's 3/8 rule.

Example 1: Calculate the integral value of following tabulated function from $x=0$ to $x=1.6$ using Simpson's 3/8 rule.

Solution :

$f(x)$	0	0.2	0.4	0.6	0.8	1.0	1.2	1.4	1.6
	0	0.24	0.55	0.92	1.63	1.84	2.37	2.95	3.56

Here, $h = 0.2$

Composite Simpson's 3/8 rule is given by;

$$I = \int_{x_0}^{x_n} f(x) dx = \frac{3}{8} h \left[f(x_0) + 3 \sum_{q=1}^{\frac{n-1}{3}} f(x_q) + 2 \sum_{q=2}^{\frac{n-1}{3}} f(x_q) + f(x_n) \right]$$

$\begin{matrix} q \bmod n \neq 0 \\ q \bmod n = 0 \end{matrix}$

$$\Rightarrow I = \frac{3}{8} h [f(x_0) + 3f(x_1) + 3f(x_2) + 2f(x_3) + 3f(x_4) + 3f(x_5) + 2f(x_6) \\ + 3f(x_7) + 3f(x_8) + f(x_9)]$$

Thus,

$$I = \frac{3}{8} h [0 + 3 \times 0.24 + 3 \times 0.55 + 2 \times 0.92 + 3 \times 1.63 + 3 \times 1.84 \\ + 2 \times 2.37 + 3 \times 2.95 + 3.56] \\ = 2.38$$

Note:- $x=0$ to $x=1.6$ in question means calculating 8 segments from $f(x_0)$ to $f(x_8)$. Values of $f(x_0)$ to $f(x_8)$ are given in table in this question if not given we have to calculate as;

$$f(x_0) = f(0) = \dots$$

$$f(x_1) = f(x_0 + h) = \dots \quad \text{Then we place values and calculate.}$$

$$f(x_8) = f(x_0 + 8h) = \dots$$

⊗ GAUSSIAN INTEGRATION:

Generalized n -point Gaussian quadrature rule is given as;

$$\int_{-1}^1 f(x) dx = \sum_{q=1}^n w_q \cdot f(x_q)$$

One-point: $\int_{-1}^1 f(x) dx = 2 \cdot f(0)$.

Two-point: $\int_{-1}^1 f(x) dx = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$.

Three-point: $\int_{-1}^1 f(x) dx = \frac{5}{9} f\left(-\sqrt{\frac{3}{5}}\right) + \frac{8}{9} f(0) + \frac{5}{9} f\left(\sqrt{\frac{3}{5}}\right)$.

Changing limits:

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

$$\text{Also, } x = \frac{b-a}{2} z + \frac{a+b}{2} = 2z$$

Example: Compute the integral $\int_{-2}^2 e^{-x^2/2} dx$ using Gaussian two-point formula.

Solution: Here, $a = -2$ and $b = 2$.

after changing limits, we get

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

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

Thus,

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

From Gaussian two-point formula, we know that,

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

Thus,

$$\begin{aligned} \int_a^b e^{-x^2} dx &= 2 \int_{-1}^1 e^{-z^2} dz \\ &= 2 \left\{ e^{-1/\sqrt{3}} + e^{1/\sqrt{3}} \right\} \\ &= 4.6854. \end{aligned}$$

Alternatively we can solve it as below:-

We have, $a = -2$ and $b = 2$

We know that,

function HT value
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$$z_1 = -0.57735, z_2 = 0.57735$$

Thus,

$$x_1 = \frac{(b-a)}{2} z_1 + \frac{(b+a)}{2} = 2 \times -0.57735 = -1.1547$$

$$x_2 = \frac{(b-a)}{2} z_2 + \frac{(b+a)}{2} = 2 \times 0.57735 = 1.1547.$$

Now,

$$V = \frac{(b-a)}{2} (f(x_1) + f(x_2)) = 2 \left(e^{-1.1547/2} + e^{-1.1547/2} \right) = 4.6854$$

④ ROMBERG INTEGRATION:-

1). Trapezoidal rule to compute $T(0,0) = \frac{h}{2} (f(x_0) + f(x_1))$.

2). Recursive trapezoidal rule for $T(q,0) = \frac{T(q-1,0)}{2} + \frac{h}{2^q} \sum_{k=1}^{2^q-1} f(x_0 + (2k-1)h/2^q)$
where, $h = (x_1 - x_0)$.

→ Romberg Integration formula is given by;

$$\int_a^b f(x) dx = T_{m+k,k} + O(h^{2(k+1)}) = \frac{4^k T_{m+k,k-1} - T_{m+k-1,k-1}}{4^k - 1} + O(h^{2(k+1)}).$$

where, m is integer.

Example: Compute Romberg estimate $T(2,2)$ for $\int_0^1 \frac{1}{1+x} dx$.

Solution

Use trapezoidal rule to compute $T(0,0)$ first;

$$\begin{aligned} T(0,0) &= \frac{h}{2} (f(x_0) + f(x_1)) \\ &= \frac{1}{2} (f(0) + f(1)) \\ &= 0.5 \times (1+0.5) \\ &= 0.75. \end{aligned}$$

Now calculate $T(1,0)$ & $T(1,1)$ using recursive trapezoidal rule;

$$\begin{aligned} T(1,0) &= \frac{T(0,0)}{2} + \frac{h}{2^1} \sum_{k=1}^{2^{1-1}} f(x_0 + (2k-1)h/2^1) = \frac{T(0,0)}{2} + \frac{h}{2} f(x_0 + h/2) \\ &= \frac{0.75}{2} + 0.5 \times f(0.5) \\ &= 0.7083 \\ T(2,0) &= \frac{T(1,0)}{2} + \frac{h}{2^2} \sum_{k=1}^{2^{2-1}} f(x_0 + (2k-1)h/2^2) = \frac{T(1,0)}{2} + \frac{h}{4} f(x_0 + h/4) \\ &\quad + \frac{h}{4} f(x_0 + 3h/4) \\ &= \frac{0.7083}{2} + \frac{1}{4} f(0.25) + \frac{1}{4} f(0.75) \\ &= 0.3541 + 0.2 + 0.1428 \\ &= 0.6969 \end{aligned}$$

Now use Romberg Integration formula to compute $T(1,1)$, $T(2,1)$ & $T(2,2)$ as below:

$$T(1,1) = \frac{4 \times T(1,0) - T(0,0)}{4-1} = \frac{4 \times 0.7083 - 0.75}{3} = 0.6944.$$

$$T(2,1) = \frac{4 \times T(2,0) - T(1,0)}{4-1} = \frac{4 \times 0.6969 - 0.7083}{3} = 0.6931$$

$$T(2,2) = \frac{16 \times T(2,1) - T(1,1)}{16-1} = \frac{16 \times 0.6931 - 0.6944}{15} = 0.6930.$$