Unit 3

Numerical Differentiation & Integration

Derivative or differentiation of a function is the process of finding the rate of change of a ~~f~~ variable with respect to another variable. For example the velocity of a moving body is defined as the rate of change of location of the body w.r.t. time. Location/displacement depends on time, so time is independent variable and location is dependent variable.

Numerical differentiation is a process of getting an approximate derivative of a function in a situation where it might be difficult or impossible to find the derivative using the analytical method. For example, if we have a set of observation values (data points) instead of a function, we can find the derivative at a point by using the numerical methods.

Following are two major applications of numerical differentiation.

(i) A continuous function is to be diffentiated but is difficult using analytical method.

(ii) A discrete (tabulated) function is to be differentiated where the function is unknown.

Differentiating Continuous Functions

Numerical method of differentiation can be used to find the derivative of a continuous function where the function itself is known. We can use the following numerical methods for this:

(a) Two-point forward difference method.
(b) Two-point backward difference method.
(c) Three-point formula

a. Two-Point Forward Difference Method:

From Taylor's theorem, we have

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

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

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

If h is considered to be very small,

$$\boxed{f'(x) = \frac{f(x+h) - f(x)}{h}}, \quad E = \frac{-h.f''(x)}{2!}$$

(Truncation error).

This equation is known as two point forward difference formula of numerical differentiation. It is also known as forward difference quotient.

Q. Find the value of derivative of a function $f(x) = x^2$ at $x = 1$ by using $h = 0.2$ & 0.05.

→ Taking $h = 0.2$,

We have the two-point forward difference formula,

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

or, $$f'(1) = \frac{f(1+0.2) - f(1)}{0.2}$$

or, $$f'(1) = \frac{(1.2)^2 - (1)^2}{0.2}$$

$$\therefore f'(1) = 2.2$$

True value $f'(1) = f'(x)\big|_{x=1}$

$$= 2x\big|_{x=1}$$

$$= 2$$

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

Taking $h = 0.05$,

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

$$= \frac{f(1.05) - f(1)}{0.05}$$

$$= \frac{1.1025 - 1}{0.05}$$

$$= 2.05$$

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

$$= 2.5\%$$

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Q. Find the value of derivative at $x = 45°$ for the function $f(x) = \sin x + 1$ by using $h = 0.1$ & 0.001.

→ Angle in radian $(x) = \dfrac{45 \times \pi}{180} = 0.785$

Taking $h = 0.1$,

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

or, $$f'(0.785) = \frac{f(0.785 + 0.1) - f(0.785)}{0.1}$$

$$= \frac{f(0.885) - f(0.785)}{0.1}$$

$$= \frac{(0.774 + 1) - (0.709 + 1)}{0.1}$$

$$= \frac{0.067}{0.1}$$

$$= 0.67$$

True value $= \cancel{\sin}\ f'(x)$

$= \cos(x)$

$= \cos(0.785)$

$= 0.707$

$\therefore$ Error $= \left| \dfrac{0.707 - 0.67}{0.707} \right| \times 100\% = 5.23\%$

Similarly, Taking $h = 0.001$, we can solve it.

b. Two-Point Backward Difference Formula:

Backward difference two point formula is,

$$\boxed{f'(x) = \frac{f(x) - f(x-h)}{h}}, \quad E = \frac{h f''(x)}{2!} \text{ (Truncation Error)}$$

This is also called as backward difference quotient.

Q. Find the derivative of $f(x) = \sin x + 1$ at $x = 45°$ using backward difference two point formula. Take $h = 0.1$ and 0.001.

→ Angle in radian $(x) = 45 \times \frac{\pi}{180} = 0.785$

Taking $h = 0.1$,

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

or, $$f'(0.785) = \frac{f(0.785) - f(0.785 - 0.1)}{0.1}$$

$$= \frac{0.707 - 0.633}{0.1}$$

$$= 0.74$$

True value $f'(x) = \cos x$

$f'(0.785) = 0.707$

$$\therefore \text{Error} = \left| \frac{0.707 - 0.74}{0.707} \right| \times 100\%$$

$$= 4.67\%$$

Similarly solve for $h = 0.001$.

C. Three-Point formula :-

The three-point formula for numerical differentiation is given by,

$$\boxed{f'(x) = \frac{f(x+h) - f(x-h)}{2h}} \quad , E = \frac{2h^2}{3!} f'''(x) \text{ (Truncation Error)}$$

Q. Find the value of $f'(x)$ at $x=1$ for $f(x) = x^2$ using three point formula. Take $h=0.2$ & 0.05.

Q. Find $f'(3)$ if $f(x) = 2e^{1.5x}$ using forward difference formula. Also find relative approximate error.

Ans: $f'(3) = \cancel{270.05}\ 291.3$

Error $= 7.8\%$.

Differentiating Tabulated Functions Using Newton's Differences :-

1. By using Forward Interpolation formula

Let the tabulated data points be $(x_0, y_0), (x_1, y_1), \ldots, (x_n, y_n)$, where the independent variable x has equally spaced values x_i with equal space h.

The forward difference formula for interpolation polynomial is,

$$f(x) = y_0 + p\,\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \ldots \quad (i)$$

where,

$$p = \frac{x - x_0}{h} \quad \text{and } \Delta^n y_0 \text{ is } n^{th} \text{ forward difference}$$

Differentiating equation (i) w.r.t. x,

$$f'(x) = \frac{\partial y}{\partial p} \cdot \frac{\partial p}{\partial x}$$

$$= \frac{1}{h}\left(\frac{\partial y}{\partial p}\right)$$

$$\therefore \boxed{f'(x) = \frac{1}{h}\left[\Delta y_0 + \frac{2p-1}{2!}\Delta^2 y_0 + \frac{3p^2-6p+2}{3!}\Delta^3 y_0 + \ldots\right]}$$

Again differentiating w.r.t. x,

$$f''(x) = \frac{\partial f'(x)}{\partial p} \cdot \frac{\partial p}{\partial x}$$

$$\boxed{f''(x) = \frac{1}{h^2}\left[\Delta^2 y_0 + (p-1)\Delta^3 y_0 + \ldots\right]}$$

Note that at $x = x_0$ (initial point), $p = 0$.

Formulae to remember,

$$f'(x) = \frac{1}{h}\left[\Delta y_0 + \frac{2p-1}{2!}\Delta^2 y_0 + \frac{3p^2-6p+2}{3!}\Delta^3 y_0 + \frac{4p^3-18p^2+22p-6}{4!}\Delta^4 y_0 + \cdots\right] \quad \text{— (i)}$$

where $p = \frac{x-x_0}{h}$

If $x = x_0$ (Initial point) then $p = 0$

$$\therefore \; f'(x_0) = \frac{1}{h}\left[\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0 - \frac{1}{4}\Delta^4 y_0 + \cdots\right] \quad \text{— (ii)}$$

Similarly for second order derivative,

$$f''(x) = \frac{1}{h^2}\left[\Delta^2 y_0 + (p-1)\Delta^3 y_0 + \frac{6p^2-18p+11}{12}\Delta^4 y_0 + \cdots\right] \quad \text{— (iii)}$$

At $x = x_0$, $p = 0$.

$$f''(x_0) = \frac{1}{h^2}\left[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12}\Delta^4 y_0 - \frac{5}{6}\Delta^5 y_0 + \cdots\right] \quad \text{— (iv)}$$

Note:-

Let the tabulated function be,

x	x_0	x_1	x_2	...	x_n
$f(x)$	y_0	y_1	y_2	...	y_n

(Better remember formula (i) & iii)

If we have to find the derivatives (1st or 2nd) at any point other than $x_0, x_1, \ldots, x_n$, we use formula (i) and (iii) above.

If we have to find derivatives at $x = x_0$, we can directly use formula (ii) and (iv);

To find derivatives at $x = x_i$ $(i = 1, 2, \ldots, n)$, we can rearrange formula for $\Delta y_i, \Delta^2 y_i, \ldots, \Delta^n y_i$.

Q. Find first and second derivatives for the given tabulated functions at $x = 1.1$.

x	1.0	1.2	1.4	1.6	1.8	2.0
$f(x)$	0	0.128	0.544	1.296	2.432	4.000

→ Since 1.1 lies in the first half of the table, we can use Newton's forward difference method to find $f'(1.1)$ & $f''(1.1)$.

The forward difference table is,

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$	$\Delta^5 y$
1.0	0	0.128	0.288	0.048	0	0
1.2	0.128	0.416	0.336	0.048	0	
1.4	0.544	0.752	0.384	0.048		
1.6	1.296	1.136	0.432			
1.8	2.432	1.568				
2.0	4.000					

The first derivative of Newton's forward interpolation polynomial is,

$$f'(x) = \frac{1}{h}\left\{\Delta y_0 + \frac{2p-1}{2!}\Delta^2 y_0 + \frac{3p^2-6p+2}{3!}\Delta^3 y_0 + \dots\right\} \quad \text{(i)}$$

Where, $h = 0.2$

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

Thus,

$$f'(1.1) = \frac{1}{0.2}\left\{0.128 + \frac{2\times 0.5 - 1}{2}\times 0.288 + \frac{3\times 0.5\times 0.5 - 6\times 0.5 + 2}{6}\times 0.048\right\}$$

$$= 0.63$$

Again for second derivative,

$$f''(x) = \frac{1}{h^2}\left\{\Delta^2 y_0 + (p-1)\Delta^3 y_0 + \frac{6p^2-18p+11}{12}\Delta^4 y_0 + \cdots\right. \quad \text{(ii)}$$

Thus

$$f''(1.1) = \frac{1}{0.2^2}\left\{0.288 + (0.5-1)\,0.048 + \frac{6\times0.25-18\times0.5+11}{12} \times 0\right\}$$

$$= 6.6$$

Q. Find dy/dx and d^2y/dx^2 at $x=1$ from the following tabulated function.

x	1	2	3	4	5	6	7
$f(x)$	0.000	0.693	1.099	1.368	1.609	1.796	1.976

Ans: $\frac{dy}{dx} = f'(1) = 0.8779$

$\frac{d^2y}{dx^2} = f''(1) = -0.186$

Q. Find the first and second derivatives at $x = 1.1$.

x	1	1.1	1.2	1.3	1.4	1.5	1.6
y	7.989	8.403	8.781	9.129	9.451	9.750	10.031

Ans: $f'(1.1) = 3.952$

$f''(1.1) = -3.740$

Q. Find $f'(1)$ from the given tabulated function.

x	1.0	1.1	1.2	1.3
$f(x)$	0.041	0.891	0.932	0.763

Ans: $f'(1) = 0.542$

Maxima & Minima of Tabulated Functions :-

The Newton's forward interpolation formula is given:

$$f(x) = y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \dots$$

Differentiating w.r.t. p, we get,

$$\frac{dy}{dp} = \Delta y_0 + \frac{2p-1}{2}\Delta^2 y_0 + \frac{3p^2-6p+2}{3!}\Delta^3 y_0 + \dots$$

For maxima or minima, $\frac{dy}{dp} = 0$.

$$\frac{dy}{dp} = 0$$

or, $$\Delta y_0 + \frac{2p-1}{2!}\Delta^2 y_0 + \frac{3p^2-6p+2}{3!}\Delta^3 y_0 = 0$$

Solving the above expression for p by the help of the difference table, we get the value of p and hence the value of x for which y is maximum or min.

Q. Find the minimum value of y from the following tabulated function.

x	0.60	0.65	0.70	0.75
$f(x)$	0.6221	0.6155	0.6138	0.6170

→ Constructing the forward difference table,

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$
0.60	0.6221			
		-0.0066		
0.65	0.6155		0.0049	
		-0.0017		0
0.70	0.6138		0.0049	
		+0.0032		
0.75	0.6170			

Newton's forward difference formula is

$$f(x) = y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \cdots \quad (i)$$

where $p = (x - x_0)/h$ &

$\Delta^n y_0$ = n^{th} forward difference.

Differentiating, eqn (i) w.r.t p,

$$f'(x) = \frac{\partial f(x)}{\partial p}$$

$$= 0 + \Delta y_0 + \frac{2p-1}{2}\Delta^2 y_0 + \frac{3p^2-6p+2}{6}\Delta^3 y_0$$

$$= 0 + (-0.0066) + \frac{(2p-1)(0.0049)}{2} + 0$$

$$= -0.0066 + \frac{(2p-1)}{2} \times 0.0049$$

for maxima or minima, $f'(x) = 0$

or, $\frac{(2p-1)}{2}(0.0049) = 0.0066$

$\therefore \; p = 1.8469$

Since $p = (x - x_0)/h$

$x = x_0 + ph$

$= 0.60 + 1.8469(0.05)$

$= 0.6923$

$\therefore$ y is minimum at $x = 0.6923$. The minimum value of y can be obtained by putting the obtained values of p and $\Delta y_0, \Delta^2 y_0, \ldots$ in eqn (i).

$$f(0.6923) = 0.6221 + 1.8469 \times (-0.0066) + \frac{1.8469 \times 0.8469 \times 0.0049}{2} + 0$$

$$= 0.6137$$

Q. Find the maximum & minimum value of y from the following data.

x	-2	-1	0	1	2	3	4
y	2	-0.25	0	-0.25	2	15.75	56

→ Constructing the forward difference table,

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$	$\Delta^5 y_0$
-2	2	-2.25	2.5	-3	6	0
-1	-0.25	0.25	-0.5	3	6	0
0	0	-0.25	2.5	9	6	
1	-0.25	2.25	11.5	15		
2	2	13.75	26.5			
3	15.75	40.25				
4	56					

Newton's forward interpolation formula is,

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

$$+ \frac{p(p-1)(p-2)(p-3)}{4!}\Delta^4 y_0 + \cdots \quad \text{——— (i)}$$

where $p = (x - x_0)/h$

Differentiating eqn (i) w.r.t. x, we get,

$$\frac{dy}{dx} = \frac{\partial y}{\partial p}\frac{\partial p}{\partial x}$$

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

Let $x_0 = 0,\ y_0 = 0$ then

$\Delta y_0 = -0.25$

$\Delta^2 y_0 = 2.5$

$\Delta^3 y_0 = 9$

$\Delta^4 y_0 = 6$

$h = 1$

$p = (x - x_0)/h = (x-0)/1 = x$

$$\therefore \frac{dy}{dx} = 1\left[-0.25 + \frac{2x-1}{2} \times 2.5 + \frac{3x^2-6x+2}{6} \times 9 + \frac{4x^3-18x^2+22x-6}{24} \times 6\right]$$

$$= -0.25 + 2.5x - 1.25 + 4.5x^2 - 9x + 3 + x^3 - 4.5x^2 + 5.5x - 1.5$$

$$= x^3 - x$$

For y to be maximum or minimum

$$\frac{dy}{dx} = 0$$

or, $x^3 - x = 0$

or, $x(x^2-1) = 0$

$\therefore x = 0, -1, +1.$

Again,

$$\frac{d^2y}{dx^2} = 3x^2 - 1$$

For $x = 0$, $\frac{d^2y}{dx^2} = -1$ (Negative)

For $x = -1$, $\frac{d^2y}{dx^2} = 2$ (Positive)

For $x = 1$, $\frac{d^2y}{dx^2} = 2$ (Positive)

$\therefore$ y is maximum at $x = 0$ and

y is minimum at $x = -1$ & $+1$.

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Q. From the given data points, determine the value of x at which y is minimum. Also find the minimum value of y.

x	3	4	5	6	7	8
y	0.205	0.240	0.259	0.262	0.250	0.224

Ans: y is minimum at $x = 5.6875$ & minimum value of y is 0.2628

Numerical Integration :-

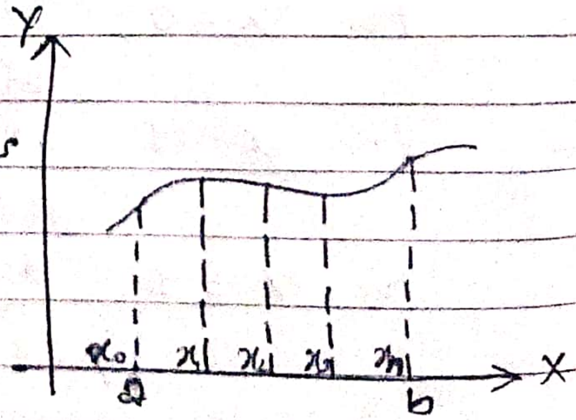
The process of evaluating a definite integral from a set of tabulated values of the integrand function is called numerical integration or quadrature. Typically, quadrature is the process of evaluating the area bounded by a curve.

Newton-Cotes Quadrature Formula :-

Let $I = \int_a^b f(x)\,dx$ be the integral to be evaluated

where $y = f(x)$ is the integrand function for the given set of tabulated data points.

Let us break the interval a-b into n different sub-intervals of size h.



Then,

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

& $x_0 = a$, $x_1 = a+h = x_0 + h$, $x_2 = x_0 + 2h$, ..., $x_n = x_0 + nh = b$

From Newton's forward interpolation, we have

$$y = y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \cdots \quad \text{(i)}$$

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

or, $x = x_0 + ph$

Now,

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

$$= h\int_0^n f(x_0 + ph)\,dp$$

or, $$\int_a^b f(x)\,dx = h\int_0^n \left[y_0 + p\Delta y_0 + \frac{p(p-1)}{2!}\Delta^2 y_0 + \frac{p(p-1)(p-2)}{3!}\Delta^3 y_0 + \cdots\right]dp$$

$$= h\left[py_0 + \frac{p^2}{2}\Delta y_0 + \frac{1}{2}\left(\frac{p^3}{3} - \frac{p^2}{2}\right)\Delta^2 y_0 + \frac{1}{6}\left(\frac{p^4}{4} - p^3 + p^2\right)\Delta^3 y_0 + \cdots\right]_0^n$$

$$= h\left[ny_0 + \frac{n^2}{2}\Delta y_0 + \left(\frac{n^3}{3} - \frac{n^2}{2}\right)\frac{\Delta^2 y_0}{2!} + \left(\frac{n^4}{4} - n^3 + n^2\right)\frac{\Delta^3 y_0}{3!} + \cdots\right]$$

Which is the required expression for the Newton-Cotes quadrature formula. This can be used to determine the integral value of a tabulated function having n integvals (ie. n+1 points).

Formula:

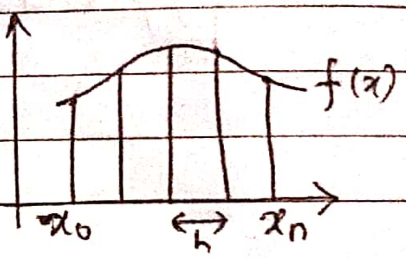
$$\int_{x_0}^{x_0+nh} f(x)\,dx = h\left[ny_0 + \frac{n^2}{2}\Delta y_0 + \left(\frac{n^3}{3} - \frac{n^2}{2}\right)\frac{\Delta^2 y_0}{2!} + \left(\frac{n^4}{4} - n^3 + n^2\right)\frac{\Delta^3 y_0}{3!} + \left(\frac{n^5}{5} - \frac{3n^4}{2} + \frac{11n^3}{3} - 3n^2\right)\frac{\Delta^4 y_0}{4!} + \cdots\right.$$

Trapezoidal Rule :-

By Newton-Cotes Quadrature formula, we have

$$\int_{x_0}^{x_0+nh} f(x)\,dx = h\left[ny_0 + \frac{n^2}{2}\Delta y_0 + \left(\frac{n^3}{3} - \frac{n^2}{2}\right)\frac{\Delta^2 y_0}{2!} + \left(\frac{n^4}{4} - n^3 + n^2\right)\frac{\Delta^3 y_0}{3!} + \cdots\right] \quad \text{—— (i)}$$

When $n=1$, the function is approximated with a polynomial of degree 1 (straight line). The integral is evaluated in the range x_0 to x_1. All the higher order forward differences except Δy_0 become zero.



So, eqn (i) gives

$$\int_{x_0}^{x_0+h} f(x)\,dx = h\left[y_0 + \frac{\Delta y_0}{2}\right]$$

$$= h\left[y_0 + \frac{y_1 - y_0}{2}\right]$$

$$= \frac{h}{2}\left[y_0 + y_1\right]$$

$$\therefore \int_{x_0}^{x_1} f(x)\,dx = \frac{h}{2}(y_0 + y_1) \quad \text{—— (ii)}$$

This is also called as one segment Trapezoidal rule.

Similarly the integral for second segment/interval is given by

$$\int_{x_1}^{x_2} f(x)\,dx = \frac{h}{2}(y_1 + y_2) \quad \text{—— (iii)}$$

For last interval, trapezoidal rule becomes

$$\int_{x_{n-1}}^{x_n} f(x)\,dx = \frac{h}{2}(y_{n-1}+y_n) \quad \text{——— (iv)}$$

Adding all the integrals, we get

$$\int_{x_0}^{x_n} f(x)\,dx = \int_{x_0}^{x_1} f(x)\,dx + \int_{x_1}^{x_2} f(x)\,dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)\,dx$$

$$= \frac{h}{2}(y_0+y_1) + \frac{h}{2}(y_1+y_2) + \cdots + \frac{h}{2}(y_{n-1}+y_n)$$

$$\therefore \int_{x_0}^{x_n} f(x)\,dx = \frac{h}{2}\left[(y_0+y_n) + 2(y_1+y_2+\cdots+y_{n-1})\right]$$

This is called as multiple segment trapezoidal rule. It can be used to find the integral of a tabulated function. It is also called as the composite trapezoidal rule.

066 Q. Evaluate $I = \int^{1} e^{-x^2}dx$ using Trapezoidal rule with $n=5$ upto 4 decimal places.

→ Here, $n=5$, $a=0$, $b=1$, $f(x) = e^{-x^2}$

$$h = \frac{b-a}{n} = \frac{1-0}{5} = 0.2$$

Tabulating the function in the interval 0,1 with $h=0.2$,

x	0	0.2	0.4	0.6	0.8	1.0
y	1	0.9607	0.8521	0.6977	0.5273	0.3679

From Trapezoidal rule,

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

For $n=5$, $a=0$, $b=1$ & $h=0.2$

$$\int_0^1 f(x)\,dx = \frac{0.2}{2}\left[(y_0+y_5)+2(y_1+y_2+y_3+y_4)\right]$$

$$= 0.1\left[1+0.3679+2(0.9607+0.8521+0.6977+0.5273)\right]$$

$$= 0.7444$$

Q. Evaluate $\int_1^2 e^{-\frac{1}{2}x}\,dx$ using Trapezoidal rule for four intervals.

Q. Use 3-segment Trapezoidal rule to find the integral $\int_{0.1}^{1.3} 5x\,e^{-2x}\,dx$.

Simpson's one-third Rule:-

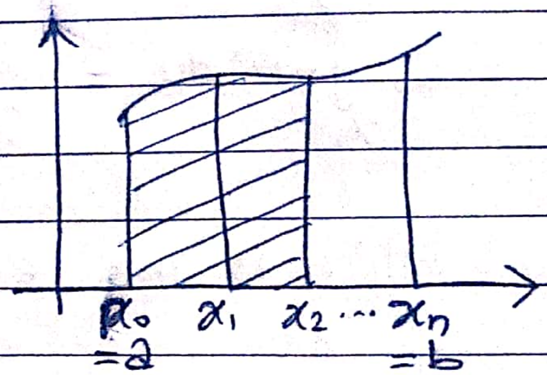
Simpson's one third rule is used to find the approximate value of a definite integral by using numerical methods. It is applicable to evaluate the value of an integral in case the usual analytical method is not applicable.

By Newton-Cotes quadrature formula, we have,

$$\int_{x_0}^{x_0+nh} f(x)\,dx = h\left[n y_0 + \frac{n^2}{2}\Delta y_0 + \left(\frac{n^3}{3} - \frac{n^2}{2}\right)\frac{\Delta^2 y_0}{2!} + \left(\frac{n^4}{4} - n^3 + n^2\right)\frac{\Delta^3 y_0}{3!} + \cdots\right] \quad \text{(i)}$$

When $n=2$, the function is approximated with a polynomial of degree 2. The integral is evaluated in the range x_0 to x_2. All the higher order forward differences except Δy_0 & $\Delta^2 y_0$ are zero.

x	y	$\Delta^2 y_0$	$\Delta^2 y$
x_0	y_0	$y_1 - y_0$	$y_2 - 2y_1 + y_0$
x_1	y_1	$y_2 - y_1$	
x_2	y_2		



For $n=2$, eqn (i) gives

$$\int_{x_0}^{x_2} f(x)\,dx = h\left[2y_0 + 2\Delta y_0 + \frac{1}{3}\Delta^2 y_0\right]$$

$$= h\left[2y_0 + 2(y_1 - y_0) + \frac{1}{3}(y_2 - 2y_1 + y_0)\right]$$

$$= h\left[\cancel{2y_0} + 2y_1 - \cancel{2y_0} + \frac{1}{3}(y_2 - 2y_1 + y_0)\right]$$

$$= h\left[2y_1 + \frac{1}{3}y_2 - \frac{2}{3}y_1 + \frac{1}{3}y_0\right]$$

$$= h\left[\frac{4}{3}y_1 + \frac{1}{3}y_2 + \frac{1}{3}y_0\right]$$

$$= \frac{h}{3}\left[y_0 + 4y_1 + y_2\right]$$

Similarly,

$$\int_{x_2}^{x_4} f(x)\,dx = \frac{h}{3}\left[y_2 + 4y_3 + y_4\right]$$

$$\int_{x_{n-2}}^{x_n} f(x)\,dx = \frac{h}{3}\left[y_{n-2} + 4y_{n-1} + y_n\right]$$

Adding all the integrals, we get

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

$$\therefore \int_{x_0}^{x_n} f(x)\,dx = \frac{h}{3}\Big[(y_0 + y_n) + 4(y_1 + y_3 + y_5 + \dots + y_{n-1}) + 2(y_2 + y_4 + y_6 + \dots + y_{n-2})\Big]$$

Which is the expression for Simpson's 1/3 rule.

Q. Evaluate $\int_0^6 1/(1+x^2)\,dx$ using Trapezoidal rule.

→ Let us divide the interval (0, 6) into 6 equal parts.
The width of each sub-interval $h = 1$.
(Note that in trapezoidal rule, no. of sub-intervals shouldn't be even}. It can be any).
Constructing the table,

x	0	1	2	3	4	5	6
y	1	0.5	0.2	0.1	0.0588	0.0385	0.0270

Here,

$x_0 = 0 = a$, $y_0 = 1 = b$, $n = 6$, $h = 1$

From Trapezoidal rule, we have

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

$$= \frac{1}{2}\left[(1+0.0270)+2(0.5+0.2+0.1+0.0588+0.0385)\right]$$

$$= 1.5323$$

Q. Evaluade $\int_0^6 1/(1+x^2)\,dx$ using Simpson's 1/3 rule.

→ In simpson's rule, the given range must be divided into sub-intervals that are multiple of 2 (even).

Let $n=6$, $h=1$.

constructing the table,

x	0	1	2	3	4	5	6
y	1	0.5	0.2	0.1	0.0588	0.0385	0.0270

From Simpson's 1/3 rule, we have

$$\int_0^6 f(x)\,dx = \frac{h}{3}\left[(y_0+y_6)+2(y_2+y_4)+4(y_1+y_3+y_5)\right]$$

$$= \frac{1}{3}\left[(1+0.0270)+2(0.2+0.0588)+4(0.5+0.1+0.0385)\right]$$

$$= 1.3662$$

T.U. Q. Using Simpson's one-third rule, evaluate

(a) $\int_0^2 (e^{x^2}-1)\,dx$ with $n=8$.

(b) $\int_{0.2}^{1.2} (x^2+\ln x-\sin x)\,dx$ with $h=0.1$

Q. Evaluate $\int_1^2 e^{-x/2}\,dx$ using Trapezoidal rule. (take four segments). Ans: 0.4725

Q. Using 3-segment Trapezoidal rule, evaluate integral

$$\int_{0.1}^{1.3} 5x\,e^{-2x}\,dx$$

Ans: 0.84385

Simson's 3/8 Rule :-

From Newton-Cotes quadrature formula, we have

$$\int_a^b f(x)\,dx = h\left[ny_0 + \frac{n^2}{2}\Delta y_0 + \left(\frac{n^3}{3} - \frac{n^2}{2}\right)\frac{\Delta^2 y_0}{2!} + \left(\frac{n^4}{4} - n^3 + n^2\right)\frac{\Delta^3 y_0}{3!} + \cdots\right] \quad \text{--- (i)}$$

For $n=3$, we take 3 subintervals.

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$
x_0	y_0			
		$y_1 - y_0$		
x_1	y_1		$y_2 - 2y_1 + y_0$	
		$y_2 - y_1$		$y_3 - 3y_2 + 3y_1 - y_0$
x_2	y_2		$y_3 - 2y_2 + y_1$	
		$y_3 - y_2$		
x_3	y_3			

From eqn (i), we have

$$\int_{x_0}^{x_3} f(x)\,dx = h\left[3y_0 + \frac{9}{2}\Delta y_0 + \left(\frac{27}{3} - \frac{9}{2}\right)\frac{\Delta^2 y_0}{2!} + \left(\frac{81}{4} - 27 + 9\right)\frac{\Delta^3 y_0}{3!}\right]$$

$$= h\left[3y_0 + \frac{9}{2}(y_1 - y_0) + \left(9 - \frac{9}{2}\right)\frac{(y_2 - 2y_1 + y_0)}{2!} + \left(\frac{81}{4} - 18\right)\frac{(y_3 - 3y_2 + 3y_1 - y_0)}{3!}\right]$$

$$= \frac{3h}{8}\left[y_0 + 3y_1 + 3y_2 + y_3\right]$$

Similarly,

$$\int_{x_3}^{x_6} f(x)\,dx = \frac{3h}{8}\left[y_3 + 3y_4 + 3y_5 + y_6\right]$$

$\cdots\cdots$

$$\int_{x_{n-3}}^{x_n} f(x)\,dx = \frac{3h}{8}\left[y_{n-3} + 3y_{n-2} + 3y_{n-1} + y_n\right]$$

Adding all the integrals, we get

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

This is known as Simpson's 3/8 rule for numerical integration. It is also called multi-segment simpson's 3/8 rule. This method can be used if n is multiple of 3.

Q. Using Simpson's 3/8 rule, evaluate $\int_0^6 \frac{1}{(1+x^2)}\,dx$.

→ For Simpson's 3/8 rule, given interval must be divided into sub-intervals that ~~are~~ is multiple of 3.

Let n = 6. The tabulated function is,

x	0	1	2	3	4	5	6
y	1	0.5	0.2	0.1	0.0588	0.0385	0.0270

By Simpson's 3/8 rule, we have

$$\int_0^6 f(x)\,dx = \frac{3h}{8}\left[(y_0+y_6) + 2(y_3) + 3(y_1+y_2+y_4+y_5)\right]$$

$$= \frac{3}{8}\left[(1+0.0270) + 2\times 0.1 + 3(0.5+0.2+0.0588+0.0385)\right]$$

$$= \cancel{0.1036}\ 1.3571$$

Gaussian Integration

An n-point Gaussian quadrature rule is a numerical integration method constructed to determine the integral of polynomials of degree 2n-1 or less. It is a method to determine integral of the polynomial in the range of [-1, 1] in the form of weighted sum as:

$$I = \int_{-1}^{1} f(x)\,dx \doteq \sum_{i=1}^{n} w_i f(x_i)$$

Where w_i are called weights and x_i are called abscissa.

Gaussian rule for three points gives value of the integral for a polynomial of degree $2\times3-1 = 5$ or less. Similarly Gaussian rule for two points gives value of the integral for a polynomial of degree $2\times2-1=3$ or less.

Two-point Gaussian formula is:

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

ie. $x_1 = -1/\sqrt{3}$, $x_2 = 1/\sqrt{3}$
$w_1 = w_2 = 1$.

Three-point Gaussian formula is:

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

ie. $x_1 = 0$, $x_2 = -\sqrt{3/5}$, $x_3 = \sqrt{3/5}$

& $w_1 = \frac{8}{9}$, $w_2 = \frac{5}{9}$, $w_3 = \frac{5}{9}$

(Above formulae also called Gauss-Legendre formula).

If the limits of the integration are a to b, it is possible to use a linear transformation to bring the limits to the standard [-1, 1] using

$$\boxed{x = \frac{1}{2}(b-a)u + \frac{1}{2}(b+a).}$$

Q. Evaluate $\int_{0.2}^{1.5} e^{-x^2} dx$ using 3-point Gaussian integration

→ Let us change the limits $a = 0.2$ to $b = 1.5$ into -1 to 1 using linear transformation formula,

$$x = \frac{1}{2}(b-a)u + \frac{1}{2}(b+a)$$

$$= 0.65u + 0.85$$

Here

$$I = \int_{0.2}^{1.5} e^{-x^2} dx$$

$$= 0.65 \int_{-1}^{1} e^{-(0.65u+0.85)^2} du$$

$$= 0.65 \int_{-1}^{1} f(u)\,du \quad \text{where } f(u) = e^{-(0.65u+0.85)^2}$$

Using Gaussian 3-pointe formula

$$\int_{-1}^{1} f(u)\,du = \frac{8}{9} f(0) + \frac{5}{9}\left[f\left(-\sqrt{\tfrac{3}{5}}\right) + f\left(\sqrt{\tfrac{3}{5}}\right)\right]$$

$$\therefore \quad I = 0.65\left[\frac{8}{9} f(0) + \frac{5}{9}\left[f\left(-\sqrt{\tfrac{3}{5}}\right) + f\left(\sqrt{3/5}\right)\right]\right]$$

$$= 0.65865$$

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CSIT-067

Q. Evaluate $I = \int_{0.2}^{1.5} e^{-x^2} dx$ using Gaussian 3-point rule.

CSIT-069

Q. Evaluate $I = \int_{1}^{2} (\ln x + x^2 \sin x) dx$ using Gaussian Integration 3-point formula.

Romberg Integration Algorithm

- Assume a h (interval size) (if not given)
- Find $I(h)$, $I(h/2)$, $I(h/4)$ using Trapezoidal rule.

$$I(h) = \frac{h}{2}\left[(y_0 + y_n) + 2(y_1 + y_2 + \cdots + y_{n-1})\right]$$

- Evaluate $I(h, h/2) = \left[\frac{4}{3} I(h/2) - \frac{1}{3} I(h)\right]$

Simillarly $I(h/2, h/4)$, $I(h/4, h/8)$, ...

- Tabulate the triangular array as:

$I(h)$

$\qquad I(h, h/2)$

$I(h/2)$ $\qquad\qquad I(h, h/2, h/4)$ ← ans

$\qquad I(h/2, h/4)$

$I(h/4)$

You may apply $I(h/8)$ also

Q. Evaluate $\int_0^8 x^2\,dx$ using Romberg method.

→ From trapezoidal rule, we have

$$I(h) = \int_a^b f(x)\,dx = \frac{h}{2}\left[(y_0 + y_n) + 2(y_1 + y_2 + \cdots + y_{n-1})\right]$$

Here, $a = 0$, $b = 8$.

Let $h = 4$. Then ⇒ $\underset{x_0}{0} — \underset{x_1}{4} — \underset{x_2}{8}$

$$I(h) = \frac{4}{2}\left[(0^2 + 8^2) + 2 \cdot 4^2\right]$$

$$= 192$$

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Again assuming $h = h/2 = 4/2 = 2$, we get the interval as

$$\underset{x_0}{0} — \underset{x_1}{2} — \underset{x_2}{4} — \underset{x_3}{6} — \underset{x_4}{8}$$

then,

$$I(h/2) = \frac{2}{2}\left[(y_0 + y_4) + 2(y_1 + y_2 + y_3)\right]$$

$$= \left[(0^2 + 8^2) + 2(2^2 + 4^2 + 6^2)\right]$$

$$= 176$$

Again assuming $h = h/4 = 4/4 = 1$,

$$\underset{x_0}{0} — \underset{x_1}{1} — \underset{x_2}{2} — \underset{x_3}{3} — \underset{x_4}{4} — \underset{x_5}{5} — \underset{x_6}{6} — \underset{x_7}{7} — \underset{x_8}{8}$$

$$I(h/4) = \frac{1}{2}\left[(0^2 + 8^2) + (1^2 + 2^2 + 3^2 + 4^2 + 5^2 + 6^2 + 7^2)\right]$$

$$= 172$$

Again assuming $h = h/8 = 4/8 = 0.5$

$$0 — 0.5 — 1 — 1.5 — 2 — 2.5 — 3 — 3.5 — 4 — 4.5 — \dots — 8$$

$$x_0 \quad x_1 \quad x_2 \quad x_3 \quad \dots \quad x_{16}$$

$$I(h/8) = \frac{0.5}{2}\left[(0^2 + 8^2) + (0.5^2 + 1^2 + 1.5^2 + 2^2 + \dots + 7.5^2)\right]$$

$$= 171$$

Gurukul

Now constructing the triangular array:

$$
\begin{array}{lll}
I(h) & & \\
 & I(h, h/2) & \\
 & & I(h, h/2, h/4) \\
I(h/2) & & \\
 & I(h/2, h/4) & \\
 & & \cancel{I(} \\
I(h/4) & & \\
 & \cancel{I(h/4, h/8)} & \\
\cancel{I(h/8)} & &
\end{array}
$$

[Better to go upto h/4 only].

where

$$I(h, h/2) = \frac{4}{3} I(h/2) - \frac{1}{3} I(h)$$

$$= \frac{4}{3} \times 176 - \frac{1}{3} \times 192$$

$$= 170.67$$

$$I(h/2, h/4) = \frac{4}{3} I(h/4) - \frac{1}{3} I(h/2)$$

$$= \frac{4}{3} \times 172 - \frac{1}{3} \times 176$$

$$= 170.67$$

$$I(h, h/2, h/4) = \frac{4}{3} I(h/2, h/4) - \frac{1}{3} I(h, h/2)$$

$$= \frac{4}{3} \times 170.67 - \frac{1}{3} \times 17[illegible].67$$

$$= 168.67$$

Ans

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Romberg Integration Method:

Step-1: Find I_1 using Trapezoidal Rule. (take h)

step-2: Find I_2 using Trapezoidal rule (take $h/2$)

step-3: Find I_3 taking $h/4$ as interval size.

Step-4: Find I_4 taking $h/8$.

step-5: Find $I_1' = I_2 + \frac{1}{3}(I_2 - I_1)$

$I_2' = I_3 + \frac{1}{3}(I_3 - I_2)$