Unit - 3

Numerical differentiation and integration :

Introduction:

Numerical differentiation is concerned with the computation of the derivatives of a function in terms of a set of given values of that function. The fundamental operation of differentiation is applied to the interpolating polynomial to evaluate the derivatives of a given tabulated function. The choice of a differentiation formula to be employed is based on the considerations as in the case of interpolation. So for finding derivatives at a point near the beginning of a table we use the differentiation of the Newton's forward interpolation formula, while for derivatives at the end of a table we use derivatives of the Newton's backward interpolation formula.

* Differentiation based on Newton's forward and backward interpolation formula:

By Newton's forward interpolation formula, we have

$$y = y_0 + u\Delta y_0 + \frac{u(u-1)}{\lfloor 2}\Delta^2 y_0 + \frac{u(u-1)(u-2)}{\lfloor 3}\Delta^3 y_0 + \cdots$$

where the fn $y = f(x)$ is tabulated for $x_i \ (= x_0 + ih)$, $i = 0, 1, 2, \ldots n$.

Differentiating both sides w.r.t. u, we have

$$\frac{dy}{du} = \Delta y_0 + \frac{2u-1}{\lfloor 2}\Delta^2 y_0 + \frac{3u^2 - 6u + 2}{\lfloor 3}\Delta^3 y_0 + \cdots$$

But $x = x_0 + uh \Rightarrow u = \dfrac{x - x_0}{h}$

$$\Rightarrow \frac{du}{dx} = \frac{1}{h}$$

Now, $\dfrac{dy}{dx} = \dfrac{dy}{du}\dfrac{du}{dx}$

$$= \frac{1}{h}\left[\Delta y_0 + \frac{2u-1}{\underline{|2}}\Delta^2 y_0 + \frac{3u^2-6u+2}{\underline{|3}}\Delta^3 y_0 + \frac{4u^3-18u^2+22u-6}{\underline{|4}}\Delta^4 y_0 + \cdots\right] \quad \text{------} (1)$$

when $x = x_0$, $u = 0$

$\therefore (1) \Rightarrow$

$$\left.\frac{dy}{dx}\right]_{x=x_0} = \frac{1}{h}\left[\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0 - \frac{1}{4}\Delta^4 y_0 + \frac{1}{5}\Delta^5 y_0 - \frac{1}{6}\Delta^6 y_0 + \cdots\right] \quad \text{----} (2)$$

Again, differentiating (1), w.r.t. x; we get,

$$\frac{d^2y}{dx^2} = \frac{d}{du}\left(\frac{dy}{dx}\right)\frac{du}{dx}$$

$$= \frac{1}{h^2}\left[\frac{2}{\underline{|2}}\Delta^2 y_0 + \frac{6u-6}{\underline{|3}}\Delta^3 y_0 + \frac{12u^2-36u+22}{\underline{|4}}\Delta^4 y_0 + \cdots\right] \quad \text{---} (3)$$

when $x = x_0$, $u = 0$

$\therefore (3) \Rightarrow$

$$\left.\frac{d^2y}{dx^2}\right]_{x=x_0} = \frac{1}{h^2}\left[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12}\Delta^4 y_0 - \frac{5}{6}\Delta^5 y_0 + \frac{137}{180}\Delta^6 y_0 + \cdots\right] \quad \text{-----} (4)$$

and similarly,

$$\left.\frac{d^3y}{dx^3}\right]_{x=x_0} = \frac{1}{h^3}\left[\Delta^3 y_0 - \frac{3}{2}\Delta^4 y_0 + \cdots\right] \quad \text{-----} (5)$$

Also, Newton's backward interpolation formula is given by

$$y = y_n + u \nabla y_n + \frac{u(u+1)}{\underline{|2}} \nabla^2 y_n + \frac{u(u+1)(u+2)}{\underline{|3}} \nabla^3 y_n + \cdots$$

Differentiating both sides w.r.t. u, we get,

$$\frac{dy}{du} = \nabla y_n + \frac{2u+1}{\underline{|2}} \nabla^2 y_n + \frac{3u^2+6u+2}{\underline{|3}} \nabla^3 y_n + \cdots$$

But, $u = \frac{x - x_n}{h} \Rightarrow \frac{du}{dx} = \frac{1}{h}$

and $\frac{dy}{dx} = \frac{dy}{du} \cdot \frac{du}{dx}$

$$= \frac{1}{h}\left[\nabla y_n + \frac{2u+1}{\underline{|2}} \nabla^2 y_n + \frac{3u^2+6u+2}{\underline{|3}} \nabla^3 y_n + \cdots\right] \quad \cdots (6)$$

But, at $x = x_n$, $u = 0$

$\therefore$ (6) $\Rightarrow$

$$\left.\frac{dy}{dx}\right]_{x=x_n} = \frac{1}{h}\left[\nabla y_n + \frac{1}{2}\nabla^2 y_n + \frac{1}{3}\nabla^3 y_n + \frac{1}{4}\nabla^4 y_n + \frac{1}{5}\nabla^5 y_n + \frac{1}{6}\nabla^6 y_n + \cdots\right] \quad \cdots (7)$$

and $\frac{d^2y}{dx^2} = \frac{d}{du}\left(\frac{dy}{dx}\right)\frac{du}{dx}$

$$= \frac{1}{h^2}\left[\nabla^2 y_n + \frac{6u+6}{\underline{|3}} \nabla^3 y_n + \frac{6u^2+18u+11}{12} \nabla^4 y_n + \cdots\right] \quad \cdots (8)$$

But at $x = x_n$, $u = 0$

$\therefore$ (8) $\Rightarrow$

$$\left.\frac{d^2y}{dx^2}\right]_{x=x_n} = \frac{1}{h^2}\left[\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12}\nabla^4 y_n + \frac{5}{6}\nabla^5 y_n + \frac{137}{180}\nabla^6 y_n + \cdots\right] \quad \cdots (9)$$

Similarly, we get,

$$\left.\frac{d^3y}{dx^3}\right]_{x=x_n} = \frac{1}{h^3}\left[\nabla^3 y_n + \frac{3}{2}\nabla^4 y_n + \cdots\right] \quad \cdots (10)$$

* Derivatives using central difference formula:

By Stirling's formula, we have

$$y_u = y_0 + \frac{u}{\lfloor 1}\left(\frac{\Delta y_0 + \Delta y_{-1}}{2}\right) + \frac{u^2}{\lfloor 2}\Delta^2 y_{-1} + \frac{u(u^2-1^2)}{\lfloor 3}\left(\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2}\right) + \frac{u^2(u^2-1^2)}{\lfloor 4}\Delta^4 y_{-2} + \cdots$$

$$\Rightarrow \frac{dy_u}{du} = \left(\frac{\Delta y_0 + \Delta y_{-1}}{2}\right) + \frac{2u}{\lfloor 2}\Delta^2 y_{-1} + \frac{3u^2-1}{\lfloor 3}\left(\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2}\right) + \frac{4u^3-2u}{\lfloor 4}\Delta^4 y_{-2} + \cdots$$

But $u = \frac{x-x_0}{h}$

$\Rightarrow \frac{du}{dx} = \frac{1}{h}$

$\therefore \frac{dy_u}{dx} = \frac{dy_u}{du}\,\frac{du}{dx}$

$$\Rightarrow \frac{dy_u}{dx} = \frac{1}{h}\left[\left(\frac{\Delta y_0 + \Delta y_{-1}}{2}\right) + u\Delta^2 y_{-1} + \frac{3u^2-1}{\lfloor 3}\left(\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2}\right) + \frac{2u^3-u}{12}\Delta^4 y_{-2} + \cdots\right] \quad \text{---}(1)$$

But at $x = x_0$, $u = 0$

$\therefore (1) \Rightarrow$

$$\left.\frac{dy_u}{dx}\right]_{x=x_0} = \frac{1}{h}\left[\left(\frac{\Delta y_0 + \Delta y_{-1}}{2}\right) - \frac{1}{6}\left(\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2}\right) + \frac{1}{30}\left(\frac{\Delta^5 y_{-2} + \Delta^5 y_{-3}}{2}\right) + \cdots\right] \quad \text{---}(2)$$

and similarly,

$$\left.\frac{d^2 y_u}{dx^2}\right]_{x=x_0} = \frac{1}{h^2}\left[\Delta^2 y_{-1} - \frac{1}{12}\Delta^4 y_{-2} + \frac{1}{90}\Delta^6 y_{-3} - \cdots\right] \quad \text{---}(3)$$

Ex) Find $f'(5)$ from the following table;

x:	0	2	3	4	7	9
$f(x)$:	4	26	58	112	466	922

Sol^n: Here, the arguments are not equally spaced.

So we shall use Newton's divided difference formula.

The divided difference table is given below:

x	$f(x)$	$\Delta f(x)$	$\Delta^2 f(x)$	$\Delta^3 f(x)$	$\Delta^4 f(x)$	$\Delta^5 f(x)$
0	4					
		11				
2	26		7			
				1		
		32				
3	58		11		0	
		54				0
4	112					
			16		0	
		118				
				1		
7	466		22			
		228				
9	922					

Newton's divided difference formula, if third differences are constant is given by,

$$f(x) = f(x_0) + (x-x_0) f(x_0,x_1) + (x-x_0)(x-x_1) f(x_0,x_1,x_2)$$
$$+ (x-x_0)(x-x_1)(x-x_2) f(x_0,x_1,x_2,x_3)$$

Now, diff. w.r.t. x, we get,

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

Putting, $x=5$, $x_0=0$, $x_1=2$, $x_2=3$, $x_3=4$, and the values of the various divided differences, we get,

$$f'(5) = 11 + \{(5-2)+(5-0)\} 7 + \{(5-0)(5-2) + (5-2)(5-3)$$
$$+ (5-3)(5-0)\} \cdot 1 \quad = 11 + 56 + 31 = 98$$

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Ex) Find $f'(6)$ from the following table:

x:	0	1	3	4	5	7	9
$f(x)$:	150	108	0	-54	-100	-144	-84

Ans: -23

Ex) Explain briefly the concept and technique of Numerical differentiation with the help of a suitable example.

Ans: Let us consider the problem of finding the 1st derivatives of the function tabulated below of the points

(i) $x = 3.0$, (ii) $x = 3.8$, (iii) $x = 3.6$

x:	3.0	3.2	3.4	3.6	3.8	4.0
y:	-14.000	-10.032	-5.296	-0.256	6.672	14.000

Now,

(i) ~~to~~ find the 1st derivatives at $x = 3.0$, i.e., to find $\left\{\frac{dy}{dx}\right\}_{x=3.0}$, we are to follow Newton-Gregory forward interpolation formula.

(ii) To find the 1st derivatives at $x = 3.8$, we are to follow Newton-Gregory backward interpolation formula.

(iii) To find the 1st derivatives at $x = 3.6$, we are to follow central difference formula.

Ex) How do you choose the proper interpolation formula for numerical differentiation? Explain.

Ans:- The problem of differentiation is solved by 1st approximating the f^n by an interpolation formula and then differentiating this formula as many times as desired. If the values of the argument are equally spaced i.e. the values of the f^n are known at equidistant values of x, we choose any one of the Newton's, Stirling's or Bessel's formula.

If the values of the f^n are not equally spaced then we shall use Newton's devided difference or Lagrange's formula.

If we desire to find the derivatives of the f^n at a point near the begining or end of a set of tabular values, we use Newton's - Gregory forward or backward formulae accordingly. To find the derivative at a point near the middle of the table, we should use a central difference formula to represent the function.

Ex) Find the first and second derivatives of the f^n tabulated below at the point $x = 3.0$:

x	$f(x)$	$\Delta f(x)$	$\Delta^2 f(x)$	$\Delta^3 f(x)$	$\Delta^4 f(x)$	$\Delta^5 f(x)$
3	-14.000					
		3.968				
3.2	-10.032		.768			
		4.736		.048		
3.4	-5.296		.816		0	
		5.552		.048		0
3.6	0.256		.864		0	
		6.416		.048		
3.8	6.672		.912			
		7.328				
4.0	14.000					

Sol^n:- Newton-Gregory forward difference interpolation formula is

$$f(a+xh) = f(a) + x\Delta f(a) + \frac{x^2-x}{2}\Delta^2 f(a) + \frac{x^3-3x^2+2x}{6}\Delta^3 f(a) + \cdots$$

Differentiating w.r.t. x twice and then putting $x=0$ we get

$$h f'(a) = \Delta f(a) - \frac{1}{2}\Delta^2 f(a) + \frac{1}{3}\Delta^3 f(a) + \cdots$$

and $h^2 f''(a) = \Delta^2 f(a) - \Delta^3 f(a)$

Here, $a=3,\ h=0.2$

$\therefore\ 0.2 \times f'(3) = 3.968 - \frac{1}{2}(.768) + \frac{1}{3}(.048)$

$= 3.6$

$\Rightarrow f'(3) = 18$

and $(0.2)^2 f''(3) = .768 - .048$

$= .72$

$\Rightarrow f''(3) = 18$

$\therefore\ \frac{dy}{dx}$ and $\frac{d^2y}{dx^2}$ at $x=3$ are both equal to 18.

Ex) Find $f'(0.1)$ from the following data:

x:	0	1	2	3	4
$f(x)$:	1	0	1	10	33

Sol^n: Newton-Gregory forward difference interpolation formula is

$$f(a+hu) = f(a) + u\Delta f(a) + \frac{u(u-1)}{\underline{|2}}\Delta^2 f(a) + \frac{u(u-1)(u-2)}{\underline{|3}}\Delta^3 f(a) + \cdots \quad (1)$$

Here, $h=1,\ u = \frac{x-0}{1} = x,\ a=0$

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

$\therefore$ (1) $\Rightarrow$

$$f(x) = f(0) + x\Delta f(0) + \frac{x(x-1)}{\lfloor 2}\Delta^2 f(0) + \cdots \quad (2)$$

Now,

x	$f(x)$	$\Delta f(x)$	$\Delta^2 f(x)$	$\Delta^3 f(x)$	$\Delta^4 f(x)$
0	1				
		-1			
1	0		2		
		1		6	
2	1		8		0
		9		6	
3	10		14		
		23			
4	33				

$\therefore$ (2) $\Rightarrow$

$$f(x) = 1 + x(-1) + \frac{x(x-1)}{\lfloor 2}2 + \frac{x(x-1)(x-2)}{\lfloor 3}6 + \cdots \quad (3)$$

$$\therefore f'(x) = -1 + (2x-1) + (3x^2 - 6x + 2)$$

$$\therefore f'(0.1) = -1 + (2\times 0.1 - 1) + \{3\times(0.1)^2 - 6\times(0.1) + 2\}$$

$$= -0.37 \quad \text{(approx)}$$

Ex) Find the derivative of $f(x)$ at $x = 0.4$ from the following table:

x :	0.1	0.2	0.3	0.4
$y = f(x)$:	1.10517	1.22140	1.34986	1.49182

Soln: Since $x = 0.4$ lies near the end of the table, therefore in this case we shall use Newton's Backward formula. The difference table is as below:

x	y	∇y	$\nabla^2 y$	$\nabla^3 y$
0·1	1·10517			
		·11623		
0·2	1·22140		·01223	
		·12846		·00127
0·3	1·34986		·01350	
		·14196		
0·4	1·49182			

Newton's Backward formula is

$$f(a+mh+xh) = f(a+mh) + x\nabla f(a+mh) + \frac{x^2+x}{\lfloor 2}\nabla^2 f(a+mh)$$
$$+ \frac{x^3+3x^2+2x}{\lfloor 3}\nabla^3 f(a+mh) \quad ---(1)$$

Here $f(a+mh)$ is the last term and h is the differencing interval.

Diff. (1) w.r.t x, we get,

$$h f'(a+mh+xh) = \nabla f(a+mh) + \frac{2x+1}{2}\nabla^2 f(a+mh)$$
$$+ \frac{3x^2+6x+2}{6}\nabla^3 f(a+mh) \quad ---(2)$$

On putting $x=0$ in (2), we get

$$0{\cdot}1 \times f'({\cdot}4) = {\cdot}14196 + \frac{1}{2}({\cdot}01350) + \frac{1}{3}({\cdot}00127)$$

$$\Rightarrow f'({\cdot}4) = 1{\cdot}4913$$

Ex) Given that

x :	1·0	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

find $\frac{dy}{dx}$ and $\frac{d^2y}{dx^2}$ at $x=1{\cdot}6$

Soln:: The difference table is

x	y	∇y	$\nabla^2 y$	$\nabla^3 y$	$\nabla^4 y$	$\nabla^5 y$	$\nabla^6 y$
1.0	7.989						
		.414					
			−.036				
1.1	8.403						
		.378		.006			
1.2	8.781		−.030		−.002		
		.348		.004		.001	
1.3	9.129		−.026		−.001		.002
		.322		.003		.003	
1.4	9.451		−.023		.002		
		.299		.005			
1.5	9.750		−.018				
		.281					
1.6	10.031						

We have,

$$\left[\frac{dy}{dx}\right]_{x=x_n} = \frac{1}{h}\left[\nabla y_n + \frac{1}{2}\nabla^2 y_n + \frac{1}{3}\nabla^3 y_n + \frac{1}{4}\nabla^4 y_n + \frac{1}{5}\nabla^5 y_n + \frac{1}{6}\nabla^6 y_n + \cdots\right] \quad \text{---} (1)$$

and

$$\left[\frac{d^2y}{dx^2}\right]_{x=x_n} = \frac{1}{h^2}\left[\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12}\nabla^4 y_n + \frac{5}{6}\nabla^5 y_n + \frac{137}{180}\nabla^6 y_n + \cdots\right] \quad \text{---} (2)$$

Here, $h = 0.1$, $x_n = 1.6$

Putting these values in (1) and (2), we get,

$$\left[\frac{dy}{dx}\right]_{x=1.6} = \frac{1}{0.1}\left[.281 + \frac{1}{2}(-.018) + \frac{1}{3}(.005) + \frac{1}{4}(.002) + \frac{1}{5}(.003) + \frac{1}{6}(.002)\right]$$

$= 2.751$

and

$$\left[\frac{d^2y}{dx^2}\right]_{x=1.6} = \frac{1}{(0.1)^2}\left[-.018 + .005 + \frac{11}{12}(.002) + \frac{5}{6}(.003) + \frac{137}{180}(.002)\right]$$

$= -.714$ //

* To establish formula for $f'(x)$ ~~and $f''(x)$~~ without using interpolation formula:

We know that

$$1+\Delta \equiv E \equiv e^{hD}$$

$$\Rightarrow hD = \log(1+\Delta) = \Delta - \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 - \frac{1}{4}\Delta^4 + \cdots$$

$$\Rightarrow D \equiv \frac{1}{h}\left[\Delta - \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 - \frac{1}{4}\Delta^4 + \cdots\right]$$

Then Dy_0 i.e $\left.\frac{dy}{dx}\right]_{x=x_0} = \frac{1}{h}\left[\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0 - \frac{1}{4}\Delta^4 y_0 + \cdots\right]$

and

$$1-\nabla \equiv E^{-1} \equiv e^{-hD}$$

$$\Rightarrow -hD = \log(1-\nabla) = -\left(\nabla + \frac{1}{2}\nabla^2 + \frac{1}{3}\nabla^3 + \frac{1}{4}\nabla^4 + \cdots\right)$$

$$\Rightarrow D \equiv \frac{1}{h}\left[\nabla + \frac{1}{2}\nabla^2 + \frac{1}{3}\nabla^3 + \frac{1}{4}\nabla^4 + \cdots\right]$$

Then Dy_n i.e $\left.\frac{dy}{dx}\right]_{x=x_n} = \frac{1}{h}\left[\nabla y_n + \frac{1}{2}\nabla^2 y_n + \frac{1}{3}\nabla^3 y_n + \frac{1}{4}\nabla^4 y_n + \cdots\right]$

Ex) A slider in a machine moves along a fixed straight rod. Its distance x cm along the rod is given below for various values of time t seconds:

t:	0	0.1	0.2	0.3	0.4	0.5	0.6
x:	30.13	31.62	32.87	33.64	33.95	33.81	33.24

Find the velocity and acc^n of the slider when $t = 0.3$ seconds.

Sol^n: Here we have to find $\frac{dx}{dt}$ and $\frac{d^2x}{dt^2}$ at $t = 0.3$ which lies in the middle of the table. So we use Stirling's formula with $t_0 = 0.3$ (so that $u = 0$)

$$\left.\frac{dx}{dt}\right]_{t_0=0.3} = \frac{1}{h}\left[\left(\frac{\Delta x_0 + \Delta x_{-1}}{2}\right) - \frac{1}{6}\left(\frac{\Delta^3 x_{-1} + \Delta^3 x_{-2}}{2}\right) + \frac{1}{30}\left(\frac{\Delta^5 x_{-2} + \Delta^5 x_{-3}}{2}\right) + \cdots\right]$$

$$\left.\frac{d^2x}{dt^2}\right]_{t_0=0.3} = \frac{1}{h^2}\left[\Delta^2 x_{-1} - \frac{1}{12}\Delta^4 x_{-2} + \frac{1}{90}\Delta^6 x_{-3} - \cdots\right]$$

with $t_0 = 0.3$ as centre we make the central difference table:

t	u	x_u	Δx_u	$\Delta^2 x_u$	$\Delta^3 x_u$	$\Delta^4 x_u$	$\Delta^5 x_u$	$\Delta^6 x_u$
0	-3	30.13						
			1.49					
0.1	-2	31.62		-.24				
			1.25		-.24			
0.2	-1	32.87		-.48		.26		
			0.77		.02		-.27	
0.3	0	33.64		-.46		-.01		0.29
			0.31		.01		-.02	
0.4	1	33.45		-.45		.01		
			-0.14		.02			
0.5	2	33.81		-.43				
			-0.57					
0.6	3	33.24						

Here $h = 0.1$

$$\therefore \left.\frac{dx}{dt}\right]_{t_0=0.3} = \frac{1}{0.1}\left[\frac{.77+.31}{2} - \frac{1}{6}\times\frac{.02+0.01}{2} + \frac{1}{30}\times\frac{-.27-.02}{2}\right]$$

$$= 5.32 \quad cm/s$$

$\therefore$ velocity $= 5.32$ cm/s at $t = 0.3$ sec.

and

$$\left.\frac{d^2x}{dt^2}\right]_{t_0=0.3} = \frac{1}{(0.1)^2}\left[-.46 - \frac{1}{12}\times(-0.01) + \frac{1}{90}\times 0.29\right]$$

$$= -45.6 \quad cm/s^2$$

$\therefore$ Acc^n at $t = 0.3$ is 45.6 cm/s^2 (in magnitude)

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