Numerical Differentiation ⇒

* It is the process of calculating the value of the derivatives of a function at some assigned val of x from the given set of values (x_i, y_i).
* To compute dy/dx, we first replace the exact relation $y = f(x)$ by the best interpolating polynomial $y = \phi(x)$ and then differentiate the latter as many times as we desire.
* If the values of x are equispaced and dy/dx is required near the begining of the table, we employ Newton's forward formula. If required near the end of the table, we use Newton's backward formula.
* If the values of x are not equispaced, we use Lagrange's formula or Newton's divided difference formula to represent the function.

Formulae for derivatives ⇒

Consider the function $y = f(x)$ which is tabulated for the values $x_i (= x_0 + ih)$ $i = 0, 1, 2, \ldots, n$

Derivatives using Newton's forward difference formula ⇒

Newton's forward interpolation formula is,

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

Differentiating (1) w.r.t. p, we get

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

~~differentiating both sides~~ w.

since $p = \frac{x - x_0}{h} \Rightarrow \frac{dp}{dx} = \frac{1}{h}$

Now $\frac{dy}{dx} = \frac{dy}{dp} \cdot \frac{dp}{dx} = \frac{1}{h}\Big[\Delta y_0 + \frac{2p-1}{2!}\Delta^2 y_0 + \frac{3p^2 - 6p + 2}{3!}\Delta^3 y_0$

$+ \frac{4p^3 - 18p^2 + 22p - 6}{4!}\Delta^4 y_0 + \cdots\Big]$ — (ii)

putting $x = x_0$, we get $p = 0$, in (ii)

$$\boxed{\left(\frac{dy}{dx}\right)\Big|_{x=x_0} = \frac{1}{h}\left[\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0 - \frac{1}{4}\Delta^4 y_0 + \cdots\right]} \quad \text{— (iii)}$$

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

$\frac{d^2y}{dx^2} = \frac{d}{dp}\left(\frac{dy}{dx}\right)\frac{dp}{dx} = \frac{1}{h}\Big[\frac{2}{2!}\Delta^2 y_0 + \frac{6p-6}{3!}\Delta^3 y_0$

$+ \frac{12p^2 - 36p + 22}{4!}\Delta^4 y_0 + \cdots\Big]\frac{1}{h}$

putting $p = 0$, we get

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

similarly

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

Otherwise $\Rightarrow$ We know that $1+\Delta = E = e^{hD}$ (73)

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

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

$$\boxed{D^2 = \frac{1}{h^2}\left[\Delta^2 - \Delta^3 + \frac{11}{12}\Delta^4 + \cdots\right]}$$

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

Now, applying the above identities to y_0, we get

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

Derivatives using Newton's backward difference formula $\Rightarrow$

Newton's Backward interpolation formula is

$$y(x) = y_n + p\nabla y_n + \frac{p(p+1)}{2!}\nabla^2 y_n + \frac{p(p+1)(p+2)}{3!}\nabla^3 y_n + \cdots$$

differentiating both sides w.r.t. p, we get

$$\frac{dy}{dp} = \nabla y_n + \frac{2p+1}{2!}\nabla^2 y_n + \frac{3p^2+6p+2}{3!}\nabla^3 y_n + \cdots \quad \text{(a)}$$

~~At $x=x_n$, $p=0$, Hence~~

since $p = \frac{x-x_n}{h} \Rightarrow \frac{dp}{dx} = \frac{1}{h}$

Now $$\frac{dy}{dx} = \frac{dy}{dp} \cdot \frac{dp}{dx} = \frac{1}{h}\left[\nabla y_n + \frac{2p+1}{2!}\nabla^2 y_n + \frac{3p^2+6p+2}{3!}\nabla^3 y_n + \cdots\cdots\right] \quad \text{—— (b)}$$

At $x = x_n$, $p = 0$. Hence putting $p = 0$, we get

$$\boxed{\left.\frac{dy}{dx}\right|_{x=x_n} = \frac{1}{h}\left[\nabla y_n + \frac{1}{2}\nabla^2 y_n + \frac{1}{3}\nabla^3 y_n + \frac{1}{4}\nabla^4 y_n + \cdots\cdots\right]} \quad \text{—— (c)}$$

Again differentiating (b) w.r.t. x, we have

$$\frac{d^2y}{dx^2} = \frac{d}{dp}\frac{dy}{dx} \cdot \frac{dp}{dx}$$

$$= \frac{1}{h^2}\left[\nabla^2 y_n + \frac{6p+6}{3!}\nabla^3 y_n + \frac{6p^2+18p+11}{12} \times \nabla^4 y_n + \cdots\right]$$

putting $p = 0$, we obtain

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

similarly

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

Otherwise ⇒

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

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

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

$$\boxed{D^2 = \frac{1}{h^2}\left[\nabla^2 + \nabla^3 + \frac{11}{12}\nabla^4 + \cdots\right]}$$

Similarly $\boxed{D^3 = \frac{1}{h^3}\left[\nabla^3 + \frac{3}{2}\nabla^4 + \cdots\right]}$

Applying these identities to y_n, we get

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

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

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

Example ⇒ 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 $\frac{dy}{dx}$ & $\frac{d^2y}{dx^2}$ at (a) $x = 1.1$ (b) $x = 1.6$

Solution ⇒ The difference table is

x	y	Δ	Δ^2	Δ^3	Δ^4	Δ^5	Δ^6
1.0	7.989						
		0.414					
1.1	8.403		-0.036				
		0.378		0.006			
1.2	8.781		-0.030		-0.002		
		0.348		0.004		0.001	
1.3	9.129		-0.026		-0.001		0.002
		0.322		0.003		0.003	
1.4	9.451		-0.023		+0.002		
		0.299		0.005			
1.5	9.750		-0.018				
		0.281					
1.6	10.031						

We have

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

here $h = 0.1$, $x_0 = 1.0$, & $x_1 = 1.1$

$$\Rightarrow \left.\frac{dy}{dx}\right|_{x=x_0=1.1} = \frac{1}{0.1}\left[\Delta y_1 - \frac{1}{2}\Delta^2 y_1 + \frac{1}{3}\Delta^3 y_1 - \frac{1}{4}\Delta^4 y_1 + \frac{1}{5}\Delta^5 y_1 - \frac{1}{6}\Delta^6 y_1 + \cdots\right]$$

$$= \frac{1}{0.1}\left[0.378 - \frac{1}{2}(-0.030) + \frac{1}{3}(0.004) - \frac{1}{4} \times (-0.001) + \frac{1}{5}(0.003)\right]$$

$$= 3.951833$$

$$\simeq 3.952$$ Ans

$$\left.\frac{d^2y}{dx^2}\right|_{x=x_1=1.1} = \frac{1}{h^2}\left[\Delta^2 y_1 - \Delta^3 y_1 + \frac{11}{12}\Delta^4 y_1 - \frac{5}{6}\Delta^5 y_1 + \cdots\right]$$

$$= \frac{1}{(0.1)^2}\left[-0.030 - 0.004 + \frac{11}{12}(-0.001) - \frac{5}{6}(0.003) + \cdots\right]$$

$$= -3.74166$$

$$\simeq -3.74 \quad \text{Ans}$$

(b) To find y' at $x = 1.6$ & y'' at $x=1.6$ we will use above difference table and backward difference operator ∇ instead of Δ.

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

$$= \frac{1}{0.1}\left[0.281 + \frac{1}{2}(-0.018) + \frac{1}{3}(0.005) + \frac{1}{4}(0.002) + \frac{1}{5}(0.003) + \frac{1}{6}(0.002)\right]$$

$$= 0.2751 / 0.1 = 2.75 \quad \text{Ans}$$

~~0.275~~

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

$$= \frac{1}{(0.1)^2}\left[-0.018 + 0.005 + \frac{11}{12}(0.002) + \frac{5}{6}(0.003) + \frac{137}{180}(0.002)\right] = -0.715 \;(-7.14)$$

Ans

Also, from

Numerical

Derivatives using unequally spaced value of argument ⇒

① Lagrange's interpolation formula is

$$f(x) = \frac{(x-x_1)(x-x_2)\cdots(x-x_n)}{(x_0-x_1)(x_0-x_2)\cdots(x_0-x_n)} f(x_0) + \frac{(x-x_0)(x-x_2)\cdots(x-x_n)}{(x_1-x_0)(x_1-x_2)\cdots(x_1-x_n)} f(x_1) + \cdots\cdots$$

differentiating both sides w.r.t. x, we get $f'(x)$.

② Newton's divided difference formula is

$$f(x) = f(x_0) + (x-x_0)[x_0, x_1] + (x-x_0)(x-x_1)[x_0, x_1, x_2] + \cdots\cdots$$

differentiating w.r.t. x, we get

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

example ⇒ Find $f'(10)$ from the following data

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

Ans. ⇒ As the values are not equispaced, we shall use Newton's divided difference formula

The divided difference table is

x	$f(x)$	1st d.d	2nd d.d	3rd d.d	4th d.d
3	-13				
		18			
5	23		16		
		146		1	
11	899		40		0
		1026		1	
27	17315		69		
		2613			
34	35606				

formula

$$f'(x) = [x_0, x_1] + (2x - (x_0+x_1)) \times [x_0, x_1, x_2] + (3x^2 - 2x(x_0+x_1+x_2) + x_0x_1 + x_1x_2 + x_2x_0)[x_0, x_1, x_2, x_3] + \cdots$$

$$\Rightarrow f'(10) = 18 + 12 \times 16 + 23 \times 1 - 0$$

$$= 233$$

Derivatives using unequally spaced value of argument ⇒

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$$f(x) = \frac{(x-x_1)(x-x_2)\cdots(x-x_n)}{(x_0-x_1)(x_0-x_2)\cdots(x_0-x_n)} f(x_0) + \frac{(x-x_0)(x-x_2)\cdots(x-x_n)}{(x_1-x_0)(x_1-x_2)\cdots(x_1-x_n)} f(x_1) + \cdots\cdots$$

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$$f(x) = f(x_0) + (x-x_0)[x_0, x_1] + (x-x_0)(x-x_1)[x_0, x_1, x_2] + \cdots$$

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$$f'(x) = [x_0, x_1] + (2x-(x_0+x_1)) \times [x_0, x_1, x_2] + (3x^2 - 2x(x_0+x_1+x_2) + x_0x_1 + x_1x_2 + x_2x_0) \cdot [x_0, x_1, x_2, x_3] + \cdots$$

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Ans