Numerical differentiation

(i) **Newton's Forward difference formula to get the derivative:**

We are given $(n+1)$ ordered pairs (x_i, y_i) $i = 0, 1, \ldots, n$. We want to find the derivative of $y = f(x)$ passing through the $(n+1)$ points, at a point nearer to the starting value $x = x_0$.

Newton's forward difference interpolation formula is

$$y(x_0 + uh) = y_0 + u\Delta y_0 + \frac{u(u-1)}{2!}\Delta^2 y_0 + \frac{u(u-1)(u-2)}{3!}\Delta^3 y_0 + \cdots \rightarrow (1)$$

Where $y(x)$ is a polynomial of degree n in x and $u = \frac{x - x_0}{h}$.

Differentiating $y(x)$ w.r.t x, we have

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

$$\frac{dy}{dx} = \frac{dy}{dx} \cdot \frac{1}{h}$$

$$\frac{dy}{dx} = \frac{1}{h}\left[\Delta y_0 + \frac{2u-1}{2}\Delta^2 y_0 + \frac{3u^2-6u+2}{6}\Delta^3 y_0 + \frac{4u^3-18u^2+22u-6}{24}\Delta^4 y_0 + \cdots\right] \rightarrow (2)$$

Equation (2) gives the value of dy/dx at general x which may be anywhere in the interval.

In special case like $x = x_0$,

i.e., $u = 0$, (2) reduces to

$$\left(\frac{dy}{dx}\right)_{x=x_0} = \left(\frac{dy}{dx}\right)_{u=0} = \frac{1}{h}\left[\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0 - \frac{1}{4}\Delta^4 y_0 + \cdots\right] \rightarrow (3)$$

Differentiating again (2) w.r.t x, we have

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

$$= \frac{d}{du}\left(\frac{dy}{dx}\right)\cdot\frac{1}{h}$$

$$\frac{d^2y}{dx^2} = \frac{1}{h^2}\left[\Delta^2 y_0 + (u-1)\Delta^3 y_0 + \frac{(6u^2-18u+11)}{12}\Delta^4 y_0 + \cdots\right] \rightarrow (4)$$

Hence, $\frac{d^3y}{dx^3} = \frac{1}{h^3}\left[\Delta^3 y_0 + \frac{12u-18}{12}\cdot\Delta^4 y_0 + \cdots\right]$ $\rightarrow$ (5)

Equations (4) and (5) give the second and third derivative value at $x = x_0$.

Setting $x = x_0$ i.e., $u = 0$ in (4) and (5)

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

$$\left(\frac{d^3y}{dx^3}\right)_{x=x_0} = \frac{1}{h^3}\left[\Delta^3 y_0 - \frac{3}{2}\Delta^4 y_0 + \cdots\right] \rightarrow (7)$$

Equations (6) and (7) give the values of second and third derivatives at the starting value $x = x_0$.

We know that $E = 1 + \Delta = e^{hD}$.

$$\therefore D = \frac{1}{h}\log(1+\Delta)$$

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

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

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

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

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

2) Newton's backward difference formula to compute the derivative:

Consider Newton's backward difference interpolation formula,

$$y(x) = y(x_n + vh) = y_n + v\nabla y_n + \frac{v(v+1)}{2!}\nabla^2 y_n + \frac{v(v+1)(v+2)}{3!}\nabla^3 y_n + \cdots \rightarrow (8)$$

where $v = \dfrac{x - x_n}{h}$

Differentiating (8) w.r.t x,

$$\frac{dy}{dx} = \frac{dy}{dv}\cdot\frac{dv}{dx} = \frac{dy}{dv}\cdot\frac{1}{h}$$

$$\frac{dy}{dx} = \frac{1}{h}\left[\nabla y_n + \frac{2v+1}{2}\nabla^2 y_n + \frac{3v^2+6v+2}{6}\nabla^3 y_n + \frac{4v^3+18v^2+22v+6}{24}\cdot\nabla^4 y_n + \cdots\right] \rightarrow (9)$$

$$\therefore \frac{d^2y}{dx^2} = \frac{1}{h^2}\left[\nabla^2 y_n + (v+1)\nabla^3 y_n + \frac{6v^2+18v+11}{12}\nabla^4 y_n + \cdots\right] \rightarrow (10)$$

$$\therefore \frac{d^3y}{dx^3} = \frac{1}{h^3}\left[\nabla^3 y_n + \frac{12v+18}{12}\nabla^4 y_n + \cdots\right] \rightarrow (11)$$

Equations (9), (10) and (11) are the first, second and third derivative at any general x.

Setting $x = x_n$ or $v = 0$ in (9), (10) and (11), we get

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

$$\left(\frac{d^2y}{dx^2}\right)_{x=x_n} = \frac{1}{h^2}\left[\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12}\nabla^4 y_n + \cdots\right] \rightarrow (13)$$

$$\left(\frac{d^3y}{dx^3}\right)_{x=x_n} = \frac{1}{h^3}\left[\nabla^3 y_n + \frac{3}{2}\nabla^4 y_n + \cdots\right] \rightarrow (14)$$

Using $E = e^{hD} = \frac{1}{1-\nabla}$, we get $D = \frac{-1}{h}\log(1-\nabla)$

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

$$D^2 = \frac{1}{h^2}\left[\nabla^2 + \nabla^3 + \frac{11}{12}\nabla^4 + \cdots\right] \rightarrow (15)$$

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

We can get the above results (12), (13) and (14).

3. Derivative using Stirling's formula:

Consider Stirling's formula,

$$y(x) = y(x_0 + uh) = y_0 + \frac{u}{2}\left[\Delta y_0 + \Delta y_{-1}\right] + \frac{u^2}{2}\Delta^2 y_{-1} + \frac{u^3-u}{12}\left(\Delta^3 y_{-1} + \Delta^3 y_{-2}\right) + \frac{u^4-u^2}{24}\Delta^4 y_{-2} + \cdots$$

where $u = \dfrac{x - x_0}{h}$. $\rightarrow$ (16)

Differentiating (16) w.r.t x

$$\frac{dy}{dx} = \frac{dy}{du} \cdot \frac{du}{dx} = \frac{1}{h} \cdot \frac{dy}{du}$$

$$= \frac{1}{h}\left[\frac{1}{2}(\Delta y_0 + \Delta y_{-1}) + u\Delta^2 y_{-1} + \frac{3u^2-1}{12}\left(\Delta^3 y_{-1} + \Delta^3 y_{-2}\right) + \frac{1}{12}(2u^3-u)\Delta^4 y_{-2} + \frac{5u^4-15u^2+4}{240}\left(\Delta^5 y_{-2} + \Delta^5 y_{-3}\right) + \cdots\right]$$

$\rightarrow$ (17)

$$\frac{d^2y}{dx^2} = \frac{1}{h^2}\left[\Delta^2 y_{-1} + \frac{u}{2}\left(\Delta^3 y_{-1} + \Delta^3 y_{-2}\right) + \frac{(6u^2-1)}{12}\Delta^4 y_{-2} + \cdots\right]$$

$\rightarrow$ (18)

$$\frac{d^3y}{dx^3} = \frac{1}{h^3}\left[\frac{1}{2}\left(\Delta^3 y_{-1} + \Delta^3 y_{-2}\right) + u \cdot \Delta^4 y_{-2} + \cdots\right]$$

$\rightarrow$ (19)

Setting $x = x_0$, ie., $u = 0$ in (17), (18) and (19), we get

$$\left(\frac{dy}{dx}\right)_{x=x_0} = \frac{1}{h}\left[\frac{1}{2}(\Delta y_0 + \Delta y_{-1}) - \frac{1}{12}\left(\Delta^3 y_{-1} + \Delta^3 y_{-2}\right) + \frac{1}{60}\left(\Delta^5 y_{-2} + \Delta^5 y_{-3}\right) + \cdots\right]$$

$\rightarrow$ (20)

$$\left(\frac{d^2y}{dx^2}\right)_{x=x_0} = \frac{1}{h^2}\left[\Delta^2 y_{-1} - \frac{1}{12}\Delta^4 y_{-2} + \cdots\right] \rightarrow (21)$$

$$\left(\frac{d^3y}{dx^3}\right)_{x=x_0} = \frac{1}{h^3}\left[\frac{1}{2}\left(\Delta^3 y_{-1} + \Delta^3 y_{-2}\right) + \cdots\right] \rightarrow (22)$$

Problems

1). Find the first two derivatives of $(x)^{1/3}$ at $x = 50$ and $x = 56$ given the table below.

x :	50	51	52	53	54	55	56
$y = x^{1/3}$:	3.6840	3.7084	3.7325	3.7563	3.7798	3.8030	3.8259

Sol:

Since we require $f'(x)$ at $x = 50$, we use Newton's forward formula and to get $f'(x)$ at $x = 56$, we use Newton's backward formula.

Difference Table :

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$
50	3.6840			
		0.0244		
51	3.7084		-0.0003	
		0.0241		0
52	3.7325		-0.0003	
		0.0238		0
53	3.7563		-0.0003	
		0.0235		0
54	3.7798		-0.0003	
		0.0232		0
55	3.8030		-0.0003	
		0.0229		
56	3.8259			

By Newton's forward formula,

$$\left(\frac{dy}{dx}\right)_{x=x_0} = \left(\frac{dy}{dx}\right)_{u=0}$$

$$= \frac{1}{h}\left[\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0 \cdots\right]$$

$$= \frac{1}{1}\left[0.0244 - \frac{1}{2}(-0.0003) + \frac{1}{3}(0)\right]$$

$$= 0.02455.$$

$$\left(\frac{d^2y}{dx^2}\right)_{x=50} = \frac{1}{h^2}\left[\Delta^2 y_0 - \Delta^3 y_0 + \cdots\right]$$

$$= 1\left[-0.0003\right]$$

$$= -0.0003$$

By Newton's backward formula,

$$\left(\frac{dy}{dx}\right)_{x=x_n} = \left(\frac{dy}{dx}\right)_{v=0} = \frac{1}{h}\left[\nabla y_n + \frac{1}{2}\nabla^2 y_n + \frac{1}{3}\nabla^3 y_n + \cdots\right]$$

$$= \frac{1}{1}\left[0.0229 + \frac{1}{2}(-0.0003) + 0\right]$$

$$\left(\frac{dy}{dx}\right)_{x=56} = 0.02275$$

$$\left(\frac{d^2y}{dx^2}\right)_{x=56} = \frac{1}{h^2}\left[\nabla^2 y_n + \nabla^3 y_n + \cdots\right]$$

$$= \frac{1}{1}\left[-0.0003\right]$$

$$= -0.0003$$

2). Find the value of $f'(0.5)$ using Stirling's formula from the following data.

x :	0.35	0.40	0.45	0.50	0.55	0.60	0.65
$y = f(x)$:	1.521	1.506	1.488	1.467	1.444	1.418	1.389

sol

x	y	Δy	Δy^2	$\Delta^3 y$	$\Delta^4 y$	$\Delta^5 y$
0.35	1.521					
		−0.015				
0.40	1.506		−0.003			
		−0.018		0		
0.45	1.488		−0.003 ($\Delta^2 y_{-2}$)		0.001	
		−0.021 (Δy_{-1})		0.001 ($\Delta^3 y_{-2}$)		−0.003 ($\Delta^5 y_{-3}$)
0.50	1.467 (y_0)		−0.002 ($\Delta^2 y_{-1}$)		−0.002	
		−0.023 (Δy_0)		−0.001 ($\Delta^3 y_{-1}$)		0.003 ($\Delta^5 y_{-2}$)
0.55	1.444		−0.003		−0.001 ($\Delta^4 y_{-1}$)	
		−0.026		0		
0.60	1.418		−0.003			
		−0.029				
0.65	1.389					

Since $x = 0.5$, is in the middle of the table, we use Stirling's formula taking 0.50 as the origin.

$\therefore x_0 = 0.50, \quad y_0 = 1.467.$

By Stirlings' formula, we have

$$\left(\frac{dy}{dx}\right)_{x=x_0} = \frac{1}{h}\left[\frac{1}{2}(\Delta y_0 + \Delta y_{-1}) - \frac{1}{12}(\Delta^3 y_{-1} + \Delta^3 y_{-2}) + \frac{1}{60}(\Delta^2 y_{-2} + \Delta^5 y_{-1}) + \cdots\right]$$

$$= \frac{1}{0.05}\left[\frac{1}{2}(-0.023 - 0.021) - \frac{1}{12}(-0.001 + 0.001) + \frac{1}{60}(0.003 - 0.003)\right]$$

$$= -0.44$$