Numerical Differentiation

Consider a set of values (x_i, y_i) ; i = 0, 1, 2,, n of a function y = f(x). The process of computing the derivative or derivatives of that function at some values of x from the given set of values is called numerical differentiation. This may be done by first approximating the function by a suitable interpolation formula and then differentiating it as many times as desired.

If the values of x are equally spaced and the derivative is required near the beginning of the table, we use Newton's forward interpolation formula. If it is required near the end of the table, we use Newton's back ward interpolation formula. For the values near the middle of the table, the derivative is calculated by means of Stirling's central difference formula.

If the values of x are not equally spaced, we use Lagrange's interpolation formula to get the derivative value.

Newton's forward difference formula for equal intervals to get the derivatives

Wkt Newton's forward difference formula for equal intervals

$$y(x) = y_0 + \frac{u}{1!} \Delta y_0 + \frac{u(u-1)}{2!} \Delta^2 y_0 + \frac{u(u-1)(u-2)}{3!} \Delta^3 y_0 + \dots$$
 where $u = \frac{x-x_0}{h}$
$$y(x) = y_0 + \frac{u}{1!} \Delta y_0 + \frac{u^2 - u}{2!} \Delta^2 y_0 + \frac{u^3 - 3u^2 + 2u}{3!} \Delta^3 y_0 + \frac{u^4 - 6u^3 + 11u^2 - 6u}{4!} \Delta^4 y_0 + \dots$$

Now differentiate the above equation with respect to x on both sides

$$\therefore \frac{dy}{dx} = \frac{1}{h} \left[\Delta y_0 + \frac{2u - 1}{2!} \Delta^2 y_0 + \frac{3u^2 - 6u + 2}{3!} \Delta^3 y_0 + \frac{4u^3 - 18u^2 + 22u - 6}{4!} \Delta^4 y_0 + \dots \right]_{------(I)}$$

Similarly
$$\frac{d^{2}y}{dx^{2}} = \frac{d}{dx} \left(\frac{dy}{dx} \right) = \frac{d}{du} \left(\frac{dy}{dx} \right) \left(\frac{du}{dx} \right) = \frac{1}{h} \frac{d}{du} \left(\frac{dy}{dx} \right)$$

$$\frac{d^{2}y}{dx^{2}} = \frac{1}{h^{2}} \left[0 + \frac{2}{2!} \Delta^{2} y_{0} + \frac{6u - 6}{3!} \Delta^{3} y_{0} + \frac{12u^{2} - 36u + 22}{4!} \Delta^{4} y_{0} + \dots \right]$$

$$\frac{d^{2}y}{dx^{2}} = \frac{1}{h^{2}} \left[\Delta^{2}y_{0} + (u - 1) \Delta^{3}y_{0} + \frac{6u^{2} - 18u + 11}{12} \Delta^{4}y_{0} + \dots \right]$$
(II)

When
$$x = x_0$$
, $u = \frac{x - x_0}{h} = 0$

Put u = 0 in the above equation (I), we get

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

Put u = 0 in the equation (II), we get

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

(OR)

Using relation between operators, wkt $E = e^{hD}$

i.e.,
$$1 + \Delta = e^{hD}$$

 $\log (1 + \Delta) = \log e^{hD}$
 $hD = \log(1 + \Delta)$
 $\log(1+x) = x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + \dots$
 $\therefore hD = \Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \frac{\Delta^4}{4} + \dots$
 $D = \frac{1}{h} \left[\Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \frac{\Delta^4}{4} + \dots \right]$
 $D^2 = \frac{1}{h^2} \left[\Delta - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \frac{\Delta^4}{4} + \dots \right]^2 = \frac{1}{h^2} \left[\Delta^2 - \Delta^3 + \frac{11}{12} \Delta^4 - \frac{5}{6} \Delta^5 + \dots \right]$

Now applying these identities to y_0 , we get

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

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

Newton's backward difference formula for equal intervals to get the derivatives

Wkt Newton's backward difference formula for equal intervals

$$y(x) = y_n + \frac{v}{1!} \nabla y_n + \frac{v(v+1)}{2!} \nabla^2 y_n + \frac{v(v+1)(v+2)}{3!} \nabla^3 y_n + \dots$$
 where $v = \frac{x - x_n}{h}$
$$y(x) = y_n + \frac{v}{1!} \nabla y_n + \frac{v^2 + v}{2!} \nabla^2 y_n + \frac{v^3 + 3v^2 + 2v}{3!} \nabla^3 y_n + \frac{v^4 + 6v^3 + 11v^2 - 6v}{4!} \nabla^4 y_n + \dots$$

Now differentiate the above equation with respect to x on both sides

$$\frac{dy}{dx} = \frac{dy}{dv} \frac{dv}{dx} \qquad \because v = \frac{x - x_n}{h}; \quad \frac{dv}{dx} = \frac{1}{h}$$

$$\frac{dy}{dx} = \frac{1}{h} \frac{dy}{dv} = \frac{1}{h} \left[0 + \nabla y_n + \frac{2v + 1}{2!} \nabla^2 y_n + \frac{3v^2 + 6v + 2}{3!} \nabla^3 y_n + \frac{4v^3 + 18v^2 + 22v + 6}{4!} \nabla^4 y_n + \dots \right]$$

$$\therefore \frac{dy}{dx} = \frac{1}{h} \left[\nabla y_n + \frac{2v+1}{2!} \nabla^2 y_n + \frac{3v^2 + 6v + 2}{3!} \nabla^3 y_n + \frac{4v^3 + 18v^2 + 22v + 6}{4!} \nabla^4 y_n + \dots \right]_{------(III)}$$

Similarly
$$\frac{d^{2}y}{dx^{2}} = \frac{d}{dx} \left(\frac{dy}{dx} \right) = \frac{d}{dv} \left(\frac{dy}{dx} \right) \left(\frac{dv}{dx} \right) = \frac{1}{h} \frac{d}{dv} \left(\frac{dy}{dx} \right)$$

$$\frac{d^{2}y}{dx^{2}} = \frac{1}{h^{2}} \left[0 + \frac{2}{2!} \nabla^{2} y_{n} + \frac{6v + 6}{3!} \nabla^{3} y_{n} + \frac{12v^{2} + 36v + 22}{4!} \nabla^{4} y_{n} + \dots \right]$$

$$\frac{d^{2}y}{dx^{2}} = \frac{1}{h^{2}} \left[\nabla^{2} y_{n} + (v + 1) \nabla^{3} y_{n} + \frac{6v^{2} + 18v + 11}{12} \nabla^{4} y_{n} + \dots \right]$$
(IV)

When
$$x = x_n$$
, $v = \frac{x - x_n}{h} = 0$

Put v = 0 in the above equation (III), we get

$$\left(\frac{dy}{dx}\right)_{x=x_{n}} = \frac{1}{h} \left[\nabla y_{n} + \frac{\nabla^{2} y_{n}}{2} + \frac{\nabla^{3} y_{n}}{3} + \frac{\nabla^{4} y_{n}}{4} + \dots \right]$$

Put v = 0 in the equation (IV), we get

$$\left(\frac{d^2 y}{dx^2}\right)_{y=y_0} = \frac{1}{h^2} \left[\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12} \nabla^4 y_n + \dots \right]$$

(OR)

Using relation between operators, wkt $E^{-1} = e^{-hD}$

i.e.,
$$1 - \nabla = e^{-hD}$$

$$\log(1-\nabla) = \log e^{-hD}$$

$$-hD = \log(1-\nabla)$$

$$\log(1-x) = -x - \frac{x^2}{2} - \frac{x^3}{3} - \frac{x^4}{4} - \dots$$

$$\therefore hD = \nabla + \frac{\nabla^2}{2} + \frac{\nabla^3}{3} + \frac{\nabla^4}{4} + \dots$$

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

$$D^2 = \frac{1}{h^2} \left[\nabla + \frac{\nabla^2}{2} + \frac{\nabla^3}{3} + \frac{\nabla^4}{4} + \dots \right]^2 = \frac{1}{h^2} \left[\nabla^2 + \nabla^3 + \frac{11}{12} \nabla^4 + \frac{5}{6} \nabla^5 + \dots \right]$$

Now applying these identities to y_n , we get

$$Dy_{n} = \left(\frac{dy}{dx}\right)_{x = x_{n}} = \frac{1}{h} \left[\nabla y_{n} + \frac{\nabla^{2} yn}{2} + \frac{\nabla^{3} y_{n}}{3} + \frac{\Delta^{4} y_{n}}{4} + \dots \right]$$

$$D^{2}y_{n} = \left(\frac{d^{2}y}{dx^{2}}\right)_{x=x} = \frac{1}{h^{2}} \left[\nabla^{2}y_{n} + \nabla^{3}y_{n} + \frac{11}{12}\nabla^{4}y_{n} + \frac{5}{6}\nabla^{5}y_{n} + \dots \right]$$

Stirling's central difference formula to get the derivatives

Wkt.

$$y(x) = y_0 + \frac{u}{1!} \left[\frac{\Delta y_0 + \Delta y_{-1}}{2} \right] + \frac{u^2}{2!} \Delta^2 y_{-1} + \frac{u(u^2 - 1^2)}{3!} \left[\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2} \right] + \frac{u^2(u^2 - 1^2)}{4!} \Delta^4 y_{-2} + \dots$$

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

Differentiate (I) with respect to 'x' on both sides

$$\frac{dy}{dx} = \frac{dy}{du}\frac{du}{dx} \qquad \qquad \because u = \frac{x - x_0}{h}; \quad \frac{du}{dx} = \frac{1}{h}$$

$$\frac{dy}{dx} = \frac{1}{h} \left[0 + \frac{1}{1!} \left[\frac{\Delta y_0 + \Delta y_{-1}}{2} \right] + \frac{2u}{2!} \Delta^2 y_{-1} + \frac{3u^2 - 1}{3!} \left[\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2} \right] + \frac{4u^3 - 2u}{4!} \Delta^4 y_{-2} + \dots \right]$$

$$\frac{dy}{dx} = \frac{1}{h} \left[\left[\frac{\Delta y_0 + \Delta y_{-1}}{2} \right] + u \Delta^2 y_{-1} + \frac{3u^2 - 1}{6} \left[\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2} \right] + \frac{2u^3 - u}{12} \Delta^4 y_{-2} + \dots \right]$$

Again differentiate with respect to 'x' on both sides

$$\begin{split} \frac{d^2 y}{dx^2} &= \frac{d}{dx} \left(\frac{dy}{dx} \right) = \frac{d}{du} \left(\frac{dy}{dx} \right) \left(\frac{du}{dx} \right) = \frac{1}{h} \frac{d}{du} \left(\frac{dy}{dx} \right) \\ \frac{d^2 y}{dx^2} &= \frac{1}{h} \left[0 + \Delta^2 y_{-1} + \frac{6u}{6} \left[\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2} \right] + \frac{6u - 1}{12} \Delta^4 y_{-2} + \dots \right] \\ \frac{d^2 y}{dx^2} &= \frac{1}{h} \left[\Delta^2 y_{-1} + u \left[\frac{\Delta^3 y_{-1} + \Delta^3 y_{-2}}{2} \right] + \frac{6u - 1}{12} \Delta^4 y_{-2} + \dots \right] \end{split}$$

When
$$x = x_0$$
, $u = \frac{x - x_0}{h} = 0$

Put u = 0 in the above equations, we get

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

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