NUMERICAL DIFFERENTIATION

Numerical Differentiation

It is the process of calculating the value of the derivative of a function at some assigned value 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.

The choice of the interpolation formula to be used, will depend on the assigned value of *x* at which *dy/dx* is desired.

If the values of x are equispaced

- dy/dx is required near the beginning of the table, we employ Newton's forward formula.
- If it is required near the end of the table, we use Newton's backward formula.
- For values near the middle of the table, dy/dx is calculated by means of Stirling's formula.

If the values of x are not equispaced,

- 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, ... n.

1. Derivatives using Newton's forward difference formula

Newton's forward interpolation formula is

$$Y(x_0 + \alpha\Delta x) = y_0 + (\alpha\Delta y_0) + \frac{\alpha(\alpha-1)}{2|}(\Delta^2 y_0) + \frac{\alpha(\alpha-1)(\alpha-2)}{3|}(\Delta^3 y_0) \ldots\ldots\ldots$$

$$\frac{\alpha(\alpha-1)(\alpha-2)\ldots\ldots\ldots(\alpha-n+1)}{n|}(\Delta^n y_0)$$

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

$$\frac{dy}{d\alpha} = \Delta y_0 + \frac{(2\alpha-1)}{2|}(\Delta^2 y_0) + \frac{(3\alpha^2-6\alpha+2)}{3|}(\Delta^3 y_0) + \ldots.$$

Since $\alpha = \frac{(x - x_0)}{\Delta x}$

Therefore $\frac{d\alpha}{dx} = \frac{1}{\Delta x} = \frac{1}{h}$

Now

$$\frac{dy}{d\alpha} \cdot \frac{d\alpha}{dx} = \frac{1}{h}[\Delta y_0 + \frac{(2\alpha-1)}{2|}(\Delta^2 y_0) + \frac{(3\alpha^2-6\alpha+2)}{3|}(\Delta^3 y_0) + \frac{(4\alpha^3-18\alpha^2+22\alpha-6)}{4|}(\Delta^4 y_0) + \ldots\ \ldots]$$

At $x = x_0$, $\alpha = 0$. Hence putting $\alpha = 0$,

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

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

$$\frac{d^2y}{dx^2} = \frac{1}{dx}\left(\frac{dy}{d\alpha}\cdot\frac{d\alpha}{dx}\right) = \frac{1}{h}\Big[\frac{2}{2|}(\Delta^2 y_0) + \frac{(6\alpha-6)}{3|}(\Delta^3 y_0) + \frac{(12\alpha^2-36\alpha+22)}{4|}(\Delta^4 y_0) + \ldots \ \ldots\Big]\frac{1}{h}$$

Putting α = 0, we obtain

$$\frac{d^2y}{dx^2} = \frac{1}{h^2}\Big[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12}(\Delta^4 y_0) - \frac{5}{6}(\Delta^5 y_0) + \frac{137}{180}(\Delta^6 y_0) + \ldots\Big]$$

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

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

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

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

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

Now applying the above identities to y_0, we get

$$Dy_0 \text{ i.e., } \left(\frac{dy}{dx}\right)_{x_0} = \frac{1}{h}\Delta y_0 - \frac{1}{2}\left[\Delta^2 y_0 \frac{1}{3}\Delta^3 y_0 - \frac{1}{4}\Delta^4 y_0 + \frac{1}{5}\Delta^5 y_0 - \frac{1}{6}\Delta^6 y_0 + \ldots\right]$$

$$\left(\frac{d^2y}{dx^2}\right) = \frac{1}{h^2}\left[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12}\Delta^4 y_0 - \frac{5}{6}\Delta^5 y_0 + \frac{137}{180}\Delta^6 y_0 - \ldots\right]$$

and $$\left(\frac{d^3y}{dx^3}\right) = \frac{1}{h^3}\left[\Delta^2 y_0 - \frac{3}{2}\Delta^4 y_0 + \ldots\right]$$

Derivatives using Newton's backward difference formula

Newton's backward interpolation formula is

$$Y(x_n + \alpha\Delta x) = y_n + \alpha(\nabla y_n) + \frac{\alpha(\alpha+1)}{2|}(\nabla^2 y_n) + \frac{\alpha(\alpha+1)(\alpha+2)}{3|}(\nabla^3 y_n) \ldots\ldots\ldots$$

$$\frac{\alpha(\alpha+1)(\alpha+2)\ldots\ldots\ldots(\alpha+n-1)}{n|}(\nabla^n y_n)$$

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

$$\frac{dy}{d\alpha} = \nabla y_n + \frac{2\alpha+1}{2|}(\nabla^2 y_n) + \frac{3\alpha^2+6\alpha+2}{3|}(\nabla^3 y_n) \ldots\ldots\ldots$$

Since $$\alpha = \frac{(x - x_n)}{\Delta x}$$

Therefore $$\frac{d\alpha}{dx} = \frac{1}{\Delta x} = \frac{1}{h}$$

Now

$$\frac{dy}{d\alpha} \cdot \frac{d\alpha}{dx} = \frac{1}{h}[\nabla y_n + \frac{2\alpha+1}{2|} (\nabla^2 y_n) + \frac{3\alpha^2+6\alpha+2}{3|} (\nabla^3 y_n) \text{ ....}]$$

At $x = x_n$, $\alpha = 0$. Hence putting $\alpha = 0$,

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

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

$$\frac{d^2 y}{dx^2} = \frac{1}{dx}\left(\frac{dy}{d\alpha} \cdot \frac{d\alpha}{dx}\right) = \frac{1}{h}[\frac{2}{2|} (\nabla^2 y_n) + \frac{6\alpha+6}{3|} (\nabla^3 y_n) + \frac{6\alpha^2+18\alpha+11}{4|} (\nabla^4 y_n) \text{ ....}] \frac{1}{h}$$

Putting $\alpha = 0$, we obtain

$$\frac{d^2y}{dx^2} = \frac{1}{h^2}[\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12}\nabla^4 y_n + \frac{5}{6}\nabla^5 y_n + \frac{137}{180}\nabla^6 y_n \ldots\ldots\ldots]$$

Else: We know that $1 - \nabla = E^{-1} = e^{-hD}$

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

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

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

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

Applying these identities to yn, we get

$$Dy_n \text{ i.e., } \left(\frac{dy}{dx}\right)_{x_n} = \frac{1}{h}\left[\nabla y_n + \frac{1}{2}\nabla^2 y_n + \frac{1}{2}\nabla^3 y_n + \frac{1}{4}\nabla^4 y_n \frac{1}{5}\nabla^5 y_n + \frac{1}{6}\nabla^6 y_n + \cdots\right]$$

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

Derivatives using Stirling's central difference formula

Stirling's central difference formula is

$$Y(x_0 + \alpha\Delta x) = y_0 + \alpha\,(\mu\delta y_0) + \frac{\alpha^2}{2|}\,(\delta^2 y_0) + \frac{\alpha(\alpha^2-1^2)}{3|}\,(\mu\delta^3 y_0) + \frac{\alpha^2(\alpha^2-1^2)}{4|}\,(\delta^4 y_0) + \frac{\alpha(\alpha^2-1^2)(\alpha^2-2^2)}{5|}\,(\mu\delta^4 y_0) \;\ldots\ldots\ldots\ldots\ldots\ldots$$

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

$$\frac{dy}{d\alpha} = \mu\delta y_0 + \frac{2\alpha}{2|}\,\delta^2 y_0 + \frac{3\alpha^2-1}{3|}\,\mu\delta^3 y_0 + \frac{4\alpha^3-2\alpha}{4|}\,\delta^4 y_0 + \frac{4\alpha^3-3\alpha^2-8\alpha+4}{5|}\,(\mu\delta^5 y_0) \;\ldots\ldots\ldots\ldots\ldots\ldots$$

Since

$$\alpha = \frac{(x - x_0)}{\Delta x}$$

Therefore

$$\frac{d\alpha}{dx} = \frac{1}{\Delta x} = \frac{1}{h}$$

Now

$$\frac{dy}{d\alpha}\cdot\frac{d\alpha}{dx} = \frac{1}{h}\Big[\mu\delta y_0 + \frac{2\alpha}{2|}\,\delta^2 y_0 + \frac{3\alpha^2-1}{3|}\,\mu\delta^3 y_0 + \frac{4\alpha^3-2\alpha}{4|}\,\delta^4 y_0 + \frac{4\alpha^3-3\alpha^2-8\alpha+4}{5|}\,(\mu\delta^5 y_0) \;\ldots\ldots\ldots\ldots\ldots\ldots\Big]$$

At $x = x_0$, $\alpha = 0$. Hence putting $\alpha = 0$,

$$\left(\frac{dy}{dx}\right)_{x_0} = \frac{1}{h}[\mu\delta y_0 - \frac{1}{6}\mu\delta^3 y_0 + \frac{1}{30}(\mu\delta^5 y_0)\ldots\ldots\ldots\ldots]$$

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

$$\frac{d^2y}{dx^2} = \frac{1}{h^2}[\delta^2 y_0 - \frac{1}{12}\delta^4 y_0 + \frac{1}{90}(\delta^6 y_0)\ldots\ldots\ldots\ldots]$$

Derivatives using unequally spaced values of argument

(i) Lagranges's interpolation formula is

$$f(x) = \frac{(x-x_1)(x-x_2)\cdots(x-x_n)}{(x_0-x_1)(x_0-x_2)\cdots(x_0-x_n)}y_0 + \frac{(x-x_0)(x-x_2)\cdots(x-x_n)}{(x_1-x_0)(x_1-x_2)\cdots(x_1-x_n)}y_1 + \cdots + \frac{(x-x_0)(x-x_1)\cdots(x-x_{n-1})}{(x_n-x_0)(x_n-x_1)\cdots(x_n-x_{n-1})}y_n$$

Differentiating both sides w.r.t. x, we get f′(x).

(ii) Newton's divided difference formula is

$$f(x) = y_0 + (x - x_0)[x_0, x_1] + (x - x_0)(x - x_1)[x_0, x_1, x_2]$$
$$+ (x - x_0)(x - x_1)(x - x_2)[x_0, x_1, x_2, x_3] + \cdots$$
$$+ (x - x_0)(x - x_1)\cdots(x - x_n)[x_0, x_1, \cdots x_n]$$

Differentiating both sides w.r.t. x, we obtain

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