Numerical Differentiation and Integration

Numerical Differentiation

It is the process of calculating the value of the derivative of a function at some assigned values of x from the given set of values (x_i, y_i). To compute dy/dx, we first replace the latter as many times as we desire. The choice of the interpolation formula to be used, will depend on the assigned values of x at which dy/dx is desired.
If the value of x are equi-spaced and 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.**

Formula for Derivatives

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

Derivatives using forward difference formula

Newton's forward interpolation formula is given by

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

where $p = \frac{x-x_0}{h}$. Then $x = x_0 + ph$.

$$y(x_0 + ph) = y_0 + p\Delta y_0 + \frac{(p^2-p)}{2!}\Delta^2 y_0 + \frac{(p^3-3p^2+2p)}{3!}\Delta^3 y_0 + ...$$

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

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

Also, $\frac{dp}{dx} = \frac{1}{h}$.

$$\frac{dy}{dx} = \frac{dy}{dp}.\frac{dp}{dx} = \frac{1}{h}\left[\Delta y_0 + \frac{(2p-1)}{2!}\Delta^2 y_0 + \frac{3p^2-6p+2}{3!}\Delta^3 y_0 + \frac{4p^3-18p^2+22p-6}{4!}\Delta^4 y_0 + ...\right] \quad (1)$$

At $x = x_0$, $p = 0$. Hence putting $p = 0$, we have

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

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

$$\frac{d^2y}{dx^2} = \frac{d}{dp}\left(\frac{dy}{dx}\right)\frac{dp}{dx} = \frac{1}{h^2}\left[\frac{2}{2!}\Delta^2 y_0 + \frac{6p-6}{3!}\Delta^3 y_0 + \frac{12p^2-36p+22}{4!}\Delta^4 y_0 + ...\right].$$

Then

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

Derivatives using backward difference formula.

Using Newton's backward interpolation formula, the formula for the first order derivative of the given function may be deduced as

$$\frac{dy}{dx} = \frac{dy}{dp}\frac{dp}{dx} = \frac{1}{h}\left[\nabla y_n + \frac{2p+1}{2!}\nabla^2 y_n + \frac{3p^2+6p+2}{3!}\nabla^3 y_n + ...\right]$$

However, for the second order derivative, we have.

$$\frac{d^2y}{dx^2} = \frac{d}{dp}\left(\frac{dy}{dx}\right)\frac{dp}{dx} = \frac{1}{h^2}\left[\nabla^2 y_n + \frac{6p+6}{3!}\nabla^3 y_n + \frac{6p^2+18p+11}{12}\nabla^4 y_n + ...\right]$$

***

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: First we start constructing the divided difference table.

x	y	Δ	Δ^2	Δ^3	$\Delta 4$	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						

From the Newton's forward difference formula, we have,

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

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

Here, $h = 0.1$, $x_0 = 1.1$, $\Delta y_0 = 0.378$, $\Delta^2 y_0 = -0.03$ etc.

Substituting these values in above equations we get

$$\left(\frac{dy}{dx}\right)_{1.1} = \frac{1}{0.1}\left[0.378 - \frac{1}{2}(-0.03) + \frac{1}{3}(0.004) - \frac{1}{4}(-0.001) + \frac{1}{5}(0.003)\right] = 3.952$$

$$\left(\frac{d^2y}{dx^2}\right)_{x=x_0} = \frac{1}{0.1^2}\left[-0.03 - (0.004) + \frac{11}{12}(-0.001) - \frac{5}{6}(0.003)\right] = -3.74$$

Again, we use the above difference table and backward difference operator ∇ instead of forward difference operator Δ. Then

$$\left(\frac{dy}{dx}\right)_{x_n} = \frac{1}{h}\left[\nabla y_n + \frac{1}{2}\nabla^2 y_n + \frac{1}{3}\nabla^3 y_n + \frac{1}{4}\nabla^4 y_n + \frac{1}{5}\nabla^5 y_5 + \frac{1}{6}\nabla^6 y_6......\right]$$

However, for the second order derivative, we have.

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

Here, $h = 0.1$, $x_n = 1.6$, $\nabla y_n = 0.281$, $\nabla^2 y_n = -0.018$ etc.

Substituting these values in above equations, we get

$$\left(\frac{dy}{dx}\right)_{1.6}=\frac{1}{0.1}\left[0.281+\frac{1}{2}(-0.018)+\frac{1}{3}(0.005)+\frac{1}{4}(0.002)+\frac{1}{5}(0.003)+\frac{1}{6}(0.002)\right]=2.75$$

$$\left(\frac{d^2y}{dx^2}\right)_{1.6}=\frac{1}{h^2}\left[-0.018+0.005+\frac{11}{12}(0.002)+\frac{5}{6}(0.003)+\frac{137}{180}(0/02)+\right]=-0.715$$

Numerical Integration

The area bounded by the curve $y=f(x)$ and the $x-axis$ between a and b is denoted by

$$I=\int_a^b ydx=\int_a^b f(x)dx$$

We need to divide the interval (a,b) into n equal length.

$$(a,b)=(a=x_0,x_1,x_2,...,x_n=b)$$

Then

$$h=\frac{b-a}{n}$$

Trapezoidal Rule

$$\int_a^b f(x)dx=\frac{h}{2}\left[y_0+2\left(y_1+y_2+y_3.....+y_{n-1}\right)+y_n\right]$$

It is applicable on any number of intervals.

Simpson's $\frac{1}{3}rd$ Rule

$$\int_a^b f(x)dx=\frac{h}{3}\left[y_0+4\left(y_1+y_3+y_5+.....\right)+2\left(y_2+y_4+y_6+.....\right)+y_n\right]$$

It is applicable when total number of interval is even.

Simpson's $\frac{3}{8}th$ Rule

$$\int_a^b f(x)dx=\frac{3h}{8}\left[y_0+3\left(y_1+y_2+y_4+y_5.....\right)+2\left(y_3+y_6+y_9+.....\right)+y_n\right]$$

It is applicable when total number of interval is multiple of 3.

EX-1: Solve $\int_0^1\frac{dx}{1+x^2}$

Solution:

Take $n=6$ then $h=\frac{b-a}{n}$.

$\Rightarrow h=\frac{1-0}{6}$.

Here $y=f(x)=\frac{1}{1+x^2}$.

$$x_0 = 0, \qquad y_0 = f(x_0) = \frac{1}{1+x_0^2} = \frac{1}{1+0^2} = 1,$$

$$x_1 = \frac{1}{6}, \qquad y_1 = f(x_1) = \frac{1}{1+x_1^2} = \frac{1}{1+(\frac{1}{6})^2} = \frac{36}{37},$$

$$x_2 = \frac{2}{6}, \qquad y_2 = f(x_2) = \frac{1}{1+x_2^2} = \frac{1}{1+(\frac{2}{6})^2} = 0.9,$$

$$x_3 = \frac{3}{6}, \qquad y_3 = f(x_3) = \frac{1}{1+x_3^2} = \frac{1}{1+(\frac{3}{6})^2} = 0.8,$$

$$x_4 = \frac{4}{6}, \qquad y_4 = f(x_4) = \frac{1}{1+x_4^2} = \frac{1}{1+(\frac{4}{6})^2} = \frac{9}{13},$$

$$x_5 = \frac{5}{6}, \qquad y_5 = f(x_5) = \frac{1}{1+x_5^2} = \frac{1}{1+(\frac{5}{6})^2} = \frac{36}{61},$$

$$x_6 = 1, \qquad y_6 = f(x_6) = \frac{1}{1+x_6^2} = \frac{1}{1+1^2} = 0.5.$$

By Trapezoidal formula

$$\int_0^1 \frac{dx}{1+x^2} = \frac{h}{2}\left[y_0 + 2\left(y_1 + y_2 + y_3. + y_4 + y_5\right) + y_6\right]$$

$$= \frac{1}{6 \times 2}\left[1 + 2\left(\frac{36}{37} + 0.9 + 0.8 + \frac{9}{13} + \frac{36}{61}\right) + 0.5\right]$$

$$= 0.784241.$$

By Simpson $\frac{1}{3}$rd formula

$$\int_0^1 \frac{dx}{1+x^2} = \frac{h}{3}\left[y_0 + 4\left(y_1 + y_3 + y_5\right) + 2\left(y_2 + y_4\right) + y_6\right]$$

$$= \frac{1}{6 \times 3}\left[1 + 4\left(\frac{36}{37} + 0.8 + \frac{36}{61}\right) + 2\left(0.9 + \frac{9}{31}\right) + 0.5\right]$$

$$= 0.785398.$$

By Simpson $\frac{3}{8}$th formula

$$\int_0^1 \frac{dx}{1+x^2} = \frac{3h}{8}\left[y_0 + 3\left(y_1 + y_2 + y_4 + y_5\right) + 2\left(y_3\right) + y_6\right]$$

$$= \frac{8}{6 \times 3}\left[1 + 3\left(\frac{36}{37} + 0.9 + \frac{9}{13} + \frac{36}{61}\right) + 2\,(0.8) + 0.5\right]$$

$$= 0.785396.$$