Numerical Differentiation

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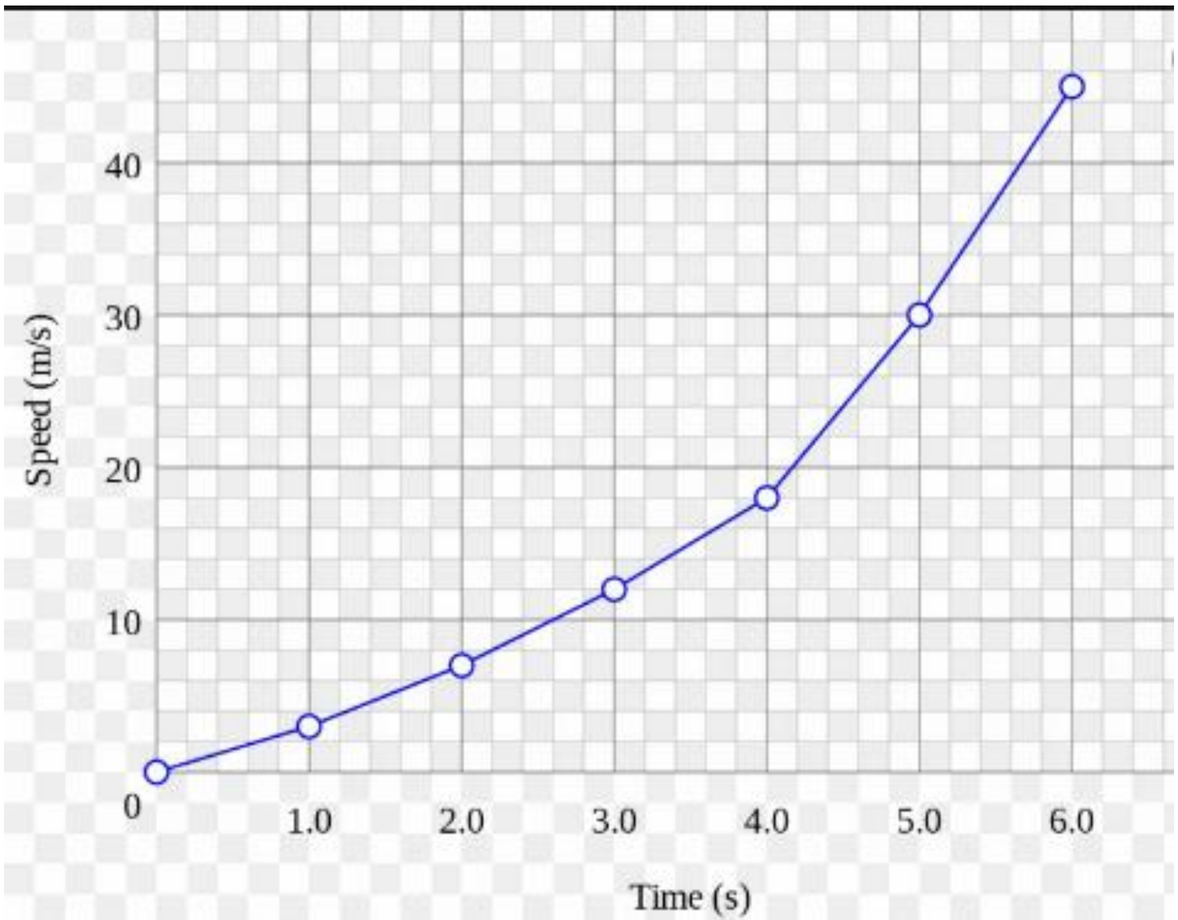

40
30
20
10
0
Speed (m/s)
1.0
2.0
3.0
4.0
5.0
6.0
Time (s)

Numerical differentiation

It is the process of calculating the values of the derivative of a function at some assigned value of x from the given set of values (x_i, y_i).

To compute this first replace the exact relation $y=f(x)$ by the best interpolating polynomial, then differentiate it as many times as required.

Gregory Newton Formula or Newton's formula for interpolation

1. Newton's Forward Difference Formula: For equal interval, we consider the more simpler formula. Let for equal spaced (h) data, We have x_0, $x_0 + h$, $x_0 + 2h, \ldots \ldots \ldots x_0 + nh$, Or $x_n = x_0 + nh$, n=0,1,2…….

$$f(x) = f\left[x_0 + \left(\frac{x - x_0}{h}\right)h\right]$$

$$Let \ldots : u = \left(\frac{x - x_0}{h}\right)$$

$$f(x) = f(x_0 + uh)$$

$$f(x) = E^u f(x_0)$$

$$f(x) = (1 + \Delta)^u f(x_0)$$

$$f(x) = f(x_0) + u\frac{\Delta f(x_0)}{1!} + u(u-1)\frac{\Delta^2 f(x_0)}{2!} + \ldots u(u-1)\ldots(u-(n-1))\frac{\Delta^n f(x_0)}{n!}$$

2. Newton's Backward Difference Formula: For equal interval, we consider the more simpler formula. Let for equal spaced (h) data, We have x_0, $x_0 + h$, $x_0 + 2h$,……… $x_0 + nh$, Or $x_n = x_0 + nh$, n=0,1,2…….

$$f(x) = f\left[x_n + \left(\frac{x - x_n}{h}\right)h\right]$$

$$let....u = \left(\frac{x - x_n}{h}\right)$$

$$f(x) = f(x_n + uh)$$

$$f(x) = E^u f(x_n)$$

$$f(x) = (1 - \nabla)^{-u} f(x_n)$$

$$f(x) = \left[1 + u\frac{\nabla}{1!} - u(-u-1)\frac{\nabla^2}{2!} + ..u(u+1)...(u+n-1)\frac{\nabla^n}{n!}\right] f(x_n)$$

$$f(x) = f(x_n) + u\frac{\nabla f(x_n)}{1!} + u(u+1)\frac{\nabla^2 f(x_n)}{2!} + ..u(u+1)...(u+n-1)\frac{\nabla^n f(x_n)}{n!}$$

Numerical differentiation using Newton's forward difference formula

$$f(x) = f(x_0) + u\frac{\Delta f(x_0)}{1!} + u(u-1)\frac{\Delta^2 f(x_0)}{2!} + u(u-1)(u-2)\frac{\Delta^3 f(x_0)}{3!} + \ldots\ldots$$

$$\ldots\ldots\ldots\ldots u(u-1)\ldots(u-(n-1))\frac{\Delta^n f(x_0)}{n!}$$

$$y = y_0 + u\frac{\Delta y_0}{1!} + u(u-1)\frac{\Delta^2 y_0}{2!} + u(u-1)(u-2)\frac{\Delta^3 y_0}{3!} + \ldots\ldots$$

$$\ldots\ldots\ldots u(u-1)\ldots(u-(n-1))\frac{\Delta^n y_0}{n!}\ldots\ldots\ldots\ldots(1)$$

Numerical differentiation using Newton's forward difference formula

$$f(x) = f(x_0) + u\frac{\Delta f(x_0)}{1!} + u(u-1)\frac{\Delta^2 f(x_0)}{2!} + u(u-1)(u-2)\frac{\Delta^3 f(x_0)}{3!} + \ldots\ldots$$

$$\ldots\ldots\ldots\ldots u(u-1)\ldots(u-(n-1))\frac{\Delta^n f(x_0)}{n!}$$

$$y = y_0 + u\frac{\Delta y_0}{1!} + u(u-1)\frac{\Delta^2 y_0}{2!} + u(u-1)(u-2)\frac{\Delta^3 y_0}{3!} + \ldots\ldots$$

$$\ldots\ldots\ldots u(u-1)\ldots(u-(n-1))\frac{\Delta^n y_0}{n!}\ldots\ldots\ldots\ldots(1)$$

$$x = x_0 + uh, u = \frac{x-x_0}{h}\ldots\ldots\ldots\ldots(2)$$

Numerical differentiation using Newton's forward difference formula

Differentiate eq (1) w.r.t u

$$\frac{dy}{du} = \frac{\Delta y_0}{1!} + (2u-1)\frac{\Delta^2 y_0}{2!} + (3u^2 - 6u + 2)\frac{\Delta^3 y_0}{3!} + \ldots\ldots\ldots$$

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

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

$$now, \frac{dy}{dx} = \frac{dy}{du} \times \frac{du}{dx}$$

$$\frac{dy}{dx} = \frac{1}{h}\left(\frac{\Delta y_0}{1!} + (2u-1)\frac{\Delta^2 y_0}{2!} + (3u^2 - 6u + 2)\frac{\Delta^3 y_0}{3!} + \ldots\ldots\ldots\right) \qquad \ldots\ldots\ldots\ldots(3)$$

Numerical differentiation using Newton's forward difference formula

At x=x_0, u=0

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

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

Differentiating eq(3) w.r.t x

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

$$\frac{d^2y}{dx^2}=\frac{1}{h}\left((2)\frac{\Delta^2 y_0}{2!}+(6u-6)\frac{\Delta^3 y_0}{3!}+\ldots\ldots..\right)\frac{du}{dx}$$

At x=x_0, u=0

$$D^2=\frac{d^2y}{dx^2}=\frac{1}{h^2}\left(\frac{\Delta^2 y_0}{1}-\frac{\Delta^3 y_0}{1}+\frac{11}{12}\Delta^4 y_0\ldots\ldots..\right)$$

Numerical differentiation using Newton's backward difference formula

$$f(x) = f(x_n) + u\frac{\nabla f(x_n)}{1!} + u(u+1)\frac{\nabla^2 f(x_n)}{2!} + \ldots u(u+1)\ldots(u+n-1)\frac{\nabla^n f(x_n)}{n!}$$

$$y_n(x) = y_n + u\frac{\nabla y_n}{1!} + u(u+1)\frac{\nabla^2 y_n}{2!} + \ldots u(u+1)\ldots(u+n-1)\frac{\nabla^n y_n}{n!}$$

$$x_n = x + uh, u = \frac{x - x_n}{h}$$

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

and

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

Numerical differentiation using difference operator

As we know

$$E = 1 + \Delta$$

$$E = (1-\nabla)^{-1} and \delta = \left(E^{1/2} - E^{-1/2}\right)$$

$$now$$

$$Ef(x) = f(x+h)$$

By taylor series,

$$Ef(x) = f(x) + hf^{'}(x) + \frac{h^2}{2!} f^{''}(x) + \ldots..$$

$$Ef(x) = f(x) + hDf \quad (x) + \frac{h^2}{2!} D^2 f \quad (x) + \ldots..$$

$$Ef(x) = \left[1 + hD + \frac{h^2}{2!} D^2 + \ldots..\right] f(x)$$

$$Ef(x) = e^{hD} f(x)$$

$$E = e^{hD}$$

$$take \log$$

$$\log E = hD \log e$$

$$D = \frac{1}{h} \log E$$

Numerical differentiation using difference operator

For forward difference operator

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

$$D = \frac{1}{h}\left(\frac{\Delta}{1} - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \ldots\ldots\right)$$

$$Df(x) = \frac{1}{h}\left(\frac{\Delta}{1} - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \ldots\ldots\right) f(x)$$

$$D^2 f(x) = \frac{1}{h^2}\left(\frac{\Delta}{1} - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \ldots\ldots\right)^2 f(x)$$

Similarly, the higher order derivatives can be calculated.

Numerical differentiation using difference operator

As we know

$$As$$

$$E=(1-\nabla)^{-1}$$

$$Ef(x)=e^{hD}f(x)$$

$$E=e^{hD}$$

$$take \log$$

$$\log E=hD\log e$$

$$D=\frac{1}{h}\log E$$

For backward Difference operator

$$D=\frac{1}{h}\log(1-\nabla)^{-1}$$

$$D=-\frac{1}{h}\log(1-\nabla)$$

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

$$Df(x)=\frac{1}{h}\left[\nabla+\frac{\nabla^2}{2}+\frac{\nabla^3}{3}+\ldots\ldots\right]f(x)$$

Forward difference Table

x	$f(x)$	Δ^1	Δ^2	Δ^3
x_0	y_0	$\Delta y_0=y_1-y_0$	$\Delta^2 y_0=\Delta y_1-\Delta y_0$	$\Delta^3 y_0=\Delta^2 y_1-\Delta^2 y_0$
x_1	y_1	$\Delta y_1=y_2-y_1$	$\Delta^2 y_1=\Delta y_2-\Delta y_1$	
x_2	y_2	$\Delta y_2=y_3-y_2$		
x_3	y_3			

Backward difference Table

x	f(x)	∇^1	∇^2	∇^3
x_0	y_0	$\nabla y_1 = y_1 - y_0$	$\nabla^2 y_2 = \nabla y_2 - \nabla y_1$	$\nabla^3 y_3 = \nabla^2 y_3 - \nabla^2 y_2$
x_1	y_1	$\nabla y_2 = y_2 - y_1$	$\nabla^2 y_3 = \nabla y_3 - \nabla y_2$	
x_2	y_2	$\nabla y_3 = y_3 - y_2$		
x_3	y_3			

Note: $\Delta y_0 = \nabla y_1$ and $\Delta^2 y_0 = \nabla^2 y_2$

Example-1

Given the values

x	1	1.1	1.2	1.3	1.4
f(x)	7.989	8.403	8.781	9.129	9.451

Calculate dy/dx at x=1

Solution

We have

x	f(x)	Δ	Δ^2	Δ^3	Δ^4	Δ^5	Δ^6
1	7.989	0.414	-0.036	-0.006	-0.002	-0.002	-0.003
1.1	8.403	0.378	-0.030	0.004	0.000	-0.001	
1.2	8.781	0.348	-0.026	0.004	-0.001		
1.3	9.129	0.322	-0.023	0.005			
1.4	9.451	0.299	-0.018				
1.5	9.750	0.281					
1,6	10.031						

Solution

x	f(x)	Δ	Δ^2	Δ^3	Δ^4	Δ^5	Δ^6
1	7.989	0.414	-0.036	-0.006	-0.002	-0.002	-0.003
1.1	8.403	0.378	-0.030	0.004	0.000	-0.001	
1.2	8.781	0.348	-0.026	0.004	-0.001		
1.3	9.129	0.322	-0.023	0.005			
1.4	9.451	0.299	-0.018				
1.5	9.750	0.281					
1,6	10.031						

$$Df(x) = \frac{1}{h}\left(\frac{\Delta}{1} - \frac{\Delta^2}{2} + \frac{\Delta^3}{3} - \ldots\ldots\ldots\right) f(x)$$

$$\frac{dy}{dx} = \frac{1}{0.1}\left[0.414 - \frac{0.0036}{2} + \frac{0.006}{3} - \frac{0.002}{4} + \frac{0.002}{5} - \frac{0.003}{6}\right]$$

Compute it by yourself

Practice Problem

Find the first derivative of the function f(x) at x=1.5

x	1.5	2.0	2.5	3.0	3.5	4.0
f(x)	3.3	7.00	13.625	24.0	38.875	59.00

Suggested books

1. Numerical Methods by **S.R.K Lyenger & R.K. Jain.**

2. Numerical Analysis by **Richard L. Burden.**

3. Introductory methods of Numerical analysis by **S.S. Sastry**.

Thank you