Lesson: Numerical Differentiation

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2. Introduction:

There are several method to determine the derivative of a function, however, when the function is complicated or when it is in the tabular form then we use the numerical methods. Thus, the process of finding the derivative or derivatives of a function at some values of the independent variable when we are given a set of value of that function is called numerical differentiation. Numerical differentiation methods are obtained using any of the following three techniques:

(i) Methods based on interpolation

(ii) Methods based on finite difference operators.

3. Numerical Differentiation:

The problem of differentiation is solved by first approximating the function by an interpolation formula and then differentiating this formula as many times as desired.

4. Numerical Differentiation Methods Based on Interpolation:

We know that the Lagrange's Interpolation formula is

$$f(x) = \ell_0(x) f(x_0) + \ell_1(x) f(x_1) + \ldots + \ell_n(x) f(x_n) \qquad (1)$$

where

$$\ell_0(x) = \frac{(x-x_1)(x-x_2)\ldots(x-x_n)}{(x_0-x_1)(x_0-x_2)\ldots(x_0-x_n)},$$

$$\ell_1(x) = \frac{(x-x_0)(x-x_2)\ldots(x-x_n)}{(x_1-x_0)(x_1-x_2)\ldots(x_1-x_n)},$$

$$\ell_n(x) = \frac{(x-x_0)(x-x_1)\ldots(x-x_{n-1})}{(x_n-x_0)(x_n-x_1)\ldots(x_n-x_{n-1})}$$

Now, $f'(x)$ can be obtained by differentiating f(x) w.r.t. x

Thus, $f'(x) = \ell_0'(x) f(x_0) + \ell_1'(x) f(x_1) + \ldots + \ell_n'(x) f(x_n)$.

4.1. Numerical Differentiation using Linear Interpolation:

We know that for a linear interpolation

$$\ell_0(x) = \frac{(x-x_1)}{(x_0-x_1)} \quad and \quad \ell_1(x) = \frac{(x-x_0)}{(x_1-x_0)}$$

$$\Rightarrow \quad f(x) = \ell_0(x) f(x_0) + \ell_1(x) f(x_1)$$

$$\Rightarrow \quad f(x) = \frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1)$$

$$\Rightarrow \quad f'(x) = \frac{1}{(x_0 - x_1)} f(x_0) + \frac{1}{(x_1 - x_0)} f(x_1)$$

$$\Rightarrow \quad f'(x) = \frac{f(x_1) - f(x_0)}{(x_1 - x_0)}.$$

which is constant for all $x \in [x_0, x_1]$.

We also have errors in approximation of the derivatives as

$$E_1'(x_0) = \frac{x_0 - x_1}{2} f''(\xi), \quad x_0 < \xi < x_1$$

and $$E_1'(x_1) = \frac{x_1 - x_0}{2} f''(\xi), \quad x_0 < \xi < x_1$$

4.2. Numerical Differentiation using Quadratic Interpolation:

We know that for a quadratic interpolation

$$\ell_0(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} \quad and \quad \ell_0'(x) = \frac{(x - x_1) + (x - x_2)}{(x_0 - x_1)(x_0 - x_2)} = \frac{(2x - x_1 - x_2)}{(x_0 - x_1)(x_0 - x_2)},$$

$$\ell_1(x) = \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} \quad and \quad \ell_1'(x) = \frac{(x - x_0) + (x - x_2)}{(x_1 - x_0)(x_1 - x_2)} = \frac{(2x - x_0 - x_2)}{(x_1 - x_0)(x_1 - x_2)},$$

$$\ell_2(x) = \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} \quad and \quad \ell_2'(x) = \frac{(x - x_0) + (x - x_1)}{(x_2 - x_0)(x_2 - x_1)} = \frac{(2x - x_0 - x_1)}{(x_2 - x_0)(x_2 - x_1)}$$

$$\Rightarrow \quad f(x) = \ell_0(x) f(x_0) + \ell_1(x) f(x_1) + \ell_2(x) f(x_2)$$

$$\Rightarrow \quad f(x) = \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2)$$

$$\Rightarrow \quad f'(x) = \frac{(2x - x_1 - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(2x - x_0 - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{(2x - x_0 - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2).$$

and $$f''(x) = \frac{2}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{2}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{2}{(x_2 - x_0)(x_2 - x_1)} f(x_2)$$

$$\Rightarrow \quad f''(x) = 2\left[\frac{f(x_0)}{(x_0 - x_1)(x_0 - x_2)} + \frac{f(x_1)}{(x_1 - x_0)(x_1 - x_2)} + \frac{f(x_2)}{(x_2 - x_0)(x_2 - x_1)}\right]$$

We also have errors in approximation of the derivatives as

$$E_2'(x_0) = \frac{1}{6}\left(x_0 - x_1\right)\left(x_0 - x_2\right) f'''(\xi), \quad x_0 < \xi < x_2$$

The error in second derivative at the tabular point x_0 is written as

$$E_2''(x_0) = \frac{1}{3}\left(2x_0 - x_1 - x_2\right) f'''(\xi) + \frac{1}{24}\left(x_0 - x_1\right)\left(x_0 - x_2\right)\left[f^{iv}(\eta_1) + f^{iv}(\eta_2)\right]$$

where $x, \eta_1, \eta_2 \in (x_0, x_1)$.

Example 1: Using the following data

x	6.0	6.1	6.2
f(x)	0.1750	-0.1998	-0.2223

Find f'(6.0) using linear interpolation also find f'(6.0) and f''(6.0) using quadratic interpolation.

Solution: (i) Using linear interpolation, we have

$$f'(x) = \frac{f(x_1) - f(x_0)}{(x_1 - x_0)}$$

$$\Rightarrow \quad f'(x) = \frac{-0.1998 - 0.1750}{(6.1 - 6.0)} = -3.748.$$

(ii) Using quadratic interpolation, we have

$$f'(x) = \frac{(2x - x_1 - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(2x - x_0 - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) + \frac{(2x - x_0 - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2)$$

and $$f''(x) = 2\left[\frac{f(x_0)}{(x_0 - x_1)(x_0 - x_2)} + \frac{f(x_1)}{(x_1 - x_0)(x_1 - x_2)} + \frac{f(x_2)}{(x_2 - x_0)(x_2 - x_1)}\right]$$

$$\Rightarrow \quad f'(6.0) = \frac{12 - 6.1 - 6.2}{(6.0 - 6.1)(6.0 - 6.2)}(0.175) + \frac{12 - 6.0 - 6.2}{(6.1 - 6.0)(6.1 - 6.2)}(-0.1998) + \frac{12 - 6.0 - 6.1}{(6.2 - 6.0)(6.2 - 6.1)}(-0.2223)$$

$$\Rightarrow \quad f'(6.0) = -5.5115$$

and $$f''(x) = 2\left[\frac{0.175}{(6.0 - 6.1)(6.0 - 6.2)} + \frac{-0.1998}{(6.1 - 6.0)(6.1 - 6.2)} + \frac{-0.2223}{(6.2 - 6.0)(6.2 - 6.1)}\right]$$

$\Rightarrow \quad f''(6.0) = 17.615$.

Example 2: Using the following data for the function $f(x) = \ln x$

x	2.0	2.2	2.6
f(x)	0.69315	0.78846	0.95551

Find f'(2.0) using linear interpolation also find f'(2.0) and f"(2.0) using quadratic interpolation. Compare with the exact solution and also obtain an upper bound on the error.

Solution: (i) Using linear interpolation, we have

$$f'(x) = \frac{f(x_1) - f(x_0)}{(x_1 - x_0)}$$

$$\Rightarrow \quad f'(x) = \frac{0.78846 - 0.69315}{(2.2 - 2.0)} = 0.47655.$$

Exact value of $f'(x)$ is

$$f'(x) = \frac{1}{x}$$

$$\Rightarrow \quad f'(2.0) = \frac{1}{2.0} = 0.5$$

The error associated with linear interpolation is

$$E_1^{'}(x_0) = \frac{x_0 - x_1}{2} f''(\xi), \quad x_0 < \xi < x_1$$

For $f(x) = \ln x$, we have

$$M_1 = \max_{x_0 < \xi < x_1} |f'(x)| = \max_{2.0 < \xi < 2.2} \left|\frac{1}{x}\right| = 0.5$$

and $$M_2 = \max_{x_0 < \xi < x_1} |f''(x)| = \max_{2.0 < \xi < 2.2} \left|-\frac{1}{x^2}\right| = 0.25$$

Thus upper bound on the error is

$$E_1^{'}(x_0) \le \left|\frac{2.0 - 2.2}{2}\right| (0.25) = 0.025$$

(ii) Using quadratic interpolation, we have

$$f'(x)=\frac{(2x-x_1-x_2)}{(x_0-x_1)(x_0-x_2)}f(x_0)+\frac{(2x-x_0-x_2)}{(x_1-x_0)(x_1-x_2)}f(x_1)+\frac{(2x-x_0-x_1)}{(x_2-x_0)(x_2-x_1)}f(x_2)$$

and $$f''(x)=2\left[\frac{f(x_0)}{(x_0-x_1)(x_0-x_2)}+\frac{f(x_1)}{(x_1-x_0)(x_1-x_2)}+\frac{f(x_2)}{(x_2-x_0)(x_2-x_1)}\right]$$

$$\Rightarrow \quad f'(2.0)=\frac{4-2.2-2.6}{(2.0-2.2)(2.0-2.6)}(0.69315)+\frac{4-2.0-2.6}{(2.2-2.0)(2.2-2.6)}(0.78846)+\frac{4-2.0-2.2}{(2.6-2.0)(2.6-2.2)}(0.95551)$$

$$\Rightarrow \quad f'(2.0)=0.49619$$

and $$f''(x)=2\left[\frac{0.69315}{(2.0-2.2)(2.0-2.6)}+\frac{0.78846}{(2.2-2.0)(2.2-2.6)}+\frac{0.95551}{(2.6-2.0)(2.6-2.2)}\right]$$

$$\Rightarrow \quad f''(2.0)=-0.19642\,.$$

Exact value of $f'(x)$ is

$$f'(x)=\frac{1}{x}$$

$$\Rightarrow \quad f'(2.0)=\frac{1}{2.0}=0.5$$

Exact value of $f''(x)$ is

$$f''(x)=-\frac{1}{x^2}$$

$$\Rightarrow \quad f''(2.0)=-\frac{1}{4.0}=-0.25$$

The error associated with linear interpolation is

$$E_2'(x_0)=\frac{1}{6}\left(x_0-x_1\right)\left(x_0-x_2\right)f'''(\xi),\quad x_0<\xi<x_2$$

The error in second derivative at the tabular point x_0 is written as

$$E_2''(x_0)=\frac{1}{3}\left(2x_0-x_1-x_2\right)f'''(\xi)+\frac{1}{24}\left(x_0-x_1\right)\left(x_0-x_2\right)\left[f^{iv}(\eta_1)+f^{iv}(\eta_2)\right]$$

For $f(x)=\ln x$, we have

$$M_1 = \max_{x_0<\xi<x_1} |f'(x)| = \max_{2.0<\xi<2.2} \left|\frac{1}{x}\right| = 0.5$$

$$M_2 = \max_{x_0<\xi<x_1} |f''(x)| = \max_{2.0<\xi<2.2} \left|-\frac{1}{x^2}\right| = 0.25$$

$$M_3 = \max_{x_0<\xi<x_1} |f'''(x)| = \max_{2.0<\xi<2.2} \left|\frac{2}{x^3}\right| = 0.25$$

and $$M_4 = \max_{x_0<\xi<x_1} |f^{iv}(x)| = \max_{2.0<\xi<2.2} \left|-\frac{6}{x^4}\right| = 0.375$$

Thus upper bound on the error is

$$E_2^{'}(x_0) \le \frac{1}{6}|(2.0-2.2)(2.0-2.6)|(0.25) = 0.005$$

and $$E_2^{'}(x_0) \le \frac{1}{3}|(4-2.2-2.6)|(0.25) + \frac{1}{24}|(2-2.2)(2-2.6)|(0.75) = 0.0704\,.$$

5. Numerical Differentiation Methods Based on Finite Difference Operators:

5.1. For Equally Spaced Values of the Arguments:

If the arguments are equally spaced then we use the following interpolation formulas to find the derivatives of a function at a point.

5.1.1. Numerical Differentiation using Newton's Forward Difference Interpolation Formula:

We know that the Newton's forward difference interpolation formula is

$$f(x) = f_0 + u\Delta f_0 + \frac{u(u-1)}{2!}\Delta^2 f_0 + \frac{u(u-1)(u-2)}{3!}\Delta^3 f_0 + \ldots \quad (1)$$

where $u = \dfrac{x-x_0}{h}$ (2)

If we take the approximation of f(x) of order (n) or $O(h^n)$, then

$$f(x) = f_0 + u\Delta f_0 + \frac{u(u-1)}{2!}\Delta^2 f_0 + \frac{u(u-1)(u-2)}{3!}\Delta^3 f_0 + \ldots + \frac{u(u-1)(u-2)\ldots(u-(n-1))}{n!}\Delta^n f_0 \quad (3)$$

and error in this approximation is

$$E(x)=\frac{u(u-1)(u-2)\ldots(u-n)}{(n+1)!}h^{n+1}f^{(n+1)}(\xi) \qquad (4)$$

On differentiating equation (1) w.r.t. u, we have

$$\frac{df(x)}{du}=\Delta f_0+\frac{2u-1}{2}\Delta^2 f_0+\frac{(3u^2-6u+2)}{6}\Delta^3 f_0+\ldots$$

On differentiating equation (2) w.r.t. x, we have

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

$$\Rightarrow \quad \frac{df(x)}{dx}=\frac{df(x)}{du}\frac{du}{dx}=\frac{1}{h}\left[\Delta f_0+\frac{2u-1}{2}\Delta^2 f_0+\frac{(3u^2-6u+2)}{6}\Delta^3 f_0+\ldots\right]$$

$$\Rightarrow \quad f'(x)=\frac{df(x)}{dx}=\frac{1}{h}\left[\Delta f_0+\frac{2u-1}{2}\Delta^2 f_0+\frac{(3u^2-6u+2)}{6}\Delta^3 f_0+\ldots\right] \qquad (5)$$

and the error in the approximation of the first derivative of order $O(h^n)$ is

$$\left|E'(x_0)\right|=\left|E'(u=0)\right|\le\frac{h^n}{(n+1)}M_{(n+1)}$$

where $\quad M_{(n+1)}=\max_{x_0\le x\le x_2}\left|f^{(n+1)}(x)\right|.$

On again differentiating equation (3) w.r.t. x we have

$$f''(x)=\frac{d}{dx}\left(\frac{df(x)}{dx}\right)=\frac{d}{dx}\left(\frac{df(x)}{dx}\right)\frac{du}{dx}$$

$$\Rightarrow \quad f''(x)=\frac{1}{h^2}\left[\Delta^2 f_0+(u-1)\Delta^3 f_0+\left(\frac{6u^2-18u+11}{12}\right)\Delta^4 f_0+\ \ldots\right]$$

5.1.2. Numerical Differentiation using Newton's Backward Difference Interpolation Formula:

We know that the Newton's backward difference interpolation formula is

$$f(x)=f_n+u\nabla f_n+\frac{u(u+1)}{2!}\nabla^2 f_n+\frac{u(u+1)(u+2)}{3!}\nabla^3 f_n+\ldots \qquad (1)$$

where $u=\dfrac{x-x_n}{h}$ (2)

If we take the approximation of f(x) of order (n) or $O(h^n)$, then

$$f(x) = f(x) = f_n + u\nabla f_n + \frac{u(u+1)}{2!}\nabla^2 f_n + \frac{u(u+1)(u+2)}{3!}\nabla^3 f_n + \ldots + \frac{u(u+1)(u+2)\ \ldots\ (u+(n-1))}{n!}\nabla^n f_0 \qquad (3)$$

and error in this approximation is

$$E(x) = \frac{u(u+1)(u+2)\ldots(u+n)}{(n+1)!}h^{n+1} f^{(n+1)}(\xi) \qquad (4)$$

On differentiating equation (1) w.r.t. u, we have

$$\frac{df(x)}{du} = \nabla f_n + \frac{2u+1}{2}\nabla^2 f_n + \frac{(3u^2+6u+2)}{6}\nabla^3 f_n + \ldots$$

On differentiating equation (2) w.r.t. x, we have

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

$$\Rightarrow \quad \frac{df(x)}{dx} = \frac{df(x)}{du}\frac{du}{dx} = \frac{1}{h}\left[\nabla f_n + \frac{2u+1}{2}\nabla^2 f_n + \frac{(3u^2+6u+2)}{6}\nabla^3 f_n + \ldots\right]$$

$$\Rightarrow \quad f'(x) = \frac{df(x)}{dx} = \frac{1}{h}\left[\nabla f_n + \frac{2u+1}{2}\nabla^2 f_n + \frac{(3u^2+6u+2)}{6}\nabla^3 f_n + \ldots\right] \qquad (5)$$

and the error in the approximation of the first derivative of order $O(h^n)$ is

$$|E'(x_0)| = |E'(u=0)| \le \frac{h^n}{(n+1)} M_{(n+1)}$$

where $\quad M_{(n+1)} = \max_{x_0 \le x \le x_2} \left| f^{(n+1)}(x) \right|.$

On again differentiating equation (3) w.r.t. x we have

$$f''(x) = \frac{d}{dx}\left(\frac{df(x)}{dx}\right) = \frac{d}{dx}\left(\frac{df(x)}{dx}\right)\frac{du}{dx}$$

$$\Rightarrow \quad f''(x) = \frac{1}{h^2}\left[\nabla^2 f_n + (u+1)\nabla^3 f_n + \left(\frac{6u^2+18u+11}{12}\right)\nabla^4 f_n + \ldots\right]$$

5.1.3. Numerical Differentiation using Stirling's Central Difference Interpolation Formula:

We know that the Stirling's Central difference interpolation formula is

$$f(x) = f_0 + u\left(\frac{\Delta f_0 + \Delta f_{-1}}{2}\right) + \frac{u^2}{2!}\Delta^2 f_{-1} + \frac{u(u^2-1^2)}{3!}\left(\frac{\Delta^3 f_{-1} + \Delta^3 f_{-2}}{2}\right) + \frac{u^2(u^2-1^2)}{4!}\Delta^4 f_{-2} + \frac{u(u^2-1^2)(u^2-2^2)}{5!}\left(\frac{\Delta^5 f_{-2} + \Delta^5 f_{-3}}{2}\right) + \ldots \quad (1)$$

where $u = \frac{x - x_0}{h}$ (2)

On differentiating equation (1) w.r.t. u, we have

$$\frac{df(x)}{du} = \left(\frac{\Delta f_0 + \Delta f_{-1}}{2}\right) + u\Delta^2 f_{-1} + \frac{(3u^2-1)}{6}\left(\frac{\Delta^3 f_{-1} + \Delta^3 f_{-2}}{2}\right) + \frac{(4u^3-2u)}{4!}\Delta^4 f_{-2} + \frac{(5u^4-15u^2+4)}{5!}\left(\frac{\Delta^5 f_{-2} + \Delta^5 f_{-3}}{2}\right) + \ldots$$

On differentiating equation (2) w.r.t. x, we have

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

$$\Rightarrow \frac{df(x)}{dx} = \frac{df(x)}{du}\frac{du}{dx} = \frac{1}{h}\left[\left(\frac{\Delta f_0 + \Delta f_{-1}}{2}\right) + u\Delta^2 f_{-1} + \frac{(3u^2-1)}{6}\left(\frac{\Delta^3 f_{-1} + \Delta^3 f_{-2}}{2}\right) + \frac{(4u^3-2u)}{4!}\Delta^4 f_{-2} + \frac{(5u^4-15u^2+4)}{5!}\left(\frac{\Delta^5 f_{-2} + \Delta^5 f_{-3}}{2}\right) + \ldots\right]$$

$$\Rightarrow f'(x) = \frac{df(x)}{dx} = \frac{1}{h}\left[\left(\frac{\Delta f_0 + \Delta f_{-1}}{2}\right) + u\Delta^2 f_{-1} + \frac{(3u^2-1)}{6}\left(\frac{\Delta^3 f_{-1} + \Delta^3 f_{-2}}{2}\right) + \frac{(4u^3-2u)}{4!}\Delta^4 f_{-2} + \frac{(5u^4-15u^2+4)}{5!}\left(\frac{\Delta^5 f_{-2} + \Delta^5 f_{-3}}{2}\right) + \ldots\right] \quad (3)$$

On again differentiating equation (3) w.r.t. x we have

$$f''(x) = \frac{d}{dx}\left(\frac{df(x)}{dx}\right) = \frac{d}{dx}\left(\frac{df(x)}{dx}\right)\frac{du}{dx}$$

$$\Rightarrow$$

$$f''(x) = \frac{1}{h^2}\left[\Delta^2 f_{-1} + u\left(\frac{\Delta^3 f_{-1} + \Delta^3 f_{-2}}{2}\right) + \frac{(6u^2-1)}{12}\Delta^4 f_{-2} + \frac{(2u^3-3u)}{12}\left(\frac{\Delta^5 f_{-2} + \Delta^5 f_{-3}}{2}\right) + \ldots\right]$$

5.1.4. Numerical Differentiation using Bessel's Central Difference Interpolation Formula:

We know that the Bessel's Central difference interpolation formula is

$$f(x)=\left(\frac{f_0+f_1}{2}\right)+\left(u-\frac{1}{2}\right)\Delta f_0+\frac{u(u-1)}{2!}\left(\frac{\Delta^2 f_{-1}+\Delta^2 f_0}{2}\right)+\frac{u(u-1)\left(u-\frac{1}{2}\right)}{3!}\Delta^3 f_{-1}$$

$$+\frac{(u+1)u(u-1)(u-2)}{4!}\left(\frac{\Delta^4 f_{-2}+\Delta^4 f_{-1}}{2}\right)+\frac{(u+1)u(u-1)(u-2)\left(u-\frac{1}{2}\right)}{5!}\Delta^5 f_{-2} \quad (1)$$

$$+\frac{(u+2)(u+1)u(u-1)(u-2)(u-3)}{6!}\left(\frac{\Delta^6 f_{-3}+\Delta^6 f_{-2}}{2}\right)+\ldots$$

where $u=\dfrac{x-x_0}{h}$ (2)

On differentiating equation (1) w.r.t. u, we have

$$\frac{df(x)}{du}=\Delta f_0+\frac{(2u-1)}{2!}\left(\frac{\Delta^2 f_{-1}+\Delta^2 f_0}{2}\right)+\frac{\left(3u^2-3u+\frac{1}{2}\right)}{3!}\Delta^3 f_{-1}$$

$$+\frac{(4u^3-6u^2-2u+2)}{4!}\left(\frac{\Delta^4 f_{-2}+\Delta^4 f_{-1}}{2}\right)+\frac{(5u^4-10u^3+5u-1)}{5!}\Delta^5 f_{-2}$$

$$+\frac{(6u^5-15u^4-20u^3+45u^2+8u-12)}{6!}\left(\frac{\Delta^6 f_{-3}+\Delta^6 f_{-2}}{2}\right)+\ldots$$

On differentiating equation (2) w.r.t. x, we have

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

$$\frac{df(x)}{dx}=\frac{df(x)}{du}\frac{du}{dx}=\frac{1}{h}\left[\Delta f_0+\frac{(2u-1)}{2!}\left(\frac{\Delta^2 f_{-1}+\Delta^2 f_0}{2}\right)+\frac{1}{3!}\left(3u^2-3u+\frac{1}{2}\right)\Delta^3 f_{-1}\right.$$

$$\Rightarrow \qquad +\frac{(4u^3-6u^2-2u+2)}{4!}\left(\frac{\Delta^4 f_{-2}+\Delta^4 f_{-1}}{2}\right)+\frac{(5u^4-10u^3+5u-1)}{5!}\Delta^5 f_{-2}$$

$$\left.+\frac{(6u^5-15u^4-20u^3+45u^2+8u-12)}{6!}\left(\frac{\Delta^6 f_{-3}+\Delta^6 f_{-2}}{2}\right)+\ldots\right]$$

$$\Rightarrow \quad f'(x) = \frac{df(x)}{dx} = \frac{1}{h}\left[\Delta f_0 + \frac{(2u-1)}{2!}\left(\frac{\Delta^2 f_{-1} + \Delta^2 f_0}{2}\right) + \frac{1}{3!}\left(3u^2 - 3u + \frac{1}{2}\right)\Delta^3 f_{-1} + \frac{(4u^3 - 6u^2 - 2u + 2)}{4!}\left(\frac{\Delta^4 f_{-2} + \Delta^4 f_{-1}}{2}\right) + \frac{(5u^4 - 10u^3 + 5u - 1)}{5!}\Delta^5 f_{-2} + \frac{(6u^5 - 15u^4 - 20u^3 + 45u^2 + 8u - 12)}{6!}\left(\frac{\Delta^6 f_{-3} + \Delta^6 f_{-2}}{2}\right) + \ldots\right] \quad (3)$$

On again differentiating equation (3) w.r.t. x we have

$$f''(x) = \frac{d}{dx}\left(\frac{df(x)}{dx}\right) = \frac{d}{dx}\left(\frac{df(x)}{dx}\right)\frac{du}{dx}$$

$$\Rightarrow \quad f''(x) = \frac{1}{h^2}\left[\left(\frac{\Delta^2 f_{-1} + \Delta^2 f_0}{2}\right) - \frac{(2u-1)}{2}\Delta^3 f_{-1} + \frac{(6u^2 - 6u - 1)}{12}\left(\frac{\Delta^4 f_{-2} + \Delta^4 f_{-1}}{2}\right) + \frac{(4u^3 - 6u^2 + 1)}{24}\Delta^5 f_{-2} + \frac{(15u^4 - 30u^3 - 30u^2 + 45u + 4)}{360}\left(\frac{\Delta^6 f_{-3} + \Delta^6 f_{-2}}{2}\right) + \ldots\right]$$

Value Addition: Note
The above interpolation formulas are used to find the derivative of a function at a point only if the arguments are equally spaced.

Example 3: Find $\frac{dy}{dx}$ at x = 0.1 from the following table:

x	0.1	0.2	0.3	0.4
y	0.9975	0.9900	0.9776	0.9604

Solution: The difference table is:

x	y	Δy	$\Delta^2 y$	$\Delta^3 y$
0.1	0.9975			
		-0.0075		
0.2	0.9900		-0.0049	
		-0.0124		0.0001
0.3	0.9776		-0.0048	
		-0.0172		
0.4	0.9604			

We know that Newton's forward difference interpolation formula is

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

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

On differentiating w.r.t. x we have

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

here x_0 =0.1, h = 0.1 and x=0.1, thus

$$u = \frac{x - x_0}{h} = \frac{0.1 - 0.1}{0.1} = 0$$

Thus, we have

$$\frac{dy}{dx} = \frac{1}{h}\left[\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0\right] = \frac{1}{0.1}\left[-0.0075 - \frac{1}{2}(-0.0049) + \frac{1}{3}(0.0001)\right]$$

$$\Rightarrow \quad \frac{dy}{dx} = -0.050167 .$$

Example 4: Find the first and second derivative of the function tabulated below at the point x = 1.1 from the following table:

x	1.0	1.2	1.4	1.6	1.8	2.0
f(x)	0	0.1280	0.5440	1.2960	2.4320	4.0000

Solution: The difference table is:

x	f(x)	Δf	$\Delta^2 f$	$\Delta^3 f$	$\Delta^4 f$	$\Delta^5 f$
1.0	0					
		0.1280				
1.2	0.1280		0.2880			
		0.4160		0.0480		
1.4	0.544		0.3360		0	
		0.7520		0.0480		0
1.6	1.2960		0.3840		0	
		1.1360		0.480		
1.8	2.4320		0.4320			
		1.5680				
2.0	4.0000					

We know that Newton's forward difference interpolation formula is

$$f(x) = f_0 + u\Delta f_0 + \frac{u(u-1)}{2!}\Delta^2 f_0 + \frac{u(u-1)(u-2)}{3!}\Delta^3 f_0 + \ldots \qquad (1)$$

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

on differentiating w.r.t. x we have

$$\frac{df}{dx} = \frac{1}{h}\left[\Delta f_0 + \frac{2u-1}{2}\Delta^2 f_0 + \frac{3u^2 - 6u + 2)}{6}\Delta^3 f_0 + \ldots\right]$$

and $$\frac{d^2 f}{dx^2} = \frac{1}{h^2}\left[\Delta^2 f_0 + (u-1)\Delta^3 f_0 + \left(\frac{6u^2 - 18u + 11}{12}\right)\Delta^4 f_0 + \ldots\right]$$

here x_0 =1.0, h = 0.2 and x=1.1, thus

$$u = \frac{x - x_0}{h} = \frac{1.1 - 1.0}{0.2} = 0.5$$

Thus, we have

$$\left(\frac{df}{dx}\right)_{x=1.1} = \frac{1}{0.2}\left[0.1280 + \frac{2(0.5)-1}{2}(0.2880) + \frac{3(0.5)^2 - 6(0.5) + 2}{6}(0.0480) + 0\right]$$

$$\Rightarrow \quad \left(\frac{df}{dx}\right)_{x=1.1} = 0.630\,.$$

and $$\left(\frac{d^2 f}{dx^2}\right)_{x=1.1} = \frac{1}{(0.2)^2}\left[0.2880 + (0.5-1)(0.0480) + 0\right] = 6.60\,.$$

Example 5: Find the first derivative of the function tabulated below at the point x = 5:

x	0	1	2	3	4	5	6
f(x)	0	2.5	8.5	15.5	24.5	36.5	50

Solution: We know that the Newton's backward difference interpolation formula is

$$f(x) = f_n + u\nabla f_n + \frac{u(u+1)}{2!}\nabla^2 f_n + \frac{u(u+1)(u+2)}{3!}\nabla^3 f_n + \frac{u(u+1)(u+2)(u+3)}{4!}\nabla^4 f_n +$$

$$\frac{u(u+1)(u+2)(u+3)(u+4)}{5!}\nabla^5 f_n + \frac{u(u+1)(u+2)(u+3)(u+4)(u+5)}{6!}\nabla^6 f_n + . . .$$

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

The backward difference table is:

x	f(x)	∇f	$\nabla^2 f$	$\nabla^3 f$	$\nabla^4 f$	$\nabla^5 f$	$\nabla^6 f$
0	0						
		2.5					
1	2.5		3.5				
		6		-2.5			
2	8.5		1		3.5		
		7		1		-3.5	
3	15.5		2		0		1
		9		1		-2.5	
4	24.5		3		-2.5		
		12		-1.5			
5	36.5		1.5				
		13.5					
6	50						

on differentiating w.r.t. x we have

$$f'(x) = \frac{1}{h}\Bigg[\nabla f_n + \frac{2u+1}{2}\nabla^2 f_n + \frac{3u^2+6u+2}{6}\nabla^3 f_n + \frac{4u^3+18u^2+22u+6}{24}\nabla^4 f_n$$

$$+\frac{5u^4+40u^3+105u^2+100u+24}{120}\nabla^5 f_n$$

$$+\frac{6u^5+75u^4+340u^3+675u^2+548u+120}{720}\nabla^6 f_n + . . .\Bigg]$$

here x_n =6, h = 1 and x=5, thus

$$u = \frac{x - x_n}{h} = \frac{5-6}{1} = -1$$

Thus, we have

$$\left(f'(x)\right)_{x=5} = \frac{1}{1}\Bigg[13.5 + \frac{2(-1)+1}{2}(1.5) + \frac{3(-1)^2+6(-1)+2}{6}(-1.5) +$$

$$\frac{4(-1)^3+18(-1)^2+22(-1)+6}{24}(-2.5) +$$

$$\frac{5(-1)^4+40(-1)^3+105(-1)^2+100(-1)+24}{120}(-2.5)+$$
$$\left.\frac{6(-1)^5+75(-1)^4+340(-1)^3+675(-1)^2+548(-1)+120}{720}(1)\right]$$

$\Rightarrow \quad \left(f'(x)\right)_{x=5}=13.0917$.

Example 6: From the following table of values of x and f(x), find the first and second derivatives of the function at the point x = 2.2:

x	1.0	1.2	1.4	1.6	1.8	2.0	2.2
f(x)	2.7183	3.3201	4.0552	4.9530	6.0496	7.3891	9.0250

Solution: The backward difference table is:

x	f(x)	∇f	$\nabla^2 f$	$\nabla^3 f$	$\nabla^4 f$	$\nabla^5 f$	$\nabla^6 f$
1.0	2.7183						
		0.6018					
1.2	3.3201		0.1333				
		0.7351		0.0294			
1.4	4.0552		0.1627		0.0067		
		0.8978		0.0361		0.0013	
1.6	4.9530		0.1988		0.0080		0.0001
		1.0966		0.0441		0.0014	
1.8	6.0496		0.2429		0.0094		
		1.3395		0.0535			
2.0	7.3891		0.2964				
		1.6359					
2.2	9.0250						

We know that the Newton's backward difference interpolation formula is

$$f(x)=f_n+u\nabla f_n+\frac{u(u+1)}{2!}\nabla^2 f_n+\frac{u(u+1)(u+2)}{3!}\nabla^3 f_n+\frac{u(u+1)(u+2)(u+3)}{4!}\nabla^4 f_n+$$
$$\frac{u(u+1)(u+2)(u+3)(u+4)}{5!}\nabla^5 f_n+\frac{u(u+1)(u+2)(u+3)(u+4)(u+5)}{6!}\nabla^6 f_n+\ldots$$

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

on differentiating w.r.t. x we have

$$f'(x)=\frac{1}{h}\left[\nabla f_n+\frac{2u+1}{2}\nabla^2 f_n+\frac{3u^2+6u+2}{6}\nabla^3 f_n+\frac{4u^3+18u^2+22u+6}{24}\nabla^4 f_n\right.$$

$$+\frac{5u^4+40u^3+105u^2+100u+24}{120}\nabla^5 f_n$$
$$\left.+\frac{6u^5+75u^4+340u^3+675u^2+548u+120}{720}\nabla^6 f_n+...\right]$$

on again differentiating w.r.t. x we have

$$f''(x)=\frac{1}{h}\left[\nabla^2 f_n+(u+1)\nabla^3 f_n+\frac{12u^2+36u+22}{24}\nabla^4 f_n\right.$$
$$+\frac{20u^3+120u^2+210u+100}{120}\nabla^5 f_n$$
$$\left.+\frac{30u^4+300u^3+1020u^2+1350u+548}{720}\nabla^6 f_n+...\right]$$

here x_n =2.2, h = 0.2 and x=2.2, thus

$$u=\frac{x-x_n}{h}=\frac{2.2-2.2}{0.2}=0$$

Thus, we have

$$\left(f'(x)\right)_{x=2.2}=\frac{1}{0.2}\left[1.6359+\frac{1}{2}(0.2964)+\frac{1}{3}(0.0535)+\frac{1}{4}(0.0094)+\frac{1}{5}(0.0014)\right.$$
$$\left.+\frac{1}{6}(0.0001)\right]$$

$$\Rightarrow \quad \left(f'(x)\right)_{x=2.2}=9.0228.$$

and $\left(f''(x)\right)_{x=2.2}=\frac{1}{0.2}\left[0.2964+0.0535+\frac{22}{24}(0.0094)+\frac{100}{120}(0.0014)+\frac{548}{720}(0.0001)\right]$

$$\Rightarrow \quad \left(f''(x)\right)_{x=2.2}=8.992.$$

Example 7: From the following table of values of x and f(x), find the first derivatives of the function at the point x = 7.5 using Bessel's formula:

x	7.47	7.48	7.49	7.50	7.51	7.52	7.53
f(x)	0.193	0.195	0.198	0.201	0.203	0.206	0.208

Solution: We know that the derivative of f(x) using Bessel's central difference interpolation formula is

$$f'(x)=\frac{df(x)}{dx}=\frac{1}{h}\Bigg[\Delta f_0+\frac{(2u-1)}{2!}\left(\frac{\Delta^2 f_{-1}+\Delta^2 f_0}{2}\right)+\frac{1}{3!}\left(3u^2-3u+\frac{1}{2}\right)\Delta^3 f_{-1}$$

$$+\frac{(4u^3-6u^2-2u+2)}{4!}\left(\frac{\Delta^4 f_{-2}+\Delta^4 f_{-1}}{2}\right)+\frac{(5u^4-10u^3+5u-1)}{5!}\Delta^5 f_{-2}$$

$$+\frac{(6u^5-15u^4-20u^3+45u^2+8u-12)}{6!}\left(\frac{\Delta^6 f_{-3}+\Delta^6 f_{-2}}{2}\right)+\ldots\Bigg]$$

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

The backward difference table is:

x	f(x)	∇f	$\nabla^2 f$	$\nabla^3 f$	$\nabla^4 f$	$\nabla^5 f$	$\nabla^6 f$
7.47	0.193						
		0.002					
7.48	0.195		0.001				
		0.003		-0.001			
7.49	0.198		0.000		0.000		
		0.003		-0.001		0.003	
7.50	0.201		-0.001		0.003		-0.01
		0.002		0.002		-0.007	
7.51	0.203		0.001		-0.004		
		0.003		-0.002			
7.52	0.206		-0.001				
		0.002					
7.53	0.208						

here $x_0 = 7.5$, h = 0.01 and x=7.5, thus

$$u=\frac{x-x_0}{h}=\frac{7.5-7.5}{0.01}=0$$

Thus, we have

$$f'(7.5)=\frac{1}{h}\Bigg[\Delta f_0-\frac{1}{2!}\left(\frac{\Delta^2 f_{-1}+\Delta^2 f_0}{2}\right)+\frac{1}{12}\Delta^3 f_{-1}+\frac{1}{12}\left(\frac{\Delta^4 f_{-2}+\Delta^4 f_{-1}}{2}\right)-\frac{1}{120}\Delta^5 f_{-2}$$

$$-\frac{1}{60}\left(\frac{\Delta^6 f_{-3}+\Delta^6 f_{-2}}{2}\right)+\ldots\Bigg]$$

$$\Rightarrow \qquad f'(7.5)=\frac{1}{0.01}\Bigg[(0.002)-\frac{1}{2}\left\{\frac{-0.001+0.001}{2}\right\}+\frac{1}{12}(0.002)+\frac{1}{12}\left\{\frac{0.003-0.004}{2}\right\}$$

$$-\frac{1}{120}(-0.007)-\frac{1}{60}\left\{\frac{-0.01}{2}\right\}\Bigg]$$

$\Rightarrow \qquad f\,'(7.5) = 0.226667$.

5.2. Numerical Differentiation For Unequally Spaced Values of the Arguments:

If the arguments are unequally spaced then we use the Newton's divided difference interpolation formulas to find the derivatives of a function at a point.

5.2.1. Numerical Differentiation using Newton's Divided Difference Interpolation Formula

We know that the Newton's divided difference interpolation formula is

$$f(x) = f_0 + (x-x_0)\Diamond f_0 + (x-x_0)(x-x_1)\Diamond^2 f_0 + (x-x_0)(x-x_1)(x-x_2)\Diamond^3 f_0 + \ldots \qquad (1)$$

On differentiating equation (1) w.r.t. x we have

$$f\,'(x) = \Diamond f_0 + (2x-x_0-x_1)\Diamond^2 f_0 + \left\{3x^2 - 2x(x_0+x_1+x_2) + (x_0x_1 + x_1x_2 + x_2x_0)\right\}$$
$$\Diamond^3 f_0 + \ldots$$

and so on.

Example 8: Find the first three derivatives of the function tabulated below at the point x = 2.5 from the following table:

x	1.5	1.9	2.5	3.2	4.3	5.9
f(x)	3.375	6.059	13.625	29.368	73.907	196.579

Solution: The difference table is:

x	y	$\Diamond y$	$\Diamond^2 y$	$\Diamond^3 y$	$\Diamond^4 y$	$\Diamond^5 y$
1.5	3.375					
		6.71				
1.9	6.059		5.90			
		12.61		1		
2.5	13.625		7.60		0	
		22.49		1		0
3.2	29.368		10.00		0	
		40.49		1		
4.3	73.9.7		13.40			
		76.67				
5.9	196.579					

We know that the Newton's divided difference interpolation formula is

$$f(x) = f_0 + (x - x_0)\Delta f_0 + (x - x_0)(x - x_1)\Delta^2 f_0 + (x - x_0)(x - x_1)(x - x_2)\Delta^3 f_0 + \ldots \quad (1)$$

On differentiating equation (1) w.r.t. x we have

$$f'(x) = \Delta f_0 + (2x - x_0 - x_1)\Delta^2 f_0 + \left\{3x^2 - 2x(x_0 + x_1 + x_2) + (x_0x_1 + x_1x_2 + x_2x_0)\right\} \Delta^3 f_0 + \ldots \quad (2)$$

on differentiating equation (2) w.r.t. x we have

$$f''(x) = 2\Delta^2 f_0 + \{6x - 2(x_0 + x_1 + x_2)\}\Delta^3 f_0 + \ldots \quad (3)$$

on differentiating equation (3) w.r.t. x we have

$$f'''(x) = 6\Delta^3 f_0 + \ldots \quad (4)$$

Thus, from equation (2), we have

$$\left(f'(x)\right)_{x=2.5} = 6.71 + (2(2.5) - 1.5 - 1.9)(5.9) + \left\{3(2.5)^2 - 2(2.5)(1.5 + 1.9 + 2.5) + ((1.5)(1.9) + (1.9)(2.5) + (2.5)(1.5)\right\} 1 + 0$$

$$\Rightarrow \quad \left(f'(x)\right)_{x=2.5} = 16.750$$

From equation (3), we have

$$\left\{f''(x)\right\}_{x=2.5} = 2(5.90) + \{6(2.5) - 2(1.5 + 1.9 + 2.5)\}(1) + 0 = 15.00\,.$$

From equation (4), we have

$$f'''(x) = 6(1) + 0 = 6\,.$$

Value Addition: Note
When the arguments are unequally spaced we can also use the Lagrange's Interpolation formula to find the derivative of a function at a point.

Example 9: Using Stirling's formula, obtain the following approximation:

$$\frac{df}{dx} = \frac{2}{3}\left[f(x+1) - f(x-1)\right] - \frac{1}{12}\left[f(x+2) - f(x-2)\right]$$

up to third differences.

Solution: We know that the Stirling's formula is

$$f(x) = f_0 + x\left(\frac{\Delta f_0 + \Delta f_{-1}}{2}\right) + \frac{x^2}{2!}\Delta^2 f_{-1} + \frac{x(x^2 - 1^2)}{3!}\left(\frac{\Delta^3 f_{-1} + \Delta^3 f_{-2}}{2}\right) + \ldots \quad (1)$$

On differentiating w.r.t. x considering the approximation up to third differences, we have

$$\frac{df(x)}{dx} = \left(\frac{\Delta f_0 + \Delta f_{-1}}{2}\right) + \frac{2x}{2!}\Delta^2 f_{-1} + \frac{(3x^2 - 1)}{3!}\left(\frac{\Delta^3 f_{-1} + \Delta^3 f_{-2}}{2}\right)$$

putting x=0, we have

$$\left(\frac{df(x)}{dx}\right)_{x=0} = \left(\frac{\Delta f_0 + \Delta f_{-1}}{2}\right) - \frac{1}{3!}\left(\frac{\Delta^3 f_{-1} + \Delta^3 f_{-2}}{2}\right)$$

$$\Rightarrow \quad \left(\frac{df(x)}{dx}\right)_{x=0} = \frac{1}{2}\left(\Delta f_0 + \Delta f_{-1}\right) - \frac{1}{12}\left(\Delta^3 f_{-1} + \Delta^3 f_{-2}\right) \quad (2)$$

Now putting

$$\Delta f_0 = f_1 - f_0,\ \Delta f_{-1} = f_0 - f_{-1},\ \Delta^3 f_{-1} = f_2 - 3f_1 + 3f_0 - f_{-1}$$
$$and\ \Delta^3 f_{-2} = f_1 - 3f_0 + 3f_{-1} - f_{-2}$$

in equation (2) and simplifying, we have

$$\left(\frac{df(x)}{dx}\right)_{x=0} = \frac{1}{2}\left(f_1 - f_{-1}\right) - \frac{1}{12}\left(f_2 - 2f_1 + 2f_{-1} - f_{-2}\right)$$

$$\Rightarrow \quad \left(\frac{df(x)}{dx}\right)_{x=0} = \frac{2}{3}\left(f_1 - f_{-1}\right) - \frac{1}{12}\left(f_2 - f_{-2}\right)$$

Shifting the origin to x, we have

$$\frac{df(x)}{dx} = \frac{2}{3}\left[f(x+1) - f(x-1)\right] - \frac{1}{12}\left[f(x+2) - f(x-2)\right].$$

Example 10: Using central difference approximations derive the formulas for the first derivative of f(x) of $O(h^2)$ and the error in this approximation.

Solution: We know that the central difference formula is given by

$$f(x) = f_0 + u\left(\frac{\Delta f_0 + \Delta f_{-1}}{2}\right) + \frac{u^2}{2!}\Delta^2 f_{-1} \quad (1)$$

where $u = \dfrac{x - x_0}{h}$ and error in the approximation is

$$E = \frac{u(u^2 - 1^2)}{3!} h^3 f'''(\xi) \qquad (2)$$

On differentiating (1) we have

$$f'(x) = \frac{df}{du}\frac{du}{dx} = \frac{1}{h}\left[\left(\frac{\Delta f_0 + \Delta f_{-1}}{2}\right) + u\Delta^2 f_{-1}\right] \qquad (3)$$

and the error in the approximation of the derivative of f(x) at x_0 is

$$|E'(x)| \le \frac{h^2}{6} M_3 .$$

where $M_3 = \max_{x_0 \le x \le x_2} |f'''(x)|$.

Example 11: Derive the following forward difference approximation for the second derivative:

$$f''(x_0) \approx \frac{f(x_0) - 2f(x_0 + h) + f(x_0 + 2h)}{h^2}$$

what is the error term associated with this formula?

Solution: We know that the Newton's forward difference formula for the second order is

$$f(x) \approx f_0 + u\Delta f_0 + \frac{u(u-1)}{2!}\Delta^2 f_0 \qquad (1)$$

where $u = \frac{x - x_0}{h}$ and $f_0 = f(x_0),\ f_1 = f(x_0 + \mathrm{h})$ and $f_2 = f(x_0 + 2\mathrm{h})$ (2)

and the error is

$$E(x) = \frac{u(u-1)(u-2)}{3!} h^3 f'''(\xi) \qquad (3)$$

on differentiating (1) w.r.t. x we have

$$f'(x) = \frac{df}{du}\frac{du}{dx} \approx \left[\Delta f_0 + \frac{(2u-1)}{2!}\Delta^2 f_0\right]\frac{1}{h}$$

$$\Rightarrow \qquad f'(x) \approx \frac{1}{h}\left[\Delta f_0 + \frac{(2u-1)}{2!}\Delta^2 f_0\right]$$

again differentiating w.r.t. x we have

$$f''(x) = \frac{df'}{du}\frac{du}{dx} \approx \left[\Delta^2 f_0\right]\frac{1}{h^2}$$

$\Rightarrow$ $$f''(x) \approx \frac{1}{h^2}\left[\Delta^2 f_0\right] \qquad (3)$$

Using forward difference we know that

$$\Delta f_0 = f_1 - f_0 \quad and \quad \Delta f_1 = f_2 - f_1$$

$\Rightarrow$ $$\Delta^2 f_0 = \Delta\{\Delta f_0\} = \Delta\{f_1 - f_0\} = \Delta f_1 - \Delta f_0 = (f_2 - f_1) - (f_1 - f_0) = f_2 - 2f_1 + f_0$$

or $$\Delta^2 f_0 = f_0 - 2f_1 + f_2$$

using equation (2) we have

$$\Delta^2 f_0 = f(x_0) - 2f(x_0 + \mathrm{h}) + f(x_0 + 2\mathrm{h})$$

Thus, from equation (3) we have

$$f''(x) \approx \frac{f(x_0) - 2f(x_0 + \mathrm{h}) + f(x_0 + 2\mathrm{h})}{h^2}$$

Error term associated with the derivative is

$$\left|E'(x_0)\right| = \left|E'(u=0)\right| \le \frac{h^2}{3} M_3$$

where $M_3 = \max_{x_0 \le x \le x_2} \left| f'''(x) \right|$.

Exercise:

1. Derive the second-order central difference approximation for the first derivative, including error term:

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0 - h)}{2h} - \frac{h^2}{6} f'''(\xi) .$$

2. Use the following data to find first two derivatives at x=1.1:

x	1.0	1.1	1.2	1.3	1.4	1.5	1.6
f(x)	7.989	8.403	8.781	9.129	9.451	9.750	10.031

3. From the following value of x and f(x), find f'(x) when (a) x=1, (b) x=3, (c) x=6 and (d) find f''(x) when x=3.

x	0	1	2	3	4	5	6
f(x)	6.9897	7.4036	7.7815	8.1291	8.4510	8.7506	9.0309

4. Find f'(6) from the table:

x	0	1	3	4	5	7	9
f(x)	150	108	0	-54	-100	-144	-84

5. Find first two derivative of f(x) at x=1 from the following table:

x	-2	-1	0	1	2	3	4
f(x)	104	17	0	-1	8	69	272

6. Derive the following difference approximation for the first derivative:

$$f'(x_0) \approx \frac{f(x_0+2h) - f(x_0-h)}{3h}$$

(a) what is the error term associated with this formula?

(b) Numerically verify the order of approximation using $f(x) = \ln x \text{ and } x_0 = 2$.

7. Derive the following backward difference approximation for the second derivative:

$$f''(x_0) \approx \frac{f(x_0-2\text{h}) - 2f(x_0-h) + f(x_0)}{h^2}$$

(a) what is the error term associated with this formula?

(b) Numerically verify the order of approximation using $f(x) = \ln x \text{ and } x_0 = 2$.

8. Using $f(x) = \ln x \text{ and } x_0 = 2$ demonstrate numerically that the central difference approximation for the second derivative given by:

$$f''(x_0) \approx \frac{f(x_0-\text{h}) - 2f(x_0) + f(x_0+\text{h})}{h^2}$$

is second order accurate.

9. Use the formula

$$f'(x_0) \approx \frac{f(x_0+\mathrm{h}) - f(x_0)}{h}$$

to approximate the derivative of $f(x) = 1 + x + x^3$ *at* $x_0 = 1$, *taking* $h = 1,\ 0.1,\ 0.01$ *and* 0.001. what is the order of approximation?

10. Use the formula

$$f'(x_0) \approx \frac{f(x_0) - f(x_0-\mathrm{h})}{h}$$

to approximate the derivative of $f(x) = \sin x$ *at* $x_0 = \pi$, *taking* $h = 1,\ 0.1,\ 0.01$ *and* 0.001. what is the order of approximation?

Summary:

In this lesson we have emphasized on the followings:

- Numerical Differentiation Methods Based on Interpolation
- Linear Interpolation
- Quadratic Interpolation
- Numerical Differentiation Methods Based on Finite Difference Operators
- For Equally Spaced Values of the Arguments
- Newton's Forward Difference Interpolation Formula
- Newton's Backward Difference Interpolation Formula
- Stirling's Central Difference Interpolation Formula
- Bessel's Central Difference Interpolation Formula
- For Unequally Spaced Values of the Arguments
- Newton's Divided Difference Interpolation Formula

References:

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