PHYS 362 : Numerical Methods and computational Physics.

Unit - II

Numerical Differentiation :

Need for differentiation of function arises quite often in engineering and science. While differentiating, we may face any one of the following problems.

(i) The function values are known but the function is unknown. Such functions are called tabulated function.

(ii) The function to be differentiated is complicated and therefore, it is difficult to differentiate.

In such situation, we seek the help of numerical techniques to obtain the estimates of function derivatives. This method of obtaining the derivative of a function using a numerical technique is known as numerical differentiation.

Approximation to the derivatives can be obtained numerically using following two approaches

(i) Methods based on finite differences for equispaced data

(ii) Methods based on divided ~~f~~ differences or Lagrange interpolation for non-uniform data.

Methods based on finite differences :

(A) **Derivatives using Newton's Forward Difference Formula :**

Let us consider the data $(x_i, f(x_i))$ given at equispaced points $x_i = x_0 + ih$, $i = 0, 1, 2, \ldots, n$; where h is the step length. The Newton's forward difference formula is given by

$$f(x) = f(x_0) + (x-x_0)\frac{\Delta f_0}{\lfloor 1\, h} + (x-x_0)(x-x_1)\frac{\Delta^2 f_0}{\lfloor 2\, h^2} + \cdots$$

$$\cdots + (x-x_0)(x-x_1)\cdots(x-x_{n-1})\frac{\Delta^n f_0}{\lfloor n\, h^n} \longrightarrow (1)$$

Let us ~~set~~ set $x = x_0 + sh$

$$\therefore f(x) = f(x_0 + sh)$$

$$= f(x_0) + (\cancel{x_0} + sh - \cancel{x_0})\frac{\Delta f_0}{h} + (\cancel{x_0}+sh-\cancel{x_0})(x_0+sh-x_1) \times \frac{\Delta^2 f_0}{\lfloor 2\, h^2}$$

$$\cdots + (\cancel{x_0}+sh-x_0)\cdot(x_0+sh-x_1)\cdots(x_0+sh-x_{n-1})\frac{\Delta^n f_0}{\lfloor n\, h^n}$$

$$= f(x_0) + s\cancel{h}\frac{\Delta f_0}{\cancel{h}} + sh(\cancel{x_0}+sh-\cancel{x_0}-h)\frac{\Delta^2 f_0}{\lfloor 2\, h^2}$$

$$+ \cdots sh(\cancel{x_0}+sh-\cancel{x_0}-h)\cdots(\cancel{x_0}+sh-\cancel{x_0}-nh+h)\frac{\Delta^n f_0}{\lfloor n\, h^n}$$

$$= f(x_0) + s\Delta f_0 + \cancel{h^2}\, s(s-1)\frac{\Delta^2 f_0}{\lfloor 2\, \cancel{h^2}}$$

$$+ \cdots s\cancel{h}(s-1)(s-2)\cdots(s-n+1)\frac{\Delta^n f_0}{\lfloor n\, \cancel{h^n}}$$

$$\therefore f(x) = f(x_0) + s\Delta f_0 + \frac{1}{\lfloor 2}s(s-1)\Delta^2 f_0 + \frac{1}{\lfloor 3}s(s-1)(s-2)\Delta^3 f_0$$

$$+ \cdots + \frac{1}{\lfloor n}s(s-1)(s-2)\cdots(s-n+1)\Delta^n f_0 \rightarrow (2)$$

Here, $s = \dfrac{(x-x_0)}{h} > 0$.

The magnitudes of the successive terms on the right hand side become smaller and smaller.

Differentiating (2) wrt x, we get

$$f'(x) = \frac{df}{dx} = \frac{df}{ds}\frac{ds}{dx}$$

$x = x_0 + sh$

$\Rightarrow \frac{dx}{dx} = 0 + h\frac{ds}{dx}$

$\Rightarrow 1 = h\frac{ds}{dx}$

$\Rightarrow \frac{ds}{dx} = \frac{1}{h}$

$$= \frac{ds}{dx}\frac{df}{ds}$$

$$= \frac{1}{h}\frac{df}{ds}$$

$$= \frac{1}{h}\Big[0 + \Delta f_0 + \frac{1}{\underline{|2}}(2s-1)\Delta^2 f_0 + \frac{1}{\underline{|3}}(3s^2-6s+2)\Delta^3 f_0 + \frac{1}{24}(4s^3-18s^2+22s-6)\Delta^4 f_0$$

$$+ \frac{1}{120}(5s^4 - 40s^3 + 105s^2 - 100s + 24)\Delta^5 f_0 + \cdots\Big] \rightarrow (3)$$

At $x = x_0$ and $s = 0$, we obtain the approximation for $f'(x)$ as

$$f'(x_0) = f'(x)\Big|_{x=x_0} = \frac{1}{h}\Big[\Delta f_0 - \frac{1}{2}\Delta^2 f_0 + \frac{1}{3}\Delta^3 f_0 - \frac{1}{4}\Delta^4 f_0 + \frac{1}{5}\Delta^5 f_0 + \cdots\Big] \rightarrow (4)$$

Differentiating (3) wrt x,

$$\frac{d^2f}{dx^2} = \frac{1}{h}\frac{d}{dx}\left(\frac{df}{ds}\right)$$

$$= \frac{1}{h}\frac{d}{ds}\left(\frac{df}{ds}\right)\frac{ds}{dx}$$

$$= \frac{1}{h}\frac{d^2f}{ds^2}\frac{1}{h}$$

$$f''(x) = \frac{d^2f}{dx^2} = \frac{1}{h^2}\frac{d^2f}{ds^2}$$

$$= \frac{1}{h^2}\Big[0 + \frac{1}{\cancel{2}}\cancel{2}\Delta^2 f_0 + \frac{1}{6}(6s-6)\Delta^3 f_0 + \cdots$$

$$\frac{1}{24}(12s^2 - 36s + 22)\Delta^4 f_0 + \frac{1}{120}(20s^3 - 120s^2 + 210s - 100)\Delta^5 f_0 + \cdots\Big] \rightarrow (5)$$

$\frac{1}{120}\times[5\times16 - 40\times8 + 105\times4 - 200 + 24]$

$= \frac{1}{120}\times[80 - 320 + 420 - 200 + 24]$

$= \frac{1}{120}[300 - 320 + 24]$ (-20)

$= \frac{4}{120} = \frac{1}{30}$

Again at $x = x_0$ and $s = 0$

$$f''(x)\Big|_{x=x_0} = f''(x_0) = \frac{1}{h^2}\left[\Delta^2 f_0 - \Delta^3 f_0 + \frac{11}{12}\Delta^4 f_0 - \frac{5}{6}\Delta^5 f_0 + \frac{137}{180} f\Delta^6 f_0 - \cdots\right] \longrightarrow (6)$$

Taking lower order approximation we have from (6)

$$f'(x) = \frac{1}{h}\Delta f_0 = \frac{1}{h}\left[f(x_1) - f(x_0)\right]$$

Generalising

$$\boxed{f'(x_k) = \frac{1}{h}\Delta f_k = \frac{1}{h}\left[f(x_{k+1}) - f(x_k)\right]} \longrightarrow (7)$$

Taking two terms of (4) we obtain

$$f'(x_0) = \frac{1}{h}\left[\Delta f_0 - \frac{1}{2}\Delta^2 f_0\right]$$

$$= \frac{1}{h}\left[\{f(x_1) - f(x_0)\} - \frac{1}{2}\{f(x_2) - 2f(x_1) + f(x_0)\}\right]$$

$$f'(x_0) = \frac{1}{2h}\left[-3f(x_0) + 4f(x_1) - f(x_2)\right] \longrightarrow (8)$$

Now generalising

$$f'(x_k) = \frac{1}{2h}\left[-3f(x_k) + 4f(x_{k+1}) - f(x_{k+2})\right] \longrightarrow (9)$$

Similarly, approximation for $f''(x_0)$ is

$$f''(x_0) = \frac{1}{h^2}\Delta^2 f_0 = \frac{1}{h^2}\left[f(x_2) - 2f(x_1) + f(x_0)\right]$$

Generalising,

$$\boxed{f''(x_k) = \frac{1}{h^2}\left[f(x_{k+2}) - 2f(x_{k+1}) + f(x_k)\right]}$$

Error of approximation : Error for $f'(x)$ at $x = x_k$ is

$$E(f, x_k) = f'(x_k) - \frac{1}{h}[f(x_k+h) - f(x_k)]$$

$$= f'(x_k) - \frac{1}{h}\left[\left\{f(x_k) + hf'(x_k) + \frac{h^2}{2}f''(x_k) + \cdots\right\} - f(x_k)\right]$$

$$= -\frac{h}{2}f''(x_k) + \cdots \longrightarrow (11) \quad [\text{for } (7)]$$

$$E(f, x_k) = f'(x_k) - \frac{1}{2h}[-3f(x_k) + 4f(x_{k+1}) - f(x_{k+2})]$$

$$= \frac{h^2}{3}f'''(x_k) + \cdots \longrightarrow (12) \quad [\text{for } (8)]$$

(11) represents error of order $O(h)$ or the formula is of first order.

(12) represents error of order $O(h^2)$ or the formula is of second order.

Error for (9) can be written as

$$E(f, x_k) = f''(x_k) - \frac{1}{h^2}[f(x_k+2h) - 2f(x_k+h) + f(x_k)]$$

$$E(f, x_k) = -hf'''(x_k) + \cdots \longrightarrow (13)$$

This error is again of first order. $(O(h))$.

$$E(f, x_k) = f'(x_k) - \frac{1}{2h}\left[-3f(x_k) + 4\left\{f(x_k) + hf'(x_k) + \frac{h^2}{2}f''(x_k) + \frac{h^3}{6}f'''(x_k) + \cdots\right\} - \left\{f(x_k) + (2h)f'(x_k) + \frac{(2h)^2}{2}f''(x_k) + \frac{(2h)^3}{\lfloor 3}f'''(x_k) + \cdots\right\}\right]$$

$$= \frac{h^2}{3}f'''(x_k).$$