B.Sc. (H) Chem Semester - IVth Generic Elective IVth Numerical Method :-

Chapter - 4 Wednesday 18/03/2020 Lec-1

* The Newton divided differences in terms of forward and backward become i.e.

$$f[x_0, x_1] = \frac{f(x_1) - f(x_0)}{h} = \frac{1}{h}\Delta f_0$$

$$f[x_0, x_1, x_2] = \frac{f[x_1, x_2] - f[x_0, x_1]}{x_2 - x_0}$$

$$= \frac{\frac{1}{h}\Delta f_1 - \frac{1}{h}\Delta f_0}{2h} = \frac{1}{2!\,h^2}\Delta^2 f_0$$

By Induction, we can show that

$$f[x_0, x_1, x_2 - - x_n] = \frac{1}{n!\,h^n}\Delta^n f_0 \qquad - (1)$$

~~By induction~~, ~~we can sh~~ Similarly

$$f[x_0, x_1] = \frac{f(x_1) - f(x_0)}{h} = \frac{1}{h}\nabla f_1$$

$$f[x_0, x_1, x_2] = \frac{f[x_1, x_2] - f[x_0, x_1]}{2h}$$

$$= \frac{1}{2h^2}(\nabla f_2 - \nabla f_1) = \frac{1}{2!\,h^2}\nabla^2 f_2$$

By induction $f[x_0, x_1, x_2 \text{ —— } x_n] = \dfrac{f[x_1, x_2, -x_n] - f[x_0, x_1, --x_{n-1}]}{nh}$

$$= \frac{1}{n!\,h^n}\nabla^n f_n \qquad - (2)$$

Relations between Differences & Derivatives:-

We have $\Delta f(x) = f(x+h) - f(x)$ By Taylor's Series is

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

$$= h f'(x) + \frac{h^2}{2} f''(x) + \cdots$$

$\Delta f(x) \simeq h f'(x)$ or $f'(x) \simeq \frac{\Delta f(x)}{h}$ The error is of $O(h)$ neglecting higher power of h.

Also $\Delta^2 f(x) = f(x+2h) - 2f(x+h) + f(x)$ By Taylor Series is

$$= \left[f(x) + 2h f'(x) + \frac{4h^2}{2} f''(x) + \cdots\right]$$

$$- 2\left[f(x) + h f'(x) + \frac{h^2}{2} f''(x) + \cdots\right] + f(x)$$

$$h^2 f''(x) + h^3 f'''(x) + \cdots$$

$\Delta^2 f(x) \simeq h^2 f''(x)$ or $f''(x) \simeq \frac{\Delta^2 f(x)}{h^2}$

The error is of $O(h)$, neglecting higher power of h.

Similarly we have

$$\nabla f(x) = f(x) - f(x-h) = h f'(x) - \frac{h^2}{2} f''(x) + \cdots$$

$$\nabla^2 f(x) = f(x) - 2f(x-h) + f(x-2h) = h^2 f''(x) - h^3 f'''(x) + \cdots$$

Hence $\nabla f(x) \simeq h f'(x)$ or $f'(x) \simeq \frac{\nabla f(x)}{h}$

$\nabla^2 f(x) \simeq h^2 f''(x)$ or $f''(x) \simeq \frac{\nabla^2 f(x)}{h^2}$

We also have $f[x_0, x_1] = \frac{1}{h} \Delta f_0 \simeq f_0'$

$$f[x_0, x_1, x_2] = \frac{1}{2!\,h^2} \Delta^2 f_0 \simeq \frac{1}{2} f_0''$$

Interpolation with Equal Intervals

Interpolating polynomials using finite Differences :-

In terms of divide difference Newton Interpolating polynomial become :-

$$P_n(x) = f[x_0] + (x-x_0) f[x_0, x_1] + \cdots (x-x_0) \cdots (x-x_{n-1}) f[x_0, x_1, \cdots x_{n-1}]$$

We also have forward divide difference

$$f[x_0, x_1, \cdots x_n] = \frac{1}{n! h^n} \Delta^n f_0$$

Substituting the divided differences in terms of forward differences in the Newton divide difference interpolation polynomial we get

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

$$+ \frac{(x-x_0)(x-x_1) \cdots (x-x_{n-1})}{n!\, h^n} \Delta^n f_0 \qquad (3)$$

Gregory-Newton Forward Difference Interpolation :- If we put $\frac{(x-x_0)}{h} = u$, then eq^n (3) becomes

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

$$= f(x_0 + uh) = E^u f(x_0)$$

Which may be written as $f(x) = (1+\Delta)^u f(x_0)$ symbolically, expanding the right hand side in binomial series we obtain :-

$$f(x) = P(x_0 + hu) = f_0 + u\Delta f_0 + \frac{u(u-1)}{2!}\Delta^2 f_0 + \text{---}$$

$$+ \cdot \frac{u(u-1) \text{--} (u-n+1)}{n!}\Delta^n f_0 + \text{---} \quad \text{---}(4)$$

Neglecting $\Delta^{n+1} f_0$ & higher order diff.

This series is known as Gregory-Newton forward difference interpolating polynomial.

Gregory-Newton Backward Difference Interpolation :-

We have backward divide difference

$$f[x_0, x_1, \text{--} x_n] = \frac{1}{n!\,h^n}\nabla^n f_n$$

From the backward difference Table 2, it can be observed that the Newton interpolation with divide differences in terms of backward differences should be in terms of the differences at the end points x_n. Thus we may write

$$f(x) = f\left(x_n + \frac{x-x_n}{h}h\right) = f(x_n + hu) = E^u f(x_n) = (1-\nabla)^{-u} f(x_n)$$

where $\frac{(x-x_n)}{h} = u$ & we have symbolically expanded $(1-\nabla)^{-u}$ in binomial series we get (1)

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

$$+ \frac{u(u+1) \text{---} (u+n-1)}{n!}\nabla^n f(x_n) + \text{---}$$

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

$$+ \text{---} \frac{u(u+1) \text{---} (u+n-1)}{n!}\nabla^n f_n \quad \text{---}(5)$$

Neglecting $\nabla^{n+1} f(x_n)$ & higher order differences.