Numerical differentiation

Motivation

- How do you evaluate the derivative of a tabulated function.
- How do we determine the velocity and acceleration from tabulated measurements.

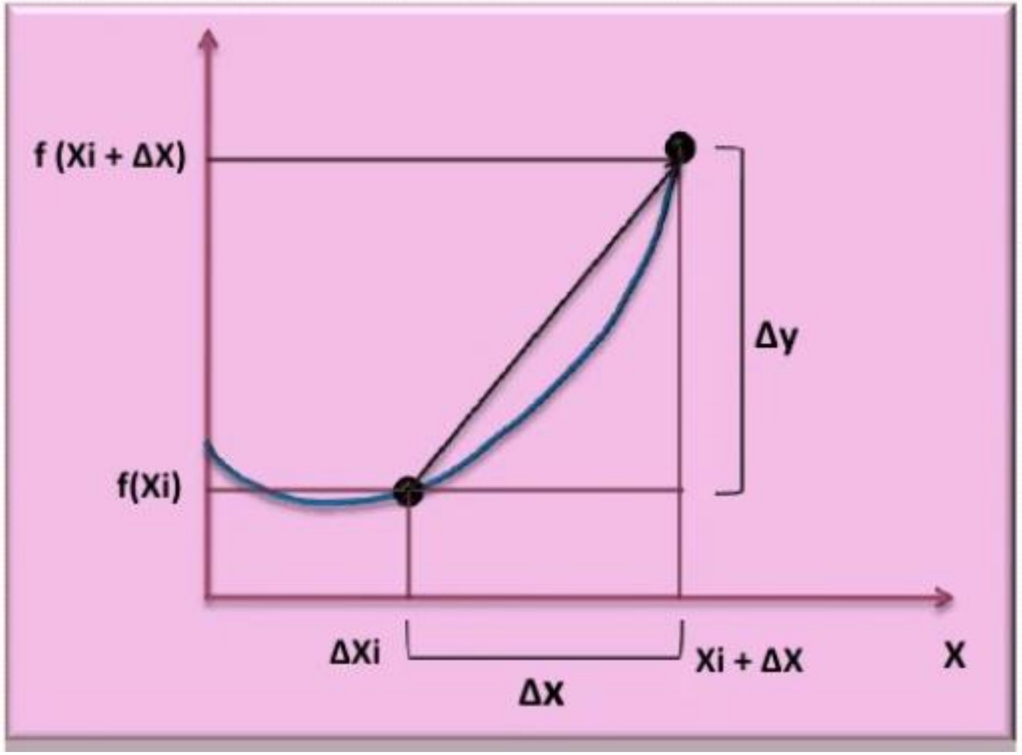
Time (second)	Displacement (meters)
0	30.1
5	48.2
10	50.0
15	40.2

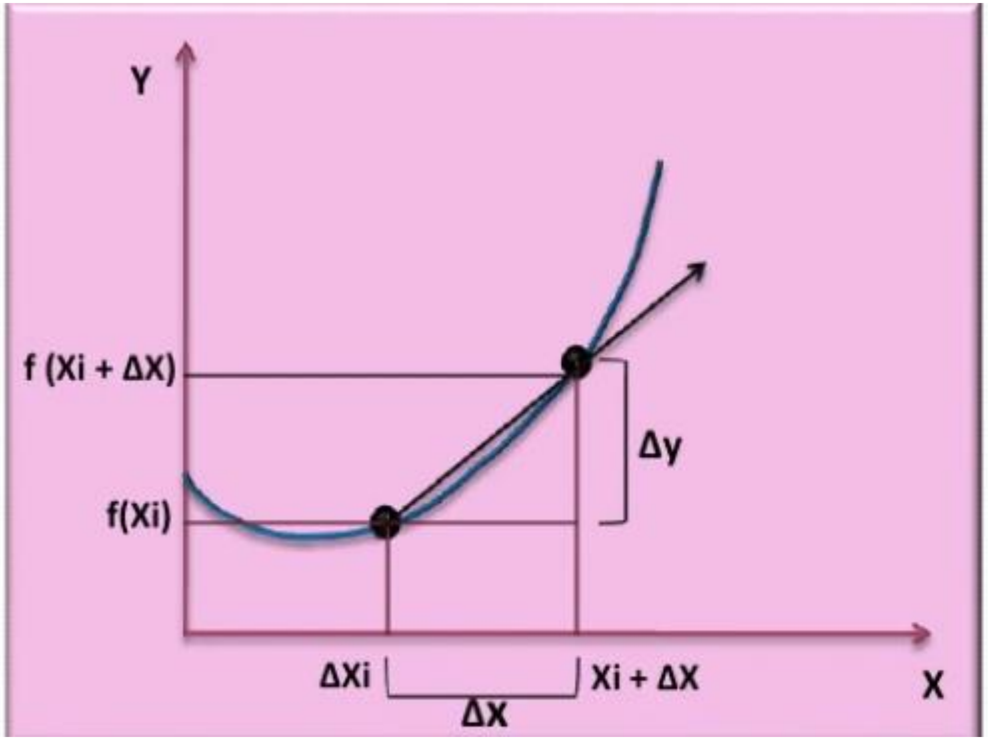
- We like to estimate the value of $f'(x)$ for a given function $f(x)$.
- The derivative represents the rate of change of a dependent variable with respect to an independent variable.
- The difference approximation is

$$\frac{\Delta y}{\Delta x} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

- If Δx is allowed to approach zero, the difference becomes a derivative:

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$


f (Xi + ΔX)
Δy
f(Xi)
ΔXi
Xi + ΔX
X
ΔX


Y
f (Xi + ΔX)
Δy
f(Xi)
ΔXi
Xi + ΔX
X
ΔX

- The Taylor series expansion of $f(x)$ about x_i is

$$f(x_{i+1}) \approx f(x_i) + f'(x_i)(x_{i+1} - x_i)$$

- From this:

$$\boxed{f'(x_i) \approx \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} = \frac{f(x_{i+1}) - f(x_i)}{h}}$$

- This formula is called the first **forward divided difference** formula and the error is of order $O(h)$.
- Or equivalently, the Taylor series expansion of $f(x)$ about x_i can be written as

$$f(x_{i-1}) \approx f(x_i) + f'(x_i)(x_{i-1} - x_i)$$

- From this:

$$\boxed{f'(x_i) \approx \frac{f(x_{i-1}) - f(x_i)}{x_{i-1} - x_i} = \frac{f(x_i) - f(x_{i-1})}{h}}$$

- This formula is called the first **backward divided difference** formula and the error is of order $O(h)$.

- A third way to approximate the first derivative is to subtract the backward from the forward Taylor series expansions:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h$$

$$-$$

$$f(x_{i-1}) = f(x_i) - f'(x_i)h$$

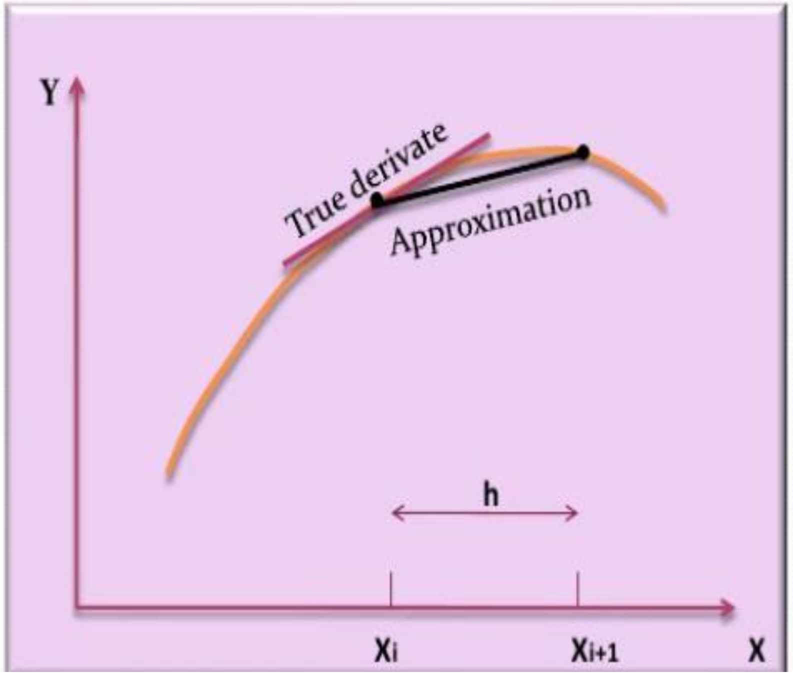
$$f(x_{i+1}) - f(x_{i-1}) = 2f'(x_i)h$$

- This yields to

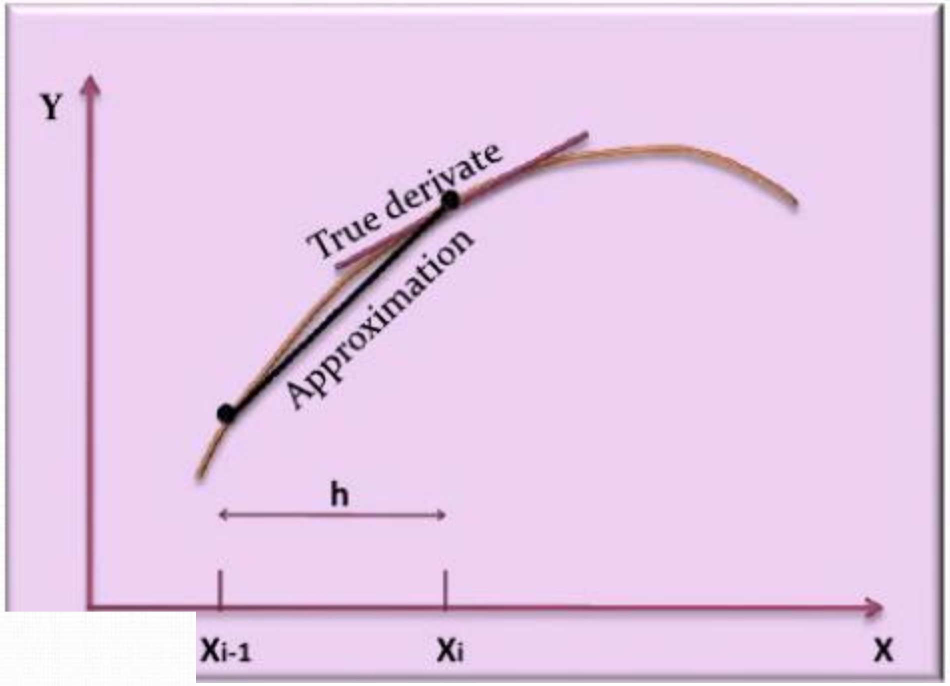
$$\boxed{f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h}}$$

- This formula is called the **centered divided difference** formula and the error is of order $O(h^2)$.

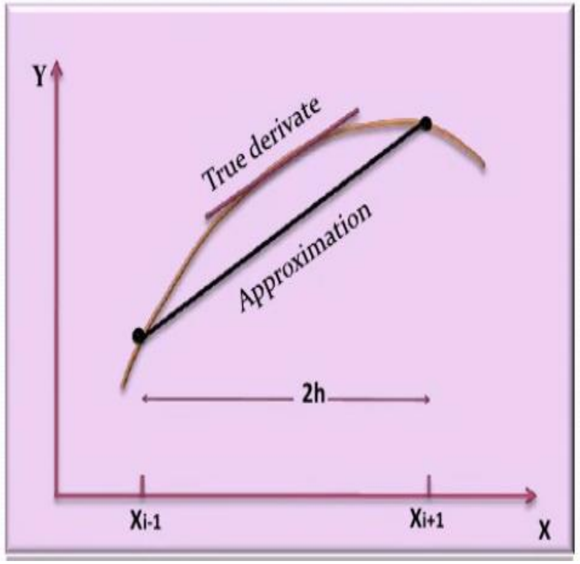
FORWARD



BACKWARD



CENTERED



FUNCTION TABULATED AT EQUAL INTERVALS

- Derivatives Using Newton's Forward Difference Formula

Newton's forward interpolation formula is

$$y = y_0 + u\Delta y_0 + \frac{u(u-1)}{2!}\Delta^2 y_0 + \frac{u(u-1)(u-2)}{3!}\Delta^3 y_0 + \ldots\ldots (8.2.1)$$

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

Differentiating both sides of Eq. (8.2.1) with respect to x, we have

$$\frac{dy}{dx} = \frac{dy}{du} \cdot \frac{du}{dx}$$

Since

$$u = \frac{x-x_0}{h} \Rightarrow \frac{du}{dx} = \frac{1}{h}$$

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

$$= \frac{1}{h}\{\Delta y_0 + \frac{\Delta^2 y_0}{2!}[(u-1)+u]$$

$$+ \frac{\Delta^3 y_0}{3!}[(u-1)(u-2) + u(u-2) + u(u-1)]$$

$$+ \frac{\Delta^4 y_0}{4!}[(u-1)(u-2)(u-3) + u(u-2)(u-3) + u(u-1)(u-3)$$

$$+ u(u-1)(u-2)] + \ldots\ldots\}$$

$$= \frac{1}{h}\Bigg[\Delta y_0 + \frac{(2u-1)}{2}\Delta^2 y_0 + \frac{(3u^2-6u+2)}{6}\Delta^3 y_0 + \frac{(4u^3-18u^2+22u-6)}{24}\Delta^4 y_0 + \frac{(5u^4-40u^3+105u^2-100u+24)}{120}\Delta^5 y_0 + \ldots\Bigg] \quad \ldots\ldots\ldots (8.2.2)$$

Differentiating Eq. (8.2.2) again with respect to x, we have

$$\frac{d^2y}{dx^2} = \frac{d}{dx}\left(\frac{dy}{dx}\right) = \frac{d}{du}\left(\frac{dy}{dx}\right)\cdot\frac{du}{dx} = \frac{1}{h}\,\frac{d}{du}\left(\frac{dy}{dx}\right)$$

$$= \frac{1}{h^2}\Bigg[\Delta^2 y_0 + (u-1)\Delta^3 y_0 + \frac{(6u^2-18u+11)}{12}\Delta^4 y_0 + \frac{(2u^3-12u^2+21u-10)}{12}\Delta^5 y_0 + \ldots\Bigg] \quad \ldots\ldots\ldots (8.2.3)$$

Differentiating Eq. (8.2.3) again with respect to x, we have

$$\frac{d^3y}{dx^3} = \frac{1}{h^3}\Bigg[\Delta^3 y_0 + \frac{(12u-18)}{12}\Delta^4 y_0 + \frac{(6u^2-24u+21)}{12}\Delta^5 y_0 + \ldots\ldots\Bigg] \quad \ldots\ldots\ldots (8.2.4)$$

The formula obtained in Eq. (8.2.2), (8.2.3) and (8.2.4) is used to calculate first, second and third derivatives respectively at any point $x = x_k$ beginning of the table of values in terms of forward differences.

The formula will be further simplified if we want to compute the derivative at the tabulated point $x = x_0$ i.e. when $u = 0$. Substitute $u = 0$ in Eqs. (8.2.2) – (8.2.4), we get

$$\left(\frac{dy}{dx}\right)_{x=x_0} = Dy_0 = \frac{1}{h}\Bigg[\Delta y_0 - \frac{1}{2}\Delta^2 y_0 + \frac{1}{3}\Delta^3 y_0 - \frac{1}{4}\Delta^4 y_0 + \frac{1}{5}\Delta^5 y_0 - \ldots\ldots\Bigg] \quad \ldots\ldots\ldots (8.2.5)$$

$$\left(\frac{d^2y}{dx^2}\right)_{x=x_0} = D^2 y_0$$

$$= \frac{1}{h^2}\left[\Delta^2 y_0 - \Delta^3 y_0 + \frac{11}{12}\ \Delta^4 y_0 - \frac{5}{6}\Delta^5 y_0 + \frac{137}{180}\Delta^6 y_0\ \ \ldots\ldots\right] \quad \ldots\ldots\ldots (8.2.6)$$

$$\left(\frac{d^3y}{dx^3}\right)_{x=x_0} = D^3 y_0$$

$$= \frac{1}{h^3}\left[\Delta^3 y_0 - \frac{3}{2}\ \Delta^4 y_0 + \frac{7}{4}\ \Delta^5 y_0 - \ \ldots\ldots\right] \quad \ldots\ldots\ldots (8.2.7)$$

$$1 + \Delta = E = e^{hD}$$

$$\therefore hD = \log(1+\Delta) = \Delta - \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 - \frac{1}{4}\Delta^4 + \ldots$$

$$\therefore\ \ D = \frac{1}{h}\left[\Delta - \frac{1}{2}\Delta^2 + \frac{1}{3}\Delta^3 - \frac{1}{4}\Delta^4 + \ldots\right]$$

From this we get,

$$D^2 = \frac{1}{h^2}\left[\Delta^2 - \Delta^3 + \frac{11}{12}\Delta^4 - \frac{5}{6}\Delta^5 + \ldots\right]$$

and

$$D^3 = \frac{1}{h^3}\left[\Delta^3 - \frac{3}{2}\Delta^4 + \ldots\right]$$

Similarly, we can derive these formulas using operators at the tabulated point $x = x_0$ which are same as Eq. (8.2.5), (8.2.6) and (8.2.7) respectively.

Example 8.1 Compute $f'(0.2)$ and $f''(0)$ from the following tabular data.

x	0.0	0.2	0.4	0.6	0.8	1.0
$f(x)$	1.00	1.16	3.56	13.96	41.96	101.00

- Derivatives Using Newton’s Backward Difference Formula

Newton’s backward interpolation formula is

$$y = y_n + u\nabla y_n + \frac{u(u+1)}{2!}\nabla^2 y_n + \frac{u(u+1)(u+2)}{3!}\Delta^3 y_n + \ldots\ldots \quad (8.2.8)$$

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

Differentiating both sides of Eq. (8.2.8) with respect to x, we have

$$\frac{dy}{dx} = \frac{dy}{du} \cdot \frac{du}{dx}$$

Since

$$u = \frac{x - x_0}{h}, \qquad \frac{du}{dx} = \frac{1}{h}$$

$$\begin{aligned}
\frac{dy}{dx} &= \frac{1}{h}\frac{dy}{du} \\
&= \frac{1}{h}\Big\{\nabla y_n + \frac{\nabla^2 y_n}{2!}[(u+1) + u] \\
&+ \frac{\nabla^3 y_n}{3!}[(u+1)(u+2) + u(u+2) + u(u+1)] \\
&+ \frac{\nabla^4 y_n}{4!}[(u+1)(u+2)(u+3) + u(u+2)(u+3) + u(u+1)(u+3) \\
&\qquad + u(u+1)(u+2)] + \ldots\ldots\Big\} \\
&= \frac{1}{h}\Big[\nabla y_n + \frac{(2u+1)}{2}\nabla^2 y_n + \frac{(3u^2+6u+2)}{6}\nabla^3 y_n \\
&\qquad + \frac{(4u^3+18u^2+22u+6)}{24}\nabla^4 y_n \\
&\qquad + \frac{(5u^4+40u^3+105u^2+100u+24)}{120}\Delta^5 y_0 + \ldots\ldots\Big]
\end{aligned}$$

$$\ldots\ldots\ (8.2.9)$$

.... (8.2.9)

Differentiating Eq. (8.2.9) again with respect to x, we have

$$\frac{d^2y}{dx^2} = \frac{d}{dx}\left(\frac{dy}{dx}\right) = \frac{d}{du}\left(\frac{dy}{dx}\right).\frac{du}{dx} = \frac{1}{h}\ \frac{d}{du}\left(\frac{dy}{dx}\right)$$

$$= \frac{1}{h^2}\Big[\nabla^2 y_n + (u+1)\nabla^3 y_n + \frac{(6u^2+18u+11)}{12}\nabla^4 y_n + \frac{(2u^3+12u^2+21u+10)}{12}\nabla^5 y_0 \ldots\Big] \quad \ldots\ldots..(8.2.10)$$

Differentiating Eq. (8.2.10) again with respect to x, we have

$$\frac{d^3y}{dx^3} = \frac{1}{h^3}\Big[\nabla^3 y_n + \frac{(12u+18)}{12}\nabla^4 y_n + \frac{(6u^2+24u+21)}{12}\Delta^5 y_0 \ldots\ldots\Big] \quad \ldots\ldots..(8.2.11)$$

The formula obtained in Eq. (8.2.9), (8.2.10) and (8.2.11) is used to calculate first, second and third derivative respectively at any point $x = x_k$ near the end points of the table in terms of backward differences.
The formula will be further simplified if we want to compute the derivative at the tabulated point $x = x_n$ i.e. when $u = 0$. Substitute $u = 0$ in Eqs. (8.2.9) – (8.2.11), we get

$$\left(\frac{dy}{dx}\right)_{x=x_n} = Dy_0 = \frac{1}{h}\Big[\nabla y_n + \frac{1}{2}\nabla^2 y_n + \frac{1}{3}\nabla^3 y_n + \frac{1}{4}\nabla^4 y_n + \frac{1}{5}\nabla^5 y_n + \ldots\ldots\Big] \quad \ldots\ldots..(8.2.12)$$

$$\left(\frac{d^2y}{dx^2}\right)_{x=x_n} = D^2 y_0$$

$$= \frac{1}{h^2}\Big[\nabla^2 y_n + \nabla^3 y_n + \frac{11}{12}\nabla^4 y_n + \frac{5}{6}\nabla^5 y_n + \frac{137}{180}\nabla^6 y_n \ldots\ldots\Big] \quad \ldots\ldots..(8.2.13)$$

$$\left(\frac{d^3y}{dx^3}\right)_{x=x_n} = D^3 y_0$$

$$= \frac{1}{h^3}\left[\nabla^3 y_n + \frac{3}{2}\ \nabla^4 y_n + \frac{7}{4}\ \nabla^5 y_n +\ \dots\dots\right] \qquad \dots\dots\dots(8.2.14)$$

Now, we know that

$$E = e^{-hD} = \frac{1}{1-\nabla}$$

$$\therefore -hD = \log(1-\nabla) = -\left[\nabla + \frac{1}{2}\nabla^2 + \frac{1}{3}\nabla^3 + \frac{1}{4}\nabla^4 + \dots\right]$$

$$\therefore\ D = \frac{1}{h}\left[\nabla + \frac{1}{2}\nabla^2 + \frac{1}{3}\nabla^3 + \frac{1}{4}\nabla^4 + \dots\right]$$

From this we get,

$$D^2 = \frac{1}{h^2}\left[\nabla^2 + \nabla^3 + \frac{11}{12}\nabla^4 + \frac{5}{6}\nabla^5 + \dots\right]$$

and

$$D^3 = \frac{1}{h^3}\left[\nabla^3 + \frac{3}{2}\nabla^4 + \dots\right]$$

Similarly, we can derive these formulas using operators at the tabulated point $x = x_0$ which are same as Eq. (8.2.12), (8.2.13) and (8.2.14) respectively.

Example 8.3 The following data give the corresponding values of pressure and specific volume V of a superheated steam.

Volume V:	2	4	6	8	10
Pressure P:	105	42.7	25.3	16.7	13.0

Find the rate of change of pressure with respect to volume when $v = 10$. Also find $\frac{d^2y}{dx^2}$ when $v = 10$.

$$y' = f'(x_0) = \frac{(x_0 - x_1) + (x_0 - x_2)}{(x_0 - x_1)(x_0 - x_2)} y_0 + \frac{(x_0 - x_0) + (x_0 - x_2)}{(x_1 - x_0)(x_1 - x_2)} y_1$$

$$+ \frac{(x_0 - x_0) + (x_0 - x_1)}{(x_2 - x_0)(x_2 - x_1)} y_2 \qquad \text{— (B)}$$

$x_1 - x_0 = h, \qquad x_2 - x_1 = h, \qquad x_2 - x_0 = 2h.$

$$y'(x_0) = f'(x_0) = \frac{-h + (-2h)}{(-h)(-2h)} y_0 + \frac{(-2h)}{h(-h)} y_1 + \frac{(-h)}{2h.h} y_2$$

$$= \frac{-3h}{2h^2} y_0 + \frac{2h}{h^2} y_1 - \frac{1}{2h} y_2$$

$$y'(x_0) = f'(x_0) = \frac{-3y_0 + 4y_1 - y_2}{2h}$$

which is first order formula.

$$y = f(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} y_0 + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} y_1$$

$$+ \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} y_2 \qquad \text{--- (A)}$$

Diffbⁿ (A) w.r.to 'x' twice, we get

$$f''(x) = \frac{2}{(x_0-x_1)(x_0-x_2)} y_0 + \frac{2}{(x_1-x_0)(x_1-x_2)} y_1$$

$$+ \frac{2}{(x_2-x_0)(x_2-x_1)} y_2 \quad \text{—} \quad C$$

$$f''(x_0) = \frac{2}{(x_0-x_1)(x_0-x_2)} y_0 + \frac{2}{(x_1-x_0)(x_1-x_2)} y_1$$

$$+ \frac{2}{(x_2-x_0)(x_2-x_1)} y_2$$

$$f''(x_0) = \frac{2}{(-h)(-2h)} y_0 + \frac{2}{h(-h)} y_1 + \frac{2}{(2h \cdot h)} y_2$$

$$\boxed{f''(x_0) = \frac{y_0 + 2y_1 + y_2}{h^2}}$$

is second order derivative formula of Lagrange interpolating polynomial based on 3 point x_0, x_1, x_2.

Now the formula of Lagrange interpolating polynomial based on 4 points x_0, x_1, x_2, x_3 is

$$y = f(x) = \frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)}\, y_0 + \frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)}\, y_1$$

$$+ \frac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)}\, y_2 + \frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)}\, y_3.$$

D

$$y' = f'(x) = \frac{(x-x_1)(x-x_2)+(x-x_3)(x-x_1)+(x-x_3)(x-x_2)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)}\, y_0$$

$+$

$$+\frac{(x-x_0)(x-x_2)+(x-x_3)(x-x_0)+(x-x_3)(x-x_2)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)}\,y_1$$

$$+\frac{(x-x_0)(x-x_1)+(x-x_3)(x-x_0)+(x-x_3)(x-x_1)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)}\,y_2$$

$$+\frac{(x-x_0)(x-x_1)+(x-x_2)(x-x_0)+(x-x_2)(x-x_1)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)}\cdot y_3$$

$$-E$$

$x_1 - x_0 = h, \quad x_2 - x_0 = 2h, \quad x_3 - x_0 = 3h.$

$x = x_0$ in E

$$y' = f'(x_0) = \frac{(-h)(-2h) + (-3h)(-h) + (-3h)(-2h)}{(-h)(-2h)(-3h)} y_0$$

$$+ \frac{0 + 0 + (-3h)(-2h)}{h(-h)(-2h)} y_1 + \frac{0 + 0 + (-3h)(-h)}{(2h).(h)(-h)} y_2$$

$$+ 0 + 0 + \frac{(-2h)(-h)}{3h.2h.h} y_3$$

$$= \frac{11h^2}{-6h^3} y_0 + \frac{6h^2}{2h^3} y_1 + \frac{3h^2}{(-2h^3)} y_2 + \frac{2h^2}{6h^3} \cdot y_3$$

$$y'(x_0) = f'(x_0) = \frac{-11y_0 + 18y_1 - 9y_2 + 2y_3}{6h}.$$

which is first order formula (L.I.P.

$$f''(x_0) = \frac{2y_0 - 5y_1 + 4y_2 - y_3}{h^2}$$