NUMERICAL DIFFERENTIATION

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FIRST DERIVATIVES

The simplest difference formulas are based on using a straight line to interpolate the given data; they use two data points to estimate the derivative. We assume that we have function values at

$$x - h \ (or\, x_{i-1}) \ , \ x \ (or\, x_i) \ and \ x + h \ (or\, x_{i+1})$$

we let

$$f(x-h) = y(x-h) \ (or\, f(x_{i-1}) = y_{i-1}) \ , \ f(x) = y(x) \ (or\, f(x_i) = y_i) \ and \ f(x+h) = y(x+h) \ (or\, f(x_{i+1}) = y_{i+1})$$

The spacing between the values of x is constant (see figure below) , so that

$$x_i - x_{i-1} = h \quad and \quad x_i - x_{i+1} = h$$

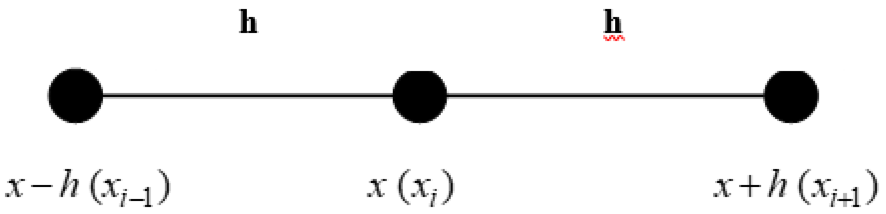


Fig.1

Forward difference formula (first derivative)

Consider the Taylor series expansion

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \ldots \quad \text{where}$$

$$hf'(x) = f(x+h) - f(x) - \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + \ldots \quad \Rightarrow f'(x) = \frac{f(x+h)-f(x)}{h} - \frac{h}{2!}f''(x) - \frac{h^2}{3!}f'''(x) + \ldots$$

$$f'(x) = \frac{f(x+h)-f(x)}{h} + E_{trunc}(f,h\Big)$$

where forward difference formula for first derivative and truncation error as follows

$$f'(x) = \frac{f(x+h)-f(x)}{h} \quad and \quad E_{trunc}(f,h) = -\frac{h}{2!}f''(x) = O(h\Big) \quad \text{(order h)}$$

Backward difference formula (first derivative)

Consider the Taylor series expansion

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + \ldots \quad \text{where}$$

$$hf'(x) = f(x) - f(x-h) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + \ldots \quad \Rightarrow f'(x) = \frac{f(x)-f(x-h)}{h} + \frac{h}{2!}f''(x) - \frac{h^2}{3!}f'''(x) + \ldots$$

$$f'(x) = \frac{f(x)-f(x-h)}{h} + E_{trunc}(f,h)$$

where backward difference formula for first derivative and truncation error as follows

$$f'(x) = \frac{f(x)-f(x-h)}{h} \quad and \quad E_{trunc}(f,h) = \frac{h}{2!}f''(x) = O(h) \quad \text{(order h)}$$

Central difference formula

Theorem: (centered formula for $O(h^2)$)

Assume that $f \in C^3[a,b]$ $\;and\;$ $that$ $\;x-h,\;\; x+h \in [a,b]$ then

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h}$$ (central difference formula for first derivative)

Furthermore , there exist a number $c = c(x) \in [a,b]$ such that

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} + E_{trunc}(f,h) \qquad where \qquad E_{trunc}(f,h) = -\frac{h^2 f^{(3)}(c)}{6} = O(h^2)\Big)$$

The term E(f,h) is called truncation error.

PROOF:

Start with second degree Taylor expansions

$$f(x) = P_2(x) + E_2(x)\ ,\ about\ \ x,\ for\ \ f(x+h)\ \ and\ \ f(x-h)$$

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x)+\ldots$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x)+\ldots$$

$$f(x+h) - f(x-h) = 2hf'(x) + 2\frac{h^3}{3!}f'''(x)+\ldots$$

$$2hf'(x) = f(x+h) - f(x-h) - \frac{h^3}{3}f'''(x)+\ldots \qquad then$$

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6}f'''(x)+\ldots$$

Central difference formula $$f'(x) = \frac{f(x+h) - f(x-h)}{2h}$$

Truncation error $$E(f,h) = -\frac{h^2}{6} f'''(x) = O(h^2)$$

Theorem: (centered formula of order $O(h^4)$)

Assume that $f \in C^5[a,b]$ and $that\, x-2h,\ x-h,\ x+h,\ x+2h \in [a,b]$ then

$$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} \qquad \textbf{(*)}$$

Furthermore there exists a number $c = c(x) \in [a,b]$ such that

$$f'(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h} + E_{trunc}(f,h\Big)$$

where

$$E(f,h) = \frac{h^4}{30} f^{(5)}(c) = O(h^4)$$

Proof:

One way to derive formula (*) is as follows. Start with the difference between fourth degree Taylor expansions $f(x) = P_4(x) + E_4(x)$, $about\ \ x,\ \ for\ \ f(x+h)\ \ and\ \ f(x-h)$

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x) + \frac{h^5}{5!}f^{(5)}(x\big)$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x) - \frac{h^5}{5!}f^{(5)}(x\big)$$

(**)

—

$$f(x+h) - f(x-h) = 2hf'(x) + \frac{h^3}{3}f'''(x) + \frac{2h^5}{5!}f^{(5)}(x)\quad\big)$$

Then use step size 2h, instead of h, and write down the following approximation

$$f(x+2h) - f(x-2h) = 2(2h)f'(x) + \frac{2(2h)^3}{3} f'''(x) + \frac{2(2h)^5}{5!} f^{(5)}(x)$$

$$f(x+2h) - f(x-2h) = 4hf'(x) + \frac{16h^3}{6} f'''(x) + \frac{64h^5}{5!} f^{(5)}(x) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (***)$$

Next multiply the terms in equation (**) by 8 and subtract (***) from it

$$8 \times \left[f(x+h) - f(x-h) = 2hf'(x) + \frac{h^3}{3} f'''(x) + \frac{2h^5}{5!} f^{(5)}(x) \right]$$

$$f(x+2h) - f(x-2h) = 4hf'(x) + \frac{16h^3}{6} f'''(x) + \frac{64h^5}{5!} f^{(5)}(x)$$

$-$

$$-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h) = 12hf'(x) - \frac{48}{5!} h^5 f^{(5)}(x)$$

Then $$f'(x) = \frac{-f(x+2h)+8f(x+h)-8f(x-h)+f(x-2h)}{12h} + E_{trunc}(f,h)$$

and

$$E(f,h) = \frac{h^4}{30} f^{(5)}(c) = O(h^4)$$

ERROR ANALYSIS AND OPTIMUM STEP SIZE

An important topic in the study of numerical differentiation is the effect of the computer's round-off error. Let us examine the formulas more closely. Assume that a computer is used to make numerical computation and that

$$f(x_0 - h) = y_{-1} + e_{-1} \qquad and \qquad f(x_0 + h) = y_1 + e_1$$

where $f(x_0 - h) \;\; and \;\; f(x_0 + h)$ are approximated by the numerical values $y_{-1} \;\; and \;\; y_1$, and $e_{-1} \;\; and \;\; e_1$ are the associated round-off errors, respectively. The following result indicates the complex nature of error analysis for numerical differentiation.

COROLLARY: Assume that f satisfies the hypotheses of

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0 - h)}{2h} \qquad \textbf{(1)}$$

and use computational formula $$f'(x_0) \approx \frac{y_1 - y_{-1}}{2h} + E(f, h) \qquad \textbf{(2)}$$

where $$E(f,h) = E_{round}(f,h) + E_{trunc}(f,h) = \frac{e_1 - e_{-1}}{2h} - \frac{h^2 f^{(3)}(c)}{6} \qquad \textbf{(3)}$$

where the total error term $E(f,h)$ has part due to round-off error plus a part due to truncation error.

COROLLARY: If $|e_1| \le \varepsilon$, $|e_{-1}| \le \varepsilon$ and $M = \max\limits_{a \le x \le b}\{|f^{(3)}(x)|\}$ then (from equation **(3)**)

$$|E(f,h)| \le \frac{|e_1| + |-e_{-1}|}{2h} + \frac{Mh^2}{6} = \frac{\varepsilon + \varepsilon}{2h} + \frac{Mh^2}{6} = \frac{\varepsilon}{h} + \frac{Mh^2}{6}$$

let total error

$$\Psi(h) = |E(f,h)| \le \frac{\varepsilon}{h} + \frac{Mh^2}{6} \qquad \textbf{(4)}$$

and setting $\Psi'(h) = 0$ and the value of h that minimizes the right hand side of **(4)**

$$\Psi'(h) = 0 \quad \Rightarrow \quad \frac{-\varepsilon}{h^2} + \frac{Mh}{3} = 0 \quad \Rightarrow \quad \frac{Mh}{3} = \frac{\varepsilon}{h^2} \quad \Rightarrow \quad h^3 = \frac{3\varepsilon}{M}$$

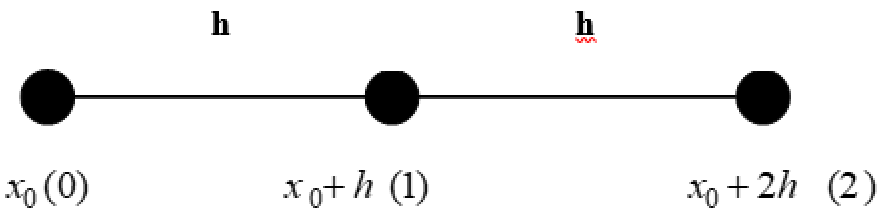
$h = \left(\frac{3\varepsilon}{M}\right)^{\frac{1}{3}}$ is the optimum step size h

Example: Derive the numerical differentiation formula

$$f'(x_0) = \frac{-3f_0 + 4f_1 - f_2}{2h} = \frac{-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)}{2h}$$

If $f(x)$ is given by $f(x) = \sin x$, find the optimum step size h to estimate the derivative at the point $x = \frac{\pi}{4}$, provided that the upper bound of the rounding error is given by $|e_k| \leq 8 \times 10^{-6}$ compare the result with exact value of the derivative at $x = \frac{\pi}{4}$.

Solution:



Taylor series expansion for $f(x_0 + h)$ *and* $f(x_0 + 2h)$ is as follows

$$4 \times \left(\quad f(x_0 + h) = f(x_0) + hf'(x_0) + \frac{h^2}{2!} f''(x_0) + \frac{h^3}{3!} f'''(x_0) + \frac{h^4}{4!} f^{(4)}(x_0) + \ldots \quad \right)$$

$$-1 \times \left(f(x_0 + 2h) = f(x_0) + 2hf'(x_0) + \frac{4h^2}{2!} f''(x_0) + \frac{8h^3}{3!} f'''(x_0) + \frac{16h^4}{4!} f^{(4)}(x_0) + \ldots \right)$$

$$+$$

$$4f(x_0 + h) - f(x_0 + 2h) = 3f(x_0) + 2hf'(x_0) - \frac{4h^3}{3!} f'''(x) + \ldots$$

then

$$f'(x_0) = \frac{-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)}{2h} + \frac{h^2}{3} f'''(x_0)$$

$$E_{trunc} = \frac{h^2}{3} f'''(x_0)$$

where

$$E(f,h) = E_{round}(f,h) + E_{trunc}(f,h) = \frac{-3e_0 + 4e_1 - e_2}{2h} + \frac{h^2}{3} f'''(x)$$

$$|E(f,h)| \leq \frac{|-3e_0| + |4e_1| + |-e_2|}{2h} + \left|\frac{h^2}{3} f'''(x)\right|$$

$$find \quad M,$$

$$f(x) = \sin x \ , \quad f'(x) = \cos x \ , \ f''(x) = -\sin x \quad and \quad f'''(x) = -\cos x$$

$$M = \max_{0 \leq x \leq 2\pi} \{|f'''(x)|\} = \max_{0 \leq x \leq 2\pi} \{|-\cos x|\} \leq 1 \quad so \quad M = 1$$

and

$$|E(f,h)| \leq \frac{3\varepsilon + 4\varepsilon + \varepsilon}{2h} + \frac{h^2}{3} = \frac{8\varepsilon}{2h} + \frac{h^2}{3}$$

$$let \ \ \Psi(h) = \frac{8\varepsilon}{2h} + \frac{h^2}{3} \quad and \ \ \Psi'(h) = \frac{-4\varepsilon}{h^2} + \frac{2h}{3} = 0$$

$$\frac{4\varepsilon}{h^2} = \frac{2h}{3} \quad \Rightarrow \ h^3 = 6\varepsilon \quad and \quad h = (6\varepsilon)^{\frac{1}{3}} \quad where \ \ \varepsilon = 8 \times 10^{-6}$$

$$then \quad h = (6 \times (8 \times 10^{-6}))^{\frac{1}{3}} = 0.0363$$

Then find

$$f'(\frac{\pi}{4}) = \frac{-3f(\frac{\pi}{4}) + 4f(\frac{\pi}{4} + 0.0363) - f(\frac{\pi}{4} + 2(0.0363))}{2(0.0363)}$$

$$= \frac{-3\sin\left(\frac{\pi}{4}\right) + 4\sin\left(\frac{\pi}{4} + 0.0363\right) - \sin\left(\frac{\pi}{4} + 2(0.0363)\right)}{0.0726}$$

$$f'(\frac{\pi}{4}) = 0.7024$$

$$f(x) = \sin x \quad and \quad f'(x) = \cos x \quad then$$

Exact value:

$$f'\left(\frac{\pi}{4}\right) = \cos\left(\frac{\pi}{4}\right) = 0.7071$$

Example: Derive the numerical differentiation formula

$$f'(x) = \frac{-3f(x) + 4f(x+h) - f(x+2h)}{2h}$$

Evaluate the derivative at the point x=1 using the above formula for the function $f(x) = 3x^2 - 2x$ such that the rounding error should not exceed $\varepsilon = 10^{-4}$ and the total error bounded by 10^{-3} and verify the result.

Solution:

From previous example

$$f'(x) = \frac{-3f(x) + 4f(x+h) - f(x+2h)}{2h} + \frac{h^2}{3} f'''(x)$$

$$E_{trunc} = \frac{h^2}{3} f'''(x)$$

$$E(f,h) = E_{round}(f,h) + E_{trunc}(f,h) = \frac{-3e_0 + 4e_1 - e_2}{2h} + \frac{h^2}{3} f'''(x))$$

$$|E(f,h)| \leq \frac{|-3e_0| + |4e_1| + |-e_2|}{2h} + \left|\frac{h^2}{3} f'''(x))\right| \leq 10^{-3}$$

$$and$$

$$|E(f,h)| \leq \frac{3\varepsilon + 4\varepsilon + \varepsilon}{2h} + \frac{h^2}{3}|f'''(x)| \leq 10^{-3} \quad \Rightarrow |E(f,h)| \leq \frac{8\varepsilon}{2h} + \frac{h^2}{3}|f'''(x)| \leq 10^{-3}$$

$$Find \quad M, \quad where$$

$$f(x) = 3x^2 - 2x \quad , \quad f'(x) = 6x - 2 \quad , \; f''(x) = 6 \quad and \quad f'''(x) = 0$$

$$that\ is \quad M = 0$$

$$|E(f,h)| \leq \frac{8\varepsilon}{2h} + 0 \leq 10^{-3} \quad where \;\; \varepsilon = 10^{-4}$$

$$|E(f,h)| \leq \frac{8 \times 10^{-4}}{2h} \leq 10^{-3} \quad \Rightarrow \qquad \boxed{h \approx 0.4}$$

$$f'(1) = \frac{-3f(1) + 4f(1+0.4) - f(1+2(0.4))}{2(0.4)} = \frac{-3(1) + 4(3.08) - 6.12}{0.8} = 4$$

$$Exact\ value\!: \;\; f'(x) = 6x - 2 \quad \Rightarrow f'(1) = 6 - 2 = 4$$

EXERCISE 1: The local truncation error of

$$f''(x_0) = \frac{-f_2 + 16f_1 - 30f_0 + 16f_{-1} - f_{-2}}{12h^2}$$

$$is \;\; E_{trunc}(f,h) = \frac{h^4}{90} f^{(6)}(c\bigg)$$

Find the best value of h to approximate $f''(x)$, for $f(x) = e^x \;\; over \;\; [-1,1]$ with rounding error bounded by 2.32×10^{-5} .

EXERCISE 2: Derive the numerical differentiation formula

$$f'(x_0) = \frac{3f_0 - 4f_{-1} + f_{-2}}{2h} = \frac{3f(x_0) - 4f(x_0 - h) + f(x_0 - 2h)}{2h}$$

and determine the truncation error

EXERCISE 3: Derive the following numerical differentiation formula

$$f^{/}(x) = \frac{-f(x+2h) + 8f(x+h) - 8f(x-h) + f(x-2h)}{12h}$$

and define the order of approximation.

DIFFERENTIATION OF THE LAGRANGE POLYNOMIAL

If the function must be evaluated at abscissas that lie on one side of x0, the central-difference formulas cannot be used. Formulas for equally spaced abscissas that lie to the right (or left) of x0 are called forward (or backward) difference formulas. These formulas can be derived by differentiation of the Lagrange interpolation polynomial.

Example: Derive the formulas

$$f'(x_0) \approx \frac{3f_0 - 4f_{-1} + f_{-2}}{2h} \quad \textbf{(Backward)}$$

Start with the Lagrange interpolation polynomial for f(t) based on the three points x_0, x_{-1}, x_{-2}.

$$x_0, x_{-1}, x_{-2}$$

$$f_0, f_{-1}, f_{-2}$$

$$f(t) \approx f_0 \frac{(t-x_{-1})(t-x_{-2})}{(x_0-x_{-1})(x_0-x_{-2})} + f_{-1} \frac{(t-x_0)(t-x_{-2})}{(x_{-1}-x_0)(x_{-1}-x_{-2})} + f_{-2} \frac{(t-x_0)(t-x_{-1})}{(x_{-2}-x_0)(x_{-2}-x_{-1})}$$

Take the derivative of f(t) w.r.t. t,

$$f'(t) \approx f_0 \frac{(t-x_{-2})+(t-x_{-1})}{(x_0-x_{-1})(x_0-x_{-2})} + f_{-1} \frac{(t-x_{-2})+(t-x_0)}{(x_{-1}-x_0)(x_{-1}-x_{-2})} + f_{-2} \frac{(t-x_{-1})+(t-x_0)}{(x_{-2}-x_0)(x_{-2}-x_{-1})}$$

$$f'(x_0) \approx f_0 \frac{(x_0-x_{-2})+(x_0-x_{-1})}{(x_0-x_{-1})(x_0-x_{-2})} + f_{-1} \frac{(x_0-x_{-2})+(x_0-x_0)}{(x_{-1}-x_0)(x_{-1}-x_{-2})} + f_{-2} \frac{(x_0-x_{-1})+(x_0-x_0)}{(x_{-2}-x_0)(x_{-2}-x_{-1})}$$

Now, we use $x = x_0 + th$,

$$x_0 = x_0 + 0h$$
$$x_{-1} = x_0 - h$$
$$x_{-2} = x_0 - 2h$$

$$f'(x_0) \approx f_0 \frac{(x_0 - x_{-2}) + (x_0 - x_{-1})}{(x_0 - x_{-1})(x_0 - x_{-2})} + f_{-1} \frac{(x_0 - x_{-2}) + (x_0 - x_0)}{(x_{-1} - x_0)(x_{-1} - x_{-2})} + f_{-2} \frac{(x_0 - x_{-1}) + (x_0 - x_0)}{(x_{-2} - x_0)(x_{-2} - x_{-1})}$$

$$f'(x_0) \approx f_0 \frac{(2h) + (h)}{(h)(2h)} + f_{-1} \frac{(2h)}{(-h)(h)} + f_{-2} \frac{(h)}{(-2h)(-h)}$$

$$f'(x_0) \approx f_0 \frac{3h}{2h^2} + f_{-1} \frac{(2h)}{-h^2} + f_{-2} \frac{(h)}{2h^2}$$

$$f'(x_0) \approx f_0 \frac{3}{2h} - f_{-1} \frac{2}{h} + f_{-2} \frac{1}{2h}$$

$$f'(x_0) \approx \frac{3f_0 - 4f_{-1} + f_{-2}}{2h}$$

Example: Derive the formulas

$$f''(x_0) \approx \frac{2f_0 - 5f_1 + 4f_2 - f_3}{h^2} \quad \textbf{(Forward)}$$

Start with the Lagrange interpolation polynomial for f(t) based on the three points x_0, x_1, x_2, x_3.

$$x_0, x_1, x_2, x_3$$

$$f_0, f_1, f_2, f_3$$

$$f(t) \approx f_0 \frac{(t-x_1)(t-x_2)(t-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)} + f_1 \frac{(t-x_0)(t-x_2)(t-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)}$$
$$+ f_2 \frac{(t-x_0)(t-x_1)(t-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)} + f_3 \frac{(t-x_0)(t-x_1)(t-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)}$$

Take the second derivative of f(t) w.r.t. t, and get

$$f''(t) \approx f_0 \frac{2\left[(t-x_1)+(t-x_2)+(t-x_3)\right]}{(x_0-x_1)(x_0-x_2)(x_0-x_3)} + f_1 \frac{2\left[(t-x_0)+(t-x_2)+(t-x_3)\right]}{(x_1-x_0)(x_1-x_2)(x_1-x_3)}$$

$$+f_2 \frac{2\left[(t-x_0)+(t-x_1)+(t-x_3)\right]}{(x_2-x_0)(x_2-x_1)(x_2-x_3)} + f_3 \frac{2\left[(t-x_0)+(t-x_1)+(t-x_2)\right]}{(x_3-x_0)(x_3-x_1)(x_3-x_2)}$$

$$f''(x_0) \approx f_0 \frac{2\left[(x_0-x_1)+(x_0-x_2)+(x_0-x_3)\right]}{(x_0-x_1)(x_0-x_2)(x_0-x_3)} + f_1 \frac{2\left[(x_0-x_0)+(x_0-x_2)+(x_0-x_3)\right]}{(x_1-x_0)(x_1-x_2)(x_1-x_3)}$$

$$+f_2 \frac{2\left[(x_0-x_0)+(x_0-x_1)+(x_0-x_3)\right]}{(x_2-x_0)(x_2-x_1)(x_2-x_3)} + f_3 \frac{2\left[(x_0-x_0)+(x_0-x_1)+(x_0-x_2)\right]}{(x_3-x_0)(x_3-x_1)(x_3-x_2)}$$

Now, we use $x = x_0 + th$,

$$x_0 = x_0 + 0h$$
$$x_1 = x_0 + h$$
$$x_2 = x_0 + 2h$$
$$x_3 = x_0 + 3h$$

$$f''(x_0) \approx f_0 \frac{2\left[(x_0 - x_1) + (x_0 - x_2) + (x_0 - x_3)\right]}{(x_0 - x_1)(x_0 - x_2)(x_0 - x_3)} + f_1 \frac{2\left[(x_0 - x_0) + (x_0 - x_2) + (x_0 - x_3)\right]}{(x_1 - x_0)(x_1 - x_2)(x_1 - x_3)}$$
$$+ f_2 \frac{2\left[(x_0 - x_0) + (x_0 - x_1) + (x_0 - x_3)\right]}{(x_2 - x_0)(x_2 - x_1)(x_2 - x_3)} + f_3 \frac{2\left[(x_0 - x_0) + (x_0 - x_1) + (x_0 - x_2)\right]}{(x_3 - x_0)(x_3 - x_1)(x_3 - x_2)}$$

$$f''(x_0) \approx f_0 \frac{2\left[(-h) + (-2h) + (-3h)\right]}{(-h)(-2h)(-3h)} + f_1 \frac{2\left[(-2h) + (-3h)\right]}{(h)(-h)(-2h)}$$
$$+ f_2 \frac{2\left[(-h) + (-3h)\right]}{(2h)(h)(-h)} + f_3 \frac{2\left[(-h) + (-2h)\right]}{(3h)(2h)(h)}$$

$$f''(x_0) \approx f_0 \frac{-12h}{-6h^3} + f_1 \frac{-10h}{2h^3} + f_2 \frac{-8h}{-2h^3} + f_3 \frac{-6h}{6h^3}$$

$$f''(x_0) \approx \frac{2f_0 - 5f_1 + 4f_2 - f_3}{h^2}$$

DIFFERENTIATION OF THE NEWTON POLYNOMIAL

The Newton Polynomial P(t) of degree N=2 that approximates f(t) using the nodes t_0, t_1, t_2 **is**

$$P(t) = a_0 + a_1(t - t_0) + a_2(t - t_0)(t - t_1)$$

where $a_0 = f(t_0), a_1 = \dfrac{f(t_1) - f(t_0)}{t_1 - t_0}$ and $a_2 = \dfrac{\dfrac{f(t_2) - f(t_1)}{t_2 - t_1} - \dfrac{f(t_1) - f(t_0)}{t_1 - t_0}}{t_2 - t_0}$

The derivative of P(t) is $P'(t) = a_1 + a_2\left[(t - t_0) + (t - t_1)\right]$

$$P'(t_0) = a_1 + a_2(t_0 - t_1) \approx f'(t_0) \quad \text{..................} \quad (1)$$

CASE1. (FORWARD) **If** $t_0 = x, t_1 = x + h, t_2 = x + 2h$

$$a_1 = \frac{f(t_1) - f(t_0)}{t_1 - t_0} = \frac{f(x+h) - f(x)}{h}$$

$$a_2 = \frac{\dfrac{f(t_2) - f(t_1)}{t_2 - t_1} - \dfrac{f(t_1) - f(t_0)}{t_1 - t_0}}{t_2 - t_0} = \frac{\dfrac{f(x+2h) - f(x+h)}{h} - \dfrac{f(x+h) - f(x)}{h}}{2h}$$

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

Substituting these values into (1) we get

$$P'(t_0) = a_1 + a_2(t_0 - t_1) \approx f'(t_0)$$

$$P'(x) = \frac{f(x+h) - f(x)}{h} + \frac{-f(x+2h) + 2f(x+h) - f(x)}{2h} \approx f'(x)$$

$f'(x) = \dfrac{-3f_0 + 4f_1 - f_2}{2h}$ which second order forward difference formula for $f'(x)$

CASE2. (CENTRAL) If $t_0 = x, t_1 = x+h, t_2 = x-h$

$$a_1 = \frac{f(x+h)-f(x)}{h}, a_2 = \frac{f(x+h)-2f(x)+f(x-h)}{2h^2}$$

Substituting these values into (1) we get

$$P'(t_0) = a_1 + a_2(t_0 - t_1) \approx f'(t_0)$$

$$P'(x) = \frac{f(x+h)-f(x)}{h} + \frac{-f(x+h)+2f(x)-f(x-h)}{2h} \approx f'(x)$$

$f'(x) = \dfrac{f_1 - f_{-1}}{2h}$ which second order central difference formula for $f'(x)$

CASE3. (BACKWARD) If $t_0 = x, t_1 = x - h, t_2 = x - 2h$

$$a_1 = \frac{f(x) - f(x-h)}{h}, a_2 = \frac{f(x) - 2f(x-h) + f(x-2h)}{2h^2}$$

Substituting these values into (1) we get

$$P'(t_0) = a_1 + a_2(t_0 - t_1) \approx f'(t_0)$$

$$P'(x) = \frac{f(x) - f(x-h)}{h} + \frac{f(x) - 2f(x-h) + f(x-2h)}{2h} \approx f'(x)$$

$f'(x) = \dfrac{3f_0 - 4f_{-1} + f_{-2}}{2h}$ which second order backward difference formula for $f'(x)$

Example: Use Newton forward interpolation for N=3 nodes to find $f'(x)$ at x=0

x	0	1	2	3
y	5	6	3	8

Newton Polynomial: $P(t) = a_0 + a_1(t-t_0) + a_2(t-t_0)(t-t_1) + a_3(t-t_0)(t-t_1)(t-t_2)$

$$P'(t) = a_1 + a_2\left[(t-t_0) + (t-t_1)\right] + a_3\left[(t-t_1)(t-t_2) + (t-t_0)(t-t_2) + (t-t_0)(t-t_1)\right]$$

$$P'(t_0) = a_1 + a_2\left[\cancel{(t_0-t_0)} + (t_0-t_1)\right] + a_3\left[(t_0-t_1)(t_0-t_2) + \cancel{(t_0-t_0)(t_0-t_2)} + \cancel{(t_0-t_0)(t_0-t_1)}\right]$$

$$\boxed{P'(t_0) = a_1 + a_2(t_0-t_1) + a_3(t_0-t_1)(t_0-t_2)}$$

$$f'(x) = P'(t_0)$$

$$f'(x) = P'(t_0) = a_1 + a_2(t_0 - t_1) + a_3(t_0 - t_1)(t_0 - t_2)$$

Use Forward Formula : $t_0 = x$, $t_1 = x+h$, $t_2 = x+2h$

$t_0 = 0$, $t_1 = h$ $t_2 = 2h$

Use Newton difference Table :

	x	y			
	0	$\boxed{5} = a_0$			
h=1	1	6	$\boxed{1} = a_1$		
h=1	2	3	-3	$\boxed{-2} = a_2$	
h=1	3	8	5	4	$\boxed{2} = a_3$

$$f'(0) = P'(0) = a_1 + a_2(t_0 - t_1) + a_3(t_0 - t_1)(t_0 - t_2)$$

$$= 1 - 2(-h) + 2(-h)(-2h)$$

$$= 1 + 2h + 4h^2$$

$$= 1 + 2 + 4$$

$$= 7$$

$$\boxed{f'(0) = P'(0) = 7}$$