We know that if f is k times continuously differentiable function on an interval $[c, d]$ containing the node points $x_0, x_1, \ldots x_k$, then

$$f[x_0, x_1, \ldots x_k] = \frac{f^{(k)}(\xi)}{k!}, \quad \xi \in [c, d].$$

Theorem: If f is $(k+1)$ times continuously differentiable function on $[c, d]$ containing the nodes $x_0, x_1, \ldots x_k$ and a point $x \in [c, d]$, then

$$f[x_0, x_1, \ldots x_k, x] = \frac{f^{(k+1)}(\xi(x))}{(k+1)!}, \quad \xi(x) \in [c, d]$$

If f is $(k+2)$ times continuously differentiable on $[c, d]$, then $f[x_0, x_1, \ldots x_k, x]$ is differentiable

and $$\frac{d}{dx} f[x_0, x_1, \ldots x_k, x] = f[x_0, x_1, \ldots x_k, x, x].$$

Furthermore

$$f[x_0, x_1, \ldots x_k, x, x] = \frac{f^{(k+2)}(\xi)}{(k+2)!}, \quad \xi \in (c, d).$$

The proof of above theorem is left.

[to see a proof, Refer to Conte, de Boor book]

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Numerical Differentiation :

Let f be continuously differentiable function on the interval $[c, d]$. If $x_0, x_1, \ldots x_k$ are distinct points in $[c, d]$, we can write

$$f(x) = P_k(x) + f[x_0, x_1, \ldots x_k, x]\, \psi_k(x) \quad \text{— (1)}$$

where $P_k(x)$ is the polynomial of degree $\leq k$ interpolating $f(x)$ at $x_0, x_1, \ldots x_k$ and

$$\psi_k(x) = \prod_{j=0}^{k} (x - x_j).$$

Differentiating (1) w.r.to x, we get

$$f'(x) = P_k'(x) + f[x_0, x_1, \ldots x_k, x]\, \psi_k'(x) + \frac{d}{dx} f[x_0, x_1, \ldots x_k, x]\, \psi_k(x)$$

$$\therefore \boxed{f'(x) = P_k'(x) + f[x_0, \ldots x_k, x]\, \psi_k'(x) + f[x_0, \ldots x_k, x, x]\, \psi_k(x)}$$

Using the theorem on page (0)

$$f'(x) = P_k'(x) + \frac{f^{(k+1)}(\xi)}{(k+1)!} \psi_k'(x) + \frac{f^{(k+2)}(\eta)}{(k+2)!} \psi_k(x)$$

where ξ, η are some points in (c, d).

Define the operator D as

$$D(f) = f'(a)$$

where a is some point in $[c, d]$ at which $f'(a)$ is approximated.

$$E(f) = D(f) - D(P_k)$$

$$E(f) = \frac{f^{(k+1)}(\xi)}{(k+1)!}\,\psi_k'(a) + \psi_k(a)\,\frac{f^{(k+2)}(\eta)}{(k+2)!}$$

(1) If a is one of the node points $x_0, x_1, \dots x_k$, then $\psi_k(a)$ is zero and the error is given by $E(f) = \frac{f^{(k+1)}(\xi)}{(k+1)!}\,\psi_k'(a)$.

(2) If a is such that $\psi_k'(a)$ is zero, then the error takes the form

$$E(f) = \frac{f^{(k+2)}(\eta)}{(k+2)!}\,\psi_k(a).$$

In the first case, when a is one of the nodes, $a = x_i$, then $\psi_k'(a) = q(a)$

where $q(x) = \frac{\psi_k(x)}{(x-x_i)} = (x-x_0)(x-x_1)\cdots(x-x_{i-1})(x-x_{i+1}) \cdots (x-x_k)$

$$q(a) = \prod_{\substack{j=0 \\ j\neq i}}^{k} (a-x_j), \text{ if } a = x_i.$$

Therefore the error takes the form in the first case

$$E(f) = \frac{f^{(k+1)}(\xi)}{(k+1)!} \prod_{\substack{j=0 \\ j\neq i}}^{k} (x_i - x_j),$$

when $a = x_i$

In the second case, i.e. when a is chosen such that $\varphi_K'(a)=0$, we can simplify the error. We can choose such ~~that~~ a point $x=a$, if the number of nodes is even, i.e. when k is odd. (3)

We can achieve this by placing x_i's symmetrically around a, that is

$$x_{k-j}-a = a - x_j, \quad j=0,1,\dots \frac{k-1}{2}.$$

Then

$$(x-x_j)(x-x_{k-j}) = (x-a+a-x_j)(x-a+a-x_{k-j})$$

$$= (x-a+a-x_j)(x-a-(a-x_j))$$

$$= (x-a)^2-(a-x_j)^2, \quad j=0,1,\dots \frac{k-1}{2}.$$

Hence

$$\varphi_k(x) = \prod_{j=0}^{(k-1)/2}\left[(x-a)^2-(a-x_j)^2\right]$$

Since

$$\frac{d}{dx}\left[(x-a)^2-(a-x_j)^2\right]\Big|_{x=a} = 2(x-a)\Big|_{x=a} = 0.$$

it follows that

$$\varphi_k'(a)=0.$$

The error then takes the form

$$E(f) = \frac{f^{(k+2)}}{(k+2)!}(\eta)\cdot\prod_{j=0}^{k}(a-x_j)$$

(or)

$$E(f) = \frac{f^{(k+2)}}{(k+2)!}(\eta)\prod_{j=0}^{(k-1)/2}\left(-(a-x_j)^2\right)$$

Specific examples:

If $k=0$, then $D(P_k)=0$, which may not be a good approximation of $f'(a) = D(f)$.

We assume $k \geq 1$.

Examples with $k=1$: $\boxed{\text{Example 1}}$

$$P_1(x) = f(x_0) + f[x_0, x_1](x - x_0).$$

Hence $D(P_1) = f[x_0, x_1]$, regardless of a.

If $a = x_0$, then we get with $h = x_1 - x_0$,

$$f'(a) \simeq f[a, a+h] = \frac{f(a+h) - f(a)}{h}$$

$$E(f) = \frac{f''(\xi)}{2} \psi_1'(a).$$

$$\psi_1(x) = (x-a)(x-(a+h)) \Rightarrow \psi_1'(a) = \left[2x - (a+a+h)\right]\Big|_{x=a}$$
$$= -h.$$

$$\therefore \boxed{E(f) = -\frac{h}{2} f''(\xi)}$$

The formula $f'(a) \approx \dfrac{f(a+h) - f(a)}{h}$

is called forward difference formula if $h>0$, backward difference formula if $h<0$.

Example 2: with $k=1$:

we choose $x_0 = a-h$, and $x_1 = a+h$, $[h>0]$.

then $a = \frac{x_0+x_1}{2}$, and $h = \frac{1}{2}(x_1 - x_0)$.

we get

$$D(P_1) = f[x_0, x_1] = \frac{f(x_1)-f(x_0)}{x_1-x_0} = \frac{f(a+h)-f(a-h)}{2h}$$

$$\boxed{f'(a) \simeq \frac{f(a+h)-f(a-h)}{2h}}$$

and the error is given by,

$$E(f) = \frac{f^{(3)}(\eta)}{2!}\psi_1(a).$$

where $\psi_1(x) = (x-x_0)(x-x_1) = (x-a+h)(x-a-h)$

$$\psi_1(a) = (h)(-h) = -h^2$$

$$\therefore \boxed{E(f) = -\frac{h^2}{6} f^{(3)}(\eta),}\quad \eta \in (a-h, a+h).$$

We now consider $k=2$:

$$P_2(x) = f[x_0] + f[x_0, x_1](x-x_0) + f[x_0, x_1, x_2](x-x_0)(x-x_1)$$

and

$$P_2'(x) = f[x_0, x_1] + f[x_0, x_1, x_2](2x - x_0 - x_1)$$

$$f'(a) \simeq P_2'(a) = f[x_0, x_1] + f[x_0, x_1, x_2](2a - x_0 - x_1)$$

6 (a)

Consider $x_0 = a,\ x_1 = a+h,\ x_2 = a+2h$, then

$$f[a, a+h, a+2h] = \frac{1}{2h}\left(f[a+h, a+2h] - f[a, a+h] \right)$$

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

$$P_2'(a) = f[a, a+h] + f[a, a+h, a+2h]\,(2a - a - (a+h))$$

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

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

The formula is

$$f'(a) \approx \frac{-3f(a) + 4f(a+h) - f(a+2h)}{2h}$$

and the error is given by

$$\boxed{E(f) = \frac{f^{(3)}(\xi)}{3!}\,\psi_2'(a) = \frac{h^2}{3} f^{(3)}(\xi)}$$

since $\psi_2(x) = (x-a)(x-a-h)(x-a-2h)$

$$\psi_2'(a) = [(x-a-h)(x-a-2h)]_{x=a}$$

$$\boxed{\psi_2'(a) = (-h)(-2h) = 2h^2}$$

$= \cancel{\left[\left(x^2 - (a+h+a+2h)x \right) \right]_{x=a}}$

$= \cancel{\left\{ 2x - (2a+3h) \right\}_{x=a}}$

$$\boxed{\psi_2'(a) = 2h^2}$$

If we choose

$x_1 = a-h$ and $x_2 = a+h$, then

$P_2'(a) = f[a, a-h] + f[a, a-h, a+h]\,(2a-a-(a-h))$

$= f[a, a-h] + f[a-h, a, a+h]\,(h).$

$f[a-h, a, a+h]\cdot(h) = \dfrac{f[a, a+h] - f[a-h, a]}{2h}\cdot h$

$= \dfrac{1}{2}\left[\dfrac{f(a+h) - f(a) - f(a) + f(a-h)}{h}\right]$

$= \dfrac{f(a+h) - 2f(a) + f(a-h)}{2h}$

$P_2'(a) = \dfrac{f(a-h) - f(a)}{-h} + \dfrac{f(a+h) - 2f(a) + f(a-h)}{2h}$

$= \dfrac{2f(a) - 2f(a-h) + f(a+h) - 2f(a) + f(a-h)}{2h}$

$= \dfrac{f(a+h) - f(a-h)}{2h}$

we get the same formula as before (with $k=1$, cetral difference).

$$f'(a) \approx \frac{f(a+h) - f(a-h)}{2h}.$$

The error is given by

$E(f) = \dfrac{f^{(3)}(\xi)}{6}\,\psi_k'(a)$; $\psi_k'(a) = -h^2$

$\psi_k(x) = (x-a)(x-(a-h))(x-(a+h)) = (x-a)((x-a)+h)((x-a)-h)$

$= (x-a)((x-a)^2 - h^2) = (x-a)^3 - (x-a)h^2$

$\psi_k'(a) = -h^2$ $\therefore$ $\boxed{E(f) = -\dfrac{h^2}{6} f^{(3)}(\xi)}$

Similarly we can derive formula for numerical differentiation for second order derivative.

Recall that

$$f'(x) = P_k'(x) + f[x_0, x_1, \cdots x_k, x]\,\psi_k'(x) + f[x_0, x_1, \cdots x_k, x, x]\,\psi_k(x)$$

Differentiating the above identity w.r.to x.

$$f''(x) = P_k''(x) + f[x_0, x_1, \cdots x_k, x]\,\psi_k''(x)$$
$$+ 2 f[x_0, x_1, \cdots x_k, x, x]\,\psi_k'(x)$$
$$+ f[x_0, x_1, \cdots x_k, x, x, x]\,\psi_k(x).$$

Using the theorem on page (0).

$$f''(x) = P_k''(x) + \frac{f^{(k+1)}(\xi)}{(k+1)!}\psi_k''(x) + 2\frac{f^{(k+2)}(\eta)}{(k+2)!}\psi_k'(x) + \frac{f^{(k+3)}(\zeta)}{(k+3)!}\psi_k(x)$$

where ξ, η, ζ are points in $[c, d]$ containing the points $x_0, x_1, \cdots x_k$ and x.

Specific examples: we assume $k \geq 2$:

Let $k=2$:

$$P_2(x) = f[x_0] + f[x_0, x_1](x-x_0) + f[x_0, x_1, x_2](x-x_0)(x-x_1)$$

$$P_2'(x) = f[x_0, x_1] + f[x_0, x_1, x_2](2x - x_0 - x_1)$$

$$P_2''(x) = 2 \cdot f[x_0, x_1, x_2]$$

$$P_2''(a) = 2 \cdot f[x_0, x_1, x_2]$$ regardless of a.

We choose $x_0 = a, \quad x_1 = a+h, \quad x_2 = a+2h$

for some $h > 0$.

Then
$$f[a, a+h, a+2h] = \frac{f[a+h, a+2h] - f[a, a+h]}{2h}$$

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

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

$$2f[a, a+h, a+2h] = \frac{f(a) + f(a+2h) - 2f(a+h)}{h^2}$$

The formula is
$$f''(a) \approx \frac{f(a) - 2f(a+h) + f(a+2h)}{h^2}$$

and the error is given by the following

$\psi_2(x) = (x-a)(x-(a+h))(x-(a+2h))$

$\psi_2'(a) = \left[(x-(a+h))(x-(a+2h))\right]_{x=a} = (-h)(-2h) = 2h^2$

$\psi_2(x) = (x^3 - 3(a+h)x^2 + \text{lower order terms in } x)$

$\psi_2''(x) = 6x - 6(a+h) \Rightarrow \psi_2''(a) = -6h.$

$$E(f) = \frac{f^{(3)}(\xi)}{3!}\psi_2''(a) + 2 \cdot \frac{f^{(4)}(\eta)}{4!}\psi_2'(a)$$

$$\therefore \boxed{E(f) = -\frac{h}{6} f^{(3)}(\xi) + \frac{h^2}{6} f^{(4)}(\eta) \qquad \xi, \eta \in [c, d]}$$

we may choose

$x_0 = a, \quad x_1 = a-h, \quad x_2 = a+h.$ Then

$$P_2(x) = f[a] + f[a, a-h](x-a) + f[a, a-h, a+h](x-a)(x-a+h)$$

$$P_2''(x) = 2 \cdot f[a, a-h, a+h] =$$

$$= 2 \cdot f[a-h, a, a+h]$$

$$= 2 \cdot \frac{f[a, a+h] - f[a-h, a]}{2h}$$

$$= \frac{1}{h}\left[\frac{f(a+h) - f(a) - f(a) + f(a-h)}{h}\right]$$

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

The formula (central difference) is given by

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

$$\psi_2(x) = (x-a)(x-(a-h))(x-(a+h))$$

$$= (x-a)((x-a)+h)((x-a)-h)$$

$$\psi_2(x) = (x-a)((x-a)^2 - h^2) = (x-a)^3 - (x-a)h^2$$

$$\psi_2'(x) = 3(x-a)^2 - h^2$$

$$\psi_2''(x) = 6(x-a)$$

$$\psi_2(a) = 0 = \psi_2''(a)$$

$$\psi_2'(a) = -h^2$$

The error is given by

$$E(f) = 2\,\frac{f^{(4)}(\eta)}{4!}\,\varphi_2'(a)$$

$$\boxed{E(f) = -\frac{h^3}{12}\,f^{(4)}(\eta), \qquad \eta \in [c, d]}$$