Properties of W_i

i) We note that $W_i(x_{2i}) = 0$

ii) $$W_i(x_{2i+2}) = \int_{x_{2i}}^{x_{2i+2}} (t - x_{2i})(t - x_{2i+1})(t - x_{2i+2})\,dt$$

$t - x_{2i+1} = u$

$$= \int_{-h}^{h} (u+h)\,u\,(u-h)\,du$$

$$= \int_{-h}^{h} u(u^2 - h)\,du = 0 \quad \left(u(u^2-h) \text{ is odd fn.} \right)$$

$\therefore \quad W_i(x_{2i+2}) = 0.$

iii) $$W_i'(x) = g_i(x) = \begin{cases} > 0, & x_{2i} < x < x_{2i+1} \\ 0, & x = x_{2i+1} \\ < 0 & , x_{2i+1} < x < x_{2i+2} \end{cases}$$

$\Rightarrow$ W_i is strictly increasing in $[x_i, x_{2i+1}]$

and W_i " " " in $[x_{2i+1}, x_{2i+2}]$

and achieves maximum at $x = x_{2i+1}$

$\Rightarrow 0 = W(x_{2i}) < W(x) \leq W(x_{2i+1}), \quad x_{2i} < x \leq x_{2i+1},$

$0 = W(x_{2i+2}) < W(x) \leq W(x_{2i+1}), \quad x_{2i+1} \leq x < x_{2i+2}.$

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$$\Rightarrow \; W_i(x) > 0 \quad , \; x_{2i} < x < x_{2i+2}.$$

Coming back to $E_{s,i}(f,h)$

$$E_{s,i}(f,h) = \int_{x_{2i}}^{x_{2i+2}} W_i'(x) \, f[x_{2i}, x_{2i+1}, x_{2i+2}, x] \, dx$$

using integration by parts formula $\rightarrow$

$$= -\int_{x_{2i}}^{x_{2i+2}} W_i(x) \left(f[x_{2i}, x_{2i+1}, x_{2i+2}, x] \right)' dx$$

$$+ \underbrace{\Big\{ W_i(x) \, f[x_{2i}, x_{2i+1}, x_{2i+2}, x] \Big\}_{x_{2i}}^{x_{2i+2}}}_{= 0}$$

(by properties of W_i (i) & (ii))

$$= -\int_{x_{2i}}^{x_{2i+2}} W_i(x) \, f[x_{2i}, x_{2i+1}, x_{2i+2}, x, x] \, dx$$

(Assuming f is 4-times continuously differentiable).

$$= - f[x_{2i}, x_{2i+1}, x_{2i+2}, \xi_i, \xi_i] \int_{x_{2i}}^{x_{2i+2}} W_i(x) \, dx$$

(using weighted M.V.T. for some $\xi_i \in [x_{2i}, x_{2i+2}]$.)

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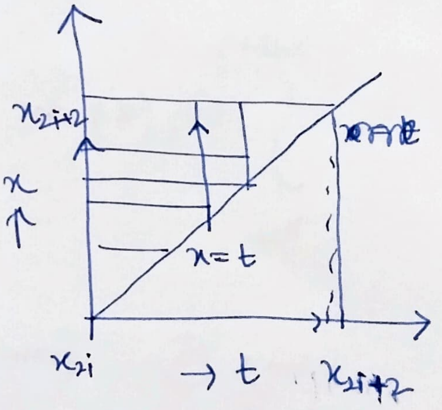
$$E_{s,i}(f,h) = -\frac{f^4(\eta_i)}{\lfloor 4}\int_{x_{2i}}^{x_{2i+2}} W_i(x)\,dx \longrightarrow (1)$$

(Again by Generalized M.V.T.

$\exists\ \eta_i \in (x_{2i}, x_{2i+2})$

$f[x_{2i}, x_{2i+1}, x_{2i+2}, \xi_i, \xi_i] = \frac{f^4(\eta_i)}{\lfloor 4}$)

$$\int_{x_{2i}}^{x_{2i+2}} W_i(x)\,dx = \int_{x_{2i}}^{x_{2i+2}}\int_{x_{2i}}^{x} g(t)\,dt\,dx$$



$$= \int_{x_{2i}}^{x_{2i+2}}\int_{t}^{x_{2i+2}} g(t)\,dx\,dt$$

$$= \int_{x_{2i}}^{x_{2i+2}} (x_{2i+2} - t)\,g(t)\,dt$$

$$= -\int_{x_{2i}}^{x_{2i+2}} (t - x_{2i})(t - x_{2i+1})(t - x_{2i+2})^2\,dt$$

$t - x_{2i+1} = r$

$$= -\int_{-h}^{h} (r+h)\,r\,(r-h)^2\,dr$$

$\boxed{\text{P-4}}$

$$= -\int_{-h}^{h} (r^2-h^2)(r^2-rh)\,dr$$

$$= -\int_{-h}^{h} \left[r^4 - r^2h^2 - r^3h + rh^3\right] dr$$

$$= -2\int_{0}^{h} \left[r^4 - r^2h^2\right] dr \qquad \left[\begin{array}{l} \int_{-h}^{h} r^3 h\,dr = 0 \\ \int_{-h}^{h} r h^3\,dr = 0 \\ \text{(odd fn.)} \end{array}\right]$$

$$= -2\cdot\left[\frac{r^5}{5} - \frac{r^3h^2}{3}\right]_0^h.$$

$$= -\frac{2}{15}\left(3h^5 - 5h^5\right)$$

$$\int_{x_{2i}}^{x_{2i+2}} w_i(x)\,dx = \frac{4h^5}{15}. \longrightarrow (2)$$

using (2) from (1) $E_{s,i}(f,h) = -\frac{f^4(\eta_i)}{\lfloor 4}\cdot\frac{4h^5}{15}$

$$= -\frac{h^5}{90} f^{iv}(\eta_i)$$

And Total Error.

$$E_s(f,h) = -\sum_{i=0}^{n-1} \frac{h^5}{90} f^{iv}(\eta_i) = -\frac{h^4}{90}\cdot h \sum_{i=0}^{n-1} f^{iv}(\eta_i)$$

$$= -\frac{h^4}{90}\cdot\frac{(b-a)}{2n}\sum_{i=0}^{n-1} f^{iv}(\eta_i).$$

$$= -\frac{h^4(b-a)}{180}\left\{\frac{1}{n}\sum_{i=0}^{n-1} f^{iv}(\eta_i)\right\}$$

$$E_s(f,h) = -\frac{h^4(b-a)}{180} f^{iv}(\eta) \quad \text{for some } \eta \in [a,b].$$

$$|E_s(f,h)| \leq \frac{h^4(b-a)}{180} \max_{x\in[a,b]} |f^{iv}(x)| = O(h^4).$$

1. Newton - Cotes integration formula

We now generalize the previous formulas for $(n+1)$ pts. formula.

Let us consider the interval $[c, d]$, $c < d$.

For $n \in \mathbb{N}$, $h = \frac{d-c}{n}$, $x_i = c + ih$

$i = 0, \ldots, n$

We define $I_n(f)$ by replacing f by its interpolating polynomial $P_n(x)$ on the nodes $x_0, x_1, \ldots, x_n$.

$$I(f) = \int_c^d f(x)\,dx, \quad I_n^c(f) = \int_c^d P_n(x)\,dx$$

Idea: $I(f) \approx I_n^c(f)$.

Using Lagrange form of interpolating polynomial

$$P_n(x) = \sum_{i=0}^{n} L_{i,n}(x) f(x_i) \quad \text{we get}$$

$$I_n^c(f) = \int_c^d P_n(x)\,dx = \sum_{i=0}^{n} f(x_i) \int_c^d L_{i,n}(x)\,dx$$

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$$I_n^c(f) = \sum_{i=0}^{n} f(x_i)\, w_{i,n}, \longrightarrow (1)$$

where $\displaystyle w_{i,n} = \int_c^d L_{i,n}(x)\,dx.$

$i = 0, 1, \ldots, n.$

The $(n+1)$ pt. closed Newton-Cotes formula is given by (1).

Theorem 1

Let $h = \frac{d-c}{n}$, $x_i = a + ih$, $i = 0, \ldots, n$.

Let $(n+1)$-pt. Newton-Cotes formula is given in (1).

(i) If n is even and f is of class C^{n+2} (i.e. f is $(n+2)$-times continuously differentiable),

Then, $\exists\ \xi \in (c,d)$ such that

$$\int_c^d f(x)\,dx = I_n^c(f) + \frac{h^{n+3}}{\lfloor n+2} f^{n+2}(\xi) \int_0^n t^2 (t-1)\cdots(t-n)\,dt$$

i.e. the error $E_n(f) = I(f) - I_n^c(f)$

$$= \frac{h^{n+3}}{\lfloor n+2} f^{n+2}(\xi) \int_0^n t^2 (t-1)\cdots(t-n)\,dt. \longrightarrow (2)$$

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(ii) If n is odd and f is of class C^{n+1},

then, $\exists\ \xi \in (c,d)$ such that

$$\int_c^d f(x)\,dx = I_n^c(f) + \frac{h^{n+2} f^{n+1}(\xi)}{\lfloor n+1}\int_0^n t(t-1)\cdots(t-n)\,dt$$

i.e. the error $E_n(f,h) = I(f) - I_n^c(f)$

$$= \frac{h^{n+2} f^{n+1}(\xi)}{\lfloor n+1}\int_0^n t(t-1)\cdots(t-n)\,dt. \longrightarrow (3)$$

proof: (i) $n =$ even

Using the error formula for interpolation we can write

$$E_n(f,h) = \int_c^d \underbrace{(x-x_0)(x-x_1)\cdots(x-x_n)}_{g_n(x)} f[x_0,x_1,\ldots,x_n,x]\,dx$$

Define $W_n : [c,d] \to \mathbb{R}$ by

$$W_n(x) = \int_c^x g_n(t)\,dt, \quad c \le x \le d.$$

properties of W

i) $W_n(c) = 0$.

ii) $W_n(d) = \int_c^d g_n(t)\,dt.$

$\boxed{\text{P-4}}$

$$W_n(d) = \int_c^d (t-x_0)\cdots(t-x_n)\,dt$$

~~n = even~~

~~n = 2k.~~

$$= \int_{x_0}^{x_n} (t-x_0)\cdots(t-x_{n/2})\cdots(t-x_n)\,dt$$

$c = x_0$

$d = x_n.$

$$= \int_{-\frac{n}{2}h}^{\frac{nh}{2}} \left(r+\tfrac{n}{2}h\right)\left(r+\left(\tfrac{n}{2}-1\right)h\right)\cdots(r+h)\,r\,(r-h)\cdots\left(r-\tfrac{n}{2}h\right)dr$$

$t - x_{n/2} = r$

$t - x_i = r + x_{n/2} - x_i$

$= r + (n/2 - i)h.$

$$= \int_{-\frac{nh}{2}}^{\frac{nh}{2}} \left(r^2 - \frac{n^2h^2}{4}\right)\left(r^2 - \left(\tfrac{n}{2}-1\right)^2 h^2\right)\cdots\left(r^2-h^2\right) r\,dr$$

$= 0$ (odd. integrand)

iii) $W_n(x) \geq 0$, $c \leq x \leq d$

$$W_n'(x) = \begin{cases} 0, & x = x_i,\ i = 0,\ldots,n. \\ >0, & x_{2k} < x < x_{2k+1},\quad k = 0,\ldots,n/2-1 \\ <0, & x_{2k+1} < x < x_{2k+2},\quad k = 0,\ldots,n/2-1 \end{cases}$$

Using similar analysis as in case of Simpson's rule

$W_n(x) \geq 0$, $c \leq x \leq d$.

Now we have

$$E_n(f) = \int_c^d W_n'(x)\, f[x_0, x_1, \dots, x_n, x]\, dx$$

$$= -\int_c^d W_n(x)\, f[x_0, x_1, \dots, x_n, x, x]\, dx$$

$$+ \underbrace{\left\{ W_n(x)\, f[x_0, x_1, \dots, x_n, x] \right\}_{x_0}^{x_n}}_{= 0}$$

(using integration by parts formula)

$$= -\int_c^d W_n(x)\, f[x_0, x_1, \dots, x_n, x, x]\, dx$$

$$= -f[x_0, x_1, \dots, x_n, \eta, \eta] \int_c^d W(x)\, dx$$

(by weighted M.V.T.)

$$= -\frac{f^{n+2}(\xi)}{\lfloor n+2} \int_c^d W_n(x)\, dx$$

(by generalized M.V.T as f is of class C^{n+2}).

P-6

$$\int_c^d W_n(x)\,dx = \int_c^d \int_c^x g_n(t)\,dt\,dx$$

$$= \int_c^d \int_t^d g_n(t)\,dx\,dt$$

$$= \int_c^d (d-t)\, g_n(t)\,dt$$

$$= \int_{x_0}^{x_n} (t-x_0)(t-x_1)\cdots(t-x_n)(x_n-t)\,dt$$

$$= -\int_{x_0}^{x_n} (t-x_0)(t-x_1)\cdots(t-x_{n-1})(t-x_n)^r\,dt$$

put $t = x_0 + rh.$

$$= -\int_0^n rh\,(r-1)h \cdots (r-n+1)h\,(r-n)^r h^r\,h\,dr$$

$$= -h^{n+3} \int_0^n r(r-1)\cdots(r-n+1)(r-n)^r\,dr$$

$$= -h^{n+3} \int_0^n (n-t)(n-1-t)\cdots(1-t)\,t^r\,dt \quad n-r=t$$

$$= -h^{n+3} \int_0^n t^r(t-1)\cdots(t-n)\,dt$$

($\because$ n is even no sign change occurs).

Hence,

$$E_n(f,h) = \frac{h^{n+3} f^{n+2}(\xi)}{\lfloor n+2} \int_0^n t^r(t-1)\cdots(t-n)\,dt.$$

$\boxed{\text{Lecture-26}}$

$\boxed{\text{P-7}}$

(ii) $n =$ odd.

As before $$E_n(f,h) = \int_c^d g_n(x)\, f[x_0, x_1, \dots, x_n, x]\,dx.$$

where $$g_n(x) = (x-x_0)\cdots(x-x_n).$$

Defined $W_n : [c,d] \to \mathbb{R}$ by

$$W_n(x) = \int_c^x g(t)\,dt, \quad c \le x \le d$$

$$E_n(f,h) = \int_c^d g_n(x)\, f[x_0, x_1, x_2, \dots, x_n, x]\,dx$$

$$= \int_c^{d-h} g_n(x)\, f[x_0, x_1, x_2, \dots, x_n, x]\,dx$$

$$+ \int_{d-h}^{d} g_n(x)\, f[x_0, x_1, x_2, \dots, x_n, x]\,dx$$

$$\cancel{= L_1 + L_2}$$

$$\cancel{L_2 = \int_{x_{n-1}}^{x_n} (x-x_0)\cdots(x-x_n)\, f[x_0, x_1, \dots, x_n, x]\,dx}$$

$$\cancel{= f[x_0, x_1, \dots, x_n, \xi_2] \int_{x_{n-1}}^{x_n} g(x)\,dx.}$$

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$$E_n(f;h) = L_1 + L_2 \longrightarrow (6)$$

where $L_1 = \int_c^{d-h} g_n(x)\, f[x_0, x_1, \ldots, x_n, x]\, dx$

and $L_2 = \int_{d-h}^{d} g_n(x)\, f[x_0, x_1, \ldots, x_n, x]\, dx$

$$= \int_{x_{n-1}}^{x_n} g_n(x)\, f[x_0, x_1, \ldots, x_n, x]\, dx$$

$\left(\because \begin{array}{l} x_{n-1} = d-h \\ x_n = d \end{array}\right)$.

Note that $g_n(x) = (x-x_0)(x-x_1)\cdots(x-x_n) < 0$

$x_{n-1} < x < x_n$

By weighted M.V.T. $\exists\ \xi_2 \in (x_{n-1}, x_n)$.

$$L_2 = f[x_0, x_1, \ldots, x_n, \xi_2] \int_{x_{n-1}}^{x_n} g_n(x)\, dx$$

$$L_2 = \frac{f^{n+1}(\eta_2)}{\lfloor n+1} \int_{x_{n-1}}^{x_n} g_n(x)\, dx. \longrightarrow (7)$$

for some $\eta_2 \in (x_{n-1}, x_n)$.

To estimate L_1.

we note that

~~$(x-x_n) f[x_0, x_1, \ldots, x_n, x] = f[x_1, x_2, \ldots, x_n, x] - f[x_0, x_1, \ldots, x_n]$~~

$$f[x_0, x_1, \ldots, x_{n-1}, x_n, x]$$

$$= \frac{f[x_0, x_1, \ldots, x_{n-1}, x] - f[x_0, x_1, \ldots, x_{n-1}, x]}{(x - x_n)}$$

$$\Rightarrow (x - x_n)\, f[x_0, x_1, \ldots, x_{n-1}, x_n, x]$$

$$= f[x_0, x_1, \ldots, x_{n-1}, x] - f[x_0, x_1, \ldots, x_{n-1}, x]$$

Now,

$$L_1 = \int_c^{d-h} g_n(x)\, f[x_0, x_1, \ldots, x_n, x]\, dx$$

$$= \int_{x_0}^{x_{n-1}} \underbrace{(x - x_0) \cdots (x - x_{n-1})}_{g_{n-1}(x)} \underbrace{(x - x_n)\, f[x_0, x_1, \ldots, x_n, x]}\, dx$$

$$= \int_{x_0}^{x_{n-1}} W_{n-1}'(x)\, f[x_0, x_1, \ldots, x_{n-1}, x]\, dx$$

$$- \int_{x_0}^{x_{n-1}} W_{n-1}'(x)\, f[x_0, x_1, \ldots, x_n]\, dx$$

$$= -\int_{x_0}^{x_{n-1}} W_{n-1}(x)\, f[x_0, x_1, \ldots, x_{n-1}, x, x]\, dx$$

$$+ \Big\{ W_{n-1}(x)\, f[x_0, x_1, \ldots, x_{n-1}, x] \Big\}_{x_0}^{x_{n-1}}$$

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$$- f[x_0, x_1, \ldots, x_n] \int_{x_0}^{x_{n-1}} W'_{n-1}(x)\, dx$$

$$\Rightarrow L_1 = - f[x_0, x_1, \ldots, x_{n-1}, \xi_1, \xi_1] \int_{x_0}^{x_{n-1}} W_{n-1}(x)\, dx$$

$$+ 0 + 0 \qquad [\because W_{n-1}(x_0) = 0 = W_{n-1}(x_{n-1})]$$

$$= \frac{-f^{n+1}(\eta_1)}{\lfloor n+1} \int_{x_0}^{x_{n-1}} W_{n-1}(x)\, dx \quad \text{for some } \eta_1 \in (x_0, x_{n-1}).$$

$$\longrightarrow (8)$$

Combining we have

$$E_n(f,h) = -\frac{f^{n+1}(\eta_1)}{\lfloor n+1} \int_{x_0}^{x_{n-1}} W_{n-1}(x)\, dx + \frac{f^{n+1}(\eta_2)}{\lfloor n+1} \int_{x_{n-1}}^{x_n} g_n(x)\, dx$$

$$= -\left[\frac{f^{n+1}(\eta_1)}{\lfloor n+1} A_n + \frac{f^{n+1}(\eta_2)}{\lfloor n+1} B_n\right]$$

where $A_n = \int_{x_0}^{x_{n-1}} W_{n-1}(x)\, dx$, $B_n = -\int_{x_{n-1}}^{x_n} g_n(x)\, dx$

Now, $$\int_{x_0}^{x_{n-1}} g_n(x)\,dx = \int_{x_0}^{x_{n-1}} g_{n-1}(x)(x-x_n)\,dx$$

$$= \int_{x_0}^{x_{n-1}} \omega_{n-1}'(x)(x-x_n)\,dx$$

$$= -\int_{x_0}^{x_{n-1}} \omega_{n-1}(x)\,dx + \underbrace{\left\{\omega_{n-1}(x)(x-x_n)\right\}_{x_0}^{x_{n-1}}}_{=0}$$

$$\int_{x_0}^{x_{n-1}} g_n(x)\,dx = -\int_{x_n}^{x_{n-1}} \omega_{n-1}(x)\,dx \longrightarrow (*)$$

$$\therefore\quad A_n + B_n = \int_{x_0}^{x_{n-1}} \omega_{n-1}(x)\,dx - \int_{x_{n-1}}^{x_n} g_n(x)\,dx$$

$$= -\int_{x_0}^{x_{n-1}} g_n(x)\,dx - \int_{x_{n-1}}^{x_n} g_n(x)\,dx \quad (\text{using } (*))$$

$$= -\int_{x_0}^{x_n} g_n(x)\,dx \longrightarrow (9)$$

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using ⑨ we have

$$E_n(f,h) = -\left[\frac{f^{n+1}(\eta_1)}{\underline{|n+1}}\frac{A_n}{A_n+B_n} + \frac{f^{n+1}(\eta_2)}{\underline{|n+1}}\frac{B_n}{A_n+B_n}\right](A_n+B_n)$$

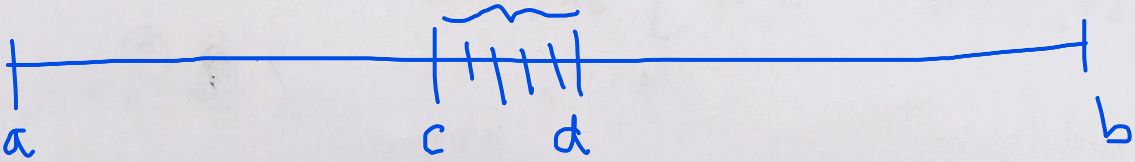
$$= -\frac{f^{n+1}(\eta)}{\underline{|n+1}}.(A_n+B_n)$$

for some $\eta \in (x_0, x_n)$.

$$E_n(f,h). = \frac{f^{n+1}(\eta)}{\underline{|n+1}}\int_{x_0}^{x_n} g_n(x)\,dx$$

$$E_n(f,h) = \frac{h^{n+2} f^{n+1}(\eta)}{\underline{|n+1}}\int_0^n t(t-1)\cdots(t-n)\,dt$$

$\eta \in (x_0, x_n)$ using a change of variable as before in case (I).



To get composite N-C formula, we divide $(b-a)/N$, where $N = kn$, $k \in \mathbb{N}$.

Lecture-26

Examples:

N=1 : Trapozoidal rule

$$I_1(f) = \frac{h}{2}\left(f(x_0) + f(x_1)\right)$$

$$E_1(f) = -\frac{h^3}{12} f''(\xi), \quad x_0 < \xi < x_1$$

N=2 : Simpson's 1/3 rule

$$I_2(f) = \frac{h}{3}\left(f(x_0) + 4f(x_1) + f(x_2)\right)$$

$$E_2(f) = -\frac{h^5}{90} f^{iv}(\xi), \quad x_0 < \xi < x_2$$

N=3 : Simpson's 3/8 rule.

$$I_3(f) = \frac{3h}{8}\left(f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)\right)$$

$$E_3(f) = -\frac{3h^5}{80} f^{iv}(\xi)$$

N=4 : ~~Milne's~~ Boole's rule

$$I_4 = \frac{2h}{45}\left(7f(x_0) + 32f(x_1) + 12f(x_2) + 32f(x_3) + 7f(x_4)\right)$$

$$E_4(f) = -\frac{8h^7}{945} f^{vi}(\xi).$$

N=6 : Weddle's rule.

P-14

2. Open Newton-Cotes Formula

The open Newton-cotes formula do not include the end points of $[c, d]$ as nodes:

It uses grids $x_i = x_0 + ih$,

$$i = 0, \ldots, n$$

$$h = \frac{d-c}{(n+2)}, \quad x_0 = c+h.$$

$$x_n = x_0 + nh$$
$$= d - h.$$

$\therefore$ ~~...~~

We lebel the end points as $x_{-1} = c$, $x_{n+1} = d$.

The open N-C quadrature formula is given by

$$I_n^o(f) = \sum_{i=0}^{n} w_{i,n} f(x_i), \longrightarrow (10)$$

$$w_{i,n} = \int_c^d L_{i,n}(x)\, dx.$$

Theorem 2 Let (10) denotes the $(n+1)$ pts open Newton-Cotes Formula with $x_{-1} = c$, and $x_{n+1} = d$, $h = \frac{d-c}{n+2}$.

(i) If n is even and f is of class C^{n+2}.

Then, $\exists\ \xi \in (c,d)$ such that

$$\int_c^d f(x)\,dx = I_n^0(f) + \frac{h^{n+3} f^{n+2}(\xi)}{\lfloor n+2} \int_{-1}^{n+1} t^2(t-1)\cdots(t-n)\,dt$$

i.e. the error term $E_n(f,h) = I(f) - I_n^0(f)$ is given by

$$E_n(f,h) = \frac{h^{n+3}}{\lfloor n+3} f^{n+2}(\xi) \int_{-1}^{n+1} t^2(t-1)\cdots(t-n)\,dt$$

(ii) If n is odd and f is of class C^{n+1}.

Then, $\exists\ \xi \in (c,d)$ such that

$$\int_c^d f(x)\,dx = I_n^0(f) + \frac{h^{n+2} f^{n+1}(\xi)}{\lfloor n+1} \int_{-1}^{n+1} t(t-1)\cdots(t-n)\,dt$$

and the error term $E_n(f,h) = I_n(f) - I_n^0(f)$ is given by

$$E_n(f,h) = \frac{h^{n+2} f^{n+1}(\xi)}{\lfloor n+1} \int_{-1}^{n+1} t(t-1)\cdots(t-n)\,dt.$$

Proof: See. (Issacson & Keller: Analysis of Numerical methods p: 313-314)

$\boxed{P-16}$

$N=0$: Midpoint rule.

$$I_0(f) = 2h\,f(x_0)$$

$$E_0(f) = \frac{h^3}{3} f''(\xi), \qquad x_{-1} < \xi < x_1$$

$N=1$,

$$I_1(f) = \frac{3h}{2}\left(f(x_0) + f(x_1)\right)$$

$$E_1(f) = \frac{3h^3}{4} f''(\xi), \qquad x_{-1} < \xi < x_2$$

$N=2$.

$$I_2(f) = \frac{4h}{3}\left(2f(x_0) - f(x_1) + 2f(x_2)\right)$$

$$E_3(f) = \frac{14h^5}{45} f^{iv}(\xi), \qquad x_{-1} < \xi < x_3.$$

$\boxed{\text{Defn.}}$ (Degree of accuracy or precision of a quadrature rule).

The degree of accuracy of a quadrature rule is the largest positive integer n such that, the formula is exact for polynomial of degree less than or equal to n. (ie. $E(x^k)=0$ for $k=0,\dots,n$.)

Eg: (1) Trapezoidal, degree of accuracy $= 1$

(2) Simpson's 1/3, " " " $= 3$

(4) Newton-Cotes $\longrightarrow$ $n+1$, n even

$\qquad\qquad\qquad\quad\ \longrightarrow$ n, n odd.

1. Gauss quadrature rule:

So far we have discussed numerical integration ~~~~ rules ~~~~ of the form

$$\int_a^b f(x)\,dx \approx w_0 f(x_0) + w_1 f(x_1) + \cdots + w_n f(x_n),$$

where we fixed the nodes/grids $x_i \in [a,b]$ and we adjust the weights. we get certain degree of accuracy. For example;

Trapozoidal rule:

$$x_0 = a,\quad x_1 = b,\quad \omega_0 = \omega_1 = \frac{b-a}{2}$$

Simpson's rule:

$$x_0 = a,\quad x_1 = \frac{a+b}{2},\quad x_2 = b,$$

$$\omega_0 = \omega_2 = \frac{1(b-a)}{6},\quad \omega_1 = \frac{2(b-a)}{3}$$

To ~~~~ increase the degree of accuracy we use the idea of Gauss.

Idea: Allow both the nodes x_i and the weights ω_i to be adjusted to achieve high accuracy.

P-2

Gaussian quadrature rule chooses the nodes x_i and weight ω_i $(i = 0, 1, \dots, n)$ such that the algorithm gives the exact value for a polynomial function p of highest possible degree m:

$$\int_a^b p(x)\,dx = \omega_0 p(x_0) + \omega_1 p(x_1) + \dots + \omega_n p(x_n),$$

$$:= G(p)$$

(1) if p is a polynomial of degree m.

Here m is called the degree of precision.

The weights $\omega_0, \omega_1, \dots, \omega_n$ in the approximation formula are arbitrary and the nodes $x_0, x_1, \dots, x_n$ are restricted only by the fact that $x_i \in [a, b]$ $\forall i = 0, \dots, n$

This gives us $2(n+1)$ parameters, to choose.

If the co-efficients of a polynomial are considered parameters, the class of polynomials of degree at most $2n+1$ also contains $2n+2$ parameters.

Therefore, this is the largest degree of polynomials for which it is reasonable to expect the formula ① (R.H.S) to be exact.

We now explain the situation for particular case.

Let us consider the interval $[-1, 1]$.

Case: 1. $n = 0$

There are two parameters ω_0, x_0. We consider requiring

$$\int_{-1}^{1} P(x)\, dx = \omega_0 P(x_0),$$

P is a polynomial of degree 1.

$(\because 2n+1 = 2\times 0+1 = 1)$

Take $P(x) = 1 \Rightarrow \int_{-1}^{1} 1\, dx = \omega_0 \Rightarrow \omega_0 = 2$

$P(x) = x \Rightarrow \int_{-1}^{1} x\, dx = \omega_0 x_0 \Rightarrow \omega_0 x_0 = 0$

$\Rightarrow x_0 = 0 \quad (\because \omega_0 = 2)$

Thus the formula becomes

$$G(P) = 2P(0).$$

$$\therefore I(f) \simeq G(f) = 2f(0). \longrightarrow ②$$

$\boxed{P-4}$ Case: 2. $n = 1$

There are four parameters $\omega_0, \omega_1, x_0, x_1$.

We consider requiring

$$\int_{-1}^{1} p(x)\,dx = \omega_0 p(x_0) + \omega_1 p(x_1),$$

for p polynomial of degree 3.

($\because 2\times 1 + 1 = 3$.)

$$\left.\begin{aligned}
&\text{Take } p(x) = 1 \Rightarrow \omega_0 + \omega_1 = \int_{-1}^{1} 1\,dx = 2 \\
&p(x) = x, \Rightarrow \omega_0 x_0 + \omega_1 x_1 = \int_{-1}^{1} x\,dx = 0 \\
&p(x) = x^2, \Rightarrow \omega_0 x_0^2 + \omega_1 x_1^2 = \int_{-1}^{1} x^2\,dx = 2/3 \\
&p(x) = x^3, \Rightarrow \omega_0 x_0^3 + \omega_1 x_1^3 = \int_{-1}^{1} x^3\,dx = 0.
\end{aligned}\right\} \rightarrow (3)$$

System (3) (non-linear) has unique soln.

$$\omega_0 = \omega_1 = 1, \quad x_0 = -\frac{1}{\sqrt{3}}, \quad x_1 = \frac{1}{\sqrt{3}}.$$

Therefore, the Gauss quadrature formula becomes

$$G(P) = P\left(-\frac{1}{\sqrt{3}}\right) + P\left(\frac{1}{\sqrt{3}}\right).$$

$$\therefore I(f) \approx G(f) = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) \longrightarrow (4)$$

Case 3. General n.

There are $2n+2$ free parameters $\{w_i\}_{i=0}^{n}$ and $\{x_i\}_{i=0}^{n}$. We would guess that there is a formula $G(f) = \sum_{i=0}^{n} w_i f(x_i)$ that uses $(n+1)$ nodes and gives a degree of precision $2n+1$.

The equation to be solved here are

$$\sum_{i=0}^{n} w_i x_i^k = \begin{cases} 0, & k = 1, 3, \dots, 2n+1 \\ \frac{2}{k+1}, & k = 0, 2, \dots, 2n \end{cases} \longrightarrow (5)$$

System (5) is a system of non-linear equations and their solvability is not at all obvious.

There is general technique to get solns of (5) (see: Atkinson, p-272).

We will describe here particular technique, which uses the Legendre polynomials.

~~The~~ This technique is used to determine the nodes and weights for $G(f)$.

P-6

Def^n. (Legendre polynomials)

It is a collection of polynomials

$\{P_0, P_1, \ldots, P_n, \ldots\}$ with the properties.

(i) For each $n \in \mathbb{N} \cup \{0\}$, P_n is a monic polynomtal of degree n.

(ii) $$\int_{-1}^{1} P(x) P_n(x)\,dx = \langle P, P_n \rangle_{L^2(-1,1)} = 0,$$

for any polynomial P of degree less than n.

There are other definitions of Legendre polynomials.

For eg. (1) They are sol^n. of the 2nd order ODE

$$(1-x^2) P_n''(x) - 2x P_n'(x) + n(n+1) P_n(x) = 0$$

$|x| \leq 1$.

(2) Rodrigues' formula:

$$P_n(x) = \frac{1}{2^n \lfloor n} \frac{d^n}{dx^n} (x^2-1)^n.$$

Other defn.s ~~a~~ are also there.

First few Legendre polynomials are:

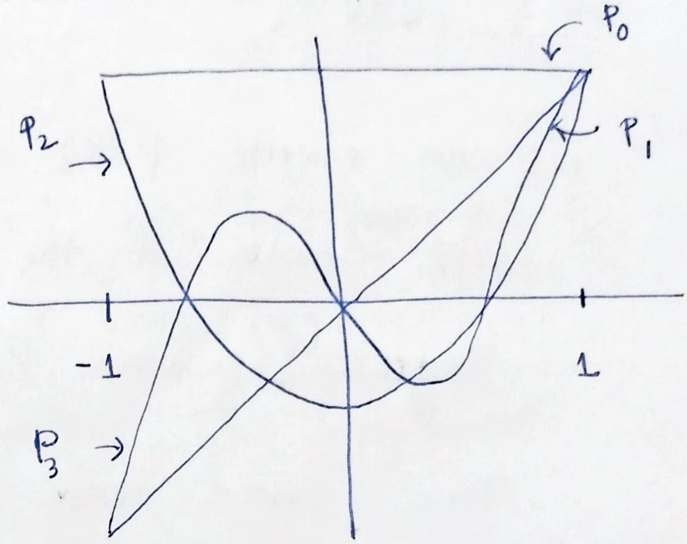
$P_0(x) = 1$

$P_1(x) = x$

$P_2(x) = x^2 - \frac{1}{3}$

$P_3(x) = x^3 - \frac{3}{5}x$

$P_4(x) = x^4 - \frac{6}{7}x^2 + \frac{3}{35}$



We observe that

(i) The roots of these polynomials are real distinct and lie in the interval $(-1, 1)$.

(ii) They are symmetrically spaced with respect to origin.

Theorem 1 Let $\{x_0, x_1, \ldots, x_n\}$ are the roots of the $(n+1)$th Legendre polynomials P_{n+1} for $n \in \mathbb{N} \cup \{0\}$.

Then,
$$\int_{-1}^{1} P(x)\,dx = \sum_{i=0}^{n} w_i P(x_i),$$

for any polynomial P of degree less than $2n+2$,

and w_i's are given by
$$w_i = \int_{-1}^{1} \prod_{\substack{k=0 \\ k \neq i}}^{n} \frac{(x - x_k)}{(x_i - x_k)}\,dx.$$

$i = 0, \ldots, n.$

P-8 proof

Case 1: ~~Let~~ P be a polynomial of degree less than $\lfloor n+1$.

We can rewrite $P(x)$ in terms of Lagrange form with nodes at the roots of the $(n+1)$th ~~degree~~ Legendre Polynomial $P_{n+1}(x)$.

The error term for this representation involves $(n+1)$ derivative of P.

Since degree of P is less than $(n+1)$, so the error term is zero.

$$P(x) = \sum_{i=0}^{n} L_{i,n}(x)\, P(x_i) + \underbrace{\frac{P^{n+1}(\xi)\,\psi_n(x)}{\lfloor n+1}}_{0}$$

$$\psi_n(x) = (x-x_0)\cdots(x-x_n).$$

$$\therefore\ P(x) = \sum_{i=0}^{n} L_{i,n}(x)\, P(x_i)$$

$$L_{i,n}(x) = \prod_{\substack{k=0\\k\neq i}}^{n} \frac{(x-x_k)}{(x_i-x_k)}$$

Now, $$\int_{-1}^{1} P(x)\,dx = \sum_{i=0}^{n} P(x_i)\int_{-1}^{1} L_{i,n}(x)\,dx = \sum_{i=0}^{n} w_i\, P(x_i).$$

(proved).

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Case 2: degree of P greater than equal to $(n+1)$ but less than $2n+2$.

Divide the polynomial by the $(n+1)$ the Legendre polynomial $P_{n+1}(x)$.

Using division algorithm, $\exists$ unique polynomial Q and R such that

$$P(x) = Q(x) P_{n+1}(x) + R(x), \quad (6)$$

so that $R(x) \equiv 0$ or $0 \leq$ degree $R < n+1$

and degree of $Q < n+1$.

As $\{x_i\}_{i=0}^{n}$ are the roots of $P_{n+1}(x)$, so we have

$$P(x_i) = Q(x_i) P_{n+1}(x_i) + R(x_i) = R(x_i) \quad (7)$$

$P_{n+1}(x_i) = 0$

$i = 0, \ldots, n$.

From (6), integrating

$$\int_{-1}^{1} P(x)\,dx = \int_{-1}^{1} Q(x) P_{n+1}(x)\,dx + \int_{-1}^{1} R(x)\,dx.$$

P-10

$$\int_{-1}^{1} P(x)\,dx = \int_{-1}^{1} R(x)\,dx$$ [$\because$ using prop (ii) of defn. of Legendre polynomial as deg $Q < n+1$]

$$= \sum_{i=0}^{n} w_i R(x_i)$$ [by case 1 as degree $R < n+1$]

$$\int_{-1}^{1} P(x)\,dx = \sum_{i=0}^{n} w_i P(x_i)$$ [by ⑦].

This proves the result.

2. Gaussian quadrature formula for arbitrary intervals.

The integral $\int_a^b f(x)\,dx$ can be transformed into an integral over $[-1, 1]$.

Take $x = \frac{1}{2}(b-a)t + \frac{(a+b)}{2}$, $dx = \frac{1}{2}(b-a)\,dt$

$x = a \Rightarrow t = -1$, $x = b \Rightarrow t = 1$

$$\int_a^b f(x)\,dx = \int_{-1}^{1} f\left(\tfrac{1}{2}(b-a)t + \tfrac{1}{2}(a+b)\right)\frac{(b-a)}{2}\,dt$$

$$= \int_{-1}^{1} g(t)\,dt;$$

where $g(t) = \frac{(b-a)}{2} f\left(\frac{1}{2}(b-a)t + \frac{1}{2}(a+b)\right)$, $-1 \le t \le 1$.

x

In polynomial interpolation we have seen approximation of a given function by using ~~polyn~~ interpolating polynomials.

For a function $f : [a,b] \to \mathbb{R}$, let $x_0, x_1, \ldots, x_n \in [a,b]$ be distinct pt.s in the interval.

Let $P_n(\cdot)$ be the polynomial which interpolates f. (Assuming degree of $P_n \leq n$).

* Existence and uniqueness of P_n is already proved in Polynomial interpolation.

P_n can be written as, $P_n : [a,b] \to \mathbb{R}$

$$P_n(x) = \begin{cases} \sum_{i=0}^{n} L_{i,n}(x) f(x_i) & \to \text{Lagrange} \\ f(x_0) + \sum_{i=1}^{n} \psi_{i-1}(x) f[x_0, x_1, \ldots, x_i] & \to \text{(Newton divided difference)} \end{cases}$$

where, $L_{i,n}(x) = \prod_{\substack{j=0 \\ j \neq i}}^{n} \frac{(x - x_j)}{(x_i - x_j)}$, $i = 0, 1, \ldots, n$

and

$$\psi_i(x) = \prod_{j=0}^{i} (x - x_j) = (x - x_0)(x - x_1) \cdots (x - x_i),$$

$i = 0, 1, \ldots, n-1.$

$\boxed{P-2}$ Let E_n be the error in this approximation.

Then E_n is given by

$$E_n(x) = \begin{cases} \dfrac{f^{n+1}(\xi(x))}{\lfloor n+1} \cdot \psi_n(x) & , \quad a < \xi(x) < b \text{ and } f \in C^{n+1}[a,b] \\ \text{or,} & \\ f[x_0, x_1, \ldots x_n, x] \, \psi_n(x) & , \text{if } \quad x \neq x_0, \ldots, x_n \\ 0 & , \text{if } \quad x = x_i \\ & \quad i = 0, \ldots, n. \end{cases}$$

① Use of Numerical differentiation:

(i) We can calculate derivatives of functions, whose values are given as data set, which is obtained empirically.

(ii) Numerical differentiation formulas are used in deriving numerical methods for solving ordinary and partial differential equations.

② Disadvantage of Numerical differentiation:

It is an unstable process. We cannot expect good accuracy even if the original data is accurate. We discuss this later in Round off Error instability.

③. Main ideas for Numerical differentiation:

The main approaches to deriving a numerical approximation to $f'(x)$ is to use the derivative of the interpolating polynomial $P_n(x)$, which interpolates f at a given set of distinct points $x_0, x_1, \ldots, x_n$.

Therefore, $\quad f(x) = P_n(x) + E_n(x), \quad x \in [a,b]$.

Assuming that the ~~differentiation~~ differentiation on both sides are justified, we get

$$f'(x) = P_n'(x) + E_n'(x).$$

To approximate derivative at $x \in [a,b]$ we use

$$f'(x) \approx P_n'(x).$$

The error in this approximation is $E_n'(x)$.

Now,

$$E_n'(x) = \begin{cases} \dfrac{\psi_n'(x)\, f^{n+1}(\xi(x))}{\lfloor n+1} + \psi_n(x) \dfrac{d}{dx}\left(f^{n+1}(\xi(x))\right) \\ \text{or,} \\ \psi_n'(x)\, f[x_0, x_1, \ldots, x_n, x] + \psi_n(x) \dfrac{d}{dx}\left(f[x_0, x_1, \ldots, x_n, x]\right) \end{cases}$$

Numerical

Hence, if $f \in C^{n+2}[a,b]$, the error for differentiation is given by

$$E_n'(x) = \psi_n'(x) \frac{f^{n+1}(\xi_1(x))}{\lfloor n+1} + \psi_n(x) \frac{f^{n+2}(\xi_2(x))}{\lfloor n+2}$$

(2) $\longleftarrow$ for $a < \xi_1(x), \xi_2(x) < b$.

~~Higher order differentiation formulas and~~

$$P_n'(x) = \begin{cases} \sum_{i=0}^{n} L_{i,n}'(x) f(x_i) \\ \text{or} \\ \sum_{i=1}^{n} \psi_{i-1}'(x) f[x_0, x_1, \ldots, x_i] \end{cases}$$

(3) $\longleftarrow$

Higher order differentiation formula and their error can be obtained by further differentiation of (3) and (2) respectively.

Formula (3) is called an $(n+1)$ pt. formula to approximate $f'(x)$.

The most common application of the above formula is used for $x = x_i$, $i = 0, \dots, n$ and the grid points are evenly spaced i.e.

$$x_i = x_0 + ih, \qquad i = 0, \dots, n.$$

In this case, $\psi_n(x_i) = 0$

$$\psi_n(x) = (x - x_0)(x - x_1) \cdots (x - x_n)$$

$$\psi_n(x) = \prod_{j=0}^{n} (x - x_j)$$

$$\psi_n'(x) = \sum_{i=0}^{n} \prod_{\substack{j=0 \\ j \neq i}}^{n} (x - x_j) \qquad \text{(Leibnitz Rule)}$$

$$\psi_n'(x_k) = \prod_{\substack{j=0 \\ j \neq k}}^{n} (x_k - x_j) \qquad k = 0, \dots, n.$$

$$\therefore\ E_n'(x_k) = \frac{f^{n+1}(\xi_1(x))}{\lfloor n+1} \prod_{\substack{j=0 \\ j \neq k}}^{n} (x_k - x_j). \longrightarrow (4)$$

P-6

$$P_n'(x_k) = \begin{cases} \sum_{i=0}^{n} L_{i,n}'(x_k)\, f(x_i) \\ \text{or} \\ \sum_{i=1}^{n} \psi_{i-1}'(x_k)\, f[x_0, \dots, x_i] \end{cases}$$

(5) $\leftarrow$

for $k = 0, \dots, n$.

(4). Let us consider particular examples.

(A) First order derivative.

Eg. (1) $n = 0$. $P_0(x) = f(x_0)$ $\therefore$ $P_0'(x) = 0$.

This is not a very good approximation.

(2) $n = 1$. $P_1(x) = f(x_0) + \psi_0(x) f[x_0, x_1]$

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

$$\therefore \quad P_1'(x) = f[x_0, x_1]$$

Let $x = x_0 = a$, $x_1 = x_0 + h = a + h$, $h > 0$.

$$\therefore \quad P_1'(a) = f[x_0, x_1] = \frac{f[x_1] - f[x_0]}{x_1 - x_0}$$

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

$$\therefore \quad f'(a) \approx P_1'(a) = \frac{f(a+h) - f(a)}{h}$$

Euler forward difference approx. of derivative.

By (4)

$$E_1'(a) = \frac{f^2(\xi_1)}{\lfloor 2}(x_0 - x_1) = -\frac{h}{2} f^2(\xi_1)$$

$a < \xi_1 < a+h.$

(ii) Again for $x = x_1 = a$,

Then, $x_1 = x_0 + h \Rightarrow a = x_0 + h$, $h > 0.$

$\Rightarrow x_0 = a - h$, $h > 0$

$$\therefore \quad P_1'(a) = f[x_0, x_1] = \frac{f(x_1) - f(x_0)}{x_1 - x_0}$$

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

(Euler backward difference formula of derivative).

By (4) $\quad E_1'(a) = \frac{f^2(\xi)}{\lfloor 2}(x_1 - x_0) = \frac{h}{2} f^2(\xi).$

(iii) For $x = \frac{x_0 + x_1}{2} = a.$ Let $x_1 - a = h = a - x_0 > 0$

$$P_1'(a) = \frac{f(x_1) - f(x_0)}{x_1 - x_0} = \frac{f(a+h) - f(a-h)}{2h}$$

(Centred difference formula).

P-48 By (2)

$$E_1'(a) = \psi_1'(a)\frac{f^2(\xi_1)}{\lfloor 2} + \frac{\psi_1(a) f^3(\xi_2)}{\lfloor 3}$$

$$= \left(\frac{x_0+x_1}{2} - x_0\right)\left(\frac{x_0+x_1}{2} - x_1\right)\frac{f^3(\xi_2)}{\lfloor 3}$$

$$\psi_1'(x) = (x-x_0)+(x-x_1)$$
$$= 2x - (x_0+x_1)$$
$$\psi_1'(a) = 2a - (x_0+x_1)$$
$$= 2\left(\frac{x_0+x_1}{2}\right) - (x_0+x_1)$$
$$= 0.$$

$$= -\frac{(x_1-x_0)^2}{4}\cdot\frac{f^3(\xi_2)}{\lfloor 3}$$

$$= -\frac{h^2 f^3(\xi_2)}{6}. \quad , \quad x_0 < \xi_2 < x_1.$$

Comparative study with $h>0$

	Derivative approx.	Error
Forward	$f'(a) \sim \frac{f(a+h) - f(a)}{h}$	$O(h)$
Backward	$f'(a) \sim \frac{f(a) - f(a-h)}{h}$	$O(h)$
Centred	$f'(a) \sim \frac{f(a+h) - f(a-h)}{2h}$	$O(h^2)$.

Eg.(3) $n = 2$ (i.e. 3 pt. formula to approximate $f'(x)$)

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

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

[3 pt. end pt. formula]

If $x = a = x_0$ and $x_1 = x_0 + h = a + h$, $h > 0$

$x_2 = x_0 + 2h = a + 2h$.

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

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

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

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

By (4).

Also, $E_2'(a) = \psi_2'(a) \dfrac{f^3(\xi)}{\lfloor\underline{3}} = \dfrac{(-h)(-2h) f^3(\xi)}{\lfloor\underline{3}} = \dfrac{h^2 f^3(\xi)}{3}.$

$\boxed{\text{P-10}}$

∴ [3 pt. mid pt. formula]

$\odot\odot$, $x = a = x_1$, $\quad x_1 = x_0 + h \Rightarrow x_0 = a - h.$

$$x_2 = x_1 + h \Rightarrow x_2 = a + h.$$

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

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

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

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

$$E_2'(a) = \psi_2'(a)\, \frac{f'''(\xi_1)}{\lfloor 3} = -\frac{h^2}{6} f'''(\xi_1).$$

[3 pt. end pt. formula]

$\odot\odot\odot$, $x = a = x_2$, $\quad x_2 = x_1 + h \Rightarrow x_1 = a - h$

$$x_1 = x_0 + h \Rightarrow x_0 = a - 2h.$$

$$f'(a) \sim P_2'(a) = f[a-2h, a-h] + 3h\, f[a-2h, a-h, a]$$

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

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

$$= \frac{2f(a-h) - 2f(a-2h) + 3f(a) - 6f(a-h) + 3f(a-2h)}{2h}$$

$$P_2'(a) = \frac{3f(a) - 4f(a-h) + f(a-2h)}{2h}.$$

and $E_2'(a) = \frac{h^2}{3} f'''(\xi).$

(B) 2nd order derivative.

We again note that

$$f(x) = P_n(x) + E_n(x)$$

$$f(x) = P_n(x) + \psi_n(x) f[x_0, x_1, \ldots, x_n, x]$$

$$f'(x) = P_n'(x) + \psi_n'(x) f[x_0, x_1, \ldots, x_n, x]$$
$$+ \psi_n(x) f[x_0, x_1, \ldots, x_n, x, x]$$

Differentiating again

$$f''(x) = P_n''(x) + \psi_n''(x) f[x_0, x_1, \ldots, x_n, x]$$
$$+ 2\psi_n'(x) f[x_0, x_1, \ldots, x_n, x, x]$$
$$+ \psi_n(x) f[x_0, x_1, \ldots, x_n, x, x, x]$$

P-~~11~~ 12 Again we ~~justify~~ assume that f is $(n+3)$ times continuously differentiable to justify the above differentiation on the R.H.S.

We use $P_n''(x)$ to approximate $f''(x)$.

Eg:(1) $n=2$, $x = x_0 = a$, For $h>0$ $x_1 = x_0 + h = a+h$, $x_2 = a+2h$.

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

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

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

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

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

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

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

$$E_2''(a) = 2f[a, a+h, a+2h, a, a]\,(a-x_1)(a-x_2)$$

$$+\ 2f[a, a+h, a+2h, a]\,(2a-x_1-x_2)$$

$$= \frac{h^2}{6} f^{iv}(\xi_1) - h f'''(\xi_2).$$

Similarly For, $x = x_1 = a$, $x_0 = a-h$, $x_2 = a+h$, with $h>0$

$$f''(a) \approx P_2''(a) = \frac{f(a-h) - 2f(a) + f(a+h)}{h^2}$$

$$E_2''(a) = -\frac{h^2}{12} f^{iv}(\xi).$$

and $x = x_2 = a$, $x_0 = a-2h$, $x_1 = a-h$, with $h>0$.

$$f''(a) \approx P_2''(a) = \frac{f(a) - 2f(a-h) + f(a+2h)}{h^2}$$

$$E_2''(a) = \frac{h^2}{6} f^{iv}(\xi_1) + h f'''(\xi_2).$$

Remark: In the above ~~[illegible]~~ we have used Newton divided difference form of interpolating polynomial to derive the approximation of ~~the~~ derivative. Similar way Lagrange form of interpolating polynomial could be ~~wse~~ use to derive the same.

5. Round off Error instability

Let us considere the centred difference formula or 3 pt. mid pt. formula.

we have $f'(a) = P_1'(a) + E_1'(a)$

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

Let us assume that in evaluating $f(a+h)$ and $f(a-h)$ we commit round off errors $e(a+h)$ and $e(a-h)$ respectively.

The computere accutally use the round off approximation $\bar{f}(a+h)$ and $\bar{f}(a-h)$ respectively.

ie $f(a+h) = \bar{f}(a+h) + e(a+h)$

$f(a-h) = \bar{f}(a-h) + e(a-h).$

$\therefore$ Total error in this approximations

$$E(f'(a)) = f'(a) - \frac{\bar{f}(a+h) - \bar{f}(a-h)}{h}$$

$$= \underbrace{\frac{e(a+h) - e(a-h)}{h}}_{\text{Round off error}} - \underbrace{\frac{h^2}{6} f'''(\xi_1)}_{\text{Truncation error.}}$$

$$\therefore \left| E(f'(a)) \right| = \left| \frac{e(a+h) - e(a-h)}{h} - \frac{h^2}{6} f'''(\xi_1) \right|$$

$$\leq \frac{|e(a+h)| + |e(a-h)|}{h} + \frac{h^2}{6} |f'''(\xi_1)|$$

$$\leq \frac{2\varepsilon}{h} + \frac{h^2}{6} M \quad \longrightarrow (6)$$

(Assume $|e(a \pm h)| \leq \varepsilon$ and $|f'''(\xi_1)| \leq M$. for some $\varepsilon, M > 0$).

We note that Round off error $\to 0$ as $h \to \infty$

and Truncation error $\to 0$ as $h \to 0$.

Therefore, we cannot take h very small to reduce the error because round off error may increase. To reduce error we use optimum value of h.

Here in the case above optimum value of h is

$$h_{opt} = \left(\frac{3\varepsilon}{M}\right)^{1/3} \longrightarrow (7)$$