Quadrature 13/4/2017

Newton divided difference

$$f[x_0, x_1] = \frac{f(x_1) - f(x_0)}{x_1 - x_0} = \frac{f(x_0)}{x_0 - x_1} + \frac{f(x_1)}{x_1 - x_0}$$

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

$$= \frac{f(x_2) - f(x_1)}{(x_2 - x_1)(x_2 - x_0)} - \frac{f(x_1) - f(x_0)}{(x_1 - x_0)(x_2 - x_0)}$$

$$= \frac{f(x_0)}{(x_0 - x_1)(x_0 - x_2)} - \frac{(x_1 - x_0 + x_2 - x_1)}{(x_2 - x_1)(x_2 - x_0)(x_1 - x_0)} + \frac{f(x_2)}{(x_2 - x_1)(x_2 - x_0)}$$

$$= \frac{f(x_0)}{(x_0 - x_1)(x_0 - x_2)} + \frac{f(x_1)}{(x_1 - x_0)(x_1 - x_2)} + \frac{f(x_2)}{(x_2 - x_0)(x_2 - x_1)}$$

$$\therefore \boxed{f[x_0, \dots, x_r] = \frac{f(x_0)}{(x_0 - x_1)\dots(x_0 - x_r)} + \dots + \frac{f(x_r)}{(x_r - x_0)\dots(x_r - x_{r-1})} = \frac{f[x_1, \dots, x_r] - f[x_0, \dots, x_{r-1}]}{x_r - x_0}}$$

proof:

$n=1$ is true, if $n=r$ is true $\Rightarrow$ $n=r+1$ true.

consider coeff. of $f(x_i)$:

$$\frac{1}{x_r - x_0}\left(\frac{1}{(x_i - x_1)\dots(x_i - x_r)} - \frac{1}{(x_i - x_0)\dots(x_i - x_{r-1})}\right)$$

$$= \frac{1}{x_r - x_0}\left(\frac{x_i - x_0 - (x_i - x_r)}{(x_i - x_0)\ \dots\ (x_i - x_r)}\right)$$

$$= \frac{1}{(x_i - x_0)\dots(x_i - x_r)} \qquad \square$$

13/4/2017

Quadrature

$$f[x+\varepsilon, x] = \frac{f(x+\varepsilon) - f(x)}{\varepsilon}$$

$$\lim_{\varepsilon\to 0} f[x+\varepsilon, x] = f[x,x] = \frac{df}{dx}$$

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

$$= \frac{1}{2}\,\frac{f[x+2\varepsilon, x+\varepsilon] - f[x+\varepsilon, x]}{\varepsilon}$$

$$\cancel{\frac{d^2f}{dx^2} = \frac{df}{dx} - \frac{df}{dx}}$$

$$\frac{d^2f}{dx^2} = \lim_{\Delta x\to 0} \frac{\left.\frac{df}{dx}\right|_{x+\frac{1}{2}\Delta x} - \left.\frac{df}{dx}\right|_{x-\frac{1}{2}\Delta x}}{\Delta x}$$

$$f[x+3\varepsilon, x+2\varepsilon, x+\varepsilon, x] = \frac{1}{3}\,\frac{f[x+3\varepsilon, x+2\varepsilon, x+\varepsilon] - f[x+2\varepsilon, x+\varepsilon, x]}{\varepsilon}$$

$$\frac{d^3f}{dx^3} = \lim_{\Delta x\to 0} \frac{\left.\frac{d^2f}{dx^2}\right|_{x+\frac{1}{2}\Delta x} - \left.\frac{d^2f}{dx^2}\right|_{x-\frac{1}{2}\Delta x}}{\Delta x}$$

by induction, $\frac{d^nf}{dx^n} = n!\, f[\overbrace{x, \ldots, x}^{n \text{ times}}]$

another proof: since we already know $f[x,x] = \frac{df}{dx}$

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

let $u_1, \ldots, u_n$ be function of x.

$$\frac{d}{dx} f[x_0, \ldots, x_k, u_1, \ldots, u_n] = \sum_{v=1}^{n} f[x_0, \ldots, x_k, u_1, \ldots, u_n, u_v]\frac{du_v}{dx}$$

if $u_1 = \cdots = u_n = x$, then

$$\frac{d}{dx} f[x_0, \ldots, x_k, \underbrace{x, \ldots, x}_{n \text{ times}}] = n\, f[x_0, \ldots, x_k, \underbrace{x, \ldots, x}_{n+1 \text{ times}}]$$

Quadrature

13/4/2017

$$\therefore \frac{d^n}{dx^n} f[x_0, \cdots, x_k, x] = n!\, f[x_0, \cdots, x_k, \underbrace{x, \cdots x}_{n+1 \text{ times}}]$$

$\square$

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

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

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

$f[x_1, x_0, x] = f[x_0, x_1, x]$ similarly for higher dimension

$\vdots$

$$\boxed{\begin{aligned} \therefore f(x) &= f(x_0) + (x - x_0) f[x_0, x_1] + (x - x_0)(x - x_1) f[x_0, x_1, x_2] \\ &+ \cdots + (x - x_0) \cdots (x - x_n) f[x_0, x_1, \cdots, x_{n+1}] + E(x) \\ E(x) &= (x - x_0) \cdots (x - x_{n+1}) f[x_0, \cdots, x_{n+1}, x] \end{aligned}}$$

Hermite Interpolation

$$\pi(x) = (x - x_1) \cdots (x - x_m) \quad , \quad x_1, x_2, \cdots, x_m$$

$$l(x) = \frac{\pi(x)}{(x - x_i)\pi'(x_i)} = \frac{(x - x_1) \cdots (x - x_{i-1})(x - x_{i+1}) \cdots (x - x_m)}{(x_i - x_1) \cdots (x_i - x_{i-1})(x_i - x_{i+1}) \cdots (x_i - x_m)}$$

$$\pi(x_j) = 0 \quad , \quad l_i(x_j) = \delta_{ij}$$

$$\therefore y(x) = \sum_{i=1}^{m} l_i(x) f(x_i)$$

$$E(x) = f(x) - y(x) = \pi(x) f[x_1, \cdots, x_m, x]$$

Quadrature

13/4/2017

~~###~~ consider $g(x) = f(x) - y(x) - K\pi(x)$

$g(x)$ vanishes at $x_1, \cdots, x_m$

K is chosen such that $g(x)$ also vanishes at x_{m+1},

$\therefore$ by Rolle's theorem, $g'(x)$ vanishes at m points,

so $g^{(m)}(x)$ vanishes at ξ.

Since $y(x)$ is polynomial of $m-1$ degree,

$$g^{(m)}(\xi) = 0 = f^{(m)}(\xi) - K\pi^{(m)}(\xi) = f^{(m)}(\xi) - m!K$$

$$\therefore K = \frac{f^{(m)}(\xi)}{m!}$$

$\therefore E(x) = \frac{f^{(m)}(\xi)}{m!}\pi(x)$ if $f(x)$ is m-differentiable

$\square$

consider interpolating polynomial at $x_1, \cdots, x_m$ so that $y(x_i) = f(x_i)$, $y'(x_i) = f'(x_i)$, $i = 1, \dots, m$

$$y(x) = \sum_{i=1}^{m} h_i(x) f(x_i) + \sum_{i=1}^{m} \bar{h}_i(x) f'(x_i)$$

$h_i(x_j) = \delta_{ij}$ $\quad \bar{h}_i(x_j) = 0$ $\quad\quad h_i(x), \bar{h}_i(x) \in P_{2m-1}$

$h_i'(x_j) = 0$ $\quad \bar{h}_i'(x_j) = \delta_{ij}$

assume $h_i(x) = r_i(x)[l_i(x)]^2$ $\quad\quad r_i(x), s_i(x) \in P_1$

$\bar{h}_i(x) = s_i(x)[l_i(x)]^2$

Quadrature 13/4/2017

$\therefore r_i(x_i) = 1 \quad s_i(x_i) = 0$

$i \neq j$ trivial

$r_i'(x_i)[l_i(x_i)]^2 + 2 l_i(x_i) l_i'(x_i) r_i(x_i)$

$= r_i'(x_i) + 2 l_i'(x_i) = 0$

$s_i'(x_i)[l_i(x_i)]^2 + 2 l_i(x_i) l_i'(x_i) s_i(x_i)$

$= s_i'(x_i) = 1$

thus, $r_i(x) = 1 - 2 l_i'(x_i)(x - x_i)$

$s_i(x) = x - x_i$

$$\therefore y(x) = \sum_{i=1}^{m} \left[\left(1 - 2 l_i'(x_i)(x - x_i)\right) l_i^2(x) \right] f(x_i) + \sum_{i=1}^{m} \left[(x - x_i) l_i^2(x) \right] f_i'(x_i)$$

Error: ~~[illegible]~~

$$F(x) = f(x) - y(x) - K[\pi(x)]^2$$

$F(x)$ vanishes at $m+1$ points, i.e. $x_1, \cdots, x_m, \bar{x}$

$F'(x)$ vanishes at $2m$ points, i.e. $x_1, \tilde{x}_1, \cdots, x_m, \tilde{x}_m$

$\therefore F^{(2m)}(x)$ vanishes at ξ

$$\therefore F^{(2m)}(\xi) = 0 = f^{(2m)}(\xi) - K(2m)!$$

$$\therefore K = \frac{f^{(2m)}(\xi)}{(2m)!}$$

Since $F(\bar{x}) = 0$, $E(\bar{x}) = f(\bar{x}) - y(\bar{x}) = \frac{f^{(2m)}(\xi)}{(2m)!}[\pi(\bar{x})]^2$ for any $\bar{x}$

$$\therefore E(x) = \frac{f^{(2m)}(\xi)}{(2m)!}[\pi(x)]^2$$

Quadrature

13/4/2017

divided diff. form of $E(x)$

consider interpolating polynomial $x_1, x_1', x_2, x_2', \ldots, x_m, x_m'$ and let $x_i' \to x_i$, thus

$$E(x) = [\pi(x)]^2 f[x_1, x_1, \ldots, x_m, x_m, x]$$

Hermite Quadrature

second term $f'(x_i)$?

$$\int_a^b w(x) f(x)\, dx = \sum_{i=1}^{m} H_i f(x_i) + \sum_{i=1}^{m} \bar{H}_i f'(x_i) + E$$

$$H_i = \int_a^b w(x) h_i(x)\, dx = \int_a^b w(x) [1 - 2 l_i'(x_i)(x - x_i)][l_i(x)]^2 dx$$

$$\bar{H}_i = \int_a^b w(x) \bar{h}_i(x)\, dx = \int_a^b w(x)(x - x_i)[l_i(x)]^2 dx$$

$$E = \frac{1}{(2m)!} \int_a^b f^{(2m)}(\xi) w(x) [\pi(x)]^2 dx$$

Gaussian Quadrature

$$\bar{H}_i = \int_a^b w(x)(x - x_i)[l_i(x)]^2 dx$$

$$= \int_a^b \frac{w(x)\pi(x)}{\pi_i'(x_i)} l_i(x)\, dx$$

$$= \frac{1}{\pi_i'(x_i)} \int_a^b w(x)\pi(x) l_i(x)\, dx$$

$\bar{H}_i = 0$ iff $\pi(x) \perp P_{m-1}, \ldots, P_0$, $\pi(x) \in P_m$

if $\pi(x) \perp P_{m-1}, \ldots, P_0$, thus $\int_a^b w(x)\pi(x) l_i(x)\, dx = 0$

$\therefore \bar{H}_i = 0$ because $l_i(x) \in P_{m-1}$

Quadrature 14/4/2017

if $\bar{H}_i = 0$, let $f(x) = \pi(x) u(x)$

$u(x) \in P_{m-1}$, or any polynomical inferior to degree $m-1$.

i.e. $u(x) \in P_q$, $q \leq m-1$

$$\therefore \int w(x) f(x)\, dx = 0 + 0 + 0 = 0$$

$$\int w(x) \pi(x) u(x)\, dx = 0$$

$$\therefore \pi(x) \perp u(x) \Rightarrow \pi(x) \perp P_{m-1}, \dots, P_0$$

$\square$

$$\boxed{\begin{aligned} &\int_a^b w(x) f(x)\, dx = \sum_{k=1}^{m} H_k f(x_k) + E \\ &E = \int_a^b \frac{f^{(2m)}(\xi)}{(2m)!} w(x) [\pi(x)]^2\, dx \\ &① : \pi(x) \perp P_{m-1}, \dots, P_0 \\ &② : x_1, \dots, x_m \text{ are zeros of } \pi(x) \end{aligned}}$$

note that
$$\begin{aligned} H_i &= \int_a^b w(x) h_i(x)\, dx \\ &= \int_a^b w(x) [l_i(x)]^2\, dx \\ &\quad - 2 l_i'(x_i) \int_a^b w(x)(x - x_i) [l_i(x)]^2\, dx \\ &= \int_a^b w(x) [l_i(x)]^2\, dx - 2 l_i'(x_i) \bar{H}_i \\ &= \int_0^b w(x) [l_i(x)]^2\, dx \end{aligned}$$

Quadrature 14/4/2017

let $f(x) = l_i(x)$

$$\therefore \int_a^b w(x) f(x)\, dx = \int_a^b w(x) l_i(x)\, dx = \sum_{k=1}^{m} H_k l_i(x_k) = H_i$$

$$= \int_a^b w(x) [l_i(x)]^2 dx$$

$$\therefore \int_a^b w(x) f(x)\, dx = \sum_{k=1}^{m} W_k f(x_k) + E$$

$$W_k = \int_a^b w(x) l_i(x)\, dx$$

Christoffel-Darboux Identity

let $\phi_k(x)$ be orthogonal polynomial

$\phi_{k+1}(x) - x\frac{A_{k+1}}{A_k}\phi_k(x) \in P_k$, and let $a_k = \frac{A_{k+1}}{A_k}$

$$\therefore \phi_{k+1}(x) - x a_k \phi_k(x) = b_k \phi_k(x) + c_k \phi_{k-1}(x) + \ldots$$

by multiplying the above equation with $w(x)\phi_i(x)$, $i \le k-2$, and integrate, we see that … terms are zero.

$$\therefore \phi_{k+1}(x) = (a_k x + b_k)\phi_k(x) + c_k \phi_{k-1}(x)$$

$\int w(x)\phi_k^2(x)\,dx = \gamma_k$

$$\therefore \gamma_{k+1} = a_k \int_a^b x\, w(x) \phi_k(x) \phi_{k+1}(x)\, dx \quad ①$$

$$0 = a_k \int_a^b x\, w(x) [\phi_k(x)]^2 dx + b_k \gamma_k \quad ②$$

$$0 = a_k \int_a^b x\, w(x) \phi_{k-1}(x) \phi_k(x)\, dx + c_k \gamma_{k-1} \quad ③$$

① and ③ $\Rightarrow$ $c_k = -\dfrac{a_k \gamma_k}{a_{k-1}\gamma_{k-1}}$

Quadrature 14/4/2017

thus $x\frac{\phi_k(x)}{\gamma_k} = \frac{\phi_{k+1}(x)}{a_k\gamma_k} + \frac{\phi_{k-1}(x)}{a_{k-1}\gamma_{k-1}} - \frac{b_k\phi_k(x)}{a_k\gamma_k}$ $\times\phi_k(y)$

$- \quad y\frac{\phi_k(y)}{\gamma_k} = \frac{\phi_{k+1}(y)}{a_k\gamma_k} + \frac{\phi_{k-1}(y)}{a_{k-1}\gamma_{k-1}} - \frac{b_k\phi_k(y)}{a_k\gamma_k}$ $\times\phi_k(x)$

$$\therefore (x-y)\frac{\phi_k(x)\phi_k(y)}{\gamma_k} = \frac{\phi_{k+1}(x)\phi_k(y)-\phi_k(x)\phi_{k+1}(y)}{a_k\gamma_k} + \frac{\phi_{k-1}(x)\phi_k(y)-\phi_k(x)\phi_{k-1}(y)}{a_{k-1}\gamma_{k-1}}$$

sum from $k=0,m$:

$$\sum_{k=0}^{m}\frac{\phi_k(x)\phi_k(y)}{\gamma_k} = \frac{\phi_{m+1}(x)\phi_m(y)-\phi_m(x)\phi_{m+1}(y)}{a_m\gamma_m(x-y)}$$

take limit $y\to x$,

$$\sum_{k=0}^{m}\frac{[\phi_k(x)]^2}{\gamma_k} = \frac{A_m}{A_{m+1}\gamma_m}\left[\phi_{m+1}'(x)\phi_m(x)-\phi_m'(x)\phi_{m+1}(x)\right]$$

Coefficients of Gaussian Quadrature

let $\phi_m = A_m\pi(x)$, and let $y=x_i$ such that $\phi_m(x_i)=0$

$$\therefore \sum_{k=0}^{m}\frac{\phi_k(x)\phi_k(x_i)}{\gamma_k} = -\frac{\phi_m(x)\phi_{m+1}(x_i)}{a_m\gamma_m(x-x_i)}$$

ϕ_0 is a constant

$$\phi_0(x_i) = -\int_a^b \frac{w(x)\phi_0(x)\phi_m(x)\phi_{m+1}(x_i)}{a_m\gamma_m(x-x_i)}\,dx$$

$$\int_a^b\frac{w(x)\phi_m(x)}{x-x_i}\,dx = -\frac{a_m\gamma_m}{\phi_{m+1}(x_i)}$$

Quadrature 14/4/2017

$$H_i = \int_a^b w(x) l_i(x) dx$$

$$= \int_a^b w(x) \frac{\phi_m(x)}{\phi_m'(x_i)(x-x_i)} dx$$

$$= -\frac{A_{m+1}\gamma_m}{A_m \phi_m'(x_i)\phi_{m+1}(x_i)}$$

$\phi_m(x_i)=0$

$\frac{a_m}{a_{m-1}} = \frac{A_{m+1}}{A_m}\cdot\frac{A_{m-1}}{A_m}$

since $\phi_{m+1}(x) = (a_m x + b_m)\phi_m(x) - \frac{a_m \gamma_m}{a_{m-1}\gamma_{m-1}}\phi_{m-1}(x)$

$$\therefore \phi_{m+1}(x_i) = -\frac{A_{m+1}A_{m-1}}{A_m^2}\frac{\gamma_m}{\gamma_{m-1}}\phi_{m-1}(x_i)$$

$$\therefore \boxed{H_i = \frac{A_m \gamma_{m-1}}{A_{m-1}\phi_m'(x_i)\phi_{m-1}(x_i)}}$$

note that $\sum_{k=0}^{m}\frac{[\phi_k(x_i)]^2}{\gamma_k} = -\frac{A_m \phi_m'(x_i)\phi_{m+1}(x_i)}{A_{m+1}\gamma_m} = \frac{1}{H_i}$

Legendre-Gauss Quadratue

some theory of orthogonal polynomial:

$$\int_a^b w(x)\phi_r(x) q_{r-1}(x) dx = 0 \quad , q_{r-1}(x) \in P_q, \ q \leq r-1$$

assume $w(x)\phi_r(x) = \frac{d^r U_r(x)}{dx^r}$

$$\therefore \int_a^b U_r^{(r)}(x) q_{r-1}(x) dx = 0$$

$$\therefore [U_r^{(r-1)} q_{r-1} - U_r^{(r-2)} q_{r-1}' + \cdots\cdots + (-1)^{r-1} U_r q_{r-1}^{(r-1)}]_a^b = 0$$

$$\phi_r(x) = \frac{1}{w(x)}\frac{d^r U_r(x)}{dx^r}$$

$$\frac{d^{r+1}}{dx^{r+1}}\left[\frac{1}{w(x)}\frac{d^r U_r(x)}{dx^r}\right] = 0 \quad \because \phi_r(x) \in P_r$$

Quadrature 14/4/2017

thus $U_r(a) = U_r'(a) = \cdots = U_r^{(r-1)}(a) = 0$

$U_r(b) = U_r'(b) = \cdots = U_r^{(r-1)}(b) = 0$

Legendre polynomial:

$$U_r = C_r (x^2-1)^r \qquad C_r = \frac{1}{2^r (r!)}$$

$$\phi_r(x) = C_r \frac{d^r}{dx^r}(x^2-1)^r \qquad w(x) = 1$$

---

let $\pi(x) = \frac{1}{A_m} P_m(x)$, $P_m(x) = \frac{1}{2^m m!} \frac{d^m}{dx^m}(x^2-1)^m$

$$A_m = \frac{(2m)!}{2^m (m!)^2}, \quad \gamma_m = \frac{2}{2m+1}$$

$$H_i = \frac{2m \cdot (2m-1) \cdot 2}{2(m)^2(2m-1)} \frac{1}{P_m'(x_i) P_{m-1}(x_i)} = \frac{2}{m P_m'(x_i) P_{m-1}(x_i)}$$

$P_0(x) = 1$

$P_1(x) = x$

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

$P_3(x) = \frac{1}{2}(5x^3 - 3x)$

$$\int_{-1}^{1} f(x)\,dx = \sum_{k=1}^{m} H_k f(x_k) + E$$

$m = 3$:

$$\pi(x) = A_3^{-1} P_3(x) = \frac{2^3 (3!)^2}{6!} \cdot \frac{1}{2}(5x^3 - 3x) = x\left(x^2 - \frac{3}{5}\right)$$

$\therefore x_1 = -\frac{\sqrt{15}}{5} \qquad x_2 = 0 \qquad x_3 = \frac{\sqrt{15}}{5}$

$H_1 = \frac{5}{9} \qquad H_2 = \frac{8}{9} \qquad H_3 = \frac{5}{9}$

$P_4(x) = \frac{1}{8}(35x^4 - 30x^2 + 3)$

$P_5(x) = \frac{1}{8}(63x^5 - 70x^3 + 15x)$

Quadrature

14/4/2017

Hermite-Gauss Quadrature

$$a = -\infty, \quad b = \infty, \quad w(x) = e^{-\alpha^2 x^2}$$

$$\phi_r(x) = e^{\alpha^2 x^2} \frac{d^r}{dx^r}\left[C_r e^{-\alpha^2 x^2}\right]$$

$$C_r = (-1)^r, \quad \alpha^2 = 1$$

$$H_r(x) = (-1)^r e^{x^2} \frac{d^r}{dx^r}\left(e^{-x^2}\right)$$

$H_0 = 1$
$H_1 = 2x$
$H_2 = 4x^2 - 2$
$H_3 = 8x^3 - 12x$

$$\pi(x) = \frac{1}{A_m} H_m(x), \quad A_m = 2^m, \quad \gamma_m = \sqrt{\pi}\, 2^m m!$$

$$\int_{-\infty}^{\infty} e^{-x^2} f(x)\,dx = \sum_{k=1}^{m} H_k f(x_k) + E$$

$$H_i = \frac{2^m}{2^{m-1}} \frac{\sqrt{\pi}\, 2^{m-1} (m-1)!}{H_m'(x_i) H_{m-1}(x_i)} = \frac{\sqrt{\pi}\, 2^m (m-1)!}{H_m'(x_i) H_{m-1}(x_i)}$$

$m = 3$:

$$\pi(x) = \frac{1}{2^3}(8x^3 - 12x) = x\left(x^2 - \frac{3}{2}\right)$$

$$x_1 = -\frac{\sqrt{6}}{2} \qquad x_2 = 0 \qquad x_3 = \frac{\sqrt{6}}{2}$$

$$H_1 = \frac{\sqrt{\pi}}{6} \qquad H_2 = \frac{2\sqrt{\pi}}{3} \qquad H_3 = \frac{\sqrt{\pi}}{6}$$