Week 7, Thursday

△ Review: numerical integration

given $\{x_j, f(x_j)\}$ find quadrature formula

$$\int_a^b f(x)dx \approx \sum_j a_j f(x_j)$$

interpolate first, then do the integration for the interpolation

$$I_h(f) := \sum_j \int_a^b L_j(x)\,dx\, f(x_j) \approx \int_a^b f(x)\,dx$$

$$E_h(f) := \frac{1}{(n+1)!}\int_a^b f^{(n+1)}(\xi(x))\, w_{n+1}(x)\,dx.$$

① trapezoidal rule:

$$\int_a^b f(x)\,dx = \boxed{\frac{b-a}{2}\left(f(a)+f(b)\right)} - \frac{(b-a)^3}{12} f''(\xi)$$

② Simpson's rule:

$$\int_a^b f(x)\,dx = \boxed{\frac{(b-a)}{6}\left(f(a)+4f\left(\frac{a+b}{2}\right)+f(b)\right)} - \frac{(b-a)^5}{2880} f^{(4)}(\xi)$$

Composite quadrature for large $[a,b]$.

(i) composite trapezoidal rule: $x_0 = a$, $x_j = x_0 + jh$, $h = \frac{b-a}{n}$.

$$\int_a^b f(x)dx = \sum_{j=0}^{n-1}\int_{x_j}^{x_{j+1}} f(x)\,dx = \frac{h}{2}\sum_{j=0}^{n}\left(f(x_j)+f(x_{j+1})\right) - \frac{h^3}{12}\sum_{j=0}^{n-1} f''(\xi_j)$$

$$= \frac{h}{2}\left(f(x_0)+2f(x_1)+\cdots+2f(x_{n-1})+f(x_n)\right) - \frac{b-a}{12}h^2 f''(\xi)$$

$\xi\in(a,b)$, $f\in C^2[a,b]$.

(ii) Composite Simpson's rule: n (even), $x_0 = a$, $x_j = x_0 + jh$, $h = \frac{b-a}{n}$

$$\int_a^b f(x)dx = \sum_{j=0}^{\frac{n}{2}-1}\int_{x_{2j}}^{x_{2j+2}} f(x)\,dx = \frac{h}{3}\sum_{j=0}^{\frac{n}{2}-1}\left(f(x_{2j})+4f(x_{2j+1})+f(x_{2j+2})\right) - \frac{h^5}{90}\sum_{j=0}^{\frac{n}{2}-1} f^{(4)}(\xi_j)$$

$$= \frac{h}{3}\left(f(a)+2\sum_{j=1}^{\frac{n}{2}-1} f(x_{2j}) + 4\sum_{j=0}^{\frac{n}{2}-1} f(x_{2j+1}) + f(b)\right) - \frac{b-a}{180}h^4 f^{(4)}(\xi)$$

$\xi\in(a,b)$, $f\in C^4[a,b]$.

Def: the degree of accuracy, or precision, of a quadrature formula is the largest positive integer n such that the formula is exact for x^k, $k=0,1,\cdots,n$.

e.g. Trapezoidal: degree of precision 1, Simpson's: degree of precision 3.

△ Newton-Cotes formula for $\int_a^b f(x)\,dx$

(closed) $x_0 = a$, $x_i = x_0 + ih$, $i=0,1,\cdots,n$, $x_n = b$, $h = \frac{b-a}{n}$

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^n a_i f(x_i), \quad a_i = \int_a^b L_i(x)\,dx = \int_{x_0}^{x_n} \prod_{\substack{j=0\\ j\neq i}}^n \frac{x-x_j}{x_i-x_j}\,dx.$$

$\boxed{\text{Thm}}$ $\sum_{i=0}^n a_i f(x_i)$ denotes the $(n+1)$-point closed Newton-Cotes quadrature with $x_0 = a$, $x_n = b$, $h = \frac{b-a}{n}$ and $x_i = x_0 + ih$. $\exists\, \xi \in (a,b)$ s.t.

(i) n is even, $f \in C^{n+2}[a,b]$

$$\int_a^b f(x)\,dx = \sum_{i=0}^n a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_0^n t^2(t-1)\cdots(t-n)\,dt.$$

(ii) n is odd, $f \in C^{n+1}[a,b]$

$$\int_a^b f(x)\,dx = \sum_{i=0}^n a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_0^n t(t-1)\cdots(t-n)\,dt.$$

RK: even, degree of precision $n+1$; odd, degree of precision n

RK: for interpolation-related quadrature rules with precision m

$$E(f) = K f^{(m+1)}(\xi), \quad K \text{ is independent of } f.$$

$f = x^{m+1}$ $\qquad \int_a^b x^{m+1} - \sum_{j=0}^n A_j f(x_j) = (m+1)!\,K$

$$\Rightarrow K = \frac{1}{(m+1)!}\left[\frac{1}{m+2}\left(b^{m+2} - a^{m+2}\right) - \sum_{k=0}^n A_k x_k^{m+1}\right].$$

Q: what if x_j are not equally spacing, can we get better formula?

e.g. $\int_{-1}^1 f(x)\,dx = c_1 f(x_1) + c_2 f(x_2)$

$$\left.\begin{array}{lll}
\text{(i)} & f=1 & c_1 + c_2 = \int_{-1}^1 1\,dx = 2 \\
\text{(ii)} & f=x & c_1x_1 + c_2x_2 = \int_{-1}^1 x\,dx = 0 \\
\text{(iii)} & f=x^2 & c_1x_1^2 + c_2x_2^2 = \int_{-1}^1 x^2\,dx = \frac{2}{3} \\
\text{(iv)} & f=x^3 & c_1x_1^3 + c_2x_2^3 = \int_{-1}^1 x^3\,dx = 0.
\end{array}\right\} \Rightarrow \begin{array}{l} c_1 = c_2 = 1 \\ x_1 = -\frac{\sqrt{3}}{3},\ x_2 = \frac{\sqrt{3}}{3}\end{array}$$

degree of precision is $\underline{3}$ (check $f = x^4$, fail!)

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same as Simpson's rule only take 2 nodes.

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

$$\approx \frac{b-a}{2}\left[f\left(\frac{b-a}{2}\left(1-\frac{\sqrt{3}}{3}\right)+a\right)+f\left(\frac{b-a}{2}\left(1+\frac{\sqrt{3}}{3}\right)+a\right)\right]$$ error: $O((b-a)^5)$

RK: $n=3$: $\int_{-1}^1 f(x)\,dx \approx \frac{5}{9}f\left(-\sqrt{\frac{3}{5}}\right)+\frac{8}{9}f(0)+\frac{5}{9}\left(\sqrt{\frac{3}{5}}\right)$

degree of precision: $\underline{5}$ (3 nodes!).

Q: more general methods to find c_i and x_i?

$\boxed{\text{Def}}$ choose suitable points $x_0<x_1<\cdots<x_n$, $\in[a,b]$, the quadrature formula $S(f)=\sum_{j=0}^n a_j f(x_j)$, where $a_j=\int_a^b L_j(x)dx$.

If $S(f)$ has $2n+1$ degree of precision. Then: $\{x_j\}$ are called Gaussian points, the quadrature $S(f)$ is called Gaussian quadrature.

Q: how to get the general formula? $\Leftarrow$ get $\{x_j\}$ $\Leftarrow$ get $W_n(x)$.

A: $E(f)=\frac{1}{(n+1)!}\int_a^b f^{(n+1)}(\xi(x))W_n(x)dx$, $W_n(x)=(x-x_0)\cdots(x-x_n)$

RK: $P_n=\{$all polynomials of degree $\le n\}$, $\forall\, P(x)\in P_{2n+1}$, $P^{(n+1)}\in P_n$.

Claim: Gaussian quadrature $\Leftrightarrow$ $\forall\, P(x)\in P_n$, $\int_a^b P(x)W_n(x)dx=0$ ($W_n\perp P_n$).

$(\Rightarrow)$ $\forall\, p(x)\in P_n$, $P(x)W_n(x)\in P_{2n+1}$, $\int_a^b P(x)W_n(x)\,dx=\sum_{j=0}^n a_j P(x_j)\underset{0}{\underset{\parallel}{W(x_j)}}=0$

$(\Leftarrow)$ $\forall\, f\in P_{2n+1}$, $f=P(x)W_n(x)+q(x)$, degree $(P,q)\le n$. $P^{(n+1)}(\xi(x))=0$

$$\int_a^b f(x)dx=\underset{0}{\underset{\parallel}{\int_a^b P(x)W_n(x)dx}}+\int_a^b q(x)dx=\int_a^b q(x)dx=\sum_{j=0}^n a_j\,q(x_j)$$

$$=\sum_{j=0}^n a_j\left(q(x_j)+P(x_j)\overset{0}{\overset{\parallel}{W_n(x_j)}}\right)=\sum_{j=0}^n a_j f(x_j),$$ precision $2n+1$!

Q: how to get Gaussian points?

$\Leftrightarrow$ find a polynomial $q(x)$ of degree $n+1$, $q(x)\perp P_n$

then its roots are Gaussian points.

Def: Legendre polynomials $\{P_0(x), P_1(x), \cdots, P_n(x)\}$.

(i) for each j, $P_j(x)$ is a monic polynomial of degree j, $a_j = 1$.

(ii) $\int_{-1}^{1} p(x) P_j(x) dx = 0$, whenever $p(x)$ is a polynomial of degree less than j.

$P_0(x) = 1$,

$P_1(x) = x - C_0^{(1)}$ $\quad \int_{-1}^{1} P_0(x) P_1(x)\, dx = 0 \Rightarrow C_0 = 0 \quad P_1(x) = x$

$P_2(x) = x^2 - C_1^{(2)} x - C_0^{(2)}$ $\quad \begin{cases} \int_{-1}^{1} P_0(x) P_2(x)\, dx = 0 \\ \int_{-1}^{1} P_1(x) P_2(x)\, dx = 0 \end{cases} \Rightarrow \quad P_2(x) = x^2 - \frac{1}{3}$.

Similarly: $P_3(x) = x^3 - \frac{3}{5}x$, $\cdots$, $P_{n+1}(x) = x P_n(x) - \frac{n(n+1)}{2n+1} P_{n-1}(x)$

Q: ① $P_n(x)$ 是否一定有 n 个实根?

② 是否有递推式?

A: Gaussian points are roots of Legendre polynoimal of degree $n+1$, thus

$q(x) = P_{n+1}(x)$!!

existence? distinct?

$\boxed{\text{Thm}}$ $x_1, x_2, \cdots, x_n$ are the roots of the n-th Legendre polynomial,

c_i is defined as $\quad c_i = \int_{-1}^{1} \prod_{\substack{j=1 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j} dx$, $\quad i = 1, 2, \cdots, n$.

For any polynomial of degree less than $2n$ ($\leq 2n-1$), we have

$$\int_{-1}^{1} f(x) dx = \sum_{i=1}^{n} c_i f(x_i) \quad \text{(exactness !)}$$

Proof: ① if $f(x)$ ($\in P_{n-1}$) is any polynomial of degree less than n, then

$$f(x) = \sum_{i=1}^{n} f(x_i) L_i(x) = \sum_{i=1}^{n} f(x_i) \prod_{\substack{j=1 \\ j \neq i}}^{n} \frac{x - x_j}{x_i - x_j}$$

$$\therefore \int_{-1}^{1} f(x) dx = \sum_{i=1}^{n} c_i f(x_i).$$

② if $n \leq \text{degree}(f) \leq 2n-1$, rewrite:

$f(x) = Q(x) P_n(x) + R(x)$, where $P_n(x)$ is the n-th Legendre polynomial and degree of Q less than n.

$$\therefore \int_{-1}^{1} f(x) dx = \underbrace{\int_{-1}^{1} Q(x) P_n(x) dx}_{0} + \int_{-1}^{1} R(x) dx = \int_{-1}^{1} R(x) dx.$$

On the other hand ...

On the other hand, $f(x_i) = Q(x_i)\underbrace{P_n(x_i)}_{\text{roots} \Rightarrow 0} + R(x_i) = R(x_i)$

In Case ①, we have shown $\int_{-1}^{1} R(x)\,dx = \sum_{i=1}^{n} c_i R(x_i)$

$$\therefore \int_{-1}^{1} f(x)\,dx = \sum_{i=1}^{n} c_i f(x_i), \quad \forall f \in P_{2n-1}.$$

RK: ① x_i roots of n-th Legendre polynomial are nodes for the quadrature and c_i are the weights

② $\sum_{i=1}^{n} c_i f(x_i)$ is one of Gaussian quadratures with degree of precision $2n-1$

③ $$\int_a^b f(x)\,dx = \frac{b-a}{2}\int_{-1}^{1} f\left(\frac{b-a}{2}(t+1)+a\right)dt \qquad \left(x = \frac{b-a}{2}(t+1)+a\right)$$
$$\approx \frac{b-a}{2}\sum_{i=1}^{n} c_i f\left(\frac{b-a}{2}(x_i+1)+a\right) \qquad O\left((b-a)^{2n+1}\right)$$

④ $n=2$, $P_2(x) = x^2 - \frac{1}{3}$, $x_1 = -\frac{\sqrt{3}}{3}$, $x_2 = \frac{\sqrt{3}}{3}$

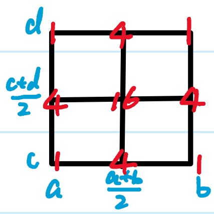
$$c_1 = \int_{-1}^{1} \frac{x - \frac{\sqrt{3}}{3}}{-\frac{\sqrt{3}}{3} - \frac{\sqrt{3}}{3}}\,dx = 1, \quad c_2 = \int_{-1}^{1} \frac{x + \frac{\sqrt{3}}{3}}{\frac{\sqrt{3}}{3} + \frac{\sqrt{3}}{3}}\,dx = 1$$

⑤ $n=3$, $P_3(x) = x^3 - \frac{4}{5}x$ $\quad x_1 = -\sqrt{\frac{4}{5}}$, $x_2 = 0$, $x_3 = \sqrt{\frac{4}{5}}$

$c_1 = \cdots$, $c_2 = \cdots$, $c_3 = \cdots$

△ multiple integrals (Simpson's rule as an example)

e.g. 1: retangular domain



$$\int_a^b \int_c^d f(x,y)\,dy\,dx$$
$$= \int_a^b \frac{d-c}{6}\left(f(x,c) + 4f\left(x, \tfrac{c+d}{2}\right) + f(x,d)\right)dx$$
$$= \frac{(b-a)(d-c)}{36}\Big[f(a,c) + 4f\left(\tfrac{a+b}{2}, c\right) + f(b,c) + 4f\left(a, \tfrac{c+d}{2}\right) + 16f\left(\tfrac{a+b}{2}, \tfrac{c+d}{2}\right) + 4f\left(b, \tfrac{c+d}{2}\right)$$
$$+ f(a,d) + 4f\left(\tfrac{a+b}{2}, d\right) + f(b,d)\Big].$$

RK: composite method for large $(b-a)$ or $(d-c)$

e.g. 2 : nonretangular domain :

$$\int_a^b \int_{c(x)}^{d(x)} f(x,y)\,dy\,dx$$

$$= \int_a^b \frac{d(x)-c(x)}{6}\left(f(x,c(x)) + 4f\left(x, \frac{c(x)+d(x)}{2}\right) + f(x,d(x))\right)dx \quad (K(x)=d(x)-c(x))$$

$$= \frac{b-a}{36}\Big[\, K(a)f(a,c(a)) + 4K\left(\tfrac{a+b}{2}\right) f\left(\tfrac{a+b}{2}, c\left(\tfrac{a+b}{2}\right)\right) + K(b)f(b,c(b)) +$$

$$4K(a)f\left(a, \frac{c(a)+d(a)}{2}\right) + 16 \cdots \Big]$$

△ Improper integrals (瑕积分)

e.g 1: left endpoint singularity

$$S = \int_a^b \frac{g(x)}{(x-a)^p}\,dx \;:\; \cancel{\approx} \; \frac{b-a}{2}\left(\frac{g(a)}{(a-a)^p} + \frac{g(b)}{(b-a)^p}\right) \qquad 0<p<1$$

$$g(x) = \boxed{g(a) + g'(a)(x-a) + \tfrac{1}{2}g''(a)(x-a)^2 + \tfrac{1}{6}g'''(a)(x-a)^3 + \tfrac{1}{24}g^{(4)}(a)(x-a)^4} + \cdots$$

$$:= P_4(x) \qquad (g \in C^5).$$

$$S = \int_a^b \frac{P_4(x) + (g(x)-P_4(x))}{(x-a)^p}\,dx = \int_a^b \frac{P_4(x)}{(x-a)^p}\,dx + \int_a^b \frac{g(x)-P_4(x)}{(x-a)^p}\,dx$$

$$= \frac{g(a)}{1-p}(b-a)^{1-p} + \frac{g'(a)}{2-p}(b-a)^{2-p} + \cdots \qquad G(x) = \frac{g(x)-P_4(x)}{(x-a)^p}$$

$$+ \frac{h}{3}\left(G(a) + 4\sum_{j=1}^{n} G(x_{2j-1}) + 2\sum_{j=1}^{n-1} G(x_{2j}) + G(b)\right)$$

e.g. 2: infinite singularity

① $\int_a^{\infty} \frac{G(x)}{x^p}\,dx = \int_0^{\frac{1}{a}} \frac{g(\frac{1}{t})}{(\frac{1}{t})^p}\, t^{-2}\,dt = \int_0^{\frac{1}{a}} t^{p-2} g(\tfrac{1}{t})\,dt \qquad (p>1) \qquad t = x^{-1}$

② $\int_1^{\infty} x^{-\frac{3}{2}} \sin\frac{1}{x}\,dx = \int_0^1 \frac{\sin(t)}{\sqrt{t}}\,dt \qquad (t = x^{-1})$

$$= \int_0^1 \frac{t - \frac{1}{6}t^3}{\sqrt{t}}\,dt + \int_0^1 \frac{\sin t - t + \frac{1}{6}t^3}{\sqrt{t}}\,dt$$

quadrature rule

HW 7-2: 4.7: 1, 3 d, 11, 14 4.8: 1, 2, 3, 4 c

4.9 1, 2 a 3, 4 a 6