Week 7, Tuesday

△ Review: numerical differentiation (finite difference formula)

given $\{x_{0\pm k}, f(x_{0\pm k})\}$, find formula to approximate the derivatives

$$\sum_{\pm k} C_{\pm k} f(x_{0\pm k}) \approx u'(x_0) \text{ or } u''(x_0)$$

first order: $\dfrac{f(x_0+h)-f(x_0)}{h} = f'(x_0) + \frac{1}{2}hf''(\xi)$

$h>0$: forward , $h<0$: backward

second-order: $\dfrac{-3f(x_0)+4f(x_0+h)-f(x_0+2h)}{2h} = f'(x_0) - \frac{1}{3}h^2 f^{(3)}(\xi)$

3-point endpoint (one-sided)

$h>0$: forward , $h<0$: backward

$$\frac{f(x_0+h)-f(x_0-h)}{2h} = f'(x_0) + \frac{1}{6}h^2 f^{(3)}(\xi)$$

central

second-order derivative:

$$\frac{f(x_0+h)-2f(x_0)+f(x_0-h)}{h^2} = f''(x_0) + \frac{1}{12}h^2 f^{(4)}(\xi)$$

Central, second-order, only 3-point

methods to derive the FD formula:

① first interpolation, then take derivative of the interpolation

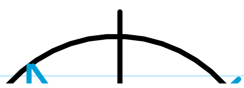
② method of undetermined coefficients

③ composite ways for high-order derivative: $D_0^2 = D_+ D_-$

△ Numerical integration (数值积分)

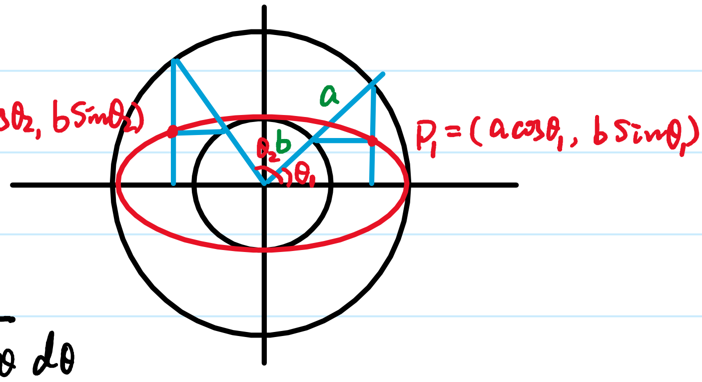
examples of integrations without analytical antiderivatives

e.g. 1: $\int e^{x^2} dx$



e.g.1: $\int e^{x^2}\,dx$

e.g.2: length of the arc from θ_1 to θ_2



$x = a\cos\theta$, $y = b\sin\theta$

$$l = \int_{\theta_1}^{\theta_2} \sqrt{dx^2+dy^2} = \int_{\theta_1}^{\theta_2} \sqrt{a^2\sin^2\theta + b^2\cos^2\theta}\, d\theta$$

$$= \int_{\theta_1}^{\theta_2} \sqrt{a^2-(a^2-b^2)\cos^2\theta}\, d\theta$$

RK: $\int \sqrt{1-m\cos^2\theta}\,d\theta$: elliptic integral of the second kind, cannot be evaluated explicitly.

Solution: numerical integration.

△ Numerical integration: use discrete datas to approximate intergrations,

i.e. use $\{(x_j, f(x_j))\}_{j=0}^{n}$, $x_j \in [a,b]$ to approximate $\int_a^b f(x)dx$

find formula: $\int_a^b f(x)dx = \sum_{j=0}^{n} a_j f(x_j)$

Also interpolate first:

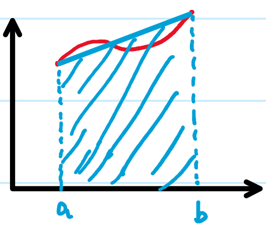
$$f(x) = P_n(x) + R_n(x) = \sum_{j=0}^{n} f(x_j) L_j(x) + \frac{f^{(n+1)}(\xi(x))}{(n+1)!}(x-x_0)(x-x_1)\cdots(x-x_n)$$

$$\int_a^b f(x)dx = \int_a^b \sum_{j=0}^{n} f(x_j) L_j(x)\,dx + \int_a^b \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{j=0}^{n}(x-x_j)\,dx$$

$$= \sum_{j=0}^{n} \underbrace{\int_a^b L_j(x)dx}_{a_j}\, f_j(x) + \underbrace{\frac{1}{(n+1)!}\int_a^b f^{(n+1)}(\xi(x)) \prod_{j=0}^{n}(x-x_j)\,dx}_{E(f)}.$$

$$:= \sum_{j=0}^{n} a_j f(x_j) + E(f)$$

△ equal spacing



① $n=1$, $x_0 = a$, $x_1 = b$

梯 $= \frac{b-a}{2}(f(a)+f(b))$

$E(f) = \int_a^b \frac{1}{2} f''(\xi(x))(x-a)(x-b)\,dx$ ↗ does not change sign

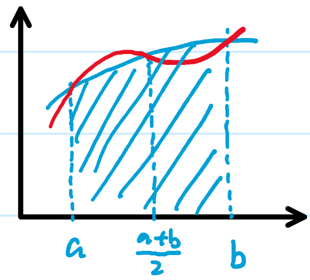
$= \frac{1}{2} f''(\xi) \int_a^b (x-a)(x-b)\,dx = -\frac{(b-a)^3}{\cdots} f''(\xi)$

$$= \frac{1}{2} f''(\xi) \int_a^b (x-a)(x-b)\, dx = -\frac{(b-a)^3}{12} f''(\xi)$$

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

Trapezoidal rule

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



$$\int_a^b f(x)\, dx = \int_{x_0}^{x_2} \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}\, dx\, f(x_0)$$

$$+ \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)}\, dx\, f(x_1)$$

$$+ \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}\, dx\, f(x_2)$$

$$+ \int_{x_0}^{x_2} \frac{1}{6} f^{(3)}(\xi(x))(x-x_0)(x-x_1)(x-x_2)\, dx \rightarrow E(f)$$

Simpson's rule

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

e.g. $\int_0^2 f(x)\, dx$

(a) x^2 (b) x^4 (c) $(1+x)^{-1}$ (d) $\sqrt{1+x}$ (e) $\sin(x)$ (f) e^x

Trape. rule : $\int_0^2 f(x)\, dx \approx f(0) + f(2)$

Simpson's rule : $\int_0^2 f(x)\, dx \approx \frac{1}{3}(f(0) + 4f(1) + f(2))$

(a) Trapezoidal: $\int_0^2 x^2\, dx \approx f(0) + f(2) = 0 + 4 = 4$

Simpson's : $\int_0^2 x^2\, dx \approx \frac{1}{3}(0+4+4) = \frac{8}{3}$

$f(x)$	x^2	x^4	$(1+x)^{-1}$	$\sqrt{1+x^2}$	$\sin x$	e^x
exact	2.667	6.400	1.099	2.958	1.416	6.389
Trapezoidal	4.000	16.000	1.333	3.326	0.909	8.389

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Simpson's	2.667	6.667	1.111	2.964	1.425	6.421

△ measuring precision

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: x^0, x^1, $E(f)=0$ due to $f''\equiv 0$, degree of precision 1.

Simpson's: x^0, x^1, x^2, x^3, $E(f)=0$, due to $f^{(4)}\equiv 0$, 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 formula, 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

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

and, degree of precision n

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

when $f \equiv x^0, x^1, \cdots, x^n$, $E(f)=0$. So at least degree of precision n.

For even n, take $f \equiv x^{n+1}$, $E(f) = \int_a^b (x-x_0)\cdots(x-x_n)\,dx = 0$

is a odd function with origin at $x_{\frac{n}{2}}$.

Q: how to make use of degree of accuracy to derive the error of Simpson's Rule as $E(f) = -\frac{(b-a)^5}{2880} f^{(4)}(\xi)$

RK: For a quadrature rule with precision m,

$$E(f) = \int_a^b f(x)\,dx - \sum_{j=0}^{n} a_j f(x_j) = K f^{(m+1)}(\xi),$$

where K is independent of f and $\xi \in (a,b)$.

△ equal spacing: $x_j = x_0 + jh$

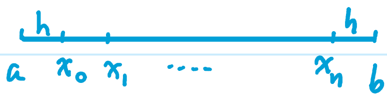
e.g. $n=1$, Trapezoidal rule: $\int_{x_0}^{x_1} f(x)\,dx = \frac{h}{2}\left(f(x_0)+f(x_1)\right) - \frac{h^3}{12} f''(\xi)$

$n=2$, Simpson's rule: $\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}\left(f(x_0)+4f(x_1)+f(x_2)\right) - \frac{h^5}{90} f^{(4)}(\xi)$

$n=3$, Simpson's three-eight rule.

$$\int_{x_0}^{x_3} f(x)\,dx = \frac{3h}{8}\left(f(x_0)+3f(x_1)+3f(x_2)+f(x_3)\right) - \frac{3h^5}{80} f^{(4)}(\xi).$$

△ open Newton-Cotes formula:



$x_i = x_0 + ih$, $i=0,1,\cdots,n$, $h = \frac{b-a}{n+2}$, $x_0 = a+h$, $x_n = b-h$

$$\int_a^b f(x)\,dx = \int_{x_{-1}}^{x_{n+1}} f(x)\,dx = \sum_{i=0}^{n} a_i f(x_i), \quad a_i = \int_a^b L_i(x)\,dx.$$

$\boxed{\text{Thm}}$ Very similar as the closed form.

e.g. $n=0$, $\int_a^b f(x)\,dx = \int_{x_{-1}}^{x_1} f(x)\,dx = 2f(x_0) + \frac{h^3}{3} f''(\xi)$ $\boxed{\text{midpoint rule}}$

degree of precision 1.

△ round-off error stability:

$$I_n(f) = \sum_{i=0}^{n} a_i f(x_i)$$

Newton-Cotes formula: $a_i = \int_a^b L_i(x)\,dx$

$$\sum_{i=0}^{n} a_i = \int_a^b \sum_{i=0}^{n} L_i(x)\,dx = b-a.$$

round-off error:

$$e = |I_n(f) - I_n(\tilde{f})| = \left|\sum_{i=0}^{n} a_i (f(x_i) - \tilde{f}(x_i))\right|$$

$$\leq \varepsilon \sum_{i=0}^{n} |a_i| \leq (b-a)\varepsilon \quad (\text{if } a_i \geq 0 \;!!!)$$

$\boxed{\text{Thm}}$ for any quadrature formula with weights $a_i \geq 0$, it is stable with respect to the round-off error.

RK: when $n \geq 8$, weights a_i of Newton-Cotes formula have negative numbers, not stable!

△ if $b-a$ is large, two ways:

① choose many $\{x_j\}$s, use very high-order polynomial to approximation

drawbacks: (i) need to calculate weights $a_j = \int_a^b \prod_{\substack{k=0 \\ k\neq j}}^{n} \frac{x-x_k}{x_j-x_k}$

(ii) $f^{(n+1)}$ may grows very rapidly or even unbounded (or ∄)

(iii) ∃ a_j s become negative, unstable respect to round off error.

② devide $[a,b]$ into small intervals $[a,b] = \bigcup_{j=0}^{n-1} [x_j, x_{j+1}]$,

do low order polynomial interpolation piecewisely: composite approach.

(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), $x_0 = a$, $x_j = x_0 + jh$, $h = \frac{b-a}{n}$

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

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

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

Lemma: $f \in C[a,b]$, $\forall x_j$ (distinct) $j = 1, 2, \cdots, n$, $\exists \xi \in (a,b)$, s.t.

$$f(\xi) = \frac{1}{n}\sum_{j=1}^{n} f(x_j)$$

proof: $f \in C[a,b]$, $\min_{x\in[a,b]} f(x)$ $\exists$, $\max_{x\in[a,b]} f(x)$ $\exists$, and

$$\min_{x\in[a,b]} f(x) \le \frac{1}{n}\sum_{j=1}^{n} f(x_j) \le \max_{x\in[a,b]} f(x)$$

by intermediate value theorem: $\exists \xi \in (a,b)$ s.t.

$$f(\xi) = \frac{1}{n}\sum_{j=1}^{n} f(x_j).$$

e.g. $\int_0^4 e^x dx$

$\int_0^4 e^x dx \approx \frac{2}{3}(e^0 + 4e^2 + e^4) = 56.76958$, err1 $= -3.17143$

$\int_0^4 e^x dx = \int_0^2 e^x dx + \int_2^4 e^x dx \approx \frac{1}{3}(e^0 + 4e^1 + e^2) + \frac{1}{3}(e^2 + 4e^3 + e^4) = 53.86385$

err2 $= -0.26570$

$\int_0^4 e^x dx = \int_0^1 e^x dx + \int_1^2 e^x dx + \int_2^3 e^x dx + \int_3^4 e^x dx$ $\qquad \frac{|err2|}{|err1|} = \frac{1}{12}$

$\approx \frac{1}{6}(e^0 + 4e^{\frac{1}{2}} + e^1) + \cdots$

$= 53.61622$ $\qquad$ err3 $= -0.01807$ $\qquad \frac{|err3|}{|err2|} = \frac{1}{14.7}$

e.g. $\int_0^\pi \sin x\, dx = 2$, determin h to let error less than 0.00002.

(a) composite trapezoidal rule:

$$|E(f)| = \left|-\frac{\pi}{12}h^2(-\sin(\xi))\right| \le \frac{\pi h^2}{12} \le 0.00002 \Rightarrow n = \frac{\pi}{h} \ge 360$$

(b) composite Simpson's rule:

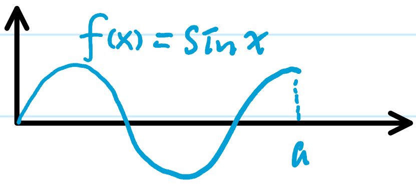
$$|E(f)| = \left| -\frac{\pi}{180} h^4 \sin(\xi) \right| \le \frac{\pi}{180} h^4 \le 0.00002 \Rightarrow n = \frac{\pi}{h} \ge 17.07.$$

take $n=18$,

$$\int_0^\pi \sin(x)\,dx \approx \frac{\pi}{54}\left(\sin(0) + 4\sin\left(\frac{\pi}{18}\right) + \cdots\right) \approx 2.0000104, \quad \text{error} = 0.00001.$$

e.g. length of sine curve:

$$l = \int_0^a \sqrt{1 + f'(x)^2}\,dx$$
$$= \int_0^a \sqrt{1 + \cos^2 x}\,dx$$



again: elliptic integral of the second kind

composite Simpson's Rule: $a = 10$

N	error	$\log_2(E(h)/E(\frac{h}{2}))$
2^3	7.10×10^{-2}	
2^4	6.42×10^{-4}	6.79
2^5	2.86×10^{-5}	4.49
2^6	3.55×10^{-6}	3.01
2^7	2.22×10^{-7}	4.00
2^8	1.39×10^{-8}	4.00

$E(h) = Ch^P$

$\log_2\left(\frac{E(h)}{E(\frac{h}{2})}\right) = P.$

$E(h) = Ch^4$ as $h \to 0$.

$\triangle$ roundoff-error: $f(x_j) \approx \tilde{f}(x_j) + e_j$

$$e(h) = \left| \frac{h}{3}\left(e_0 + 4\sum_{j=1}^{n} e_{2j-1} + 2\sum_{j=1}^{n-1} e_{2j} + e_{2n}\right) \right| \le \frac{h}{3} \cdot 6n \max_j |e_j| \le (b-a)\varepsilon$$

$$|\tilde{E}(f)| \le (b-a)\varepsilon + \frac{b-a}{180} h^4 |f^{(4)}(\xi)|,$$ stable w.r.t round-off error.

HW 7-1

Sec 4.3 $\underline{1, 3, 5, 7, 9, 11}$ a 15 $\underline{a, d}$ 19 21 23 25

Sec 4.4 $\underline{1, 3}$ b 11 15