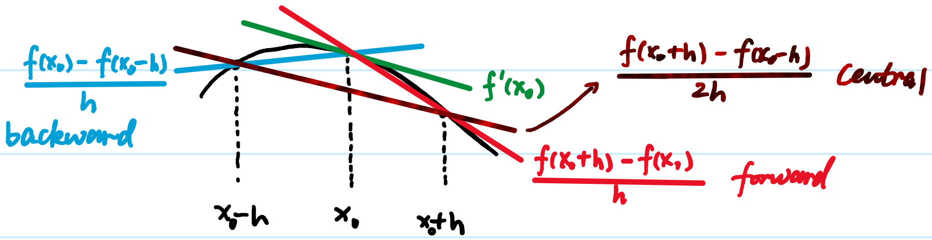
Week 6, Thursday

#2 quiz 20 mins

△ Def: $f'(x_0) = \lim_{h\to 0} \frac{f(x_0+h)-f(x_0)}{h}$

thus for small h $\quad \frac{f(x_0+h)-f(x_0)}{h} \approx f'(x_0)$

$h>0$: forward difference formula; $h<0$: backward difference formula



By Taylor's expansion: if $f \in C^2(x_0, x_0+h)$

$$\frac{f(x_0+h)-f(x_0)}{h} = f'(x_0) + \frac{h}{2} f''(\xi), \quad \xi \in (x_0, x_0+h)$$

Hence, we call $\frac{f(x_0+h)-f(x_0)}{h}$ a first order accurate approximation of $f'(x_0)$.

Q: how to get more accurate approximation.

A: central finite difference

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

RK: second-order if $f \in C^3(x_0-h, x_0+h)$.

Q: more general form?

△ Numerical differentiation: use discrete datas to approximate derivatives. i.e. use $\{(x_j, f(x_j))\}_{j=0}^{n}$ to approximate $f'(x_k)$

find formula $f'(x_k) \approx \sum_{j=0}^{n} a_{kj} f(x_j)$ → finite difference formula

interpolate first :

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

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

then take derivative:

$$f'(x_k) = \boxed{\sum_{j=0}^{n} L_j'(x_k) f(x_j)} + \frac{f^{(n+1)}(\xi(x))}{(n+1)!} \prod_{\substack{j=0 \\ j\neq k}}^{n} (x_k - x_j)$$

the formula $\qquad a_{kj}$

e.g. two-point formula: $(x_0, f(x_0))$, $(x_1, f(x_1))$

$$f(x) = f(x_0)\frac{x-x_1}{x_0-x_1} + f(x_1)\frac{x-x_0}{x_1-x_0} + \frac{1}{2}f''(\xi(x))(x-x_0)(x-x_1)$$

$$f'(x_0) = \frac{f(x_1)-f(x_0)}{x_1-x_0} + \frac{1}{2}(x_0-x_1)f''(\xi_0) \quad : \text{forward}$$

$$f'(x_1) = \frac{f(x_1)-f(x_0)}{x_1-x_0} + \frac{1}{2}(x_1-x_0)f''(\xi_1) \quad : \text{backward}$$

Three-point formula:

$$L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} \qquad L_0'(x) = \frac{2x-x_1-x_2}{(x_0-x_1)(x_0-x_2)}$$

$$L_1(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} \qquad L_1'(x) = \frac{2x-x_0-x_2}{(x_1-x_0)(x_1-x_2)}$$

$$L_2(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} \qquad L_2'(x) = \frac{2x-x_0-x_1}{(x_2-x_0)(x_2-x_1)}$$

$$f'(x_j) = \boxed{f(x_0)\frac{2x_j-x_1-x_2}{(x_0-x_1)(x_0-x_2)} + f(x_1)\frac{2x_j-x_0-x_2}{(x_1-x_0)(x_1-x_2)} + f(x_2)\frac{2x_j-x_0-x_1}{(x_2-x_0)(x_2-x_1)}}$$

$$+ \frac{f^{(3)}(\xi(x))}{6}\prod_{\substack{k=0 \\ k\neq j}}^{2}(x_j-x_k)$$

equal spacing: x_0, $x_1 = x_0+h$, $x_2 = x_0+2h$,

$$f'(x_0) = \frac{-3f(x_0)+4f(x_1)-f(x_2)}{\ldots} + \frac{h^2}{\ldots} f^{(3)}\ldots$$

$$f'(x_0) = \frac{-3f(x_0)+4f(x_1)-f(x_2)}{2h} + \frac{h^2}{3} f^{(3)}(\xi_0)$$

$$f'(x_1) = \frac{f(x_2)-f(x_0)}{2h} - \frac{h^2}{6} f^{(3)}(\xi_1)$$

$$f'(x_2) = \frac{f(x_0)-4f(x_1)+3f(x_2)}{2h} + \frac{1}{3}h^2 f^{(3)}(\xi_2)$$

or:

$$f'(x_0) = \frac{-3f(x_0)+4f(x_0+h)-f(x_0+2h)}{2h} + \frac{h^2}{3} f^{(3)}(\xi_0) \text{, forward}$$

$$f'(x_0) = \frac{f(x_0-2h)-4f(x_0-h)+3f(x_0)}{2h} + \frac{h^2}{3} f^{(3)}(\xi_2) \text{, backward}$$

$$f'(x_0) = \frac{f(x_0+h)-f(x_0-h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi_1) \text{, central}$$

In summary:

Two-point (first-order)

$$D_+ f(x_0) := \frac{f(x_0+h)-f(x_0)}{h} = f'(x_0) + \frac{h}{2} f''(\xi) \text{, } \xi \in (x_0, x_0+h) \text{, forward}$$

$$D_- f(x_0) := \frac{f(x_0)-f(x_0-h)}{h} = f'(x_0) - \frac{h}{2} f''(\xi) \text{, } \xi \in (x_0-h, x_0) \text{, backward.}$$

Three-point endpoint formula:

$$f'(x_0) = \boxed{\frac{-3f(x_0)+4f(x_0+h)-f(x_0+2h)}{2h}} + \frac{h^2}{3} f^{(3)}(\xi_0) \text{, } \quad \xi_0 \in (x_0, x_0+2h) \text{ or } (x_0+2h, x_0)$$

$$:= D_{+/-,(2)} f(x_0) \qquad +(h>0): \text{forward}, \qquad -(h<0): \text{backward}$$

Three-point midpoint formula

$$f'(x_0) = \boxed{\frac{f(x_0+h)-f(x_0-h)}{2h}} - \frac{h^2}{6} f^{(3)}(\xi_1), \quad \xi_1 \in (x_0-h, x_0+h).$$

$$:= D_0 f(x_0)$$

$\triangle$ another way to derive the finite difference formula:

: method of undermined coefficients

e.g. $D_{-,2} f(x) = af(x_0) + bf(x_0-h) + cf(x_0-2h)$

$$= (a+b+c)f(x_0) - (b+2c)hf'(x_0) + \frac{1}{2}(b+4c)h^2 f''(x_0) - \frac{1}{6}(b+8c)h^3 f'''(x_0) + \cdots$$

$$\begin{cases} a+b+c=0 \\ -h(b+2c)=1 \\ b+4c=0 \end{cases} \Rightarrow \begin{cases} a=\frac{3}{2h} \\ b=-\frac{2}{h} \\ c=\frac{1}{2h} \end{cases}$$

$$E(h) = \frac{1}{6}(b+8c)h^3 f'''(x_0) + \cdots = \boxed{\frac{1}{3} f'''(x_0) h^2} + O(h^3).$$

(leading term)

$\triangle$ Second order derivative:

standard central finite difference:

$$u''(\bar{x}) \approx D_0^2 u(\bar{x}) = \frac{u(\bar{x}+h) - 2u(\bar{x}) + u(\bar{x}-h)}{h^2}$$

By Taylor expansion:

$$D_0^2 u(\bar{x}) = u''(\bar{x}) + \frac{1}{12} h^2 u^{(4)}(\bar{x}) + O(h^4), \quad \text{second order.}$$

In fact: $D_0^2 = D_+ D_-$

$$D_+ D_- u(\bar{x}) = \frac{1}{h}\left[D_- u(\bar{x}+h) - D_- u(\bar{x})\right]$$

$$= \frac{1}{h}\left[\frac{u(\bar{x}+h)-u(\bar{x})}{h} - \frac{u(\bar{x})-u(\bar{x}-h)}{h}\right]$$

$$= \frac{u(\bar{x}+h) - 2u(\bar{x}) + u(\bar{x}-h)}{h^2} := D_0^2 u(\bar{x})$$

$$D_+D_+u(\bar{x}) = \frac{u(\bar{x}+2h)-2u(\bar{x}+h)+u(\bar{x})}{h^2}, \quad \text{only first order} \quad \times$$

$$D_-D_-u(\bar{x}) = \frac{u(\bar{x}-2h)-2u(\bar{x}-h)+u(\bar{x})}{h^2}, \quad \text{only first order} \quad \times$$

$$D_0D_0\,u(\bar{x}) = \frac{u(\bar{x}+2h)-2u(\bar{x})+u(\bar{x}-2h)}{4h^2}, \quad \text{second order, but not compact} \quad \times$$

Again by interpolation: $\bar{x}$, $\bar{x}+h_1$, $\bar{x}+h_1+h_2$

$$P(x) = u(\bar{x})\frac{(x-(\bar{x}+h_1))(x-(\bar{x}+h_1+h_2))}{h_1(h_1+h_2)} + u(\bar{x}+h_1)\frac{\cdots}{-h_1h_2} + u(\bar{x}+h_1+h_2)\frac{\cdots}{h_2(h_1+h_2)}$$

$$P''(x) = \frac{2h_2u(\bar{x})-2(h_1+h_2)u(\bar{x}+h_1)+2h_1u(\bar{x}+h_1+h_2)}{h_1h_2(h_1+h_2)} = \text{constant !}$$

$$\frac{2h_2u(\bar{x})-2(h_1+h_2)u(\bar{x}+h_1)+2h_1u(\bar{x}+h_1+h_2)}{h_1h_2(h_1+h_2)} - u''(\bar{x}+h_1)$$

$$= \frac{1}{3}(h_2-h_1)u^{(3)}(x_2) + \frac{1}{12}\frac{h_1^3+h_2^3}{h_1+h_2}u^{(4)}(x_2) + \cdots$$

Hence, for $h_1 \neq h_2$, only first order

but if $h_1 = h_2$, it becomes second-order, and the formula:

$$D_0^2u(\bar{x}) = \frac{u(\bar{x}-h)-2u(\bar{x})+u(\bar{x}+h)}{h^2}, \quad E(h) = \frac{1}{12}h^2u^{(4)}(\xi), \ \xi \in (\bar{x}-h, \bar{x}+h)$$

△ Round-off error instability: e.g. midpoint formula:

$f(x_0+h) = \tilde{f}(x_0+h)+e^+$, $f(x_0-h) = \tilde{f}(x_0-h)+e^-$, $\tilde{f} = fl(f)$

$$\left|f'(x_0) - \frac{\tilde{f}(x_0+h)-\tilde{f}(x_0-h)}{2h}\right| \le \left|f'(x_0) - \frac{f(x_0+h)-f(x_0-h)}{2h}\right| + \left|\frac{(f(x_0+h)-\tilde{f}(x_0+h))-(f(x_0-h)-\tilde{f}(x_0-h))}{2h}\right|$$

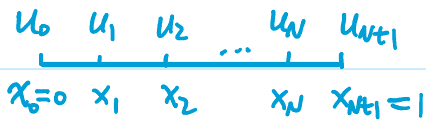
$$\leq \frac{h^2}{6}M + \frac{\varepsilon}{h} \quad (\varepsilon:\ \text{bound of round-off error})$$

RK: if we take very small h such as $h \sim \varepsilon$ then total error is $O(1)$.

in above case, optimal $h \sim \sqrt[3]{\frac{3\varepsilon}{M}}$

Δ one application of finite difference formula:

$$\begin{cases} u''(x) = f(x), & x \in (0,1) \\ u(0) = u(1) = 0 \end{cases}$$



① set $x_j = jh$, $h = \frac{1}{N+1}$, $u_j \approx u(x_j)$, $f_j = f(x_j)$

$u_0 = u_{N+1} = 0$, unknown $U = [u_1, u_2, \cdots, u_N]^T$

② at x_j, approximate the original differential equation by FD.

$$\frac{u_{j-1} - 2u_j + u_{j+1}}{h^2} = f_j, \quad j = 1, 2, \cdots, N.$$

③ matrix–vector form: $AU = F$, where

$$A = \frac{1}{h^2}\begin{bmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{bmatrix}, \quad U = \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ u_N \end{bmatrix}, \quad F = \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ f_N \end{bmatrix}$$

④ Solve the linear system $AU = F$. (Chap. 6, 7).

RK: A is the differentiation matrix which maps the value of a function to its derivative:

$$A: \mathbb{R}^N \to \mathbb{R}^N \qquad [u(x_j)] \to [\approx u''(x_j)]$$

HW6-1: Sec 4.1   2 $\underline{a}$ 4 $\underline{a}$ 6 $\underline{a}$ 8 $\underline{a}$ 24   29