

# Discussion 1.

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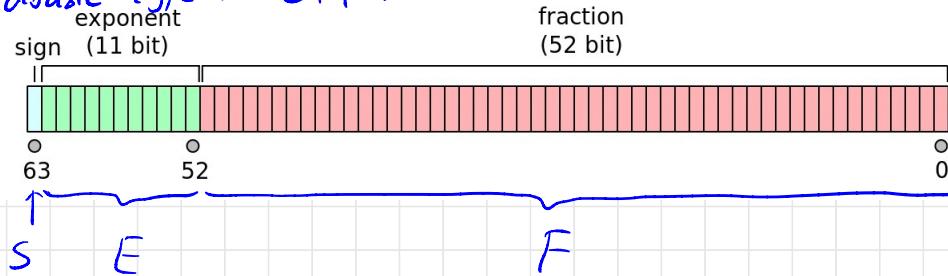
Error types :

① Round-off error : due to limitness of floating point representation

$$(-1)^S \times 2^{E-e} \times (1.F)_2$$

sign      exponent      mantissa

e.g. double type in C++,  $e = 1023$



$$\begin{aligned} 1 1000000001 1010 (+ 48 \text{ more } 0) &\equiv (-1)^1 \times 2^{(1024+1)-1023} \times (1.1010)_2 \\ &= -2^2 \times (2^0 + 2^{-1} + 2^{-3}) \\ &= -(4 + 2 + 0.5) = -6.5 \end{aligned}$$

Definition of round-off error :

The smallest (in magnitude) floating point number  $\epsilon_m$ , such that  $1.0 \text{ (floating point)} + \epsilon_m \neq 1.0 \text{ (floating point)}$

$\epsilon_m$  : machine accuracy, depend on hardware. we

can do nothing about it! float  $\sim 10^{-7}$  double  $\sim 10^{-16}$

② Truncation error: due to "discrete" approximation of "continuous" quantity. We can reduce it!

Numerical derivative of a continuous function:

Most important tool: Taylor series

single variable:

$$f(x) = f(a) + f'(a)(x-a) + \frac{1}{2!} f''(a)(x-a)^2 + \frac{1}{3!} f'''(a)(x-a)^3 + \dots = \sum_{n=0}^{\infty} \frac{1}{n!} f^{(n)}(a)(x-a)^n$$

multivariable:

$$f(\vec{x}) = f(\vec{a}) + \left. \frac{\partial f(\vec{x})}{\partial x_i} \right|_{\vec{a}} (x_i - a_i) + \frac{1}{2!} \left. \frac{\partial^2 f(\vec{x})}{\partial x_i \partial x_j} \right|_{\vec{a}} (x_i - a_i)(x_j - a_j) + \dots$$

3 variable  $\vec{x}: x, y, z$

$$+ \frac{1}{3!} \left. \frac{\partial^3 f(\vec{x})}{\partial x_i \partial x_j \partial x_k} \right|_{\vec{a}} (x_i - a_i)(x_j - a_j)(x_k - a_k) + \dots$$

Another version (expand  $x+h$  around  $x$ ):

single variable:

$$\text{let } y = x+h \\ a = x$$

$$f(x+h) = f(x) + f'(x)h + \frac{1}{2!} f''(x)h^2 + \frac{1}{3!} f'''(x)h^3 + \dots$$

multivariable:

$$f(\vec{x}+\vec{h}) = f(\vec{x}) + \left. \frac{\partial f(\vec{x})}{\partial x_i} \right| h_i + \frac{1}{2!} \left. \frac{\partial^2 f(\vec{x})}{\partial x_i \partial x_j} \right| h_i h_j + \frac{1}{3!} \left. \frac{\partial^3 f(\vec{x})}{\partial x_i \partial x_j \partial x_k} \right| h_i h_j h_k + \dots$$

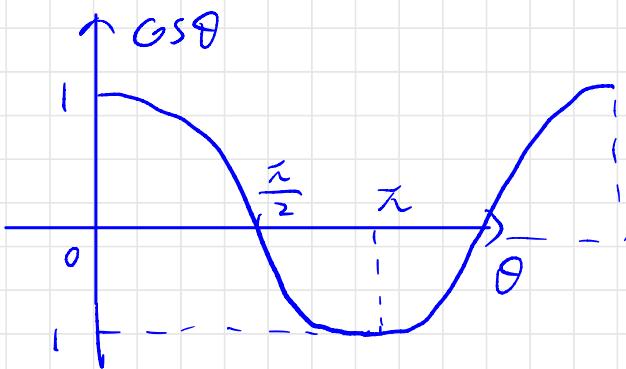
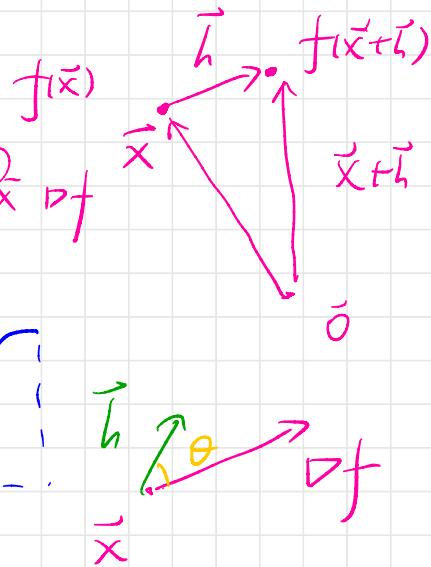
$$f(\vec{x}+\vec{h}) - f(\vec{x}) = \left. \frac{\partial f(\vec{x})}{\partial x_i} \right| h_i = \vec{h} \cdot \nabla f(\vec{x}) \quad \vec{h} = h_1 \hat{e}_1 + h_2 \hat{e}_2 + \dots$$

$$df = \vec{h} \cdot \nabla f = \left. \frac{\partial f}{\partial x_1} \right| \hat{e}_1 + \left. \frac{\partial f}{\partial x_2} \right| \hat{e}_2 + \dots \quad \hat{e}_i \cdot \hat{e}_j = \delta_{ij} = \begin{cases} 1 & i=j \\ 0 & i \neq j \end{cases}$$

$$df = \vec{h} \cdot \nabla f$$

$$= |\vec{h}| |\nabla f| \cos \theta$$

$\theta$  is angle between  $\vec{h}$  &  $\nabla f$



Numerical derivative for single variable function:

$$f(x+h) = f(x) + f'(x)h + \frac{1}{2!} f''(x)h^2 + \frac{1}{3!} f'''(x)h^3 + \dots \quad \textcircled{1}$$

$$f(x-h) = f(x) - f'(x)h + \frac{1}{2!} f''(x)h^2 - \frac{1}{3!} f'''(x)h^3 + \dots \quad \textcircled{2}$$

from \textcircled{1} :

$$\begin{aligned}\frac{f(x+h) - f(x)}{h} &= f'(x) + \frac{1}{2!} f''(x)h + \frac{1}{3!} f'''(x)h^2 + \dots \\ &= f'(x) + O(h)\end{aligned}$$

$$\Rightarrow f'(x) \approx \frac{f(x+h) - f(x)}{h} + \underbrace{O(h)}_{\text{truncation error}}$$

from  $\frac{\textcircled{1} - \textcircled{2}}{2h}$  :

$$\frac{f(x+h) - f(x-h)}{2h} = f'(x) + \frac{1}{3!} f'''(x)h^2 + \dots$$

$$\Rightarrow f'(x) = \frac{f(x+h) - f(x-h)}{2h} + \underbrace{O(h^2)}_{\text{truncation error}}$$

We can reduce  $h$  to decrease truncation error!

but not too small. Eg. for first method

round-off error  $E_r \approx \frac{|\Sigma_m| |f(x)|}{h}$  increases as we decrease  $h$

$$1 + \varepsilon_m \approx 1 \quad f(x) \approx f(x)(1 + \varepsilon_m) = f(x) + f(x)\varepsilon_m$$

$$\text{error of } f(x+h) \sim \pm |f'(x)| |\varepsilon_m|$$

$$\text{error of } f(x) \sim \pm |f'(x)| |\varepsilon_m|$$

$$\varepsilon_{\text{tot}} = |\varepsilon_h| + |\varepsilon_t| = |\varepsilon_m| |f'(x)| \cdot \frac{1}{h} + \frac{|f''(x)|}{2} \cdot h$$

$\uparrow$  round error       $\uparrow$  truncation error

$$h_0 = \sqrt{\frac{2|\varepsilon_m||f'(x)|}{|f''(x)|}}$$



Force evaluation:

finite difference:

$$-F_{x_j} = \frac{\partial E}{\partial x_j} = \frac{E[x_j + h, \{R_{i \neq j}\}] - E[x_j - h, \{R_{i \neq j}\}]}{2h}$$

$$E = \sum_{i \neq j} \varepsilon_{ij} \left\{ \left( \frac{\sigma_{ij}}{R_{ij}} \right)^2 - 2 \left( \frac{\sigma_{ij}}{R_{ij}} \right)^6 \right\}$$

Suppose  $N$  atoms, need  $\binom{N}{2} = \frac{N(N-1)}{2} \sim O(N^2)$  eval

each atom has 3 force component, each need 2 energy evaluation

$$\Rightarrow 6N \times O(N^2) \sim O(N^3)$$

analytical force:

$$\frac{\partial E}{\partial x_k} = \sum_{i \neq j} \varepsilon_{ij} \left\{ -12 \frac{\sigma_{ij}^{12}}{R_{ij}^{13}} + 12 \frac{\sigma_{ij}^6}{R_{ij}^7} \right\} \frac{\partial R_{ij}}{\partial x_k}$$

$$R_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2} \quad \text{if } i=1, j=2, k=3$$

$$\frac{\partial R_{ij}}{\partial x_k} = \frac{2(x_i - x_j)(\delta_{ik} - \delta_{jk})}{2R_{ij}} = \frac{(x_i - x_j)(\delta_{ik} - \delta_{jk})}{R_{ij}}$$

we only need these pairs with one atom is  $k$  atom

$$\Rightarrow \frac{\partial E}{\partial x_k} = \sum_{i \neq k} \epsilon_{ik} \left\{ -12 \frac{\sigma_{ik}^1}{R_{ik}^3} + 12 \frac{\sigma_{ik}^b}{R_{ik}} \right\} \frac{(x_i - x_k)(-1)}{R_{ik}}$$

takes  $\mathcal{O}(N)$  evaluation

total force:  $6N \times \mathcal{O}(N) \sim \mathcal{O}(N^2)$

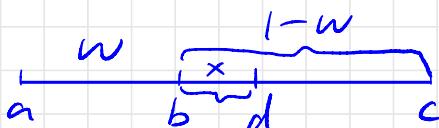
1D minimization:

Golden section search:

for  $a < b < c$ , if  $f(b) < f(a)$

$f(b) < f(c)$ ,  $\exists$  local minimal in  $(a, c)$

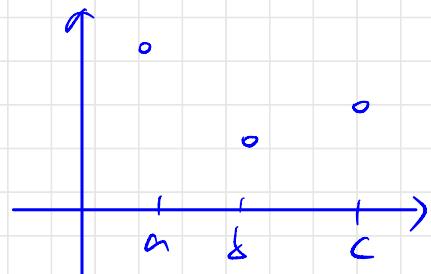
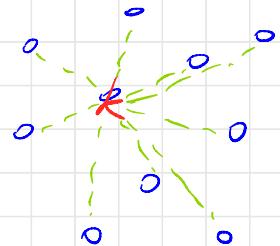
how to shrink the interval? Suppose  $a, c = 1$



$$ab = w$$

draw  $d$  between  $b, c$ , evaluate  $f(d)$

if  $f(d) > f(b)$ , then  $f(b) < f(c)$  by definition  
 $f(b) < f(d)$



$\Rightarrow$  minimal  $\in (a, d)$

if  $f(d) < f(b)$ , then  $f(d) < f(b) < f(c)$   
 $f(d) < f(b)$

$\Rightarrow$  minimal  $\in (b, c)$

want to guarantee the two case give the same  
shrinkage:  $w+x=1-w \Rightarrow x=1-2w \quad \textcircled{1}$

need  $x>0 \Rightarrow w < \frac{1}{2}$

also want to guarantee we draw new point in the  
same "place" as previous:

$$\frac{x}{1-w} = w \quad \textcircled{2}$$

$$\Rightarrow \frac{1-2w}{1-w} = w \Rightarrow 1-2w = w-w^2 \Rightarrow w^2 - 3w + 1 = 0$$

$$w = \frac{3 \pm \sqrt{5}}{2} = \frac{3-\sqrt{5}}{2} \quad (w < \frac{1}{2})$$

$$\Rightarrow \frac{w}{1-w} = \frac{\sqrt{5}-1}{2} \quad \text{Golden ratio}$$