Discussion 1.

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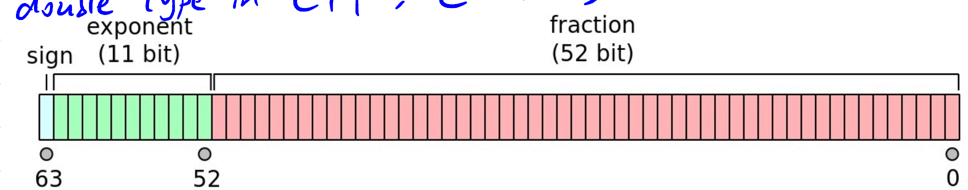
Error types:

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

$$\underbrace{(-1)^S}_{\text{sign}} \times \underbrace{2^{E-e}}_{\text{exponent}} \times \underbrace{(1.F)_2}_{\text{mantissa}}$$

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



S E F

$$1\ 10000000001\ 1010\ (+48 \text{ more } 0) \equiv (-1)^1 \times 2^{(1024+1-1023)} \times (1.1010)_2$$

$$= -2^2 \times (2^0 + 2^{-1} + 2^{-3})$$

$$= -(4+2+0.5) = -6.5$$

Definition of round-off error:

The smallest (in magnitude) floating point number ε_m, such that 1.0 (floating point) $+ \varepsilon_m \neq 1.0$ (floating point)

ε_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:

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

multivariable:

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

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

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

single variable:

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

multivariable:

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

$$+ \cdots$$

Numerical derivative for single variable function:

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

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

from (1):

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

$$= f'(x) + O(h)$$

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

from $\frac{(1)-(2)}{2h}$:

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

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

we can reduce h to decrease truncation error!

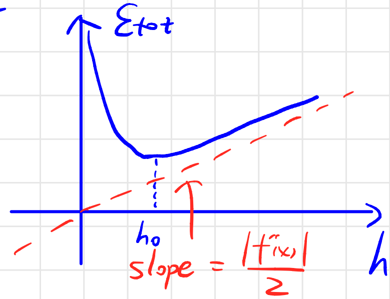
but not too small. Eg. for first method

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

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

round error

truncation error



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

Force evaluation:

finite difference:

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

$$E = \sum_{i\neq j} \varepsilon_{ij} \left\{ \left(\frac{\sigma_{ij}}{R_{ij}}\right)^{12} - 2\left(\frac{\sigma_{ij}}{R_{ij}}\right)^{6} \right\}$$

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

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

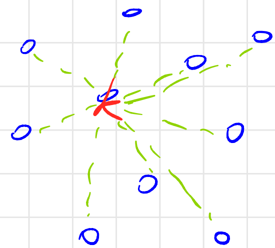
analytical force:

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

$$R_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2}$$

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

we only need these pairs with one atom is k atom

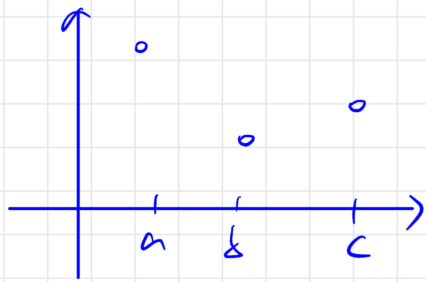


$$\Rightarrow \frac{\partial E}{\partial x_k} = \sum_{i \neq k} \varepsilon_{ik} \left\{ -12 \frac{\sigma_{ik}^{12}}{R_{ik}^{13}} + 12 \frac{\sigma_{ik}^{6}}{R_{ik}^{7}} \right\} \frac{(x_i - x_k)(-1)}{R_{ik}}$$

takes $O(N)$ evaluation

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

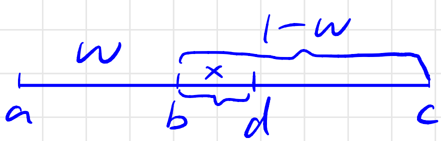
1D minimization:



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 $ac = 1$
$ab = w$



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

if $f(d) > f(b)$, then $f(b) < f(a)$ 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:

$$w + x = 1 - w \Rightarrow x = 1 - 2w \quad (1)$$

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

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

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

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

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

$$\Rightarrow \frac{w}{1-w} = \frac{\sqrt{5}-1}{2}$$ golden ratio