Computational Physics
計算物理

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This Lecture will cover:

1. Introduction
2. Numerical Differentiation
3. Numerical Integration

Approximation of Derivatives (Numerical Differentiation)

Quite often, the analytic derivatives of some function cannot be obtained very easily

For example

$$f(E) = \beta\cos(\alpha a) - \alpha\sin(\alpha a)$$

$$\alpha = \sqrt{\frac{2mE}{\hbar^2}} \qquad \beta = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

$$\frac{df(E)}{dE} = ?$$

In other cases, we only have a table of function values.

In both cases, numerical derivative can be performed.

$$f(x)$$

$$f'(x) = \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}, \text{ forward difference}$$

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

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

$$= \frac{f(x+h) - f(x)}{h} + E(h)$$

$$E(h) \simeq \frac{h}{2} f''(x) \qquad \text{Error estimate}$$

Similarly for backward difference, $h \to -h$

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

The average of forward and backward diff. gives the central diff.

$$f'(x) = \frac{1}{2h}\left[\, f(x+h) - f(x-h) \,\right] - \frac{h^2}{3!} f'''(x) - \frac{h^4}{5!} f^{(5)}(x)$$

$$\cong \frac{1}{2h}\left[\, f(x+h) - f(x-h) \,\right] + O(h^2) \qquad E(h) \approx h^2$$

When h is smaller than certain value, the error becomes worse due to the limited precision of data representation in the computer. Both numerator and denominator are subject to large round-off errors.

For higher derivatives

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} + \left(-\frac{h^2}{12}\right) f^{(4)}(x) - \frac{h^4}{360} f^{(6)}(x)$$

3-point formula for the second derivative

Richardson Extrapolation

$$D_1(h) \equiv f'(x) = \frac{f(x+h) - f(x-h)}{2h} - \frac{h^2}{6} f'''(x) - \frac{h^4}{5!} f^{(5)}(x)$$

$$D_1(2h) \equiv f'(x) = \frac{f(x+2h) - f(x-2h)}{4h} - \frac{4h^2}{6} f'''(x) - \frac{16h^4}{5!} f^{(5)}(x)$$

$$4 \times D_1(h) - D_1(2h):$$

$$3f'(x) = \frac{f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)}{4h} + \frac{12h^4}{5!} 5^{(5)}(x)$$

$$D_2(h) \equiv f'(x) = \frac{f(x-2h) - 8f(x-h) + 8f(x+h) - f(x+2h)}{12h} + \frac{h^4}{30} f^{(5)}(x)$$

$$D_2(h) = \frac{4D_1(h) - D_1(2h)}{4-1}$$

$$D_{i+1}(h) = \frac{4^i D_i(h) - D_i(2h)}{4^i - 1}$$

Iteration Steps

$$\begin{matrix} f(x-h) \\ f(x+h) \end{matrix} \;\rightarrow\; f'(x) = \frac{f(x+h)-f(x-h)}{2h} \equiv D_1(h)$$

$$\begin{matrix} f\left(x-\frac{h}{2}\right) \\ f\left(x+\frac{h}{2}\right) \end{matrix} \;\rightarrow\; D_1\left(\frac{h}{2}\right) = \frac{f\left(x+\frac{h}{2}\right)-f\left(x-\frac{h}{2}\right)}{h}$$

$$D_2\left(\frac{h}{2}\right) = \frac{4D_1\left(\frac{h}{2}\right)-D_1(h)}{4-1}$$

Iteration Steps (cont)

$$f\left(x-\frac{h}{4}\right)$$

$$f\left(x+\frac{h}{4}\right)$$

$$\rightarrow \quad D_1\left(\frac{h}{4}\right) = \frac{f\left(x+\frac{h}{4}\right)-f\left(x-\frac{h}{4}\right)}{\frac{h}{2}}$$

$$D_2\left(\frac{h}{4}\right) = \frac{4D_1\left(\frac{h}{4}\right)-D_1\left(\frac{h}{2}\right)}{4-1}$$

$$D_3\left(\frac{h}{4}\right) = \frac{4^2 D_2\left(\frac{h}{4}\right)-D_2\left(\frac{h}{2}\right)}{4^2-1}$$

Iteration Steps (cont)

$$f\left(x-\frac{h}{8}\right)$$

$$f\left(x+\frac{h}{8}\right)$$

$$\rightarrow \quad D_1\left(\frac{h}{8}\right) = \frac{f\left(x+\frac{h}{8}\right)-f\left(x-\frac{h}{8}\right)}{\frac{h}{4}}$$

$$D_2\left(\frac{h}{8}\right) = \frac{4D_1\left(\frac{h}{8}\right)-D_1\left(\frac{h}{4}\right)}{4-1}$$

$$D_3\left(\frac{h}{8}\right) = \frac{4^2D_2\left(\frac{h}{8}\right)-D_2\left(\frac{h}{4}\right)}{4^2-1}$$

$$D_4\left(\frac{h}{8}\right) = \frac{4^3D_3\left(\frac{h}{8}\right)-D_3\left(\frac{h}{4}\right)}{4^3-1}$$

Iteration Steps (cont)

$$
\begin{array}{ccccc}
h & D_1(h) & & & \\
\dfrac{h}{2} & D_1\left(\dfrac{h}{2}\right) & D_2\left(\dfrac{h}{2}\right) & & \\
\dfrac{h}{4} & D_1\left(\dfrac{h}{4}\right) & D_2\left(\dfrac{h}{4}\right) & D_3\left(\dfrac{h}{4}\right) & \\
\dfrac{h}{8} & D_1\left(\dfrac{h}{8}\right) & D_2\left(\dfrac{h}{8}\right) & D_3\left(\dfrac{h}{8}\right) & D_4\left(\dfrac{h}{8}\right)
\end{array}
$$

$$
D_{i+1}\left(\frac{h}{2}\right) = \frac{4^i D_i\left(\frac{h}{2}\right) - D_i(h)}{4^i - 1}
$$

Example

Example $\quad f(x) = x\exp(x)$

Use Richardson extrapolation to obtain $\dfrac{df(x)}{dx}$ at $x = 2$, and compare its value to the exact solution 22.1671682967919506816912823817

$f'(2)$

h	D_1	D_2	D_3	D_4
0.4	23.16346 42931			
0.2	22.41416 06570	22.16439 27783		
0.1	22.22878 68803	22.16699 56214	22.16716 91443	
0.05	22.18256 48578	22.16715 75170	22.16716 83100	22.16716 82968