Computational Physics
計算物理

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This Lecture will cover:

1. Introduction
2. Numerical Differentiation
3. Numerical Integration

Numerical Integration

$$I = \int_a^b f(x)\, dx \simeq \sum_{i=0}^{N} w_i f_i$$

$$\text{For } N = 1, \quad I \simeq w_0 f_0 + w_1 f_1$$

$$\text{Require it to be exact for } f(x) = 1,\ x$$

$$\int_{x_0}^{x_1} dx = x_1 - x_0 = w_0 + w_1$$

$$w_0 = w_1 = \frac{x_1 - x_0}{2}$$

$$\int_{x_0}^{x_1} x dx = \frac{1}{2}\left(x_1^{\ 2} - x_0^{\ 2}\right) = w_0 x_0 + w_1 x_1$$

$$\int_{x_0}^{x_1} f(x)\, dx \cong \frac{h}{2}\left(f_0 + f_1\right), \quad h \equiv x_1 - x_0$$

Error = ?

$$f(x) = f(x_0) + (x - x_0)\, f'(x_0) + \frac{(x - x_0)^2}{2!}\, f''(x_0) + \frac{(x - x_0)^3}{3!}\, f'''(x_0) + \cdots$$

$$= f(x_0) + (x - x_0)\, f'(x_0) + \frac{(x - x_0)^2}{2!}\, f''(\xi)$$

$x_0 < \xi < x$ (mean-value theorem)

$$f(x) = f(x_1) + (x - x_1)\, f'(x_1) + \frac{(x - x_1)^2}{2!}\, f''(\eta) \qquad x < \eta < x_1$$

$$\int_{x_0}^{x_1} f(x)\, dx = h\, f(x_0) + \frac{h^2}{2!} f'(x_0) + \frac{h^3}{3!}\, f''(x_0) + \frac{h^4}{4!}\, f'''(x_0) + \frac{h^5}{5!}\, f^{(4)}(x_0) + \cdots$$

$$\int_{x_0}^{x_1} f(x)\, dx = h\, f(x_1) - \frac{h^2}{2!}\, f'(x_1) + \frac{h^3}{3!}\, f''(x_1) - \frac{h^4}{4!}\, f^{(3)}(x_1) + \frac{h^5}{5!}\, f^{(4)}(x_1) + \cdots$$

Add together $\int_{x_0}^{x_1} f(x)\,dx = \frac{h}{2}\left[f(x_0)+f(x_1)\right]+\frac{h^2}{4}\left[f'(x_0)-f'(x_1)\right]$

$$+\frac{h^3}{12}\left[f''(x_0)+f''(x_1)\right]+\frac{h^4}{48}\left[f'''(x_0)-f'''(x_1)\right]$$

$$+\frac{h^5}{240}\left[f^{(4)}(x_0)+f^{(4)}(x_1)\right]+\cdots$$

Use $f'(x_1)=f'(x_0)+h\,f''(x_0)+\frac{h^2}{2}f'''(x_0)+\frac{h^3}{6}f^{(4)}(x_0)+\cdots$

$$f'(x_0)=f'(x_1)-h\,f''(x_1)+\frac{h^2}{2}f'''(x_1)-\frac{h^2}{6}f^{(4)}(x_1)+\cdots$$

It gives the Trapezoidal rule

$$\int_{x_0}^{x_1} f(x)dx=\frac{h}{2}\left[f(x_0)+f(x_1)\right]+\frac{h^2}{12}\left[f'(x_0)-f'(x_1)\right]-\frac{h^4}{720}\left[f'''(x_0)-f'''(x_1)\right]+\cdots$$

$$\text{Error} \approx -\frac{h^3}{12}f''(\xi)\,, \quad x_0<\xi<x_1$$

For N = 2 (i.e., 3 points) , require the integral to be exact for $f(x) = 1, \; x, \; x^2$

$$2h = \int_{x_0}^{x_2} dx = x_2 - x_0 = w_0 + w_1 + w_2, \qquad x_1 - x_0 = x_2 - x_1 = h$$

$$\int_{x_0}^{x_2} x \, dx = \frac{1}{2}\left(x_2^{\,2} - x_0^{\,2}\right) = w_0 x_0 + w_1 x_1 + w_2 x_2$$

$$\int_{x_0}^{x_2} x^2 dx = \frac{1}{3}\left(x_2^{\,3} - x_0^{\,3}\right) = w_0 x_0^{\,2} + w_1 x_1^{\,2} + w_2 x_2^{\,2}$$

$$\begin{pmatrix} 1 & 1 & 1 \\ x_0 & x_1 & x_2 \\ x_0^{\,2} & x_1^{\,2} & x_2^{\,2} \end{pmatrix} \begin{pmatrix} w_0 \\ w_1 \\ w_2 \end{pmatrix} = \begin{pmatrix} 2h \\ h(x_2 + x_0) \\ 2h(x_2^2 + x_2 x_0 + x_0^2)/3 \end{pmatrix}$$

$$w_0 = \frac{h}{3}, \quad w_1 = \frac{4h}{3}, \quad w_2 = \frac{h}{3}$$

$$\int_{x_0}^{x_2} f(x)\,dx = \frac{h}{3}\left(f_0 + 4f_1 + f_2\right) - \frac{h^5}{90} f^{(4)}(\xi)$$

$$= h\left[\frac{4\left(\frac{f_0 + f_1}{2} + \frac{f_1 + f_2}{2}\right) - \left(f_0 + f_2\right)}{4-1}\right] - \frac{h^5}{90} f^{(4)}(\xi)$$

Romberg Integration !

$$\int_{x_0}^{x_3} f(x)\,dx = \frac{3h}{8}\left(f_0 + 3f_1 + 3f_2 + f_3\right) - \frac{3h^5}{80} f^{(4)}(\xi) \qquad \text{(4 points)}$$

$$\int_{x_0}^{x_4} f(x)\,dx = \frac{2h}{45}\left[7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4\right] - \frac{8h^7}{945} f^{(6)}(\xi) \quad \text{(5 points)}$$

Composite Formulas

$$\int_{x_0}^{x_N} f(x)\,dx \cong \frac{h}{2}(f_0 + f_1) + \frac{h}{2}(f_1 + f_2) + \cdots + \frac{h}{2}(f_{N\text{-}1} + f_N)$$

$$= h\left[\frac{f_0}{2} + f_1 + f_2 + \cdots + f_{N\text{-}1} + \frac{f_N}{2}\right] + \frac{h^2}{12}\left(f_0' - f_N'\right)$$

Trapezoidal

$$\int_{x_0}^{x_N} f(x)\,dx \approx \frac{h}{3}\left[f_0 + 4f_1 + 2f_2 + \cdots + 2f_{N\text{-}2} + 4f_{N\text{-}1} + f_N\right] + \text{Error } (?)$$

Simpson

weights $\frac{h}{3}$ $\frac{4h}{3}$ $\frac{h}{3}$

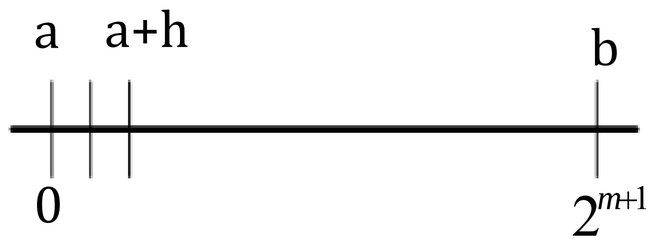
$$\begin{array}{ccccccccccc}
i = & 0 & 1 & 2 & 3 & 4 & & & & & \\
 & 1 & 4 & 1 & & & & & & & \\
 & & & 1 & 4 & 1 & & & & & \\
 & & & & & 1 & 4 & 1 & & & \\
\hline
 & 1 & 4 & 2 & 4 & 2 & 4 & \cdots & 2 & 4 & 1
\end{array}$$

Romberg Integration

$$n = 2^m$$

$$T_{m,0} = h\left(\frac{f_0}{2} + f_1 + \cdots + f_{n\text{-}1} + \frac{f_n}{2}\right), \qquad \text{Error} \approx \frac{h^2}{12}\left[f'(a) - f'(b)\right]$$

$$n \to 2^{m+1}, \quad h \to \left(\frac{h}{2}\right)$$



$$T_{m+1,0} = \frac{h}{2}\left(\frac{f_0}{2} + f_1 + \cdots + f_{n\text{-}1} + \frac{f_n}{2}\right), \quad \text{Error} \approx \left(\frac{1}{4}\right)\frac{h^2}{12}\left[f'(a) - f'(b)\right]$$

$$T_{m+1,1} = \frac{4T_{m+1,0} - T_{m,0}}{4-1} \qquad \text{Error} \approx h^4 \qquad T_{m+2,2} = \frac{4^2 T_{m+2,1} - T_{m+1,1}}{4^2 - 1}$$

$$T_{m+k,k} = \frac{4^k T_{m+k,k-1} - T_{m+k-1,k-1}}{4^k - 1}$$

$$\int_a^b f(x)dx \approx \; T_{m,0} = \frac{1}{2} T_{m-1,0} + h \sum_{i=1,3}^{2^m-1} f\left(a + ih\right) \qquad h = \left(\frac{b-a}{2^m}\right)$$

2^m	$T_{m,0}$			
2^{m+1}	$T_{m+1,0}$	$T_{m+1,1}$		
2^{m+2}	$T_{m+2,0}$	$T_{m+2,1}$	$T_{m+2,2}$	
2^{m+3}	$T_{m+3,0}$	$T_{m+3,1}$	$T_{m+3,2}$	$T_{m+3,3}$

$$T_{m+k,k} = \frac{4^k T_{m+k,k-1} - T_{m+k-1,k-1}}{4^k - 1}$$

$$\int_a^b f(x)dx \approx T_{m,0} = \frac{1}{2} T_{m-1,0} + h \sum_{i=1,3}^{2^m-1} f\left(a+ih\right) \qquad h = \left(\frac{b-a}{2^m}\right)$$

$$\begin{array}{lllll}
2^m & T_{m,0} & & & \\
2^{m+1} & T_{m+1,0} & T_{m+1,1} & & \\
2^{m+2} & T_{m+2,0} & T_{m+2,1} & T_{m+2,2} & \\
2^{m+3} & T_{m+3,0} & T_{m+3,1} & T_{m+3,2} & T_{m+3,3}
\end{array}$$

$$T_{m+k,k} = \frac{4^k T_{m+k,k-1} - T_{m+k-1,k-1}}{4^k - 1}$$

$$\int_a^b f(x)dx \approx T_{m,0} = \frac{1}{2} T_{m-1,0} + h \sum_{i=1,3}^{2^m - 1} f(a+ih) \qquad h = \left(\frac{b-a}{2^m}\right)$$

$$\begin{array}{lllll}
2^m & T_{m,0} & & & \\
2^{m+1} & T_{m+1,0} & T_{m+1,1} & & \\
2^{m+2} & T_{m+2,0} & T_{m+2,1} & T_{m+2,2} & \\
2^{m+3} & T_{m+3,0} & T_{m+3,1} & T_{m+3,2} & T_{m+3,3}
\end{array}$$

$$T_{m+k,k} = \frac{4^k T_{m+k,k-1} - T_{m+k-1,k-1}}{4^k - 1}$$

$$\int_a^b f(x)dx \approx T_{m,0} = \frac{1}{2} T_{m-1,0} + h \sum_{i=1,3}^{2^m-1} f\left(a + ih\right) \qquad h = \left(\frac{b-a}{2^m}\right)$$

$$\begin{tikzcd}
2^m & T_{m,0} \arrow[dr] & & & \\
2^{m+1} & T_{m+1,0} \arrow[r] \arrow[dr] & T_{m+1,1} \arrow[dr] & & \\
2^{m+2} & T_{m+2,0} \arrow[r] & T_{m+2,1} \arrow[r] & T_{m+2,2} & \\
2^{m+3} & T_{m+3,0} & T_{m+3,1} & T_{m+3,2} & T_{m+3,3}
\end{tikzcd}$$

$$T_{m+k,k} = \frac{4^k T_{m+k,k-1} - T_{m+k-1,k-1}}{4^k - 1}$$

$$\int_a^b f(x)dx \approx T_{m,0} = \frac{1}{2} T_{m-1,0} + h \sum_{i=1,3}^{2^m - 1} f(a + ih) \qquad h = \left(\frac{b-a}{2^m}\right)$$

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2^m & T_{m,0} \arrow[dr] & & & \\
2^{m+1} & T_{m+1,0} \arrow[r] \arrow[dr] & T_{m+1,1} \arrow[dr] & & \\
2^{m+2} & T_{m+2,0} \arrow[r] \arrow[dr] & T_{m+2,1} \arrow[r] & T_{m+2,2} & \\
2^{m+3} & T_{m+3,0} \arrow[r] & T_{m+3,1} & T_{m+3,2} & T_{m+3,3}
\end{tikzcd}$$

$$T_{m+k,k} = \frac{4^k T_{m+k,k-1} - T_{m+k-1,k-1}}{4^k - 1}$$

$$\int_a^b f(x)dx \approx T_{m,0} = \frac{1}{2} T_{m-1,0} + h \sum_{i=1,3}^{2^m-1} f\left(a+ih\right) \qquad h = \left(\frac{b-a}{2^m}\right)$$

$$\begin{tikzcd}
2^m & T_{m,0} \arrow[d, dash] & & & \\
2^{m+1} & T_{m+1,0} \arrow[r] \arrow[d, dash] & T_{m+1,1} \arrow[d, dash] & & \\
2^{m+2} & T_{m+2,0} \arrow[r] \arrow[d, dash] & T_{m+2,1} \arrow[r] \arrow[d, dash] & T_{m+2,2} & \\
2^{m+3} & T_{m+3,0} \arrow[r] & T_{m+3,1} \arrow[r] & T_{m+3,2} & T_{m+3,3}
\end{tikzcd}$$

$$T_{m+k,k} = \frac{4^k T_{m+k,k-1} - T_{m+k-1,k-1}}{4^k - 1}$$

$$\int_a^b f(x)dx \approx \; T_{m,0} = \frac{1}{2} T_{m-1,0} + h \sum_{i=1,3}^{2^m-1} f\left(a + ih\right) \qquad h = \left(\frac{b-a}{2^m}\right)$$

$$\begin{tikzcd}
2^m & T_{m,0} \arrow[d, dash] & & & \\
2^{m+1} & T_{m+1,0} \arrow[r] \arrow[d, dash] & T_{m+1,1} \arrow[d, dash] & & \\
2^{m+2} & T_{m+2,0} \arrow[r] \arrow[d, dash] & T_{m+2,1} \arrow[r] \arrow[d, dash] & T_{m+2,2} \arrow[d, dash] & \\
2^{m+3} & T_{m+3,0} \arrow[r] & T_{m+3,1} \arrow[r] & T_{m+3,2} \arrow[r] & T_{m+3,3}
\end{tikzcd}$$

To check whether Romberg integration works properly,

$$R_m = \frac{T_{m\text{-}1,0} - T_{m,0}}{T_{m,0} - T_{m+1,0}} \approx 4$$

since

$$T_{m,0} = h\left[\frac{f_0}{2} + f_1 + f_2 + \cdots + f_{n\text{-}1} + \frac{f_n}{2}\right] + E(h), \qquad E(h) \approx \frac{h^2}{12}\left[f'(a) - f'(b)\right]$$

$$T_{m\text{-}1,0} = 2h\left[\frac{f_0}{2} + f_2 + \cdots + \frac{f_n}{2}\right] + E(h), \qquad E(h) \approx \frac{4h^2}{12}\left[f'(a) - f'(b)\right]$$

$$T_{m\text{-}1,0} - T_{m,0} \approx \frac{3h^2}{12}\left[f'(a) - f'(b)\right]$$

similarly $\quad T_{m,0} - T_{m+1,0} \approx \dfrac{3}{12}\left(\dfrac{h}{2}\right)^2 \left[f'(a) - f'(b)\right]$

hence $\quad R_m = \dfrac{T_{m\text{-}1,0} - T_{m,0}}{T_{m,0} - T_{m+1,0}} \approx 4$