

$$\# \sum f(a+k_i h) = f_{\text{cen}} = \sum_{k=1}^{m-1} f(a+k_i h) = \sum_{k=1}^{m-1} f(a+k h_i)$$

$$T_i = \frac{1}{2} h_{i-1} \left[\frac{1}{h_i} f(a) + \frac{1}{h_i} f(b) + \sum_{k=1}^{m-1} f(a+k h_i) \right] + h_i \sum_{k=0}^{m-1} f(a+k h_i)$$

Adaptive rule

$$T_i = T_{i-1} + h_i \sum_{k=0}^{m-1} f(a+k h_i)$$

Magnetic

2-state

$z = \sum$

What is

$$E = -\vec{H} \cdot \vec{\mu}$$

CH^2

$$\int p(x) dx$$

$P(x, p)$

$$P(x)$$

Simpson

$$\epsilon = \frac{1}{90} h^4 [f'''(a) - f'''(b)] \approx \underline{\underline{O(h^4)}}$$

→ Error dependent on the number of steps.

$$\left. \begin{array}{l} N_1 \Rightarrow h_1 = \frac{b-a}{n_1} \Rightarrow I_1 \\ N_2 \Rightarrow h_2 = \frac{b-a}{n_2} \Rightarrow I_2 \\ n_2 = 2n_1 \end{array} \right\}$$

$$h_1 \gg h_2 \rightarrow \text{Error } \left| \frac{I_2 - I_1}{3} \right|$$

$$\left. \begin{array}{l} I_2 \approx I_1 + ch_1^2 \\ I_2 \approx I_2 + ch_2^2 \end{array} \right\} \begin{array}{l} I_2 - I_1 \approx c(h_1^2 - h_2^2) \\ (I_2 - I_1) \approx 3ch_2^2 \quad \epsilon \approx ch_2^2 \end{array}$$

$$\epsilon = ch_2^2 = \frac{1}{3} (I_2 - I_1)$$

Adaptive rules

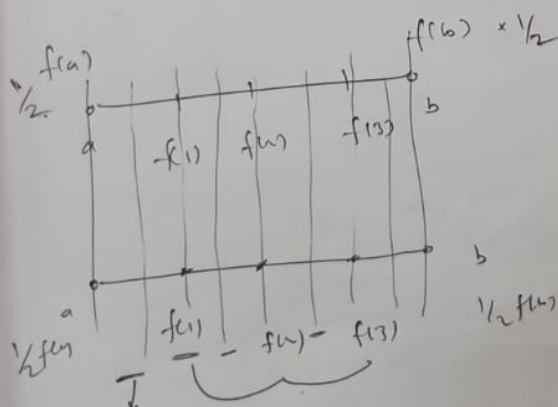
$$N_1, N_2 \approx 2N_1, N_3 \approx 2N_2, \dots$$

$$G_i = \frac{1}{3} (I_i - I_{i-1})$$

$$\left\{ \begin{array}{l} h_i = \frac{b-a}{n_i} \\ h_{i-1} = 2h_i \\ n_{i-1} = \frac{n_i}{2} \end{array} \right\}$$

$$I_i = h_i \left[\frac{1}{2} f(a) + \frac{1}{2} f(b) + \sum_{k=1}^{n_i-1} f(a + b h_i k) \right]$$

$$+ \sum_{k=1}^{n_i} f(a + b h_i k)$$



These new points are added on by itself.

[dp] as this part are along interval.

Computational Physics

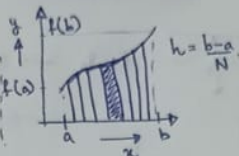
1. Integration:

Numerical:

Trapezoidal Rule:

k^{th} slice area: $\frac{1}{2} [f(a+kh) + f(a+(k-1)h)] h$

A_k



$$I(a, b) = \sum_{k=1}^N A_k = \int_a^b f(x) dx$$

$$= \frac{1}{2} h \left[\sum_{k=1}^N [f(a+kh) + f(a+(k-1)h)] \right] = h \left[\frac{1}{2} f(a) + \frac{1}{2} (f(a+h) + f(a+h)) + f(a+2h) + \dots + \frac{1}{2} f(b) \right]$$

$$= h \left[\frac{f(a)}{2} + f(a+h) + f(a+2h) + \dots + \frac{1}{2} f(b) \right]$$

$$= h \left[\frac{f(a)}{2} + \frac{f(b)}{2} + \sum_{k=1}^{N-1} f(a+kh) \right]$$

Ex: $\int_0^2 (x^4 - 2x + 1) dx \rightarrow f(x) = x^4 - 2x + 1$

$a=0, b=2, N: ??$ (how to choose)

Code:

def f(x):

return x**4 - 2*x + 1

N=10

a=0.0, b=2.0

h=(b-a)/N

s=0.5*f(a)+0.5*f(b)

for k in range(1, N):

s+=f(a+kh)

print(h*s)

$N \uparrow \Rightarrow$ better approx.

Error: $O(h^2) \rightarrow$ correct upto $O(h)$

$$C \cdot \left(\frac{f(b)-f(a)}{b-a} \right)^2$$

2. Simpson's Rule: (or one-third rule)

Fit a quadratic curve through three points.

Quadratic: $Ax^2 + Bx + C$

$$f(-h) = Ah^2 - Bh + C$$

$$f(0) = C$$

$$f(h) = Ah^2 + Bh + C$$

$$A = \frac{1}{12} [f(-h) - f(0) + f(h)]$$

$$B = \frac{1}{2h} [f(h) - f(-h)], C = f(0)$$

Area under the curve of $f(x)$ from $-h$ to h :

$$\int_{-h}^h (Ax^2 + Bx + C) dx = \frac{2}{3} Ah^3 + 2Ch = \frac{1}{3} h [f(-h) + 4f(0) + f(h)] \rightarrow \textcircled{1}$$

First three points:

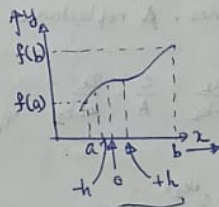
$x = a, a+h, a+2h$

Then: $x = a+2h, a+3h, a+4h$

$$I(a, b) \approx \frac{1}{3} h [f(a) + 4f(a+h) + f(a+2h)] + \frac{1}{3} h [f(a+2h) + 4f(a+3h) + f(a+4h)] + \dots + \frac{1}{3} h [f(a+(N-2)h) + 4f(a+(N-1)h) + f(b)]$$

$$\Rightarrow I(a, b) \approx \frac{1}{3} h [f(a) + f(b)] + \left[4 \sum_{\substack{k \text{ odd} \\ k \neq a, b}} f(a+kh) + 2 \sum_{\substack{k \text{ even} \\ k \neq a, b}} f(a+kh) \right]$$

Expand



Take three points for each $\frac{1}{3}$ rd portion of the actual curve (or $\frac{1}{3}h$ too!)

N=10

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→ Error in numerical calculations, (integration)

$$I(a, b) = \int_a^b f(x) \cdot dx = \frac{h}{2} [f(x_0) + 2f(x_1) + \dots + 2f(x_{n-1}) + f(x_n)]$$

$h = \frac{b-a}{n}$

→ x_{k-1} point

$$f(x) = f(x_{k-1}) + (x - x_{k-1}) f'(x_{k-1}) + \frac{1}{2} (x - x_{k-1})^2 f''(x_{k-1}) + \dots$$

$$\int_{x_{k-1}}^{x_k} f(x) \cdot dx = f(x_{k-1}) \int_{x_{k-1}}^{x_k} dx + f'(x_{k-1}) \int_{x_{k-1}}^{x_k} (x - x_{k-1}) dx + \frac{1}{2} f''(x_{k-1}) \int_{x_{k-1}}^{x_k} (x - x_{k-1})^2 dx + \dots$$

$$x - x_{k-1} = u \quad \Rightarrow \quad \int_{x_{k-1}}^{x_k} f(x) \cdot dx = f(x_{k-1}) \int_0^h du + f'(x_{k-1}) \int_0^h u du + \frac{1}{2} f''(x_{k-1}) \int_0^h u^2 du + \dots$$

$$= hf(x_{k-1}) + f'(x_{k-1}) \frac{h^2}{2} + \frac{f''(x_{k-1})}{2} \times \frac{h^3}{6} + O(h^4)$$

$$\int_{x_{k-1}}^{x_k} f(x) \cdot dx = hf(x_{k-1}) + \frac{1}{2} h^2 f'(x_{k-1}) + \frac{1}{6} h^3 f''(x_{k-1}) + O(h^4)$$

$$\int_{x_{k-1}}^{x_k} f(x) \cdot dx = \frac{1}{2} [h(f(x_{k-1}) + f(x_k))] + \frac{1}{4} h^2 [f'(x_{k-1}) + f'(x_k)] + \frac{h^3}{24} [f''(x_{k-1}) + f''(x_k)] + O(h^4)$$

$$\# = \frac{1}{2} h \sum_{k=1}^N [f(x_{k-1}) + f(x_k)] + \frac{1}{2} h^2 [f'(a) - f'(b)] + \frac{1}{12} h^3 [f''(x_{k-1}) - f''(x_k)] + O(h^4)$$

→ calculation accurate in order.

for the 2nd order derivative

$$\int_a^b f''(x) \cdot dx = \frac{1}{2} \left[\sum_{k=1}^N [f''(x_{k-1}) + f''(x_k)] + O(h^2) \right]$$

$$= \frac{1}{12} h^3 \left[\sum_{k=1}^N [f''(x_{k-1}) + f''(x_k)] \right]$$

$$= \frac{1}{6} h^2 \int_a^b f''(x) \cdot dx$$

$$= \frac{1}{6} h^2 [f'(b) - f'(a)] + O(h^4)$$

$$\left[\int_a^b f(x) dx = \frac{1}{2} h \sum_{k=1}^N [f(x_{k-1}) + f(x_k)] + \frac{1}{2} h^2 [f'(a) - f'(b)] + O(h^4) \right]$$

$$E = \frac{1}{2} h^2 [f'(a) - f'(b)]$$

$$= O(h^4)$$

→ ~~error~~
~~dynamic~~
~~what's that?~~
 first order approx
 error

Simpson

→ Error

N₁

N₂
= 2N₁

b₁, 772

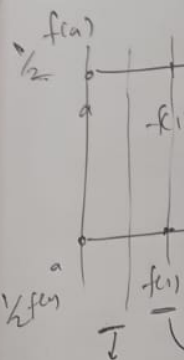
→ I₂

I₃

Adaptive

N₁, N₂

G₁₀



Three
new pts
on by
adapting.

Computational Physics

1. Romberg Integration:-

Practical error estimation: $N \rightarrow 2N$, check $I_2 - I_1$. If it is less than 10^{-8} , just stop.
 ^ helps to get higher accuracy even while using Trapezoidal rule.

Trapezoidal: Accurate upto $O(h^2) \approx C h^2$ no only accurate upto first-order.

$$\begin{aligned} \text{Simpson: Accurate upto } O(h^4) \\ U_1^2 = \frac{1}{3}(I_1 - I_{-1}) \Rightarrow I = I_1 + U_1^2 + O(h^4) \\ = I_1 + \frac{1}{3}(I_1 - I_{-1}) + O(h^4) \rightarrow (A) \end{aligned}$$

Integral is now accurate upto third-order, by adding a few terms.

Generalisation: (only for Trapezoidal)

$$R_{1,1} = I_1, R_{1,2} = I_1 + \frac{1}{3}(I_1 - I_{-1})$$

$$\Rightarrow R_{1,2} = R_{1,1} + \frac{1}{3}(R_{1,1} - R_{-1,1})$$

$$(A): I = R_{1,2} + O(h_1^4) = R_{1,2} + 16c_2 h_1^4 + O(h_1^6)$$

$$\text{PF: } I = R_{1,2} + O(h_1^4) = R_{1,2} + 16c_2 h_1^4 + O(h_1^6)$$

$$\Rightarrow S h_1^4 = \frac{1}{15}(R_{1,2} - R_{-1,2}) + O(h_1^6)$$

$$I = R_{1,2} + \frac{1}{15}(R_{1,2} - R_{-1,2}) + O(h_1^6) \rightarrow \text{Accurate in 5th order.}$$

With an error of order h^{2m} ,

$$I = R_{1,m} + C h_1^{2m} + O(h_1^{2m+2})$$

$$\text{Also, } I = R_{-1,m} + C h_{-1}^{2m} + O(h_{-1}^{2m+2}) = R_{-1,m} + C h_1^{2m} + O(h_1^{2m+2})$$

$$C h_1^{2m} = \frac{1}{4^m - 1}(R_{1,m} - R_{-1,m}) + O(h_1^{2m+2})$$

$$\therefore I = R_{1,m+1} + O(h_1^{2m+2}); R_{1,m+1} = R_{1,m} + \frac{1}{4^m - 1}(R_{1,m} - R_{-1,m})$$

Algorithm:-

$$I_1 = R_{1,1}, I_2 = R_{2,1} \rightarrow R_{2,2}$$

$$I_1 = R_{1,1}$$

$$I_2 = R_{2,1} \rightarrow R_{2,2}$$

$$I_3 = R_{3,1} \rightarrow R_{3,2} \rightarrow R_{3,3}$$

$$I_4 = R_{4,1} \rightarrow R_{4,2} \rightarrow R_{4,3} \rightarrow R_{4,4}$$