$$I = \int_a^b f(x)\,dx = A_1 + A_2 + \dots + A_{N-1}$$

$$= h\left(\frac{f_1}{2} + \frac{f_2}{2} + \frac{f_2}{2} + \frac{f_3}{2} + \dots + \frac{f_{N-1}}{2} + \frac{f_N}{2}\right)$$

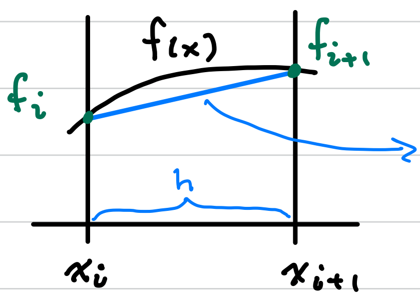
$$= h\left(f_1/2 + f_2 + f_3 + \dots + f_{N-1} + f_N/2\right)$$

(each point, except first and last, is involved with two trapezoids)

$$I_T = \sum_{i=1}^{N} f(x_i)\,\omega_i \quad , \quad \{\omega_i\} = \left\{\frac{h}{2}, h, h, \dots h, h/2\right\}$$

What is the truncation error?

$$f(x_i + h) = f(x_i) + h f'(x_i) + \frac{h^2}{2} f''(x_i) + \dots$$




eq$^{n}$ of top of trapezoid

$$f_t = f_i + (x - x_i)\,\frac{f_{i+1} - f_i}{h}$$

expand $f_{i+1}$ in Taylor series

$$f_t = f_i + \frac{(x - x_i)}{h}\left[f_i + h f_i' + \frac{h^2}{2} f_i'' + \frac{h^3}{3!} f_i''' + \dots - f_i\right]$$

$$= f_i + (x - x_i) f_i' + (x - x_i)\frac{h}{2} f_i'' + (x - x_i)\frac{h^2}{3!} f_i'''$$

$$\int_{x_i}^{x_{i+1}} f_t\,dx = h f_i + \frac{h^2}{2} f_i' + \frac{h^2}{2}\frac{h}{2} f_i'' + \frac{h^2}{2}\frac{h^2}{3!} f_i''' + \dots$$

$$= h f_i + \frac{h^2}{2} f_i' + \frac{h^3}{\underline{4}} f_i'' + \frac{h^4}{2 \cdot 3!} f_i'''$$

this is important

Compare with integral of $f(x) = f(x_i) + (x-x_i)f'(x_i) + \dots$

$$\int_{x_i}^{x_{i+1}} f\,dx = \int_{x_i}^{x_{i+1}} \left(f_i + (x-x_i)f_i' + \frac{(x-x_i)^2}{2} f_i'' + \dots\right) dx$$

$$= h f_i + \frac{h^2}{2} f_i' + \frac{h^3}{6} f_i'' + \dots$$

$h^3$ term using $f_t$ differs from result based on Taylor series expansion of $f$

$\therefore$ Truncation error in one step is $\mathcal{O}(h^3)$

Error over $N$ steps is $N \cdot \mathcal{O}(h^3)$

$N \approx \frac{b-a}{h}$ $\therefore$ $\epsilon_{trunc}$ is $\mathcal{O}(h^2)$

What about roundoff error? What is best $h$?

At each step $\sim \epsilon_M$ of roundoff
- sometimes positive, sometimes negative

so it turns out $\epsilon_{ro} \neq N \epsilon_M$ but rather $\sqrt{N}\,\epsilon_M$

$\epsilon_{ro} \sim \sqrt{\frac{b-a}{h}}\,\epsilon_M$

For $\epsilon_M \sim 10^{-16}$ and $b-a \sim 1 \sim f \sim f' \sim f'' \to N \sim \frac{1}{h}$

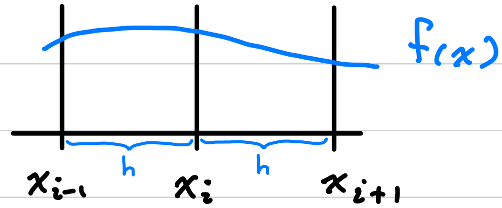
smallest error occurs when $\epsilon_{ro} \simeq \epsilon_{trunc}$

$\frac{\epsilon_M}{\sqrt{h}} \approx h^2 \to h^{5/2} \simeq \epsilon_M$ $\quad h_{optimal} \sim 4\times 10^{-7} \sim 10^{-6}$

$\epsilon_{best} \sim \frac{\epsilon_M}{\sqrt{h_{opt}}} \sim 10^{-12}$ or $10^{-13}$

# Simpson's Rule

Consider a portion of an integral from $x_{i-1}$ to $x_{i+1}$




Approximate $f(x)$ with a cubic $f^n$

$$f(x) = f(x_i) + (x-x_i)f'(x_i) + \frac{1}{2}(x-x_i)^2 f''(x_i) + \frac{1}{3!}(x-x_i)^3 f'''(x_i) + \mathcal{O}\left((x-x_i)^4\right)$$

$$I = \int_{x_{i-1}}^{x_{i+1}} dx \left[ f_i + f_i'(x-x_i) + \frac{1}{2} f_i''(x-x_i)^2 + \frac{1}{3!} f_i'''(x-x_i)^3 + \mathcal{O}(x-x_i)^4 \right]$$

$$= (x_{i+1}-x_{i-1})f_i + 0 + \frac{1}{6} f_i''\left[ (\overset{h}{x_{i+1}-x_i})^3 - (\overset{-h}{x_{i-1}-x_i})^3 \right]$$

$$+ 0 + \mathcal{O}\left( (x-x_i)^5 \Big|_{x_{i-1}}^{x_{i+1}} \right)$$

$$= 2hf_i + \frac{f_i''}{6} 2h^3 + \mathcal{O}(h^5)$$

rewrite $f_i'' = \dfrac{f_{i-1} - 2f_i + f_{i+1}}{h^2} + \mathcal{O}(h^2)$

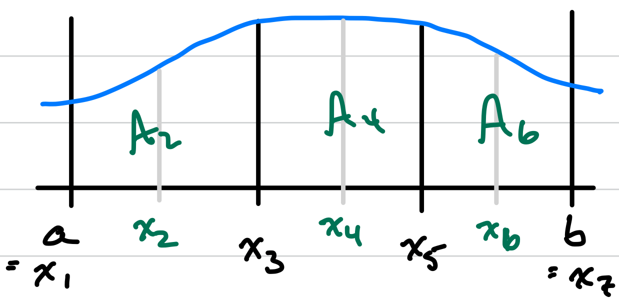
$$= 2hf_i + \frac{h}{3}\left( f_{i-1} - 2f_i + f_{i+1} \right) + \mathcal{O}(h^5)$$

$$= \frac{h}{3}\left( f_{i-1} + 4f_i + f_{i+1} \right) + \mathcal{O}(h^5)$$

truncation error in one step

Note: This is equivalent to fitting a quadratic function through $(x_{i-1}, f_{i-1})$, $(x_i, f_i)$ and $(x_{i+1}, f_{i+1})$ (cubic term contributes zero to the integral).

Break up entire integral into such portions (width $2h$).
Break up entire integral into an even number of slabs of width $h$.




$N$ is the number of points.
$N$ must be odd.

$$I_s = \frac{h}{3}\left(f_1 + 4f_2 + f_3\right) + \frac{h}{3}\left(f_3 + 4f_4 + f_5\right) + \ldots + \frac{h}{3}\left(f_{N-2} + 4f_{N-1} + f_N\right)$$

$$= \frac{h}{3}\left[f_1 + 4f_2 + 2f_3 + 4f_4 + 2f_5 + \ldots + 2f_{N-2} + 4f_{N-1} + f_N\right]$$

truncation error is $\sim \mathcal{O}(h^5)$

$N \sim \frac{b-a}{h}$ so $\epsilon_{trunc}$ is $\mathcal{O}(h^4)$

In terms of general form for numerical integration

$$I_s = \sum_{i=1}^{N} f_i\, w_i\,, \quad w_i = \left\{\frac{h}{3}, \frac{4h}{3}, \frac{2h}{3}, \frac{4h}{3}, \ldots \frac{2h}{3}, \frac{4h}{3}, \frac{h}{3}\right\}$$

Note: consider $N = 3$

$$\{\omega_i\} = \left\{ \frac{h}{3}, \frac{4h}{3}, \frac{h}{3} \right\}$$

$$\sum_{i=1}^{N} \omega_i = \frac{h}{3}(1+4+1) = 2h = (N-1)h$$

This is generally true for all integration algorithms

$$\sum_{i=1}^{N} \omega_i = (N-1)h$$

Best error, optimal $h$:

as always $\quad \epsilon_{ro} \simeq \epsilon_{trunc}$

(again, for $b-a \sim f \sim etc \sim 1$)

$$\frac{\epsilon_M}{\sqrt{h}} \simeq h^4$$

$$\epsilon_M \simeq h^{9/2}$$

$$h_{optimal} \simeq \epsilon_M^{2/9} \simeq 3 \times 10^{-4} \sim 10^{-3} \quad (N \sim 10^3)$$

$$\epsilon_{best} \approx \frac{\epsilon_M}{\sqrt{h_{opt}}} \sim 6 \times 10^{-15} \sim 10^{-14}$$

# Method of Undetermined Coefficients

Consider writing $f(x)$ as a polynomial of order $p$

$$f(x) \approx \sum_{n=0}^{p} c_n x^n$$

on a small interval $x \in [\tilde{a}, \tilde{b}]$

General integration formula

$$\int_{\tilde{a}}^{\tilde{b}} f(x)\,dx = \sum_i f(x_i)\,\omega_i$$

with $i = 1, 2, \dots p+1$

$\rightarrow p$ (sub)intervals

becomes

$$\int_{\tilde{a}}^{\tilde{b}} \sum_{n=0}^{p} c_n x^n\,dx = \sum_{n=0}^{p} c_n \int_{\tilde{a}}^{\tilde{b}} dx\, x^n = \sum_{i=1}^{p+1} \sum_{n=0}^{p} c_n x_i^n \omega_i$$

$$= \sum_{n=0}^{p} c_n \sum_{i=1}^{p+1} x_i^n \omega_i$$

$$\rightarrow \quad \int_{\tilde{a}}^{\tilde{b}} dx\, x^n = \sum_{i=1}^{p+1} x_i^n \omega_i$$

for each $n \in 0, \dots p$

$\rightarrow p+1$ equations

$p+1$ unknowns : $\omega_i$'s

$$\frac{\tilde{b}^{n+1} - \tilde{a}^{n+1}}{n+1} = \sum_{i=1}^{p+1} x_i^n \omega_i$$

$$n=0 \qquad \tilde{b}-\tilde{a} = \omega_1 + \omega_2 + \dots + \omega_{p+1}$$

$$n=1 \qquad \frac{\tilde{b}^2-\tilde{a}^2}{2} = x_1\omega_1 + x_2\omega_2 + \dots + x_{p+1}\omega_{p+1}$$

$$n=2 \qquad \frac{\tilde{b}^3-\tilde{a}^3}{3} = x_1^2\omega_1 + x_2^2\omega_2 + \dots + x_{p+1}^2\omega_{p+1}$$

$$\vdots$$

$$n=p \qquad \frac{\tilde{b}^{p+1}-\tilde{a}^{p+1}}{p+1} = x_1^p\omega_1 + x_2^p\omega_2 + \dots + x_{p+1}^p\omega_{p+1}$$

or, in matrix form

$$\begin{pmatrix} 1 & 1 & \dots & 1 \\ x_1 & x_2 & \dots & x_{p+1} \\ x_1^2 & x_2^2 & \dots & x_{p+1}^2 \\ & & \vdots & \\ x_1^p & x_2^p & \dots & x_{p+1}^p \end{pmatrix} \begin{pmatrix} \omega_1 \\ \omega_2 \\ \omega_3 \\ \vdots \\ \omega_{p+1} \end{pmatrix} = \begin{pmatrix} \tilde{b}-\tilde{a} \\ (\tilde{b}^2-\tilde{a}^2)/2 \\ (\tilde{b}^3-\tilde{a}^3)/3 \\ \vdots \\ (\tilde{b}^{p+1}-\tilde{a}^{p+1})/(p+1) \end{pmatrix}$$

solve for $\omega_i$'

- gives integration formula on fitting $f(x)$ with a polynomial of degree $p$ on each interval $\tilde{b}-\tilde{a}$

In terms of dividing up domain of integration, can let

$$\tilde{b}-\tilde{a} = ph \quad , \quad h = \frac{b-a}{N-1}$$

E.g. For Simpson's rule, $\tilde{b}-\tilde{a} = 2h$ $(p=2)$