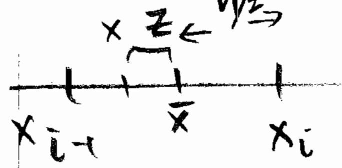
$$f(x) = f(\bar{x}) + z f'(\bar{x}) + \frac{z^2}{2} f''(\bar{x}) + \ldots$$

$$\begin{cases} z = x - \bar{x} \\ \bar{x} = \dfrac{x_i + x_{i-1}}{2} \end{cases}$$



Now, <u>1st term</u> :

$$\int_{x_{i-1}}^{x_i} f(x)\,dx = \int_{-h/2}^{h/2} \left[f(\bar{x}) + z f'(\bar{x}) + \frac{z^2}{2} f''(\bar{x}) + \ldots \right] dz$$

change of variable from x to z

$$= h f(\bar{x}) + \cancel{\left[\frac{z^2}{2} f'(\bar{x}) \right]_{-h/2}^{h/2}}^{\,0} + \left[\frac{z^3}{6} f''(\bar{x}) \right]_{-h/2}^{h/2} + \ldots$$

all even terms cancel!

$$= h f(\bar{x}) + \frac{h^3}{24} f''(\bar{x}) + \ldots$$

<u>2nd term</u> :

$$\frac{h}{2}\left(f(x_{i-1}) + f(x_i) \right) = \frac{h}{2} \Big[f(\bar{x}) - \frac{h}{2} f'(\bar{x}) + \frac{1}{2}\left(\frac{h}{2}\right)^2 f''(\bar{x}) - \ldots$$

$$+ f(\bar{x}) + \frac{h}{2} f'(\bar{x}) + \frac{1}{2}\left(\frac{h}{2}\right)^2 f''(\bar{x}) + \ldots \Big]$$

$$= h f(\bar{x}) + \frac{1}{8} h^3 f''(\bar{x}) + \ldots$$

Thus,

$$\boxed{E = -\frac{1}{12} h^3 f''(\bar{x})}$$

- proportional to $f''(\bar{x})$
- step-wise error decreases as h^3!

- Error for the entire range $[a, b]$:

sum of the previous result:

$$E_T \simeq -\frac{1}{12} \frac{(b-a)^3}{N^3} \sum_1^N f''(\bar{x}_i) \qquad \boxed{h = \frac{b-a}{N}}$$

$$= -\frac{1}{12} \frac{(b-a)^3}{N^2} \underbrace{\sum_1^N \frac{f''(\bar{x}_i)}{N}}$$

$$= -\frac{1}{12} (b-a) h^2 \bar{f}''$$

So, the total error is ~ range of integration $(b-a)$

~ h^2 step-size square!

* Note: - Since we use Taylor expansion, E make sense only if $f(x)$ is analytic in $[a, b]$!

☆ – by knowing E_i, we can do a better estimate by extrapolation to $h \to 0$

Romberg's rule (next lecture).

(2) Simpson's rule (2nd order)

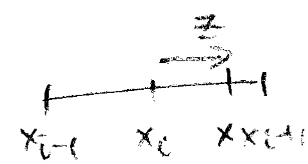
– app. $f(x) \in [x_{i-1}, x_{i+1}]$ by a quadratic polynomial.

(see notes) next page also on pdf

☆ recall from interpolation, for quadratic polynomial, we need 3 pts → two intervals

let look at $I_{[i-1, i+1]}$ by expanding $f(x)$ around x_i!

$$I_{[i-1,i+1]} = \int_{x_{i-1}}^{x_{i+1}} f(x)\,dx$$



$z = x - x_i$

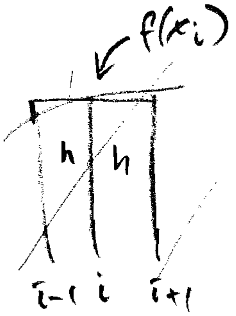
$$= \int_{-h}^{+h} \left[f(x_i) + z f'(x_i) + \frac{z^2}{2} f''(x_i) + \frac{z^3}{6} f'''(x_i) + \ldots\right] dz$$

$$= 2h f(x_i) + \cancel{\left[\frac{z^2}{2} f'(x_i)\right]_{-h}^{h}}^{\to 0} + \left[\frac{z^3}{6} f''(x_i)\right]_{-h}^{h} + O(h^5 f_i^4)$$

all even terms $\to 0$

$$I_{[i-1,i+1]} = 2h\,f(x_i) + \frac{2}{6}h^3 f''(x_i) + O(h^5 f_i^4)$$

$\uparrow$



to $O(h^3)$, this is equal to N integral with rect rule in $[i-1,i+1]$.

☆ Now, if we include $f''(x_i)$ info into our N integral, we can in principle improve accuracy to $O(h^5)$ per step

$O(h^4)$ whole interval

$$\Rightarrow f''(x_i) = \frac{d}{dx}\left(f'(x)\right)\Big|_{x=x_i} \quad \left[\begin{array}{l} x_i, x_{i-1} \to f'_{i-1/2} \\ x_i, x_{i+1} \to f'_{i+1/2} \end{array} \right\} \to f''_i$$

use (I) to numerically find using x_{i-1}, x_i, x_{i+1} (central diff.)

$$f'_{i-1/2} = \frac{f_i - f_{i-1}}{h} \qquad f'_{i+1/2} = \frac{f_{i+1} - f_i}{h}$$

$$f''_i = \frac{f'_{i+1/2} - f'_{i-1/2}}{h} = \boxed{\frac{f_{i+1} - 2f_i + f_{i-1}}{h^2}}$$

Substitute into $I_{[i-1,i+1]}$:

$$I_{[i-1,i+1]} = 2hf_i + \frac{1}{3}h^3\left(\frac{f_{i+1} - 2f_i + f_{i-1}}{h^2}\right) + \mathcal{O}(h^5 f_i^{4})$$

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

simpson's rule

For a complete interval:

$$\boxed{\begin{aligned} I_{[a,b]} &= \sum_{i=1}^{N-1} I_{[i-1,i+1]} \\ &= \frac{1}{3}h\left(f_0 + 4f_1 + 2f_2 + 4f_3 + \cdots + 2f_{N-2} + 4f_{N-1} + f_N\right) \end{aligned}}$$

Rule summary:

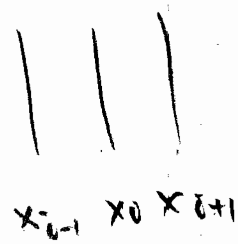
$$W_i = \begin{cases} \frac{1}{3} & \text{end pts} \\ \frac{4}{3} & \text{odd pts} \\ \frac{2}{3} & \text{even pts} \end{cases}$$

i	0	1	2	3	4	
	1	4	1			
			1	4	1	
					1	4
	1	4	2	4	2	4 ..

Note: # of intervals must be <u>even</u>!

(need a pair to get f_i'')

$\Rightarrow$ # of pts is <u>odd</u>:



Implementation: (See Box 2-2)

① Subdivide interval into small but reasonable # of intervals

$N_1 \sim 6$ (eval pts = 7)

② Calculate $f(x_i)$, $i = 0, \ldots, 6$

③ Calculate

$$S_d(N) = f_0 + f_N$$

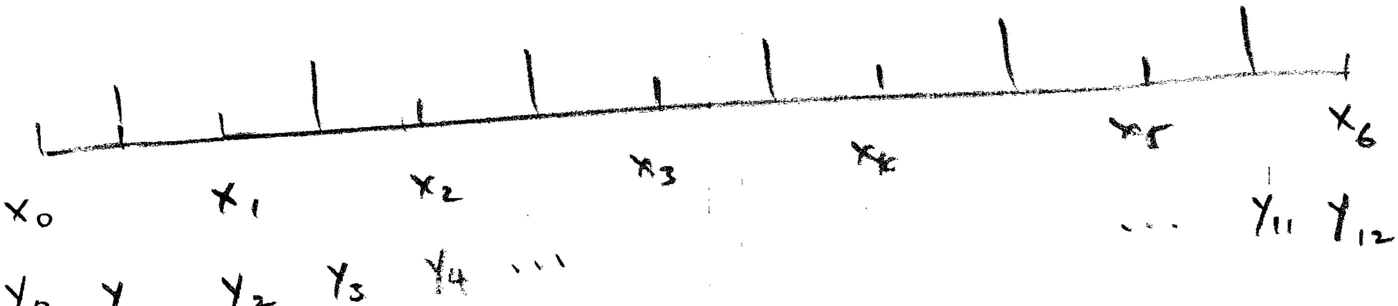
$$S_o(N) = f_1 + f_3 + \ldots + f_{N-1}$$

$$S_e(N) = f_2 + f_4 + \ldots + f_{N-2}$$

④ $I_{[a,b]}(N) = \frac{1}{3} h \{ S_d + 2 S_e + 4 S_o \}$

(check for convergence)

5 Subdivide (half) intervals



→ $h \to h/2$ $\{x_i\} \to \{y_i\}$

→ End pts stay the same

→ even pts stay even

→ previous odd pts → even

→ new pts → odd.

$$\Rightarrow \left.\begin{aligned} S_e(N_2) &= S_e(N_1) + S_o(N_1) \\ S_d(N_2) &= S_d(N_1) \end{aligned}\right\} \text{ all done before.}$$

$S_o(N_2)$ ← need new eval.

☆ advantage : can use old calculations.

General Comments :

- There are other choices for $\{W_i\}$ in Newton-Cotes (even step size)
  - high order $O(h^7)$ ...

    (high order does not necessary mean more accurate!)

    (depend on the function & h_{min})

- it can be open or close

  open → No end pts

  close → use end pts

  (might be useful for improper integral)

(B) Gaussian Quadrature

☆ We are free to choose <u>BOTH</u> $\{x_i\}$ and $\{w_i\}$!

General Statement :

If $f(x) \in P_{2n-1}(x)$

then $\int f(x)\,dx = \sum_{i=1}^{n} w_i f(x_i)$

this can be <u>exact</u> !

☆ → there are $2n$ degrees of freedom ! with $2N$ unknowns !

→ If $f(x) \approx P_{2n-1}(x)$ only

GQ will still give good app. to $\int f(x)\,dx$ up to a polynomial of order $2n-1$!

In other words, if we have <u>n data pts</u> (eval pts),

- in general, we can fit $P_{n-1}(x)$ to them & I will be <u>exact</u> for $f(x)$ being a polynomial of deg $\underline{\underline{<N}}$.

- But, if we use Gaussian grid pts, we have a formula for I which is <u>exact</u> for $f(x)$ being a polynomials of deg $\underline{\underline{<2N}}$!

N=2 example : $f(x) \in P_3(x)$

$$\int_a^b f(x)\,dx = w_1 f(x_1) + w_2 f(x_2) \qquad (*)$$

$\uparrow$

Four unknowns

→ need four equations!

Any $P_3(x)$ can be written as :

$$P_3(x) = a_0 1 + a_1 x + a_2 x^2 + a_3 x^3$$

– a linear combinations of the four basis functions : $\{1, x, x^2, x^3\} = \{e_i\}$

☆ If we require $(*)$ to be exact for $\{e_i\}_1^4$

then we can solve for w_1, w_2, x_1, x_2

And the Quadrature is exact for all $P_3(x)$!

→ reasoning: any $P_3(x)$ can be written as a linear combination of these four e_i's.