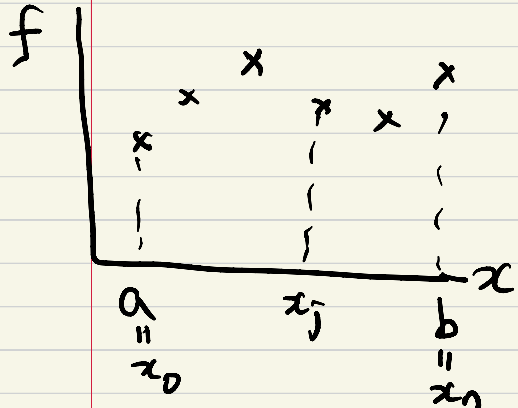
Ch.3 Numerical integration (quadrature)



$$I = \int_a^b f(x)\,dx = \sum_{j=0}^{n} f_j w_j$$ ← weight

3.1 Trapezoidal and Simpson's rule

Lagrange polynomial $P(x) = \sum_{j=0}^{n} f_j L_j(x)$

$$I = \int_a^b f(x)\,dx = \int_a^b P(x)\,dx = \int_a^b \sum_{j=0}^{n} f_j L_j\,dx = \sum_{j=0}^{n} f_j \overbrace{\int_a^b L_j\,dx}^{w_j}$$

$$= \boxed{(b-a)\sum_{j=0}^{n} c_j^n f_j}$$ where $c_j^n = \frac{1}{b-a}\int_a^b L_j(x)\,dx$

Newton-Cotes formula

Cotes number

$$c_j^n = \frac{1}{b-a}\int_a^b L_j(x)\,dx$$

$$I = (b-a)\sum_{j=0}^{n} c_j^n f_j$$

For $n=1$, $x_0 = a$, $x_1 = b$

$$L_0(x) = \frac{x-b}{a-b}, \quad L_1(x) = \frac{x-a}{b-a}$$

$$c_0^1 = \frac{1}{b-a}\int_a^b L_0(x)\,dx = \frac{1}{2}, \quad c_1^1 = \frac{1}{b-a}\int_a^b L_1(x)\,dx = \frac{1}{2}$$

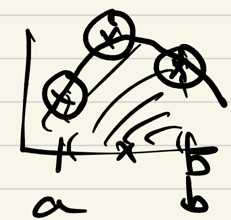
$$I = (b-a)\left(\frac{1}{2}f_0 + \frac{1}{2}f_1\right) = \boxed{(b-a)\left[\frac{1}{2}f(a) + \frac{1}{2}f(b)\right]}$$

trapezoidal method

For $n=2$, $x_0=a$, $x_1=\frac{1}{2}(a+b)$, $x_2=b$

$$\rightarrow L_0, L_1, L_2 \rightarrow c_0^2, c_1^2, c_2^2$$

$$\rightarrow I = \boxed{\frac{b-a}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right]}$$

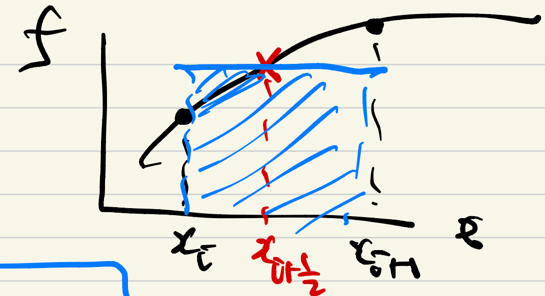


Simpson's rule

n	N	NC_0^n	NC_1^n	NC_2^n	NC_3^n	NC_4^n	NC_5^n	NC_6^n	error
1	2	1	1	0					$8.3\times10^{-2}\,\Delta^3 f''$
2	6	1	4	1					$3.5\times10^{-4}\,\Delta^5 f^{iv}$
3	8	1	3	3	1				$1.6\times10^{-4}\,\Delta^5 f^{iv}$
4	90	7	32	12	32	7			$5.2\times10^{-7}\,\Delta^7 f^{vi}$
5	288	19	75	50	50	75	19		$3.6\times10^{-7}\,\Delta^7 f^{vi}$
6	840	41	216	27	272	27	216	41	$6.4\times10^{-10}\,\Delta^9 f^{viii}$
$\vdots$									$\vdots$

3.2 Error analysis

* Rectangle (or midpoint) rule



$y_i = \frac{1}{2}(x_i + x_{i+1})$: midpoint

$$\boxed{\int_{x_i}^{x_{i+1}} f(x)\,dx = (x_{i+1}-x_i)\,f(y_i) = h_i\,f(y_i)}$$

$h_i = x_{i+1} - x_i$

$$f(x) = f(y_i) + (x-y_i)f'(y_i) + \frac{1}{2}(x-y_i)^2 f''(y_i) + \frac{1}{6}(x-y_i)^3 f'''(y_i) + \cdots$$

$$\int_{x_i}^{x_{i+1}} f(x)\,dx = f(y_i)\cdot h_i + \frac{1}{2}(x-y_i)^2\Big|_{x_i}^{x_{i+1}} f'(y_i) + \frac{1}{6}(x-y_i)^3\Big|_{x_i}^{x_{i+1}} f''(y_i) + \cdots$$

$$= \boxed{f(y_i)\cdot h_i} + \underline{\frac{1}{24}h_i^3 f''(y_i)} + \frac{1}{1920}h_i^5 f^{iv}(y_i) + \cdots \quad (*)$$

mid-point rule (MR)

leading error

3rd-order accurate for one interval

* Trapezoidal rule
$$\boxed{\int_{x_i}^{x_{i+1}} f(x)\,dx = \frac{h_i}{2}\left[f(x_i) + f(x_{i+1})\right]} \quad \text{TR}$$

$$f(x_i) = f(y_i) + (x_i - y_i) f'(y_i) + \frac{1}{2}(x_i - y_i)^2 f''(y_i) + \frac{1}{6}(x_i - y_i)^3 f'''(y_i) + \cdots$$

$$+ \quad f(x_{i+1}) = f(y_i) + (x_{i+1} - y_i) f'(y_i) + \frac{1}{2}(x_{i+1} - y_i)^2 f''(y_i) + \frac{1}{6}(x_{i+1} - y_i)^3 f'''(y_i) + \cdots$$

$$\frac{1}{2}\left(f(x_i) + f(x_{i+1})\right) = f(y_i) + \frac{1}{8} h_i^2 f''(y_i) + \frac{1}{384} h_i^4 f^{iv}(y_i) + \cdots$$

$$\rightarrow f(y_i) = \frac{1}{2}\left(f(x_i) + f(x_{i+1})\right) - \frac{1}{8} h_i^2 f''(y_i) - \frac{1}{384} h_i^4 f^{iv}(y_i) \cdots$$

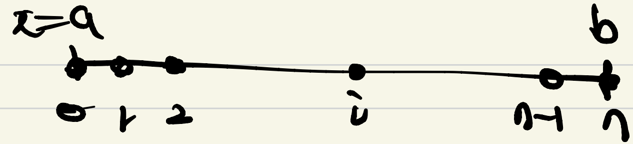
Substitute this into (*).

$$\rightarrow \underbrace{\boxed{\int_{x_i}^{x_{i+1}} f(x)\,dx = \frac{1}{2} h_i \left(f(x_i) + f(x_{i+1})\right)}}_{\text{trapezoidal method (TR)}} \underbrace{- \frac{1}{12} h_i^{3} f''(y_i)}_{\text{leading error}} - \frac{1}{480} h_i^5 f^{iv}(y_i) \cdots$$

3rd-order accurate for one interval

$\Rightarrow$ The error of TR is twice bigger than that of MR!

Global interval [a, b]



$$I = \int_a^b f(x)\,dx$$

$h_i = h$ uniform spacing

$\rightarrow nh = b-a$

TR $$= \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} f(x)\,dx$$

$$= \sum_{i=0}^{n-1} \left[\frac{1}{2}h\left(f(x_i)+f(x_{i+1})\right) - \frac{1}{12}h_i^3 f''(y_i) - \frac{1}{480}h_i^5 f^{iv}(y_i) + \cdots \right]$$

$$= \boxed{\frac{h}{2}\left[f(a)+f(b)+2\sum_{i=1}^{n-1} f(x_i)\right]} - \frac{1}{12}h^3 \sum_{i=0}^{n-1} f''(y_i) - \frac{1}{480}h^5 \sum_{i=0}^{n-1} f^{iv}(y_i) + \cdots$$

(Mean value theorem $\sum_{i=0}^{n-1} f''(y_i) = n f''(\bar{x})$ where $a \le \bar{x} \le b$

$\sum_{i=0}^{n-1} f^{iv}(y_i) = n f^{iv}(\xi)$ $\quad a \le \xi \le b$

$n = \dfrac{b-a}{h}$)

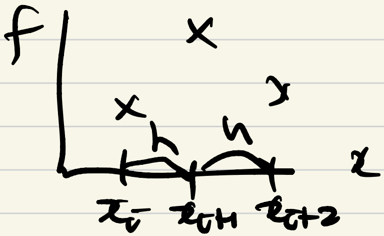
$$= \boxed{\frac{h}{2}\left[f(a)+f(b)+2\sum_{i=1}^{n-1} f(x_i)\right]} - (b-a)\frac{h^2}{12} f''(\bar{x}) - (b-a)\frac{h^4}{480} f^{iv}(\xi) + \cdots$$

2nd-order accurate for entire interval

leading error

$\Rightarrow$ TR is second-order accurate.

- Simpson's rule



$$\int_{x_i}^{x_{i+2}} f(x)\,dx = \frac{(2h)}{6}\left[f(x_i) + 4f(x_{i+1}) + f(x_{i+2})\right] \equiv S(f)$$

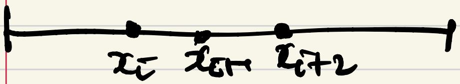
$$\int_{x_i}^{x_{i+2}} f(x)\,dx = \frac{(2h)}{2}\left[f(x_i) + f(x_{i+2})\right] \equiv T(f)$$

$$\int_{x_i}^{x_{i+2}} f(x)\,dx = (2h)\, f(x_{i+1}) \equiv R(f)$$

$$\rightarrow \boxed{S(f) = \frac{2}{3}R(f) + \frac{1}{3}T(f)}$$

Recall that the truncation error of TR is twice that of MR with opposite signs.

$\rightarrow$ Simpson's rule is 5th order accurate for one interval and 4th order accurate for entire interval.



even numbers of panels
and odd " of grid pts.

$$\int_{x_i}^{x_{i+2}} f(x)\,dx = \frac{h}{3}\left(f_i + 4f_{i+1} + f_{i+2}\right)$$

$$\int_{x_{i+2}}^{x_{i+4}} \quad = \frac{h}{3}\left(f_{i+2} + 4f_{i+3} + f_{i+4}\right)$$

$$\vdots$$

$$I = \int_a^b f(x)\,dx = \frac{h}{3}\left[f(a) + f(b) + 4\sum_{\substack{1\\ \text{odd}}}^{n-1} f_j + 2\sum_{\substack{2\\ \text{even}}}^{n-2} f_j\right]$$

$$-\frac{h^4}{180}(b-a)\,f^{iv}(\bar{x}) + \cdots$$

leading error $\Rightarrow$ 4th-order accurate

3.3 TR w/ end correction

$$\int_{x_i}^{x_{i+1}} f(x)\,dx = \underbrace{\frac{h_i}{2}(f_i + f_{i+1})}_{TR} - \frac{1}{12} h_i^3 f''(y_i) - \frac{1}{480} h_i^5 f^{iv}(y_i) + \cdots$$

h_i^5

CD2

$$f'' = \frac{f'_{i+1} - f'_i}{h_i} - \frac{1}{6}\left(\frac{h_i}{2}\right)^2 f^{iv}(y_i) + \cdots$$

$$= \frac{h_i}{2}(f_i + f_{i+1}) - \frac{1}{12} h_i^2 (f'_{i+1} - f'_i) + \frac{1}{720} h_i^5 f^{iv}(y_i) + \cdots$$

Sum over the entire domain

$$I = \int_a^b f(x)\,dx = \boxed{\frac{h}{2}\sum_{0}^{n-1}(f_i + f_{i+1}) - \frac{1}{12} h^2 (f'(b) - f'(a))} + \frac{b-a}{720} h^4 f^{iv}(\xi) + \cdots$$

TR w/ end correction

$\therefore$ 4th-order accurate!

ex) $f(x) = e^x$ $\quad \int_0^4 e^x\,dx = e^4 - 1 = 53.59815\cdots$

9pts

$I_{TR} = 54.71015$ error $= -1.112$

$I_{SR} = 53.61622$ $= -0.01807$

$I_{TC} = 53.59352$ $= +0.00463$!

3.4 Romberg integration and Richardson extrapolation

Romberg integration: integral method + Richardson extrapolation

Richardson extrapolation: technique for obtaining an accurate sol. by combining two or more less accurate sols.

TR: $I = \int_a^b f(x)\,dx = \underbrace{\frac{h}{2}\left[f(a)+f(b)+2\sum_{1}^{n-1} f_j\right]}_{TR \;=\; \tilde{I}_1} + c_1 h^2 + c_2 h^4 + \cdots$

$\rightarrow \tilde{I}_1 = I - c_1 h^2 - c_2 h^4 - \cdots$: second-order accurate.

Apply TR w/ $h_1 = h/2$ → call this $\tilde{I}_2$.

$\rightarrow \tilde{I}_2 = I - c_1\left(\frac{h}{2}\right)^2 - c_2\left(\frac{h}{2}\right)^4 - \cdots$

Idea: $4\tilde{I}_2 - \tilde{I}_1 = 3I + \frac{3}{4}c_2 h^4 + \cdots$

$\rightarrow \frac{4\tilde{I}_2 - \tilde{I}_1}{3} = I + \frac{1}{4}c_2 h^4 + \cdots$: 4th-order accurate.

HW2 announced tomorrow

by Next Tuesday

Suppl. lecture

Oct. 5 6pm ~

Video lecture

Combine two 2nd-order estimates of I → 4th-order accurate estimate

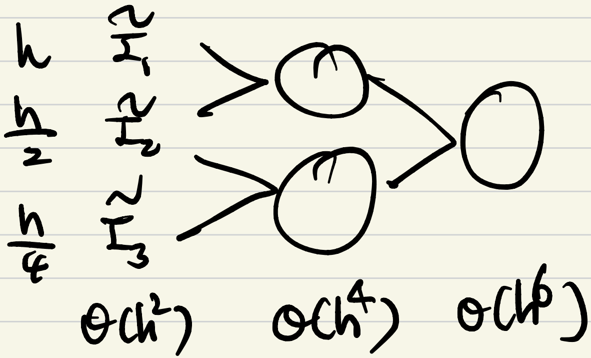
Evaluate I w/ $h_2 = h/4$ → $\tilde{I}_3$

$$\rightarrow \tilde{I}_3 = I - c_1\left(\frac{h}{4}\right)^2 - c_2\left(\frac{h}{4}\right)^4 - \cdots$$

$$\rightarrow \frac{4\tilde{I}_3 - \tilde{I}_2}{3} = I + \frac{1}{64}c_2 h^4 + \frac{5}{1026}c_3 h^6 + \cdots$$

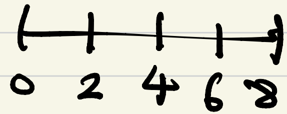
$$\Rightarrow \frac{16}{15}\left(\frac{4\tilde{I}_3 - \tilde{I}_2}{3}\right) - \frac{1}{15}\left(\frac{4\tilde{I}_2 - \tilde{I}_1}{3}\right) = I + O(h^6) + \cdots$$

6th-order accurate!



---> Romberg integration

ex) $I = \int_0^8 \left(\frac{5}{8}x^4 - 4x^3 + 2x + 1\right) dx = 72$



TR : $\tilde{I}_1 = \frac{8-0}{2}\left(f(8) + f(0)\right) = 2120$

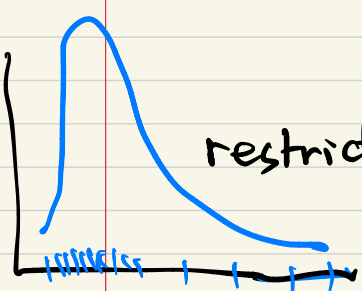
h/2 : $\tilde{I}_2 = \frac{8-0}{4}\left(f(8) + f(0) + 2f(4)\right) = 712$

h/4 : $\tilde{I}_3 = \frac{8-0}{8}\left(f(8) + f(0) + 2f(2) + 2f(4) + 2f(6)\right) = 240$

$$\left.\begin{array}{ll} h: & 2120 \\ h/2: & 712 \\ h/4: & 240 \end{array}\right\rangle \quad \begin{array}{l} \frac{4\times 712 - 2120}{3} = \frac{728}{3} \\ \\ \cdots = \frac{248}{3} \end{array} \Big\rangle \; 72 \leftarrow \text{exact sol}$$

$$O(h^2) \qquad\qquad O(h^4) \qquad O(h^6)$$

$$\varepsilon \propto h^6 \underbrace{f^{vi}(\xi)}_{=\,0}$$



restriction : points are evenly distributed throughout the interval of integration.

3.5 Adaptive quadrature

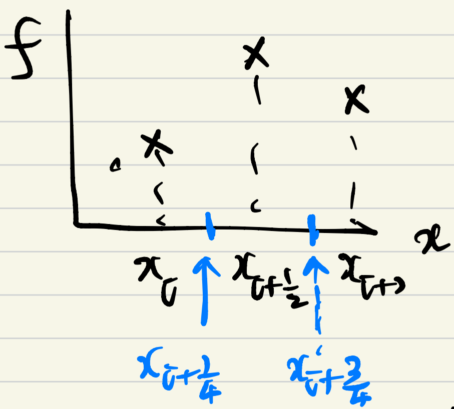
$\varepsilon = 10^{-5}$

→ user provides the error tolerance.

Then, the program automatically subdivides the interval to achieve the prescribed accuracy.

error ε $\quad \left| I - \int_a^b f(x)dx \right| \le \varepsilon$.

Base: Simpson's rule



For (x_i, x_{i+1}), $S_i = \frac{h_i}{6}\left(f_i + 4f_{i+\frac{1}{2}} + f_{i+1}\right)$

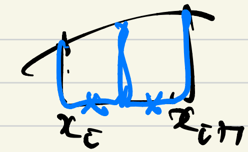
$h_i = x_{i+1} - x_i$

Subdivide into 4 panels.

$$S_i^{(2)} = \frac{h_i}{12}\left(f_i + 4f_{i+\frac{1}{4}} + 2f_{i+\frac{1}{2}} + 4f_{i+\frac{3}{4}} + f_{i+1}\right)$$

idea: compare two estimates, S_i and $S_i^{(2)}$, and get an estimate for actual accuracy of $S_i^{(2)}$.

Let I_i be the exact integral in $(x_i, x_{i+1}]$.



$$I_i - S_i = c\, h_i^5 f^{iv}\left(x_i+\frac{h_i}{2}\right) + \cdots \quad \text{— ①}$$

$$I_i - S_i^{(2)} = c\left(\frac{h_i}{2}\right)^5\left[f^{iv}\left(x_i+\frac{h_i}{4}\right) + f^{iv}\left(x_i+\frac{3h_i}{4}\right)\right] + \cdots$$

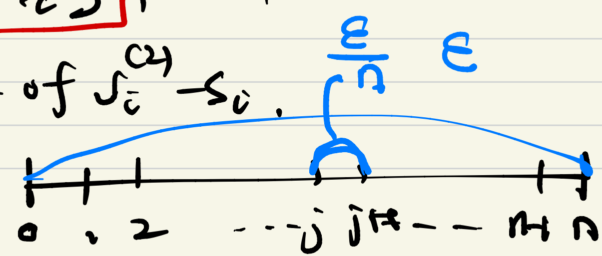
$$\left(f^{iv}\left(x_i+\frac{h_i}{2}\right) - \frac{h_i}{4} f^{v}\left(x_i+\frac{h_i}{2}\right) + \cdots \qquad f^{iv}\left(x_i+\frac{h_i}{2}\right) + \frac{h_i}{4} f^{v}\left(x_i+\frac{h_i}{2}\right) + \cdots \right)$$

$$= c\left(\frac{h_i}{2}\right)^5 \cdot 2 f^{iv}\left(x_i+\frac{h_i}{2}\right) + \cdots \quad \text{— ②}$$

① − ②: $$S_i^{(2)} - S_i = \frac{15}{16}\, c\, h_i^5 f^{iv}\left(x_i+\frac{h_i}{2}\right) + \cdots \quad \text{— ③}$$

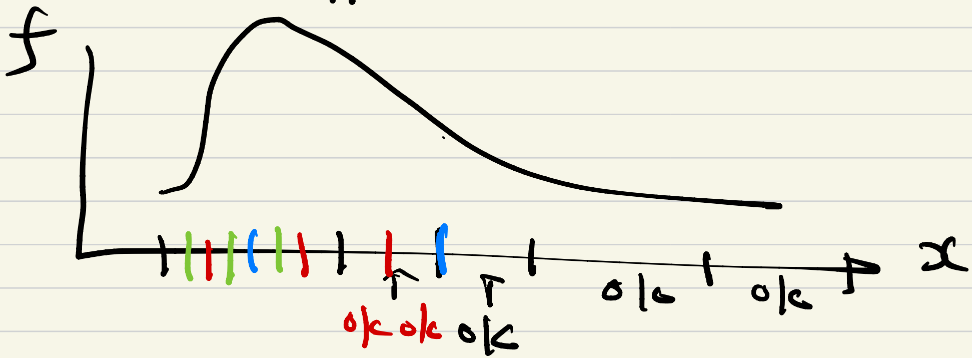
③ → ②: $$\boxed{I_i - S_i^{(2)} = \frac{1}{15}\left(S_i^{(2)} - S_i\right)} + \cdots$$

error of $S_i^{(2)}$ is $\frac{1}{15}$ of $S_i^{(2)} - S_i$.



$$\frac{1}{15}\left|S_i^{(2)} - S_i\right| \le \frac{\varepsilon}{n} \rightarrow \text{ok}$$

$$> \frac{\varepsilon}{n} \rightarrow \text{subdivide further.}$$



ε !

adaptive quadrature

3.6 Gauss quadrature

Method that is optimum in the sense of maximum accuracy for a given number of function evaluations.

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

$n+1$ grid pts, $n+1$ weights $\rightarrow$ $2n+2$ adjustable parameters

construct a polynomial of degree $2n+1$!

choose x_i and w_i for highest accuracy.

Let f be a polynomial of degree $2n+1$.

Select grid pts. $x_0, x_1, \cdots, x_n$

$f(x_0)\ f(x_1)\ \cdots\ f(x_n)$

(so far, we don't know where x_i's are

Interpolate w/ Lagrange polynomial of degree n.

$$P(x) = \sum_{j=0}^{n} f_j L_j(x)$$

$f-p$: polynomial of degree $2n+1$.

& $f-p=0$ @ $x = x_0, x_1, \cdots, x_n$.

$\Rightarrow F(x) = (x-x_0)(x-x_1)\cdots(x-x_n)$: poly. of degree $n+1$.

$$\Rightarrow f-p = F(x) \sum_{l=0}^{n} q_l x^l$$

$$\int f\,dx - \int p\,dx = \int F(x) \sum_{l=0}^{n} q_l x^l dx = \sum_{l=0}^{n} q_l \underbrace{\int F x^l dx}_{0} = 0$$

We demand $\boxed{\int F(x)\, x^l dx = 0}$ for $l = 0, 1, 2, \cdots, n$

→ $F(x)$ is orthogonal to all polynomials of degree n or less.

Then, $\int f(x)\,dx = \int p(x)\,dx = \int \sum_{j=0}^{n} f_j L_j\, dx = \sum_{j=0}^{n} f_j \underbrace{\int L_j\, dx}_{w_j}$

Here, F belongs to class of Legendre polynomials.

x_j are the zeros of " "

$$\int_{-1}^{1} F_n F_m\, dx = \delta_{mn} = \begin{cases} 0 & m \neq n \\ 1 & m = n \end{cases}$$

$F_0(x) = 1$, $F_1(x) = x$, $F_2(x) = \frac{1}{2}(3x^2 - 1)$, $F_3(x) = \frac{1}{2}(5x^3 - 3x)$,

$F_4(x) = \frac{1}{8}(35x^4 - 30x^2 + 3)$, $F_5(x) = \frac{1}{8}(63x^5 - 70x^3 + 15x)$, ...

F_5 : $x_0 = -0.9061$, $x_1 = -0.5384$, $x_2 = 0$, $x_3 = 0.5384$, $x_4 = 0.9061$

One can transform $a \le x \le b$ to $-1 \le \xi \le 1$.

using $x = \frac{1}{2}(a+b) + \frac{1}{2}(b-a)\xi$.

ex) $I = \int_0^4 e^x dx = 53.59815003$

5 pts. $x = \frac{1}{2}(0+4) + \frac{1}{2}(4-0)\xi = 2+2\xi \rightarrow dx = 2d\xi$

$I = \int_0^4 e^x dx = 2\int_{-1}^1 f(\xi) d\xi$. $f(\xi) = e^{2+2\xi}$

ξ_j	w_j
-0.9061	0.2369
-0.5384	0.4786
0	0.5688
$+0.5384$	0.4786
$+0.9061$	0.2369

$I = 2\sum_0^4 f_j w_j = 53.59813663$!

$\varepsilon = 0.0000134$

cf. $\varepsilon = 0.018$ using Simpson's rule w/ 9 pts.

Disadvantage: lack of simple method for systematic error reduction

- $\int_0^\infty e^{-x} f(x)\,dx = \sum_j f_j w_j$: Gauss-Laguerre quadrature

  orthogonality $\int_0^\infty L_n L_m e^{-x} dx = \delta_{nm}$

$\int_{-\infty}^\infty e^{-x^2} f(x)\,dx = \sum_j f_j w_j$: Gauss-Hermite quadrature

" $\int_{-\infty}^\infty H_n H_m e^{-x^2} dx = \delta_{nm}$

$\int_{-1}^1 \frac{1}{\sqrt{1-x^2}} f(x)\,dx = \sum_j f_j w_j$: Chebyshev-Gauss quadrature

" $\int_{-1}^1 T_n T_m \frac{1}{\sqrt{1-x^2}} dx = \delta_{nm}$

* Singularity $\quad I = \int_0^1 \frac{e^x}{\sqrt{x}}\, dx$

① substitution : let $x = t^2 \rightarrow dx = 2t\,dt \rightarrow I = 2\int_0^1 \sqrt{x}\, e^x dx$

② integration by parts : $u = e^x$, $v = 2\sqrt{x}$

$$\rightarrow I = 2\sqrt{x}\, e^x \Big|_0^1 - 2\int_0^1 \sqrt{x}\, e^x dx$$

* Integral w/ ∞ limits

$I = \int_0^\infty e^{-x^2} dx \longrightarrow$ ① Gauss quadrature

② change the indep. variable

$t = \frac{1}{1+x}$ maps $[0, \infty)$ to $[0, 1]$