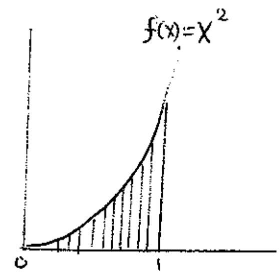
Numerical Integration

Motivation.

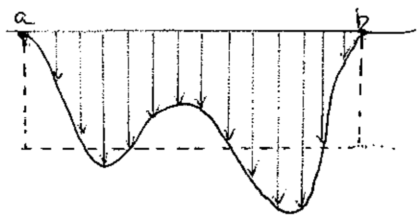
$$\int_0^1 x^2 \cdot dx = \left[\frac{x^3}{3}\right]_0^1 = \frac{1}{3}$$



Note. 1. f(x) is a positive function

2. $\int_a^b f(x)\cdot dx$ is the area under the curve.

Ex. Cross-sectional area of a river.



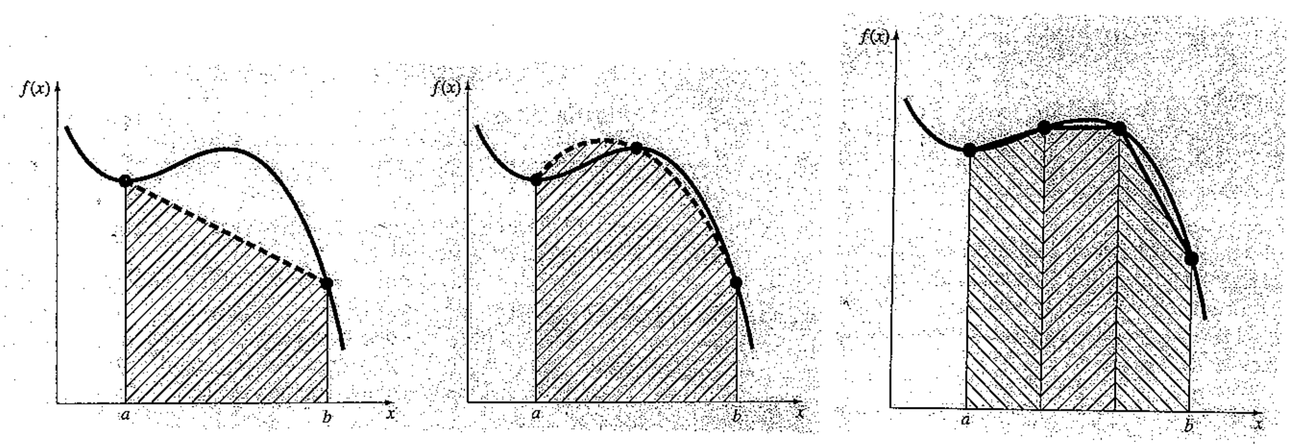
$$\text{mean} = \frac{\int_a^b f(x)\cdot dx}{b-a}$$

Note. Closed-form f(x) does not exist.

$\Rightarrow$ numerical method.

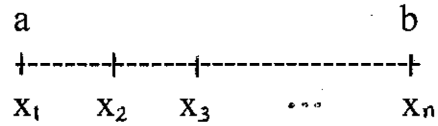
Newton – Cotes Formulas

$$\int_a^b f(x)\cdot dx \longrightarrow \int_a^b f_n(x)\, dx \qquad // f_n : \text{polynomial} //$$



Lower and Upper Sum

Partition P of interval [a,b] :

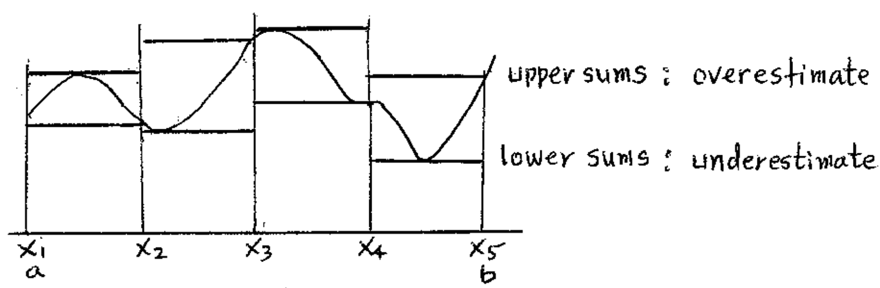


m_i (infimum) $= \inf \{f(x) \mid x_i \le x \le x_{i+1}\}$: greatest lower bound

M_i(supremum) $= \inf \{f(x) \mid x_i \le x \le x_{i+1}\}$: least upper bound

lower sums $L(f; P) = \sum_{i=1}^{n-1} m_i (x_{i+1} - x_i)$

upper sums $U(f; P) = \sum_{i=1}^{n-1} M_i (x_{i+1} - x_i)$



$$L(f; P) \le \int_a^b f(x)\,dx \le U(f; P)$$

Ex. $f(x) = x^2$, $0 \le x \le 1$, $P = \{0, ¼, ½, ¾, 1\}$

$U(f; P) = M_1(x_2 - x_1) + M_2(x_3 - x_2) + M_3(x_4 - x_3) + M_4(x_5 - x_4)$

$f(x)$ is increasing in the interval [0,1]. Therefore,

$M_1 = f(x_2) = 1/16$, $M_2 = f(x_3) = ¼$, $M_3 = f(x_4) = 9/16$, $M_4 = f(x_5) = 1$

$U(f; P) = ¼\,(1/16 + ¼ + 9/16 + 1) = \underline{15/32}$

$m_1 = f(x_1) = 0$, $m_2 = f(x_2) = 1/16$, $m_3 = f(x_3) = ¼$, $m_4 = f(x_4) = 9/16$

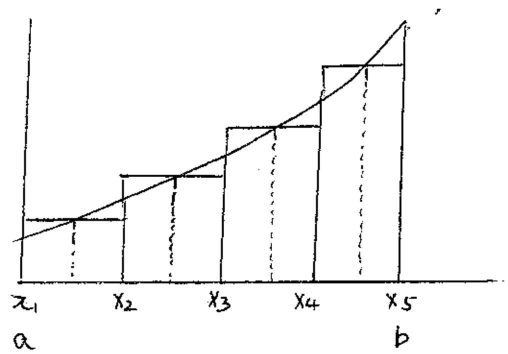
$L(f; P) = ¼\,(0 + 1/16 + ¼ + 9/16) = \underline{7/32}$

$$\int_0^1 x^2\,dx \cong ½\,(15/32 + 7/32) = 11/32$$

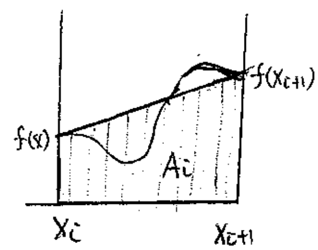
$$E_t = 1/3 - 11/32 = -\frac{1}{96}$$

Rectangle Rule (Midpoint Rule)

$$\int_a^b f(x)\,dx \approx h \cdot \sum_{i=1}^{n-1} f_{i+\frac{1}{2}}$$



Trapezoidal Rule - piecewise linear interpolation



$$A_i = \frac{1}{2}(x_{i+1} - x_{i-1})\,[f(x_i) + f(x_{i+1})]$$

$$T(f;P) = \sum_{i=1}^{n-1} A_i = \frac{1}{2}\sum_{i=1}^{n-1}(x_{i+1} - x_i)\,[f(x_i) + f(x_{i+1})]$$

Uniform spacing case: $x_i = a + (i-1)\cdot h \quad 1 \le i \le n, \quad h = \frac{b-a}{n-1}$

$$T(f;P) = \frac{1}{2}\sum_{i=1}^{n-1}[f(x_i) + f(x_{i+1})] = h \cdot \sum_{i=2}^{n-1} f(x_i) + \frac{h}{2}[f(\overset{a}{\overset{\parallel}{x_1}}) + f(\overset{b}{\overset{\parallel}{x_n}})]$$

Exercise (1) Estimate $\int_0^2 x^3\,dx$ by midpoint rule using the partition $P = \{0, 1, 2\}$

(2) Estimate $\int_0^2 x^3\,dx$ by trapezoid rule using the same partition.

(3) Which rule gives better estimate? Why?

Error Analysis

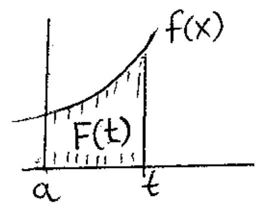
I : $\int_a^b f(x)\cdot dx$ // true value

T : result from Trapezoid method (uniform spacing) // approximate value

Error: $\boxed{I - T = -\frac{1}{12}(b-a)\cdot h^2 f''(\xi)}$ $E = O(h^2)$, $h = \frac{b-a}{n-1}$, $a < \xi < b$

Proof.

Let $F(t) = \int_a^t f(x)\,dx$



From Taylor series,

$$F(a+h) = \underbrace{F(a)}_{0} + h\cdot\underbrace{F'(a)}_{f(a)} + \frac{h^2}{2}\underbrace{F''(a)}_{f'(a)} + \frac{h^3}{3!}\underbrace{F'''(a)}_{f''(a)} + \ldots$$

Note. $F' = f$, $F'' = f'$, $F''' = f''$ …

$$I: \int_a^{a+h} f(x)\,dx = F(a+h)$$
$$= \underline{h\,f(a) + \frac{h^2}{2} f'(a) + \frac{h^3}{6} f''(a) + \frac{h^4}{24} f'''(a) + \ldots} \qquad (1)$$

Taylor:

$$f(a+h) = f(a) + h\,f'(a) + \frac{h^2}{2} f''(a) + \frac{h^3}{6} f'''(a) + \cdots$$

add f(a):

$$f(a) + f(a+h) = 2\,f(a) + h\,f'(a) + \frac{h^2}{2} f''(a) + \frac{h^3}{6} f'''(a) + \ldots$$

multiply h/2

$$T: \; h/2\,[f(a) + f(a+h)] = \underline{h\,f(a) + \frac{h^2}{2} f'(a) + \frac{h^3}{4} f''(a) + \frac{h^4}{12} f'''(a) + \cdots} \qquad (2)$$

$$(1)-(2): \; \underbrace{\int_a^{a+h} f(x)\,dx}_{I} - \underbrace{h/2\,[f(a) + f(a+h)]}_{T} = -\frac{1}{12} h^3 f''(a) - \frac{1}{24} h^4 f'''(a) \cdots \qquad (3)$$

Let $a + h = b$ (2-points, or one interval case)

$$\int_a^b f(x)\,dx - \frac{b-a}{2}[f(a) + f(b)] = -\frac{1}{12}(b-a)^3 f''(\xi), \quad a < \xi < b \qquad (4)$$

n points, or (n – 1) intervals case: $h = \frac{b-a}{n-1}$

Apply (4) to subinterval i, we have

$$\int_{x_i}^{x_{i+1}} f(x)\cdot dx = \frac{h}{2}\left[f(x_i) + f(x_{i+1})\right] - \frac{1}{12} h^3 f'(\xi), \qquad x_i < \xi < x_{i+1}$$

$$\therefore \int_a^b f(x)\, dx = \sum_{i=1}^{n-1} \int_{x_i}^{x_{i+1}} f(x)\, dx = \frac{h}{2} \sum_{i=1}^{n-1} \left[f(x_i) + f(x_{i+1})\right] \underbrace{- \frac{h^3}{12} \sum_{i=1}^{n-1} f''(\xi_i)}_{E}$$

$$E = -\frac{h^3}{12} \sum_{i=1}^{n-1} f'(\xi_i) = -\frac{b-a}{12} h^2 \left[\frac{1}{n-1} \sum_{i=1}^{n-1} f''(\xi_i)\right]$$

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

q.e.d.

Ex. $F(x) = \int_0^1 e^{-x^2} dx$. error $\le \frac{1}{2}\cdot 10^{-4}$

How many points should be used?

Solution. $-\frac{1}{12} h^2 f''(\xi)$

$$f(x) = e^{-x^2}$$
$$f'(x) = -2x\cdot e^{-x^2}$$
$$f''(x) = (4x^2-2)\, e^{-x^2} \quad \rightarrow \quad |f''(x)| \le 2 \text{ in } [0,1]$$

$$\therefore \frac{h^2}{6} < \frac{1}{2}\cdot 10^{-4}$$

$h = \frac{1}{n-1} \in h < 0.01732$

$\therefore n \ge 59$

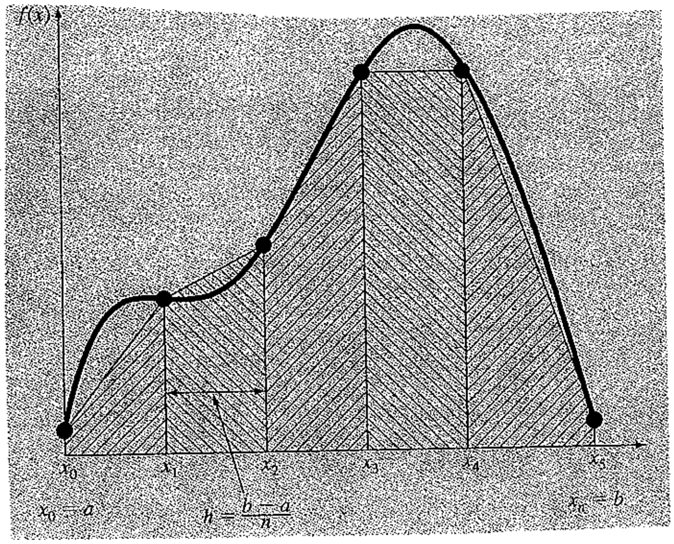
$\left(\frac{1}{n-1}\right)$

$$\frac{\left(\frac{1}{n-1}\right)^2}{6} < \frac{1}{2}\cdot 10^{-4}$$

$\Rightarrow n \ge 59$

Composite Trapezoidal Rule

Divide [a, b] into n intervals ((n+1) points) - $\boxed{h = \frac{b-a}{n}}$



$$I = \int_{x_0}^{x_1} f(x)\,dx + \int_{x_1}^{x_2} f(x)\,dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)\cdot dx$$

$$= h\cdot\frac{f(x_0)+f(x_1)}{2} + h\cdot\frac{f(x_1)+f(x_2)}{2} + \cdots + h\cdot\frac{f(x_{n-1})+f(x_n)}{2}$$

$$= \frac{h}{2}\left[f(x_0) + 2\cdot\sum_{i=1}^{n-1} f(x_i) + f(x_n)\right]$$

$$= \underbrace{(b-a)}_{\text{width}}\cdot\underbrace{\frac{\left[f(x_0) + 2\cdot\sum_{i=1}^{n-1} f(x_i) + f(x_n)\right]}{2n}}_{\text{average height}}$$

Error.
$$E_t = -\frac{(b-a)^3}{12n^3}\sum_{i=1}^{n} f''(\xi_i)$$

$$\text{Let } \bar{f''} \cong \frac{\sum_{i=1}^{n} f''(\xi_i)}{n}$$

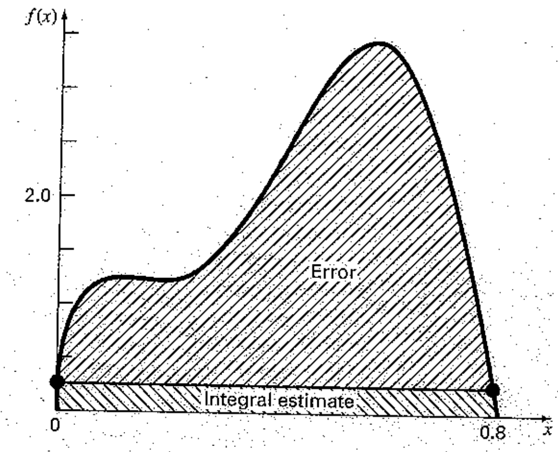
$$E_a = -\frac{(b-a)^3}{12n^2}\bar{f''}$$

Example.
$$\int_0^{0.8} (0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5) \quad (= 1.640533)$$

(1) One-interval

$n = 1,\ h = 0.8$

$f(0) = 0.2,\ f(0.8) = 0.232$



$$I = (0.8 - 0)\frac{0.2 + 0.232}{2} = 0.1728$$

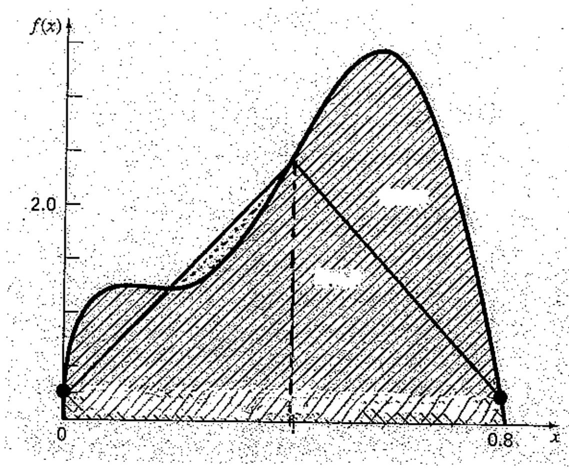
$$E_t = 1.640533 - 0.1728 = 1.467733$$

(89.5% error)

(2) Two-intervals

$n = 2,\ h = 0.4$

$f(0) = 0.2,\ f(0.4) = 2.456,\ f(0.8) = 0.232$



$$I = (0.8 - 0)\frac{0.2 + 2(2.456) + 0.232}{4} = 1.0688$$

$$E_t = 1.640533 - 1.0688 = 0.57173$$

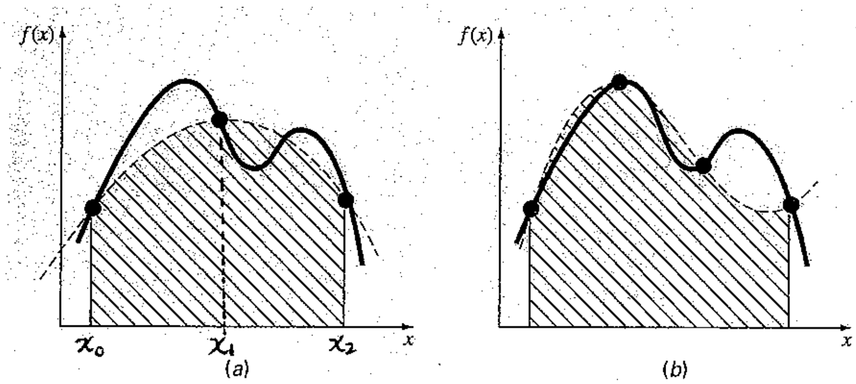
(34.9 % error)

⋮

n	h	I	ε_t (%)	
2	0.4	1.0688	34.9	←
3	0.2667	1.3695	16.5	
4	0.2	1.4848	9.5	←
5	0.16	1.5399	6.1	
6	0.1333	1.5703	4.3	
7	0.1143	1.5887	3.2	
8	0.1	1.6008	2.4	←
9	0.0889	1.6091	1.9	
10	0.08	1.6150	1.6	

Simpson's Rule

Idea



Lagrange Interpolation

$$I = \int_{x_0}^{x_2} \left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \right] \cdot dx$$

$$= \frac{h}{3} \left[f(x_0) + 4f(x_1) + f(x_2) \right] \quad \text{where } h = \frac{a-b}{2}$$

$$E_t = -\frac{1}{90} h^5 f^{(4)}(\xi) \quad \text{or} \quad E_t = -\frac{(b-a)^5}{2880} f^{(4)}(\xi)$$

Ex. $\int_0^{0.8} (0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5)\, dx$

$n = 2$, $(h = 0.4)$

$f(0) = 0.2$, $f(0.4) = 2.456$, $f(0.8) = 0.232$

$$I = \frac{0.4}{3} \left[0.2 + 4(2.456) + 0.232 \right] = 1.367467$$

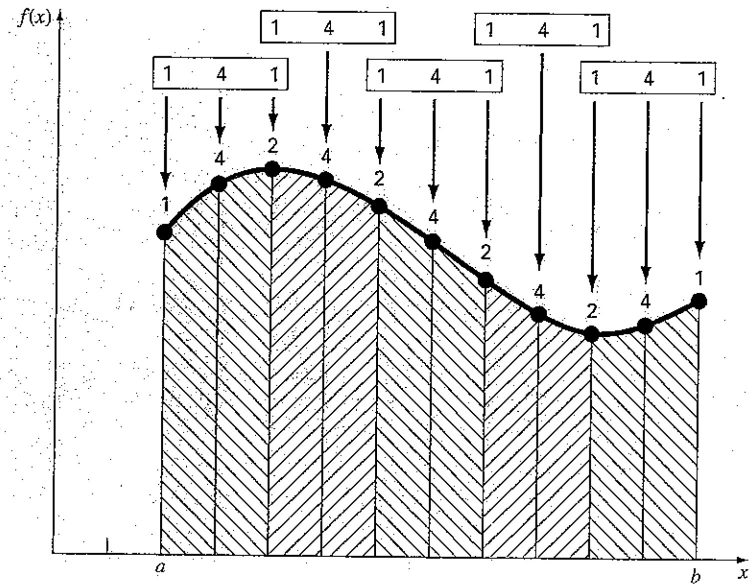
$$E_t = 1.640533 - 1.367467 = 0.2730667$$

(16.6% error)

Composite Simpson's Rule

Idea

$$I = \int_{x_0}^{x_2} f(x)\,dx + \int_{x_2}^{x_4} f(x)\,dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)\cdot dx$$



$$I = 2h\,\frac{f(x_0)+4f(x_1)+f(x_2)}{6} + 2h\cdot\frac{f(x_2)+4f(x_3)+f(x_4)}{6} + \cdots + \frac{f(x_{n-2})+4f(x_{n-1})+f(x_n)}{6}$$

or $$I = (b-a)\,\frac{f(x_0) + 4\sum_{i=1,3,5}^{n-1} f(x_i) + 2\cdot\sum_{j=2,4,6}^{n-2} f(x_j) + f(x_n)}{3n}$$

$$E_a = -\frac{(b-a)^5}{180\,n^4}\,\bar{f}^{(4)}$$

Ex. $\int_0^{0.8} (0.2 + 25x - 200x^2 + 675x^3 - 900x^5 + 400x^5)\,dx$

$n = 4 \quad (h = 0.2)$

$f(0) = 0.2,\; f(0.2) = 1.288,\; f(0.4) = 2.456,\; f(0.6) = 3.464,\; f(0.8) = 0.232$

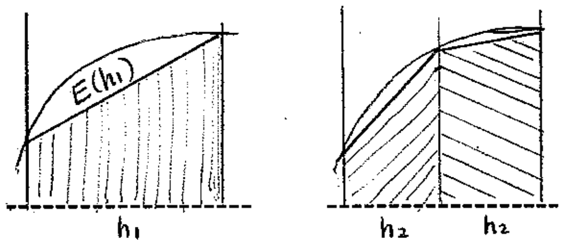
$$I = 0.8\,\frac{0.2 + 4(1.288 + 3.464) + 2(2.456) + 0.232}{12} = 1.623467$$

$$E_t = 1.640533 - 1.623467 = 0.017067$$

(1.04% error)

Richardson Extrapolation

Idea:



$\Rightarrow$ $I = I(h_2) + 1/3\,[I(h_2) - I(h_1)]$

$E = O(h^4)$

$$I(h_1) + E(h_1) = I(h_2) + E(h_2) \qquad \ldots\ldots\ldots\ldots\ldots (1)$$

Note. $E \cong -\frac{b-a}{12} h^2 \bar{f}''$

Assume $\bar{f}''$ is constant.

$$\frac{E(h_1)}{E(h_2)} \cong \frac{h_1^2}{h_2^2}$$

$$E(h_1) \cong \left(\frac{h_1}{h_2}\right)^2 E(h_2)$$

plug in (1)

$$I(h_1) + \left(\frac{h_1}{h_2}\right)^2 E(h_2) = I(h_2) + E(h_2)$$

$$\therefore\ E(h_2) = \frac{I(h_1) - I(h_2)}{1 - \left(\frac{h_1}{h_2}\right)^2}$$

plug in (1),

$$I = I(h_2) + \frac{I(h_2) - I(h_1)}{\left(\frac{h_1}{h_2}\right)^2 - 1} \qquad \ldots\ldots\ldots\ldots (2)$$

If $h_2 = \frac{1}{2} h_1$

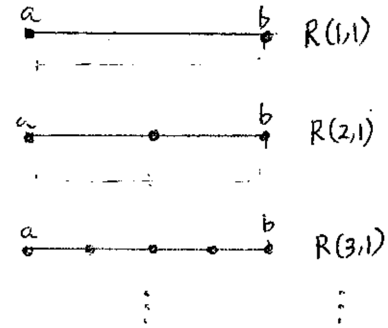
$$\boxed{I = I(h_2) + \frac{I(h_2) - I(h_1)}{3}} \text{ or}$$

$$\underline{I = 4/3\ I(h_2) - 1/3\ I(h_1)}$$

Romberg Method

- Application of Richardson extrapolation on the trapezoidal rule.

$$
\begin{array}{ccccccc}
R(1,1) & & & & & & \\
R(2,1) & \rightarrow & R(2,2) & & & & \\
R(3,1) & \rightarrow & R(3,2) & \rightarrow & R(3,3) & & \\
\vdots & & \vdots & & \vdots & \ddots & \\
R(n,1) & \rightarrow & R(n,2) & \rightarrow & R(n,3) & \cdots & R(n,n) \\
\hline
\text{Error: } O(h^2) & & O(h^4) & & O(h^6) & \cdots & O(h^{2n})
\end{array}
$$



$$\boxed{R(n+1,m+1) = R(n+1,m) + \frac{1}{4^m-1}\left[R(n+1,m) - R(n,m)\right],} \quad n > 1,\ m > 1$$

Ex. $\int_0^{0.8} (0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5)\, dx$

segment	h		$\frac{\Delta}{3}$	$\frac{\Delta}{15}$	...
1	0.8	R(1,1): 0.1728			
2	0.4	R(2,1): 1.0688	R(2,2): 1.367467		
4	0.2	R(3,1): 1.4848	R(3,2): 1.623467	R(3,3): **1.640533**	
				$O(h^6)$	

$R(2,2) = R(2,1) + \frac{1}{3}[R(2,1) - R(1,1)]$
$= 1.0688 + \frac{1}{3}(1.0688 - 0.1728)$
$= 1.367467$

$R(3,2) = R(3,1) + \frac{1}{3}(R(3,1) - R(2,1))$
$= 1.4848 + \frac{1}{3}(1.4848 - 1.0688)$
$= 1.623467$

$R(3,3) = R(3,2) + \frac{1}{15}(R(3,2) - R(2,2))$
$= 1.623467 + \frac{1}{15}(1.623467 - 1.367467)$
$= \underline{1.640533}$