Numerical integration (数値積分)

How to calculate $F(x)=\int_{x_0}^{x} g(x')dx'$ **by computer**

Replace integral with summation of small mesh area
(積分 を和 で置き換える)

$$\int_{x_0}^{x} g(x')dx' = \sum_{i=0}^{x_i=x} g(x_i)h$$

Derivation from difference approximation (差分式からの導出) :

$$\frac{df(x)}{dx} \sim \frac{f(x+h)-f(x)}{h} \quad \Rightarrow \quad g(x) \sim \frac{F(x+h)-F(x)}{h}$$

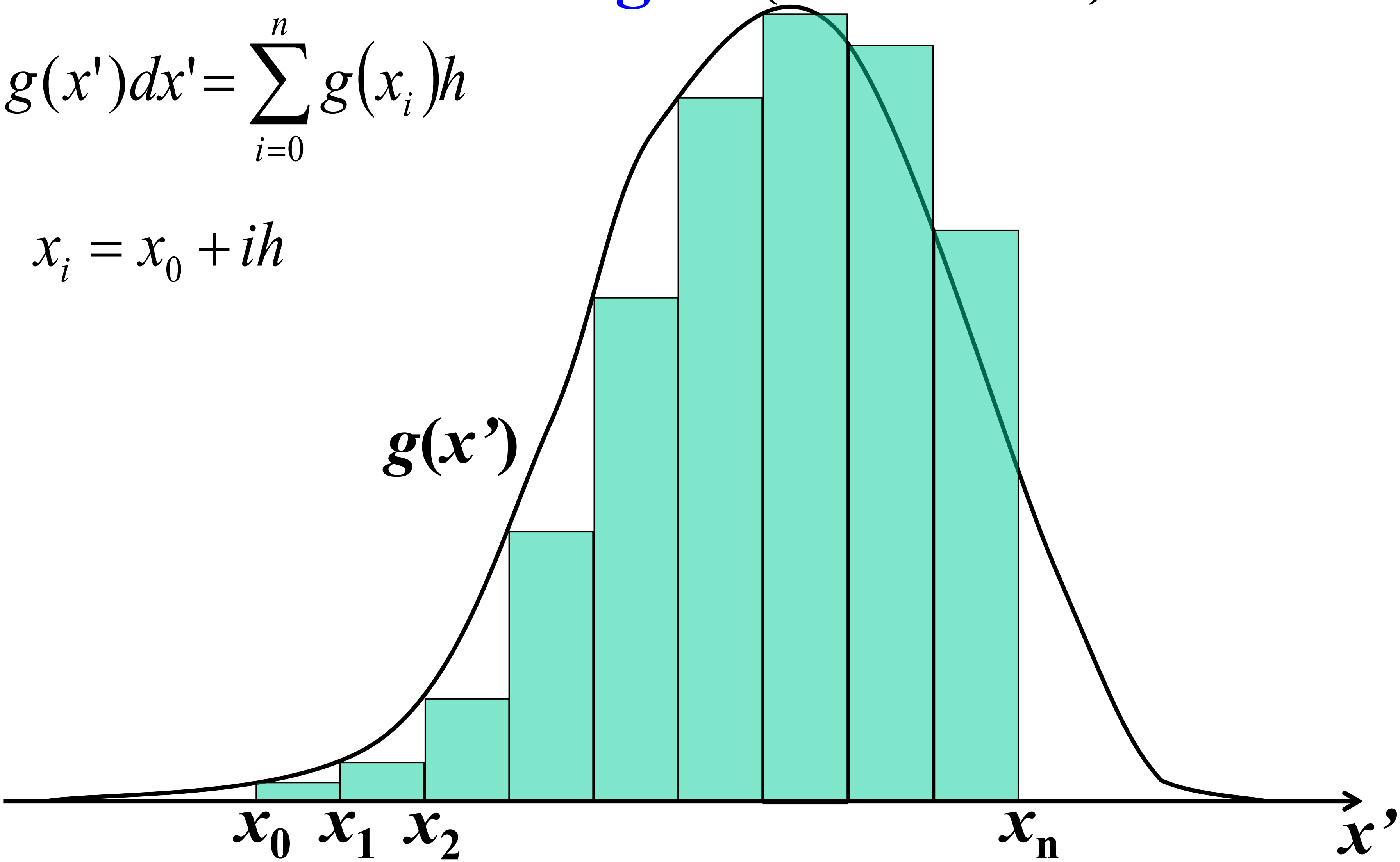
$$F(x+h) = F(x) + g(x)h = F(x-h) + \left[g(x) + g(x-h)\right]h$$

$$= \sum_{i=0}^{x_i=x} g(x_i)h$$

Rieman integral (Rieman積分)

$$\int_{x_0}^{x} g(x')dx' = \sum_{i=0}^{n} g(x_i)h$$

$$x_i = x_0 + ih$$



Asymmetric formula:

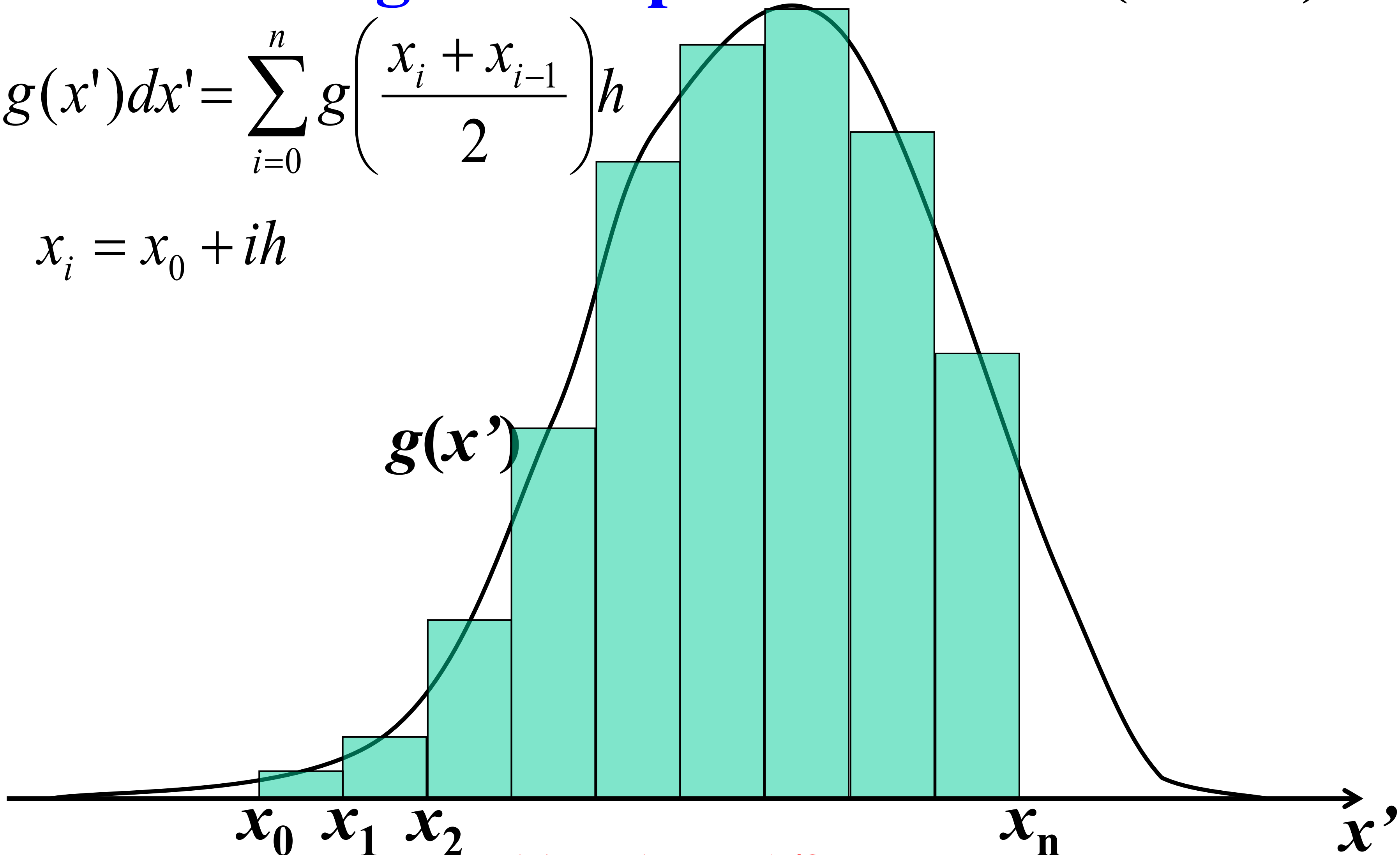
monotone increasing $g(x)$ => Underestimation (過小評価)

monotone decreasing $g(x)$ => Overestimation (過大評価)

Take average: Mid-point formula (中点則)

$$\int_{x_0}^{x} g(x')dx' = \sum_{i=0}^{n} g\left(\frac{x_i + x_{i-1}}{2}\right)h$$

$$x_i = x_0 + ih$$



Necessary to know $g(x)$ at $(x_i+x_{i-1})/2$.

=> Unavailable for $g(x)$ given only by numerical data

($g(x)$が数値データで与えられている場合は使えない)

Trapezoid formula (台形公式)

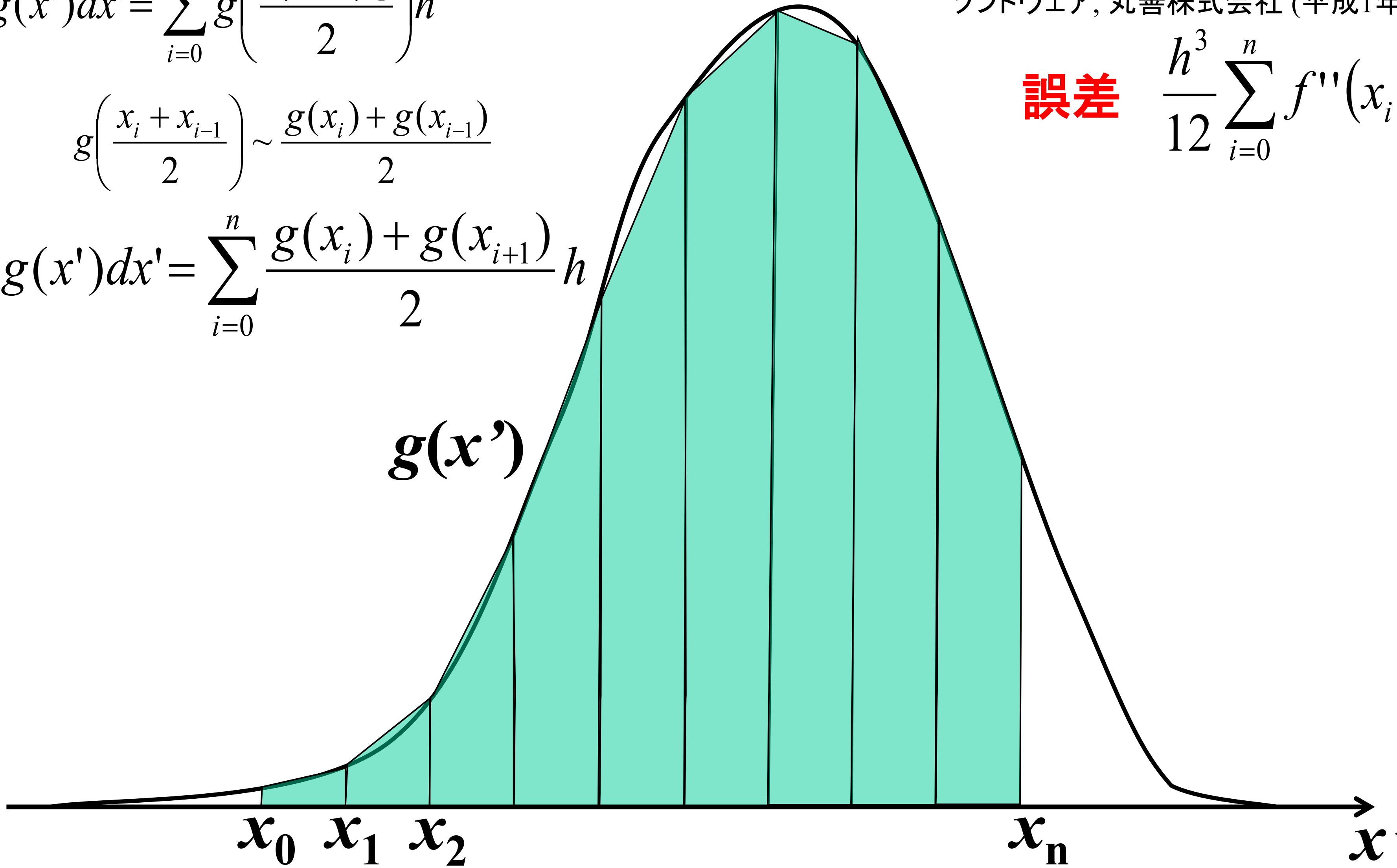
渡部力ら監修、Fortran77による数値計算ソフトウェア, 丸善株式会社 (平成1年)

$$\int_{x_0}^{x} g(x')dx' = \sum_{i=0}^{n} g\left(\frac{x_i + x_{i-1}}{2}\right)h$$

$$g\left(\frac{x_i + x_{i-1}}{2}\right) \sim \frac{g(x_i) + g(x_{i-1})}{2}$$

$$\int_{x_0}^{x} g(x')dx' = \sum_{i=0}^{n} \frac{g(x_i) + g(x_{i+1})}{2} h$$

誤差 $\frac{h^3}{12}\sum_{i=0}^{n} f''(x_i)$



Simpson formula

1. Approximate by $g(x_i) \sim g(x_1) + a_1(x_i - x_1) + a_2(x_i - x_1)^2$**,**
and determine a_i **so as to reproduce** $f(x_0)$**,** $f(x_1)$**, and** $f(x_2)$**.**
($x_i = x_1 - h, x_1, x_1 + h$**)**

2. Integrate the above approximation analytically for a range $x = x_0 \sim x_0 + 2h$**:**

$$\int_{x_0}^{x_2} g(x')dx' \sim \frac{1}{3}h\left[g(x_0) + 4g(x_1) + g(x_2)\right]$$

3. For multiply divided range ($x = x_0 \sim x_n = x_0 + nh$**):**

$$\int_{x_0}^{x_n} g(x')dx' \sim \frac{h}{3}\left[g(x_0) + 4g(x_1) + 2g(x_2) + 4g(x_3) + 2g(x_4) + \cdots + g(x_n)\right]$$

Derivation of the Simpson formula

1. Approximate by $g(x_i) \sim g(x_1) + a_1(x_i - x_1) + a_2(x_i - x_1)^2$**,**
and determine a_i so as to reproduce $f(x_0)$, $f(x_1)$, and $f(x_2)$.
($x_i = x_1 - h, x_1, x_1 + h$)

$$g(x_0) \sim g(x_1) - a_1 h + a_2 h^2$$
$$g(x_2) \sim g(x_1) + a_1 h + a_2 h^2$$

$$\Rightarrow \quad a_1 = \frac{g(x_2) - g(x_0)}{2h} \qquad a_2 = \frac{g(x_2) - 2g(x_1) + g(x_0)}{2h^2}$$

$$\int_{x_0}^{x_2} g(x')dx' \sim g(x_1)x_2 + \frac{1}{2}\frac{g(x_2) - g(x_0)}{2h}(x_2 - x_1)^2 + \frac{1}{3}\left[\frac{g(x_2) - 2g(x_1) + g(x_0)}{2h^2}\right](x_2 - x_1)^3$$
$$- \left\{ g(x_1)x_0 + \frac{1}{2}\frac{g(x_2) - g(x_0)}{2h}(x_0 - x_1)^2 + \frac{1}{3}\left[\frac{g(x_2) - 2g(x_1) + g(x_0)}{2h^2}\right](x_0 - x_1)^3 \right\}$$
$$= 2g(x_1)h + 2\left[\frac{g(x_2) - 2g(x_1) + g(x_0)}{6}\right]h$$
$$= \frac{1}{3}\left[g(x_2) + 4g(x_1) + g(x_0)\right]$$

片岡勲 他、数値解析入門, コロナ社

Error $\le \dfrac{nh^5}{180}\left|f^{(4)}(x_i)\right|$

Rieman/Trapezoid formula are better than Simpson formula for infinite-range integration

Simpson則より単純和/台形則の方が良い

$$\int_{x_0}^{x_n} g(x')dx' \sim \frac{h}{3}\left[g(x_0)+4g(x_1)+2g(x_2)+4g(x_3)+2g(x_4)+\cdots+g(x_n)\right]$$

For infinite-range integration (-∞ ~ ∞), x_0 and x_n are not essential.

$$\int_{x_0}^{x_n} g(x')dx' \sim \frac{h}{3}\left[g(x_{-1})+4g(x_0)+2g(x_1)+4g(x_2)+2g(x_3)+\cdots+g(x_{n-1})\right]$$

also provides the essentially the same result.

$$\int_{x_0}^{x_n} g(x')dx' \sim \frac{h}{3}\left[0.5g(x_{-1})+2.5g(x_0)+3g(x_1)+3g(x_2)+3g(x_3)+3g(x_4)+\cdots+0.5g(x_n)\right]$$

Considering g(x_{-1}) and $g(x_n)$ are negligible for infinite integration leads to

$$\int_{x_0}^{x_n} g(x')dx' \sim h\left[g(x_1)+g(x_2)+g(x_3)+g(x_4)+\cdots+g(x_{n-2})\right]$$

, which is the same as the Rieman sum and the Trapezoid formula.

Extrapolation method: Romberg integration

戸田英雄, 小野令美, 入門 数値計算, オーム社 (昭和58年)

Good for finite range integration without anomaly points

・Start from the Trapezoid formula, and sequentially apply higher order Newton-Cotes precision formula.

(台形則から出発し、高次のニュートン・コーツ型に相当する公式を自動的に適用し、要求精度を満たすまで続ける)

1. **Integrate by the Trapezoid formula in [a, b] with the mesh h_0 => $S_{0,0}$**
2. **Decrease mesh to $h_1 = (1/2)h_0$ and integrate all the range => $S_{1,0}$**
3. **Decrease mesh to $h_k = (1/2)h_{k-1}$ and integrate all the range => $S_{k,0}$, and calculate $S_{k,d}$ ($d = 1, 2, \cdots, k$) by**

$$S_{k,d} = \frac{4^d S_{k,d-1} - S_{k-1,d-1}}{4^d - 1}$$

4. **$S_{k,k}$ will be the approximated integration values.
Stop if $|S_{k,k} - S_{k-1,k-1}|$ becomes smaller than the required accuracy.**

Error of numerical integration: Monotone increasing function

$$S = \int_{-1}^{1} \exp(x)dx$$

Exact: exp(1) - exp(-1) = 2.3504023872876

nDivide	Rieman	Trapezoid	Simpson	Simpson 3/8	Bode	Romberg	Cubic Spline	Order 3 Gauss-Legendre
1	1.61E+00	-7.36E-01				-7.36E-01		
2	9.83E-01	-1.93E-01	-1.17E-02			-1.17E-02		6.55E-05
3	6.97E-01	-8.64E-02		-5.25E-03				
4	5.39E-01	-4.88E-02	-7.92E-04		-6.85E-05	-6.85E-05	7.19E-03	1.13E-06
5	4.39E-01	-3.13E-02					3.75E-03	
6	3.70E-01	-2.17E-02	-1.59E-04	-3.53E-04			2.35E-03	1.01E-07
7	3.20E-01	-1.60E-02					1.54E-03	
8	2.82E-01	-1.22E-02	-5.06E-05		-1.18E-06	-1.07E-07	1.07E-03	1.81E-08
9	2.51E-01	-9.66E-03		-7.08E-05			7.73E-04	
10	2.27E-01	-7.83E-03	-2.08E-05				5.77E-04	4.75E-09
11	2.07E-01	-6.47E-03					4.41E-04	
12	1.90E-01	-5.44E-03	-1.00E-05	-2.25E-05	-1.05E-07		3.45E-04	1.59E-09
13	1.76E-01	-4.63E-03					2.75E-04	
14	1.64E-01	-4.00E-03	-5.43E-06				2.23E-04	6.32E-10
15	1.53E-01	-3.48E-03		-9.25E-06			1.83E-04	
16	1.44E-01	-3.06E-03	-3.18E-06		-1.88E-08	-4.21E-11	1.52E-04	2.84E-10
17	1.36E-01	-2.71E-03					1.28E-04	
18	1.28E-01	-2.42E-03	-1.99E-06	-4.46E-06			1.08E-04	1.40E-10
19	1.22E-01	-2.17E-03					9.27E-05	
20	1.16E-01	-1.96E-03	-1.30E-06		-4.95E-09		7.99E-05	7.45E-11
32						-3.55E-15		