

Lecture 8

Numerical Integration



- Trapezoid Method (Newton-Cotes Methods)
- Simpson Method
- Romberg Method
- Gauss Quadrature

Integration

Indefinite Integrals (antiderivatives)

$$\int x \, dx = \frac{x^2}{2} + c$$

Indefinite Integrals of a function are functions that differ from each other by a constant.

Definite Integrals

$$\int_0^1 x \, dx = \left. \frac{x^2}{2} \right|_0^1 = \frac{1}{2}$$

Definite Integrals are numbers.

Fundamental Theorem of Calculus

If f is continuous on an interval $[a, b]$,

F is antiderivative of f (i.e., $F'(x) = f(x)$)

$$\int_a^b f(x)dx = F(b) - F(a)$$

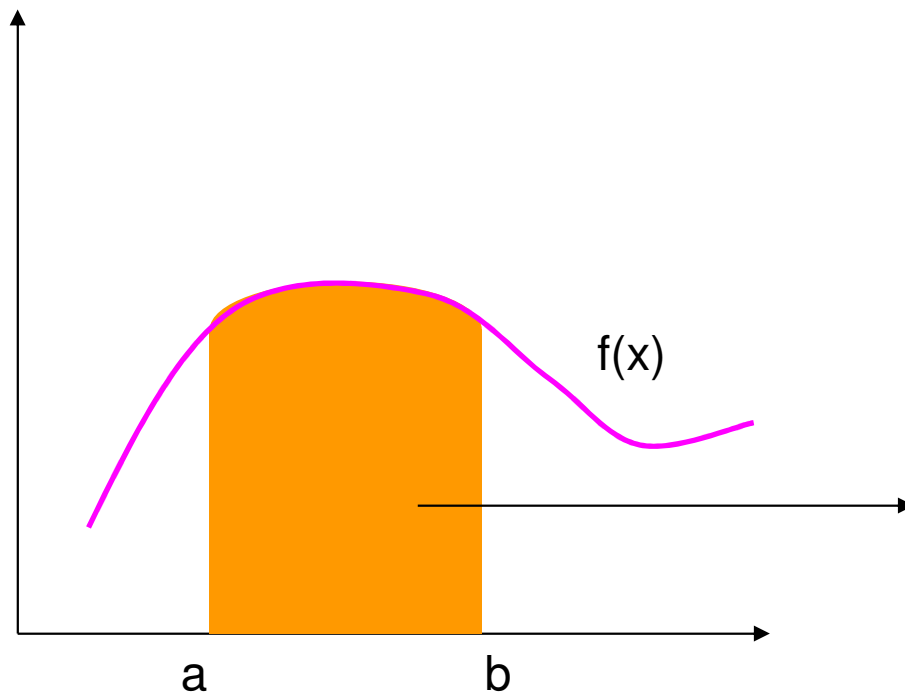
There is no antiderivative for : e^{x^2}

No "closed form" solution for : $\int_a^b e^{x^2} dx$

The Area Under the Curve

One interpretation of the definite integral is:

Integral = area under the curve



$$Area = \int_a^b f(x) dx$$

Upper and Lower Sums

The interval is divided into subintervals.

$$\text{Partition } P = \{a = x_0 \leq x_1 \leq x_2 \leq \dots \leq x_n = b\}$$

Define

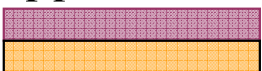
$$m_i = \min \{f(x) : x_i \leq x \leq x_{i+1}\}$$

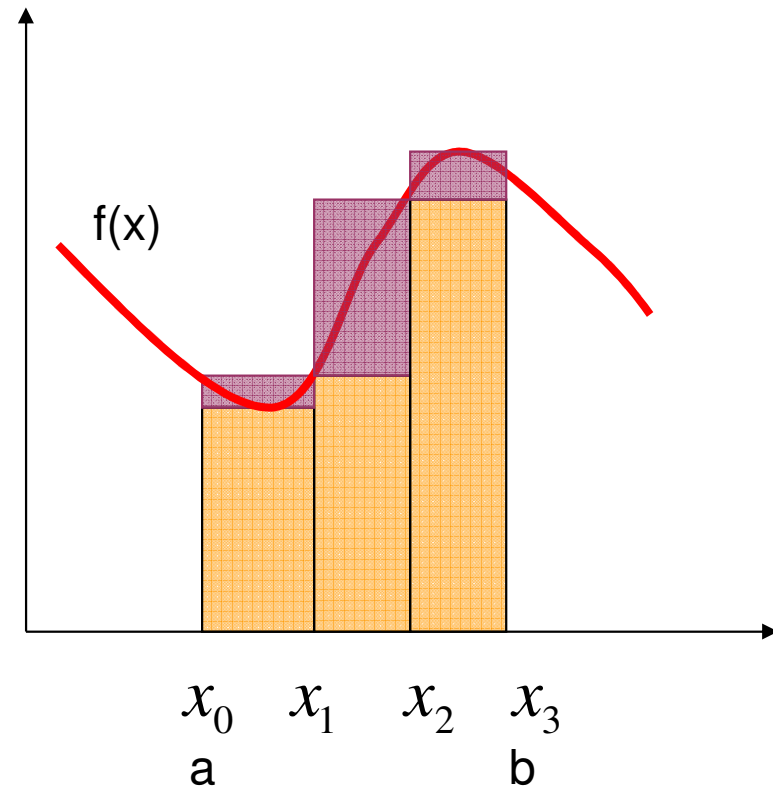
$$M_i = \max \{f(x) : x_i \leq x \leq x_{i+1}\}$$

Lower sum


$$L(f, P) = \sum_{i=0}^{n-1} m_i (x_{i+1} - x_i)$$

Upper sum


$$U(f, P) = \sum_{i=0}^{n-1} M_i (x_{i+1} - x_i)$$



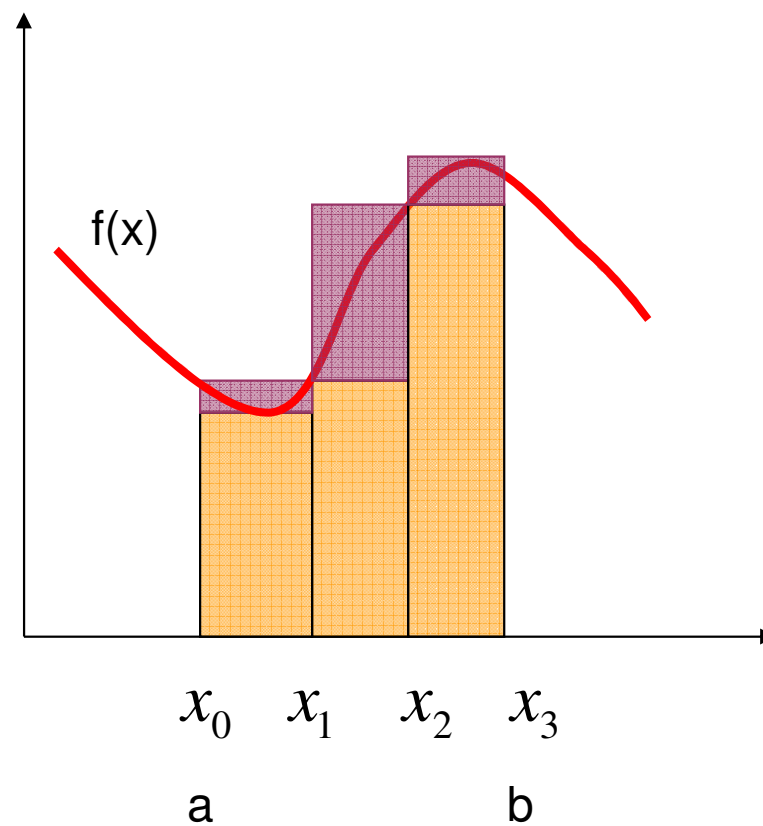
Upper and Lower Sums

Lower sum $L(f, P) = \sum_{i=0}^{n-1} m_i (x_{i+1} - x_i)$

Upper sum $U(f, P) = \sum_{i=0}^{n-1} M_i (x_{i+1} - x_i)$

Estimate of the integral $= \frac{L+U}{2}$

Error $\leq \frac{U-L}{2}$



Example

$$\int_0^1 x^2 dx$$

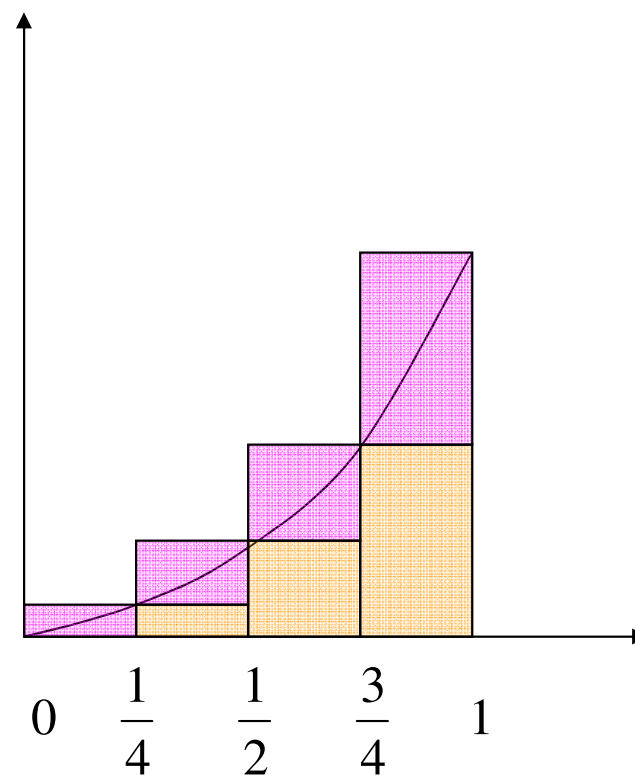
$$\text{Partition : } P = \left\{ 0, \frac{1}{4}, \frac{2}{4}, \frac{3}{4}, 1 \right\}$$

$n = 4$ (four equal intervals)

$$m_0 = 0, \quad m_1 = \frac{1}{16}, \quad m_2 = \frac{1}{4}, \quad m_3 = \frac{9}{16}$$

$$M_0 = \frac{1}{16}, \quad M_1 = \frac{1}{4}, \quad M_2 = \frac{9}{16}, \quad M_3 = 1$$

$$x_{i+1} - x_i = \frac{1}{4} \quad \text{for } i = 0, 1, 2, 3$$



Example

$$\text{Lower sum } L(f, P) = \sum_{i=0}^{n-1} m_i (x_{i+1} - x_i)$$

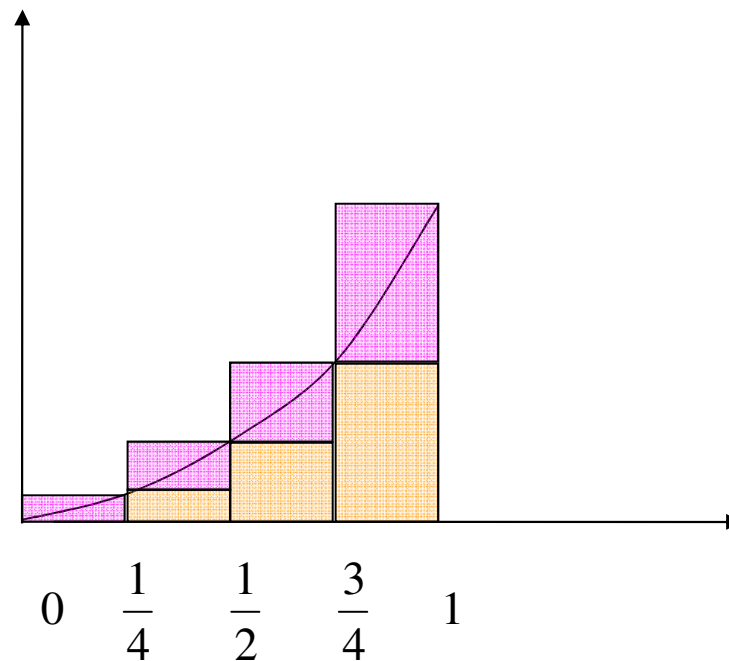
$$L(f, P) = \frac{1}{4} \left[0 + \frac{1}{16} + \frac{1}{4} + \frac{9}{16} \right] = \frac{14}{64}$$

$$\text{Upper sum } U(f, P) = \sum_{i=0}^{n-1} M_i (x_{i+1} - x_i)$$

$$U(f, P) = \frac{1}{4} \left[\frac{1}{16} + \frac{1}{4} + \frac{9}{16} + 1 \right] = \frac{30}{64}$$

$$\text{Estimate of the integral} = \frac{1}{2} \left(\frac{30}{64} + \frac{14}{64} \right) = \frac{11}{32}$$

$$\text{Error} < \frac{1}{2} \left(\frac{30}{64} - \frac{14}{64} \right) = \frac{1}{8}$$



Upper and Lower Sums

- Estimates based on Upper and Lower Sums are easy to obtain for **monotonic** functions (**always increasing or always decreasing**).
- For non-monotonic functions, finding maximum and minimum of the function can be difficult and other methods can be more attractive.

Midpoint Rule

- Recall that

$$\int_a^b f(x)dx = \lim_{\Delta x \rightarrow 0} \sum_{i=1}^n f(x_i)\Delta x; a < x_i < b$$

- In **Midpoint Rule**, the function is approximated by a **value of function at midpoint**.

- Thus, for the midpoint rule with n equal segments and define $h = (b-a)/n$,

$$\int_a^b f(x)dx \approx \sum_{i=1}^n f(x_i)h; x_i = a + (2i-1)\frac{h}{2}$$

Newton-Cotes Methods

- In **Newton-Cotes Methods**, the function is approximated by a **polynomial of order n** .
- Computing the integral of a polynomial is easy.

$$\int_a^b f(x)dx \approx \int_a^b (a_0 + a_1x + \dots + a_nx^n)dx$$

$$\int_a^b f(x)dx \approx a_0(b-a) + a_1 \frac{(b^2 - a^2)}{2} + \dots + a_n \frac{(b^{n+1} - a^{n+1})}{n+1}$$

Newton-Cotes Methods

- **Trapezoid Method** (First Order Polynomials are used)

$$\int_a^b f(x)dx \approx \int_a^b (a_0 + a_1x)dx$$

- **Simpson 1/3 Rule** (Second Order Polynomials are used)

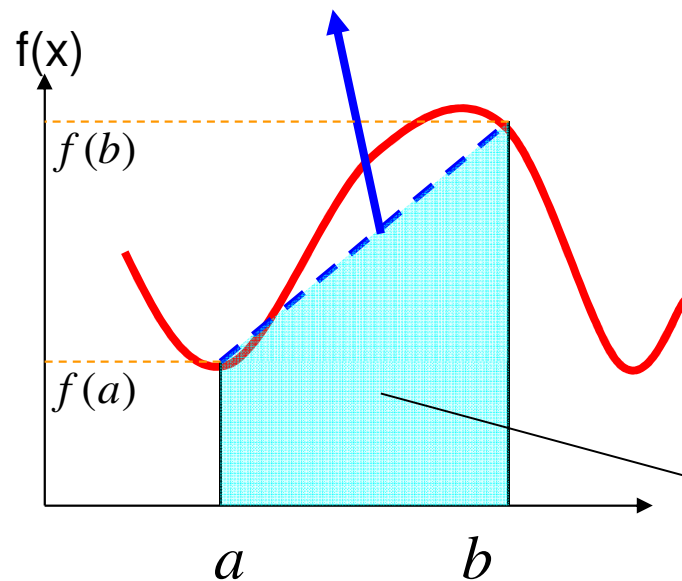
$$\int_a^b f(x)dx \approx \int_a^b (a_0 + a_1x + a_2x^2)dx$$

- Note that midpoint rule is equivalent to using zeroth order.

$$\int_a^b f(x)dx \approx \int_a^b a_0 dx$$

Trapezoid Method

$$f(a) + \frac{f(b) - f(a)}{b - a}(x - a)$$



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

$$I \approx \int_a^b \left(f(a) + \frac{f(b) - f(a)}{b - a}(x - a) \right) dx$$

$$= \left(f(a) + \frac{f(b) - f(a)}{b - a}x \right) \Big|_a^b$$

$$+ \frac{f(b) - f(a)}{b - a} \frac{x^2}{2} \Big|_a^b$$

$$= (b - a) \frac{f(b) + f(a)}{2}$$

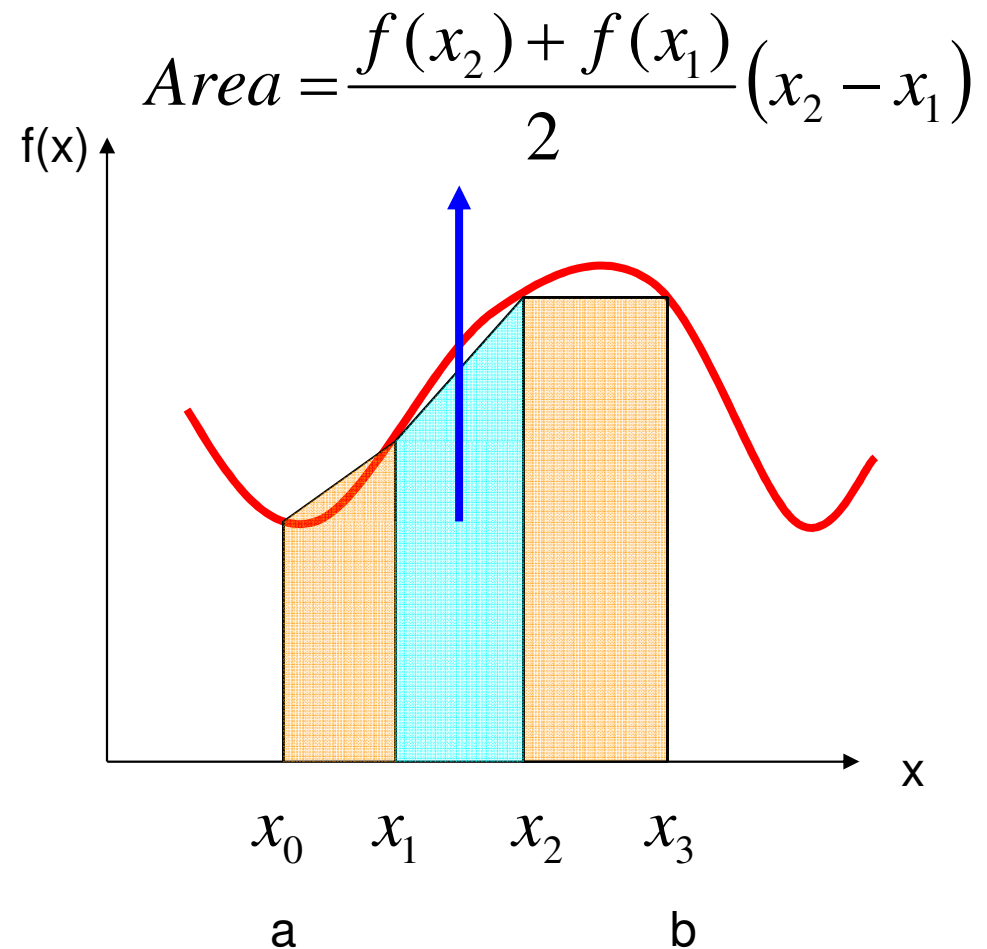
Trapezoid Method

Multiple Segments Application Rule

The interval $[a, b]$ is partitioned into n segments

$$a = x_0 \leq x_1 \leq x_2 \leq \dots \leq x_n = b$$

$\int_a^b f(x) dx = \text{sum of the areas of the trapezoids}$



Trapezoid Method

General Formula and Special Case

If the interval is divided into n segments (not necessarily equal)

$$a = x_0 \leq x_1 \leq x_2 \leq \dots \leq x_n = b$$

$$\int_a^b f(x)dx \approx \sum_{i=0}^{n-1} \frac{1}{2} (x_{i+1} - x_i) (f(x_{i+1}) + f(x_i))$$

Special Case (Equally spaced base points)

$$x_{i+1} - x_i = h \quad \text{for all } i$$

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

Example

Given a tabulated values of the velocity of an object.

Time (s)	0.0	1.0	2.0	3.0
Velocity (m/s)	0.0	10	12	14

Obtain an estimate of the distance traveled in the interval [0,3].

Distance = integral of the velocity

$$\text{Distance} = \int_0^3 V(t) dt$$

Example 1

The interval is divided
into 3 subintervals

Base points are $\{0,1,2,3\}$

Time (s)	0.0	1.0	2.0	3.0
Velocity (m/s)	0.0	10	12	14

Trapezoid Method

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

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

$$\text{Distance} = 1 \left[(10 + 12) + \frac{1}{2} (0 + 14) \right] = 29$$

Error in estimating the integral

Theorem

Assumption: $f''(x)$ is continuous on $[a, b]$

Equal intervals (width = h)

Theorem: If Trapezoid Method is used to

approximate $\int_a^b f(x)dx$ then

$$Error = -\frac{b-a}{12} h^2 f''(\xi) \quad \text{where } \xi \in [a, b]$$

$$|Error| \leq \frac{b-a}{12} h^2 \max_{x \in [a, b]} |f''(x)|$$

An alternative derivation of the trapezoidal rule is possible by integrating the forward Newton-Gregory interpolating polynomial. Recall that for the first-order version with error term, the integral would be (Box 18.2)

$$I = \int_a^b \left[f(a) + \Delta f(a)\alpha + \frac{f''(\xi)}{2}\alpha(\alpha - 1)h^2 \right] dx \quad (\text{B21.2.1})$$

To simplify the analysis, realize that because $\alpha = (x - a)/h$,

$$dx = h d\alpha$$

Inasmuch as $h = b - a$ (for the one-segment trapezoidal rule), the limits of integration a and b correspond to 0 and 1, respectively. Therefore, Eq. (B21.2.1) can be expressed as

$$I = h \int_0^1 \left[f(a) + \Delta f(a)\alpha + \frac{f''(\xi)}{2}\alpha(\alpha - 1)h^2 \right] d\alpha$$

If it is assumed that, for small h , the term $f''(\xi)$ is approximately

constant, this equation can be integrated:

$$I = h \left[\alpha f(a) + \frac{\alpha^2}{2} \Delta f(a) + \left(\frac{\alpha^3}{6} - \frac{\alpha^2}{4} \right) f''(\xi) h^2 \right]_0^1$$

and evaluated as

$$I = h \left[f(a) + \frac{\Delta f(a)}{2} \right] - \frac{1}{12} f''(\xi) h^3$$

Because $\Delta f(a) = f(b) - f(a)$, the result can be written as

$$I = h \underbrace{\frac{f(a) + f(b)}{2}}_{\text{Trapezoidal rule}} - \underbrace{\frac{1}{12} f''(\xi) h^3}_{\text{Truncation error}}$$

Thus, the first term is the trapezoidal rule and the second is an approximation for the error.

Estimating the Error

For Trapezoid Method

How many equally spaced intervals are needed to compute $\int_0^{\pi} \sin(x) dx$ to 5 decimal digit accuracy?

Example

$$\int_0^{\pi} \sin(x) dx, \quad \text{find } h \text{ so that } |\text{error}| \leq \frac{1}{2} \times 10^{-5}$$

$$|\text{Error}| \leq \frac{b-a}{12} h^2 \max_{x \in [a,b]} |f''(x)|$$

$$b = \pi; \quad a = 0; \quad f'(x) = \cos(x); \quad f''(x) = -\sin(x)$$

$$|f''(x)| \leq 1 \Rightarrow |\text{Error}| \leq \frac{\pi}{12} h^2 \leq \frac{1}{2} \times 10^{-5}$$

$$\Rightarrow h^2 \leq \frac{6}{\pi} \times 10^{-5} \Rightarrow h \leq 0.00437$$

$$\Rightarrow n \geq \frac{(b-a)}{h} = \frac{\pi}{0.00437} = 719 \text{ intervals}$$

Example

x	1.0	1.5	2.0	2.5	3.0
f(x)	2.1	3.2	3.4	2.8	2.7

Use Trapezoid method to compute: $\int_1^3 f(x)dx$

$$\text{Trapezoid } T(f, P) = \sum_{i=0}^{n-1} \frac{1}{2} (x_{i+1} - x_i) (f(x_{i+1}) + f(x_i))$$

Special Case: $h = x_{i+1} - x_i$ for all i ,

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

Example

x	1.0	1.5	2.0	2.5	3.0
f(x)	2.1	3.2	3.4	2.8	2.7

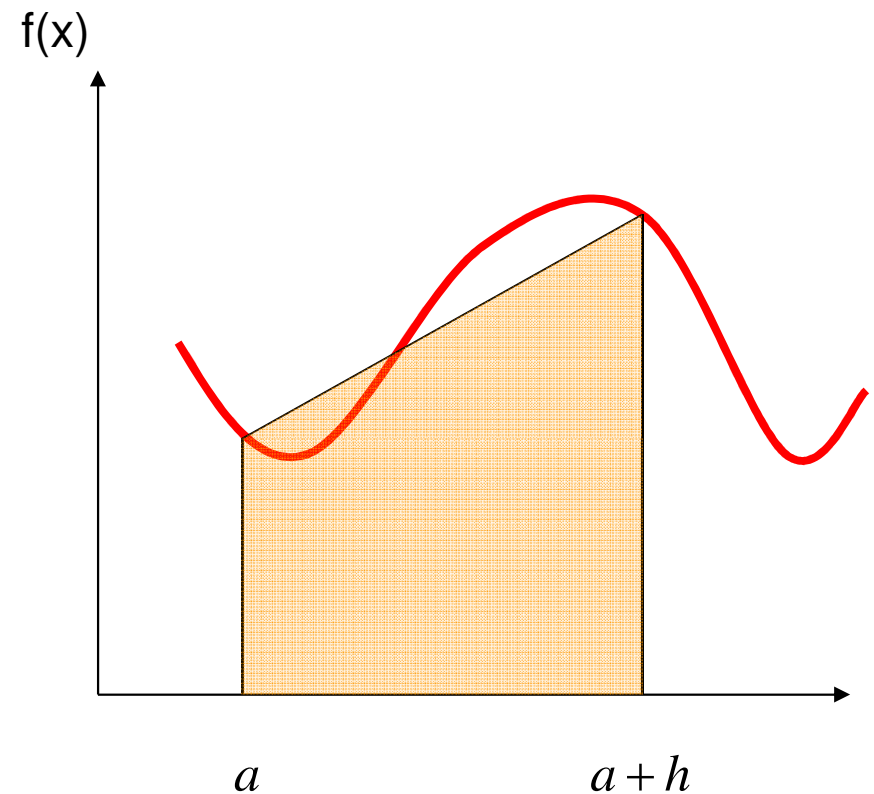
$$\begin{aligned}\int_1^3 f(x)dx &\approx h \left[\sum_{i=1}^{n-1} f(x_i) + \frac{1}{2}(f(x_0) + f(x_n)) \right] \\ &= 0.5 \left[3.2 + 3.4 + 2.8 + \frac{1}{2}(2.1 + 2.7) \right] \\ &= 5.9\end{aligned}$$

Recursive Trapezoid Method

Estimate based on one interval :

$$h = b - a$$

$$R(0,0) = \frac{b-a}{2} (f(a) + f(b))$$



Recursive Trapezoid Method

Estimate based on 2 intervals :

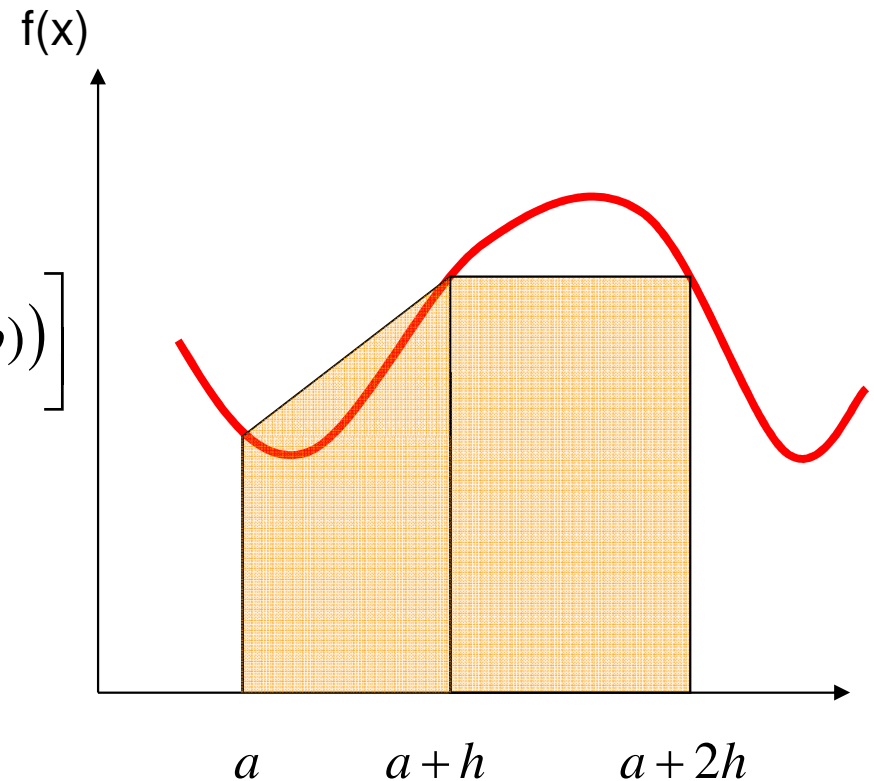
$$h = \frac{b-a}{2}$$

$$R(1,0) = \frac{b-a}{2} \left[f(a+h) + \frac{1}{2}(f(a) + f(b)) \right]$$

$$R(1,0) = \frac{1}{2} R(0,0) + h[f(a+h)]$$

Based on previous estimate

Based on new point



Recursive Trapezoid Method

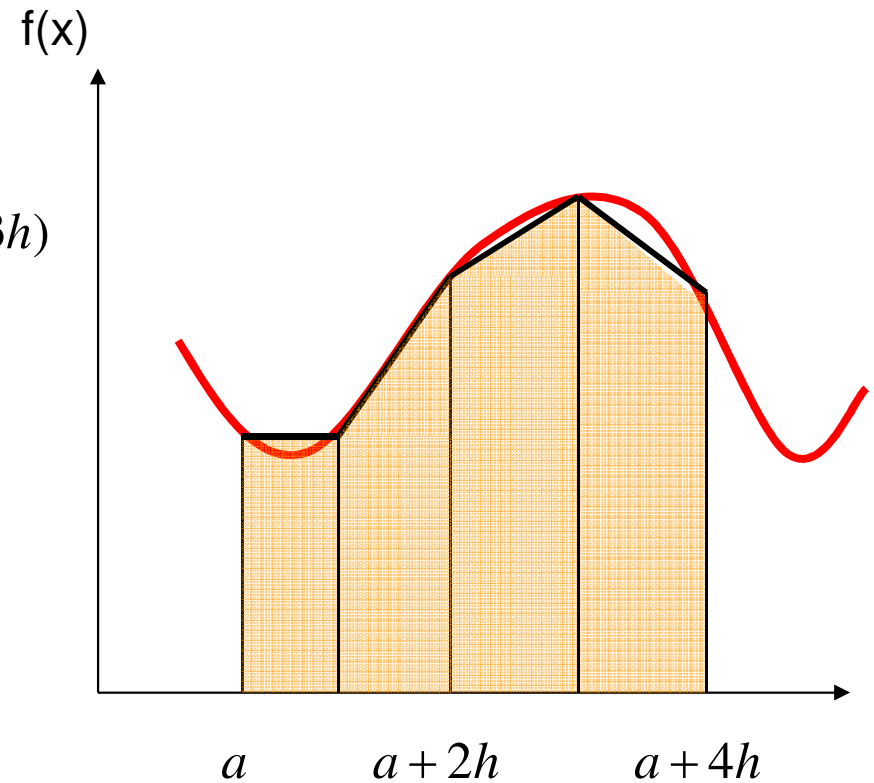
$$h = \frac{b-a}{4}$$

$$R(2,0) = \frac{b-a}{4} \left[f(a+h) + f(a+2h) + f(a+3h) + \frac{1}{2}(f(a) + f(b)) \right]$$

$$R(2,0) = \frac{1}{2} R(1,0) + h[f(a+h) + f(a+3h)]$$

Based on previous estimate

Based on new points



Recursive Trapezoid Method

Formulas

$$R(0,0) = \frac{b-a}{2} [f(a) + f(b)]$$

$$R(n,0) = \frac{1}{2} R(n-1,0) + h \left[\sum_{k=1}^{2^{(n-1)}} f(a + (2k-1)h) \right]$$

$$h = \frac{b-a}{2^n}$$

Recursive Trapezoid Method

$$h = b - a, \quad R(0,0) = \frac{b-a}{2} [f(a) + f(b)]$$

$$h = \frac{b-a}{2}, \quad R(1,0) = \frac{1}{2} R(0,0) + h \left[\sum_{k=1}^1 f(a + (2k-1)h) \right]$$

$$h = \frac{b-a}{2^2}, \quad R(2,0) = \frac{1}{2} R(1,0) + h \left[\sum_{k=1}^2 f(a + (2k-1)h) \right]$$

$$h = \frac{b-a}{2^3}, \quad R(3,0) = \frac{1}{2} R(2,0) + h \left[\sum_{k=1}^{2^2} f(a + (2k-1)h) \right]$$

.....

$$h = \frac{b-a}{2^n}, \quad R(n,0) = \frac{1}{2} R(n-1,0) + h \left[\sum_{k=1}^{2^{(n-1)}} f(a + (2k-1)h) \right]$$

Example on Recursive Trapezoid

Use Recursive Trapezoid method to estimate :

$$\int_0^{\pi/2} \sin(x) dx \text{ by computing } R(3,0) \text{ then estimate the error}$$

n	h	R(n,0)
0	(b-a)= $\pi/2$	$(\pi/4)[\sin(0) + \sin(\pi/2)]=0.785398$
1	(b-a)/2= $\pi/4$	$R(0,0)/2 + (\pi/4) \sin(\pi/4) = 0.948059$
2	(b-a)/4= $\pi/8$	$R(1,0)/2 + (\pi/8)[\sin(\pi/8)+\sin(3\pi/8)] = 0.987116$
3	(b-a)/8= $\pi/16$	$R(2,0)/2 + (\pi/16)[\sin(\pi/16)+\sin(3\pi/16)+\sin(5\pi/16)+\sin(7\pi/16)] = 0.996785$

$$\text{Estimated Error} = |R(3,0) - R(2,0)| = 0.009669$$

Advantages of Recursive Trapezoid

Recursive Trapezoid:

- ❑ Gives the same answer as the standard Trapezoid method.
- ❑ Makes use of the available information to reduce the computation time.
- ❑ Useful if the number of iterations is not known in advance.

Basis of Simpson's 1/3rd Rule

Trapezoidal rule was based on approximating the integrand by a first order polynomial, and then integrating the polynomial in the interval of integration. Simpson's 1/3rd rule is an extension of Trapezoidal rule where the integrand is approximated by a second order polynomial.

Hence

$$I = \int_a^b f(x)dx \approx \int_a^b f_2(x)dx$$

Where $f_2(x)$ is a second order polynomial.

$$f_2(x) = a_0 + a_1x + a_2x^2$$

Basis of Simpson's 1/3rd Rule

Choose $\left(\frac{a+b}{2}, f\left(\frac{a+b}{2}\right)\right), (a, f(a)), (b, f(b))$

as the three points of the function to evaluate a_0 , a_1 and a_2 .

$$f(a) = f_2(a) = a_0 + a_1a + a_2a^2$$

$$f\left(\frac{a+b}{2}\right) = f_2\left(\frac{a+b}{2}\right) = a_0 + a_1\left(\frac{a+b}{2}\right) + a_2\left(\frac{a+b}{2}\right)^2$$

$$f(b) = f_2(b) = a_0 + a_1b + a_2b^2$$

Solving the previous equations for a_0 , a_1 and a_2 give

$$a_0 = \frac{a^2 f(b) + abf(b) - 4abf\left(\frac{a+b}{2}\right) + abf(a) + b^2 f(a)}{a^2 - 2ab + b^2}$$

Basis of Simpson's 1/3rd Rule

$$a_1 = - \frac{af(a) - 4af\left(\frac{a+b}{2}\right) + 3af(b) + 3bf(a) - 4bf\left(\frac{a+b}{2}\right) + bf(b)}{a^2 - 2ab + b^2}$$

$$a_2 = \frac{2\left(f(a) - 2f\left(\frac{a+b}{2}\right) + f(b)\right)}{a^2 - 2ab + b^2}$$

Then

$$I \approx \int_a^b f_2(x)dx = \int_a^b (a_0 + a_1x + a_2x^2)dx$$

$$= \left[a_0x + a_1 \frac{x^2}{2} + a_2 \frac{x^3}{3} \right]_a^b$$

$$= a_0(b-a) + a_1 \frac{b^2 - a^2}{2} + a_2 \frac{b^3 - a^3}{3}$$

Basis of Simpson's 1/3rd Rule

Substituting values of a_0, a_1, a_2 give

$$\int_a^b f_2(x)dx = \frac{b-a}{6} \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]$$

Since for Simpson's 1/3rd Rule, the interval $[a, b]$ is broken into 2 segments, the segment width $h = (b - a)/2$

Hence

$$\int_a^b f_2(x)dx = \frac{h}{3} \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right]$$

Because the above form has 1/3 in its formula, it is called Simpson's 1/3rd Rule.

Example 1

The distance covered by a rocket from $t=8$ to $t=30$ is given by

$$x = \int_8^{30} \left(2000 \ln \left[\frac{140000}{140000 - 2100t} \right] - 9.8t \right) dt$$

- a) Use Simpson's 1/3rd Rule to find the approximate value of x
- b) Find the true error, E_t
- c) Find the absolute relative true error, $|\epsilon_t|$

Solution

$$\begin{aligned} \text{a)} \quad x &= \int_8^{30} f(t) dt x = \left(\frac{b-a}{6} \right) \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right] \\ &= \left(\frac{30-8}{6} \right) [f(8) + 4f(19) + f(30)] \\ &= \left(\frac{22}{6} \right) [177.2667 + 4(484.7455) + 901.6740] = 11065.72 \text{ m} \end{aligned}$$

b) The exact value of the above integral is

$$x = \int_8^{30} \left(2000 \ln \left[\frac{140000}{140000 - 2100t} \right] - 9.8t \right) dt = 11061.34 \text{ m}$$

$$E_t = 11061.34 - 11065.72 = -4.38 \text{ m}$$

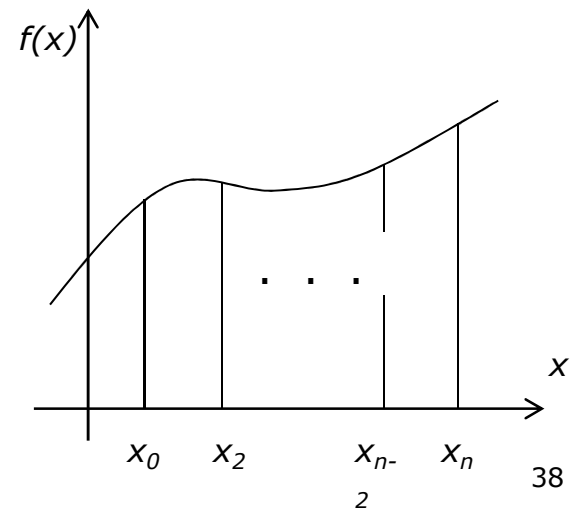
$$\text{c)} \quad |\epsilon_t| = \left| \frac{11061.34 - 11065.72}{11061.34} \right| \times 100\% = 0.0396\%$$

Multiple Segment Simpson's 1/3rd Rule

Just like in multiple segment Trapezoidal Rule, one can subdivide the interval $[a, b]$ into n segments and apply Simpson's 1/3rd Rule repeatedly over every two segments. Note that n needs to be even. Divide interval $[a, b]$ into equal segments, hence the segment

width $h = \frac{b-a}{n}$ $\int_a^b f(x)dx = \int_{x_0}^{x_n} f(x)dx; x_0 = a; x_n = b$

$$\int_a^b f(x)dx = \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx + \dots + \int_{x_{n-4}}^{x_{n-2}} f(x)dx + \int_{x_{n-2}}^{x_n} f(x)dx$$



Multiple Segment Simpson's 1/3rd Rule

Apply Simpson's 1/3rd Rule over each interval,

$$\begin{aligned}\int_a^b f(x)dx &= (x_2 - x_0) \left[\frac{f(x_0) + 4f(x_1) + f(x_2)}{6} \right] \\ &+ (x_4 - x_2) \left[\frac{f(x_2) + 4f(x_3) + f(x_4)}{6} \right] + \dots \\ &+ (x_{n-2} - x_{n-4}) \left[\frac{f(x_{n-4}) + 4f(x_{n-3}) + f(x_{n-2})}{6} \right] \\ &+ (x_n - x_{n-2}) \left[\frac{f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)}{6} \right]\end{aligned}$$

Since $x_i - x_{i-2} = 2h, i = 2, 4, \dots, n$

Multiple Segment Simpson's 1/3rd Rule

Then

$$\int_a^b f(x)dx = 2h \left[\frac{f(x_0) + 4f(x_1) + f(x_2)}{6} \right]$$
$$+ 2h \left[\frac{f(x_2) + 4f(x_3) + f(x_4)}{6} \right] + \dots$$
$$+ 2h \left[\frac{f(x_{n-4}) + 4f(x_{n-3}) + f(x_{n-2})}{6} \right]$$
$$+ 2h \left[\frac{f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)}{6} \right]$$

Multiple Segment Simpson's 1/3rd Rule

$$\begin{aligned}\int_a^b f(x)dx &= \frac{h}{3} [f(x_0) + 4\{f(x_1) + f(x_3) + \dots + f(x_{n-1})\} \\ &\quad + 2\{f(x_2) + f(x_4) + \dots + f(x_{n-2})\} + f(x_n)] \\ &= \frac{h}{3} \left[f(x_0) + 4 \sum_{\substack{i=1 \\ i=\text{odd}}}^{n-1} f(x_i) + 2 \sum_{\substack{i=2 \\ i=\text{even}}}^{n-2} f(x_i) + f(x_n) \right] \\ &= \frac{b-a}{3n} \left[f(x_0) + 4 \sum_{\substack{i=1 \\ i=\text{odd}}}^{n-1} f(x_i) + 2 \sum_{\substack{i=2 \\ i=\text{even}}}^{n-2} f(x_i) + f(x_n) \right]\end{aligned}$$

Example 2

Use 4-segment Simpson's 1/3rd Rule to approximate the distance covered by a rocket from $t=8$ to $t=30$ as given by

$$x = \int_8^{30} \left(2000 \ln \left[\frac{140000}{140000 - 2100t} \right] - 9.8t \right) dt$$

- a) Use four segment Simpson's 1/3rd Rule to find the approximate value of x .
- b) Find the true error, E_t for part (a).
- c) Find the absolute relative true error, $|\epsilon_a|$ for part (a).

Solution

a) Using n segment Simpson's 1/3rd Rule,

$$h = \frac{30-8}{4} = 5.5$$

So $f(t_0) = f(8)$

$$f(t_1) = f(8 + 5.5) = f(13.5)$$

$$f(t_2) = f(13.5 + 5.5) = f(19)$$

$$f(t_3) = f(19 + 5.5) = f(24.5)$$

$$f(t_4) = f(30)$$

Solution (cont.)

$$\begin{aligned}x &= \frac{b-a}{3n} \left[f(t_0) + 4 \sum_{\substack{i=1 \\ i=\text{odd}}}^{n-1} f(t_i) + 2 \sum_{\substack{i=2 \\ i=\text{even}}}^{n-2} f(t_i) + f(t_n) \right] \\&= \frac{30-8}{3(4)} \left[f(8) + 4 \sum_{\substack{i=1 \\ i=\text{odd}}}^3 f(t_i) + 2 \sum_{\substack{i=2 \\ i=\text{even}}}^2 f(t_i) + f(30) \right] \\&= \frac{22}{12} [f(8) + 4f(t_1) + 4f(t_3) + 2f(t_2) + f(30)] \\&= \frac{11}{6} [f(8) + 4f(13.5) + 4f(24.5) + 2f(19) + f(30)] \\&= \frac{11}{6} [177.2667 + 4(320.2469) + 4(676.0501) + 2(484.7455) + 901.6740] \\&= 11061.64 \text{ m}\end{aligned}$$

Solution (cont.)

- b) In this case, the true error is

$$E_t = 11061.34 - 11061.64 = -0.30 \text{ m}$$

- c) The absolute relative true error

$$\begin{aligned} |\epsilon_t| &= \left| \frac{11061.34 - 11061.64}{11061.34} \right| \times 100\% \\ &= 0.0027\% \end{aligned}$$

Solution (cont.)

Table 1: Values of Simpson's 1/3rd Rule for Example 2 with multiple segments

n	Approximate Value	E_t	$ \epsilon_t $
2	11065.72	4.38	0.0396%
4	11061.64	0.30	0.0027%
6	11061.40	0.06	0.0005%
8	11061.35	0.01	0.0001%
10	11061.34	0.00	0.0000%

Error in the Multiple Segment Simpson's 1/3rd Rule

The true error in a single application of Simpson's 1/3rd Rule is given as

$$E_t = -\frac{(b-a)^5}{2880} f^{(4)}(\zeta), \quad a < \zeta < b$$

In Multiple Segment Simpson's 1/3rd Rule, the error is the sum of the errors in each application of Simpson's 1/3rd Rule. The error in n segment Simpson's 1/3rd Rule is given by

$$E_1 = -\frac{(x_2 - x_0)^5}{2880} f^{(4)}(\zeta_1) = -\frac{h^5}{90} f^{(4)}(\zeta_1), \quad x_0 < \zeta_1 < x_2$$

$$E_2 = -\frac{(x_4 - x_2)^5}{2880} f^{(4)}(\zeta_2) = -\frac{h^5}{90} f^{(4)}(\zeta_2), \quad x_2 < \zeta_2 < x_4$$

Error in the Multiple Segment Simpson's 1/3rd Rule

$$E_i = -\frac{(x_{2i} - x_{2(i-1)})^5}{2880} f^{(4)}(\zeta_i) = -\frac{h^5}{90} f^{(4)}(\zeta_i), x_{2(i-1)} < \zeta_i < x_{2i}$$

⋮

$$E_{\frac{n}{2}-1} = -\frac{(x_{n-2} - x_{n-4})^5}{2880} f^{(4)}\left(\zeta_{\frac{n}{2}-1}\right) = -\frac{h^5}{90} f^{(4)}\left(\zeta_{\frac{n}{2}-1}\right), x_{n-4} < \zeta_{\frac{n}{2}-1} < x_{n-2}$$

$$E_{\frac{n}{2}} = -\frac{(x_n - x_{n-2})^5}{2880} f^{(4)}\left(\zeta_{\frac{n}{2}}\right) = -\frac{h^5}{90} f^{(4)}\left(\zeta_{\frac{n}{2}}\right), x_{n-2} < \zeta_{\frac{n}{2}} < x_n$$

Hence, the total error in Multiple Segment Simpson's 1/3rd Rule is

$$E_t = \sum_{i=1}^{\frac{n}{2}} E_i = -\frac{h^5}{90} \sum_{i=1}^{n/2} f^{(4)}(\zeta_i) = -\frac{(b-a)^5}{90n^5} \sum_{i=1}^{n/2} f^{(4)}(\zeta_i) = -\frac{(b-a)^5}{90n^4} \frac{\sum_{i=1}^{n/2} f^{(4)}(\zeta_i)}{n}$$

Error in the Multiple Segment Simpson's $1/3^{\text{rd}}$ Rule

The term $\frac{\sum_{i=1}^{\frac{n}{2}} f^{(4)}(\zeta_i)}{n}$ is an approximate average value of

$$f^{(4)}(x), a < x < b$$

Hence

$$E_t = -\frac{(b-a)^5}{90n^4} \overline{f}^{(4)}$$

where

$$\overline{f}^{(4)} = \frac{\sum_{i=1}^{\frac{n}{2}} f^{(4)}(\zeta_i)}{n}$$

As was done in Box 21.2 for the trapezoidal rule, Simpson's 1/3 rule can be derived by integrating the forward Newton-Gregory interpolating polynomial (Box 18.2):

$$I = \int_{x_0}^{x_2} \left[f(x_0) + \Delta f(x_0)\alpha + \frac{\Delta^2 f(x_0)}{2}\alpha(\alpha - 1) + \frac{\Delta^3 f(x_0)}{6}\alpha(\alpha - 1)(\alpha - 2) + \frac{f^{(4)}(\xi)}{24}\alpha(\alpha - 1)(\alpha - 2)(\alpha - 3)h^4 \right] dx$$

Notice that we have written the polynomial up to the fourth-order term rather than the third-order term as would be expected. The reason for this will be apparent shortly. Also notice that the limits of integration are from x_0 to x_2 . Therefore, when the simplifying substitutions are made (recall Box 21.2), the integral is from $\alpha = 0$ to 2:

$$\begin{aligned}
 I = h \int_0^2 & \left[f(x_0) + \Delta f(x_0)\alpha + \frac{\Delta^2 f(x_0)}{2}\alpha(\alpha - 1) \right. \\
 & + \frac{\Delta^3 f(x_0)}{6}\alpha(\alpha - 1)(\alpha - 2) \\
 & \left. + \frac{f^{(4)}(\xi)}{24}\alpha(\alpha - 1)(\alpha - 2)(\alpha - 3)h^4 \right] d\alpha
 \end{aligned}$$

which can be integrated to yield

$$\begin{aligned}
 I = h & \left[\alpha f(x_0) + \frac{\alpha^2}{2}\Delta f(x_0) + \left(\frac{\alpha^3}{6} - \frac{\alpha^2}{4} \right) \Delta^2 f(x_0) \right. \\
 & + \left(\frac{\alpha^4}{24} - \frac{\alpha^3}{6} + \frac{\alpha^2}{6} \right) \Delta^3 f(x_0) \\
 & \left. + \left(\frac{\alpha^5}{120} - \frac{\alpha^4}{16} + \frac{11\alpha^3}{72} - \frac{\alpha^2}{8} \right) f^{(4)}(\xi)h^4 \right]_0^2
 \end{aligned}$$

and evaluated for the limits to give

$$I = h \left[2 f(x_0) + 2 \Delta f(x_0) + \frac{\Delta^2 f(x_0)}{3} + (0) \Delta^3 f(x_0) - \frac{1}{90} f^{(4)}(\xi) h^4 \right] \quad (\text{B21.3.1})$$

Notice the significant result that the coefficient of the third divided difference is zero. Because $\Delta f(x_0) = f(x_1) - f(x_0)$ and $\Delta^2 f(x_0) = f(x_2) - 2f(x_1) + f(x_0)$, Eq. (B21.3.1) can be rewritten as

$$I = \underbrace{\frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)]}_{\text{Simpson's 1/3 rule}} - \underbrace{\frac{1}{90} f^{(4)}(\xi) h^5}_{\text{Truncation error}}$$

Thus, the first term is Simpson's 1/3 rule and the second is the truncation error. Because the third divided difference dropped out, we obtain the significant result that the formula is third-order accurate.

Simpson's 3/8 Rule

- Simpson's 3/8 rule uses a **third order polynomial**
 - need 3 intervals (4 data points)

$$f(x) \approx p_3(x) = a_0 + a_1x + a_2x^2 + a_3x^3$$

$$I = \int_{x_0}^{x_3} f(x)dx \approx \int_{x_0}^{x_3} p_3(x)dx$$

- Determine a 's with Lagrange polynomial
- For evenly spaced points

$$I = \frac{3}{8}h[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)]$$

$$h = \frac{b-a}{3}$$

Error

- Same order as 1/3 Rule.
 - More function evaluations.
 - Interval width, h , is smaller.

$$E_t = -\frac{3}{80}h^5 f^{(4)}(\xi) \quad O(h^4)$$

- Integrates a cubic exactly:

$\Rightarrow$

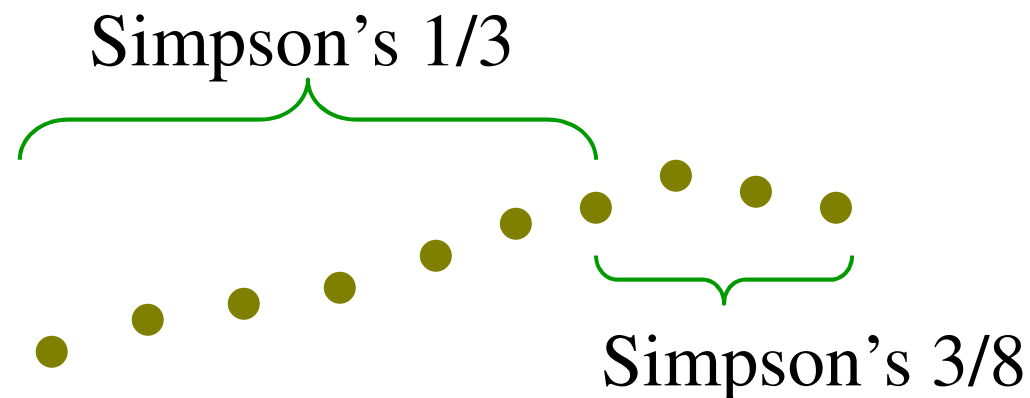
$$f^{(4)}(\xi) = 0$$

Comparison

- Simpson's 1/3 rule and Simpson's 3/8 rule have the same order of error
 - $O(h^4)$
 - trapezoidal rule has an error of $O(h^2)$
- Simpson's 1/3 rule requires **even number** of segments.
- Simpson's 3/8 rule requires multiples of **three segments**.
- Both Simpson's methods require **evenly spaced** data points

Mixing Techniques

- $n = 10$ points $\Rightarrow$ 9 intervals
 - First 6 intervals - Simpson's 1/3
 - Last 3 intervals - Simpson's 3/8



Adaptive Simpson's Scheme

- Recall Simpson's 1/3 Rule:

$$I \approx \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)]$$

- Where initially, we have $a=x_0$ and $b=x_2$.
- Subdividing the integral into two:

$$I \approx \frac{h}{6} [f(a) + 4f(x_1) + 2f(x_2) + 4f(x_3) + f(b)]$$

Adaptive Simpson's Scheme

- We want to keep subdividing, until we reach a desired error tolerance, ε .
- Mathematically:

$$\left| \int_a^b f(x) dx - \left[\frac{h}{3} [f(a) + 4f(x_1) + f(b)] \right] \right| \leq \varepsilon$$

$$\left| \int_a^b f(x) dx - \left[\frac{h}{6} [f(a) + 4f(x_1) + 2f(x_2) + 4f(x_3) + f(b)] \right] \right| \leq \varepsilon$$

Adaptive Simpson's Scheme

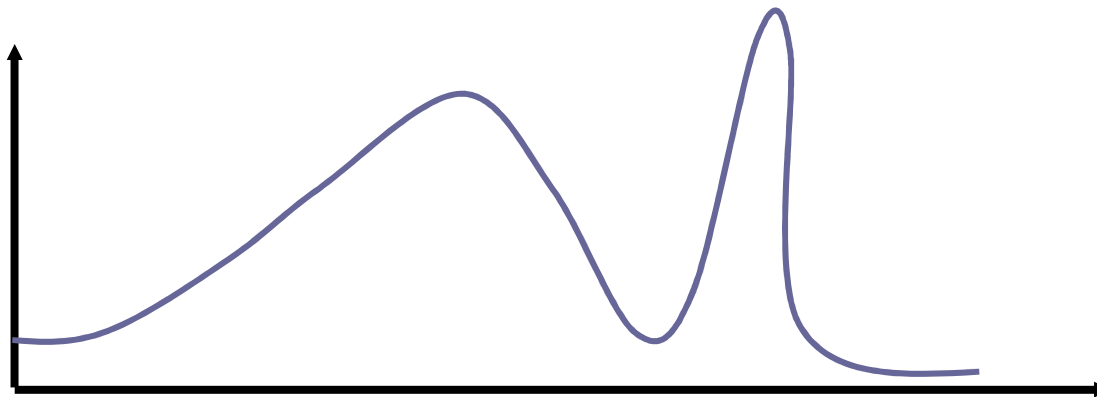
- This will be satisfied if:

$$\left| \int_a^c f(x) dx - \left[\frac{h}{6} [f(a) + 4f(x_1) + f(x_2)] \right] \right| \leq \frac{\varepsilon}{2}, \text{ and}$$
$$\left| \int_c^b f(x) dx - \left[\frac{h}{6} [f(x_2) + 4f(x_3) + f(b)] \right] \right| \leq \frac{\varepsilon}{2}, \text{ where}$$
$$c = x_2 = \frac{a+b}{2}$$

- The left and the right are within one-half of the error.

Adaptive Simpson's Scheme

- Okay, now we have two separate intervals to integrate.
- What if one can be solved accurately with an $h=10^{-3}$, but the other requires many, many more intervals, $h=10^{-6}$?



Adaptive Simpson's Scheme

- Adaptive Simpson's method provides a divide and conquer scheme until the appropriate error is satisfied everywhere.
- Very popular method in practice.
- Problem:
 - We do not know the exact value, and hence do not know the error.

Adaptive Simpson's Scheme

- How do we know whether to continue to subdivide or terminate?

$$I \equiv \int_a^b f(x) dx = S(a, b) + E(a, b), \text{ where}$$

$$S(a, b) = \frac{b-a}{6} \left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right], \text{ and}$$

$$E(a, b) = -\frac{1}{90} \left(\frac{b-a}{2} \right)^5 f^{(4)}$$

Adaptive Simpson's Scheme

- The first iteration can then be defined as:

$$I = S^{(1)} + E^{(1)}, \text{ where}$$
$$S^{(1)} = S(a, b), E^{(1)} = E(a, b)$$

- Subsequent subdivision can be defined as:

$$S^{(2)} = S(a, c) + S(c, b)$$

Adaptive Simpson's Scheme

- Now, since $E^{(2)} = E(a, c) + E(c, b)$
- We can solve for $E^{(2)}$ in terms of $E^{(1)}$.

$$\begin{aligned} E^{(2)} &= -\frac{1}{90} \left(\frac{h/2}{2} \right)^5 f^{(4)} - \frac{1}{90} \left(\frac{h/2}{2} \right)^5 f^{(4)} \\ &= -\left(\frac{1}{2^4} \right) \frac{1}{90} \left(\frac{h}{2} \right)^5 f^{(4)} = \frac{E^{(1)}}{16} \end{aligned}$$

Adaptive Simpson's Scheme

- Finally, using the identity:

$$I = S^{(1)} + E^{(1)} = S^{(2)} + E^{(2)}$$

- We have:

$$S^{(2)} - S^{(1)} = E^{(1)} - E^{(2)} = 15E^{(2)}$$

- Plugging into our definition:

$$I = S^{(2)} + E^{(2)} = S^{(2)} + \frac{1}{15} \left(S^{(2)} - S^{(1)} \right)$$

Adaptive Simpson's Scheme

- Our error criteria is thus:

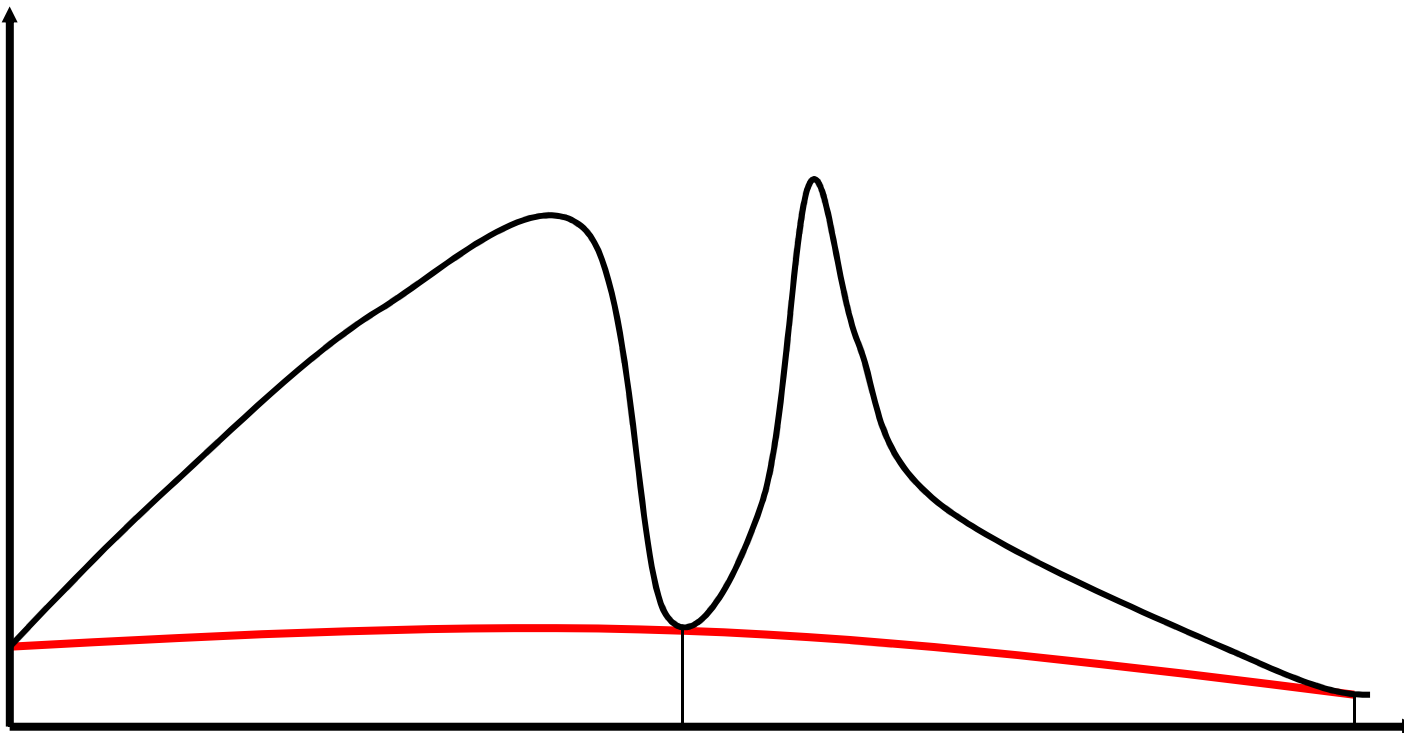
$$\left| I - S^{(2)} \right| = \left| \frac{1}{15} \left(S^{(2)} - S^{(1)} \right) \right| \leq \varepsilon$$

- Simplifying leads to the termination formula:

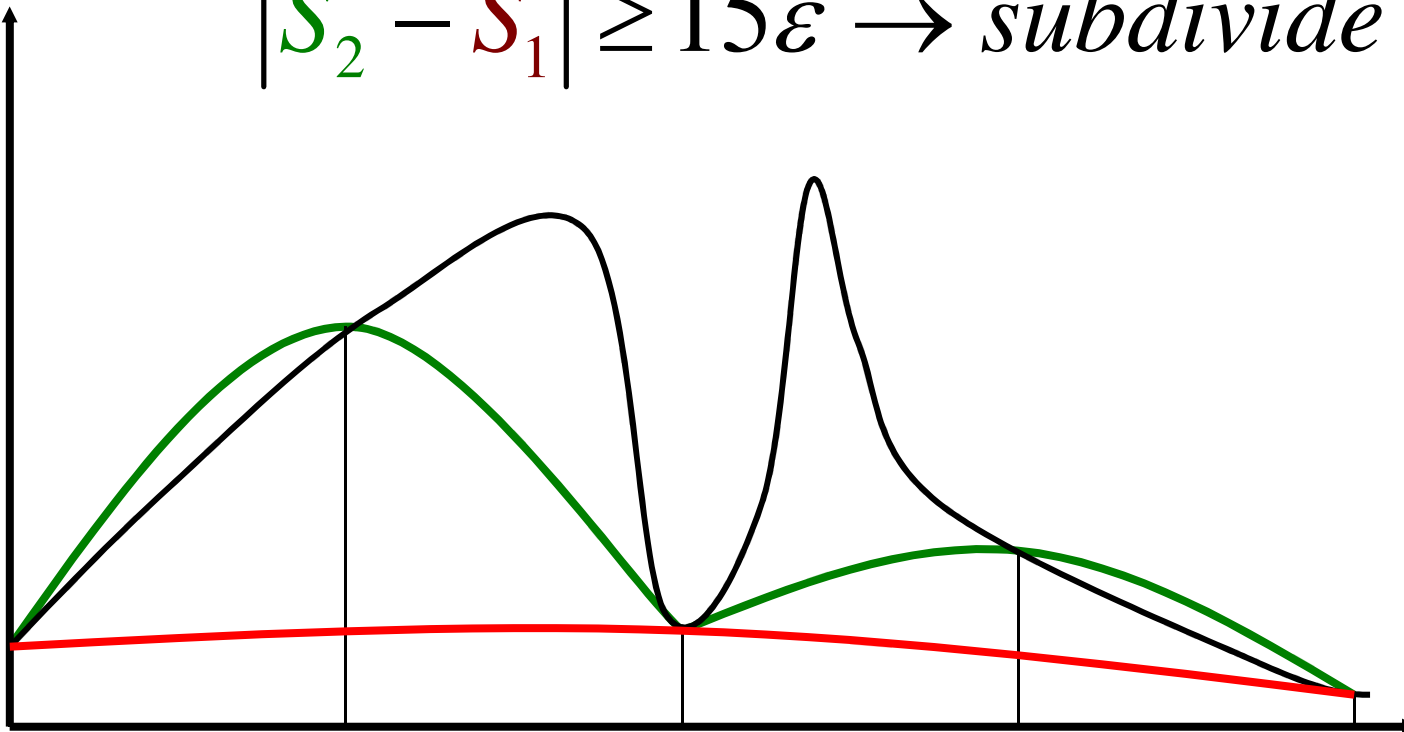
$$\left| \left(S^{(2)} - S^{(1)} \right) \right| \leq 15\varepsilon$$

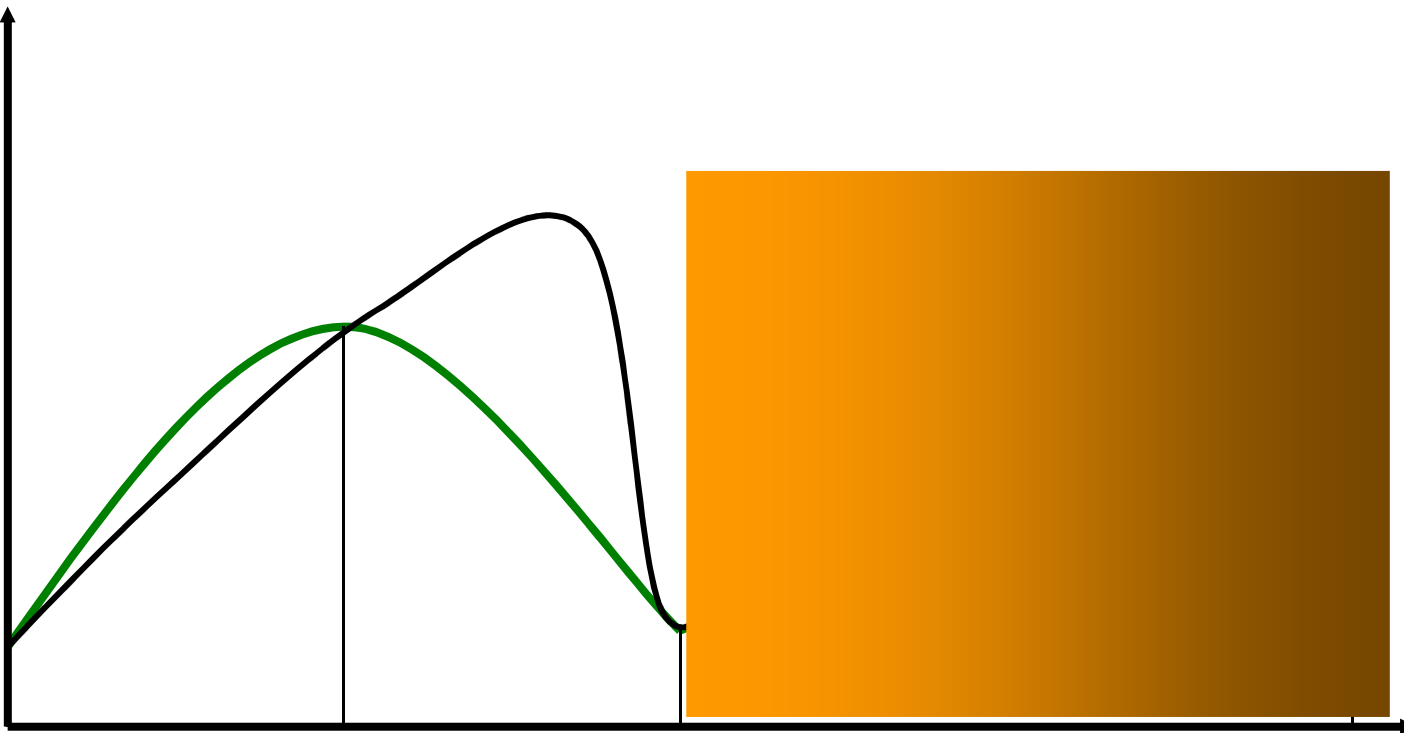
Adaptive Simpson's Scheme

- What happens graphically:

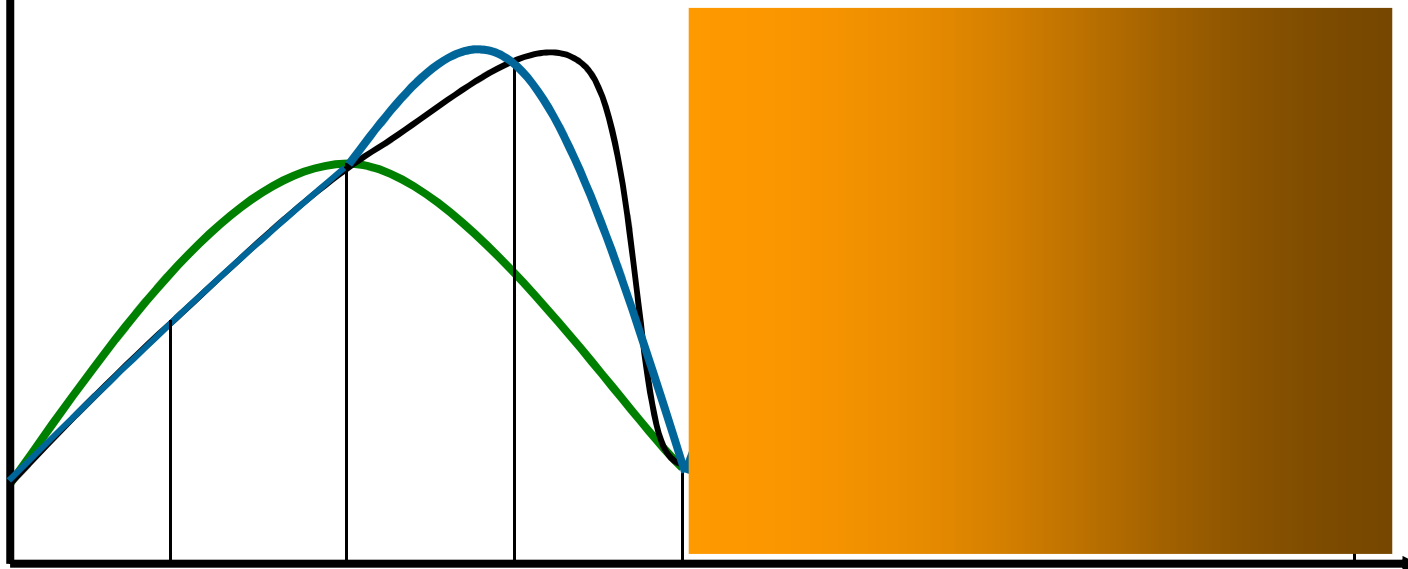


$|S_2 - S_1| \geq 15\varepsilon \rightarrow \textit{subdivide}$

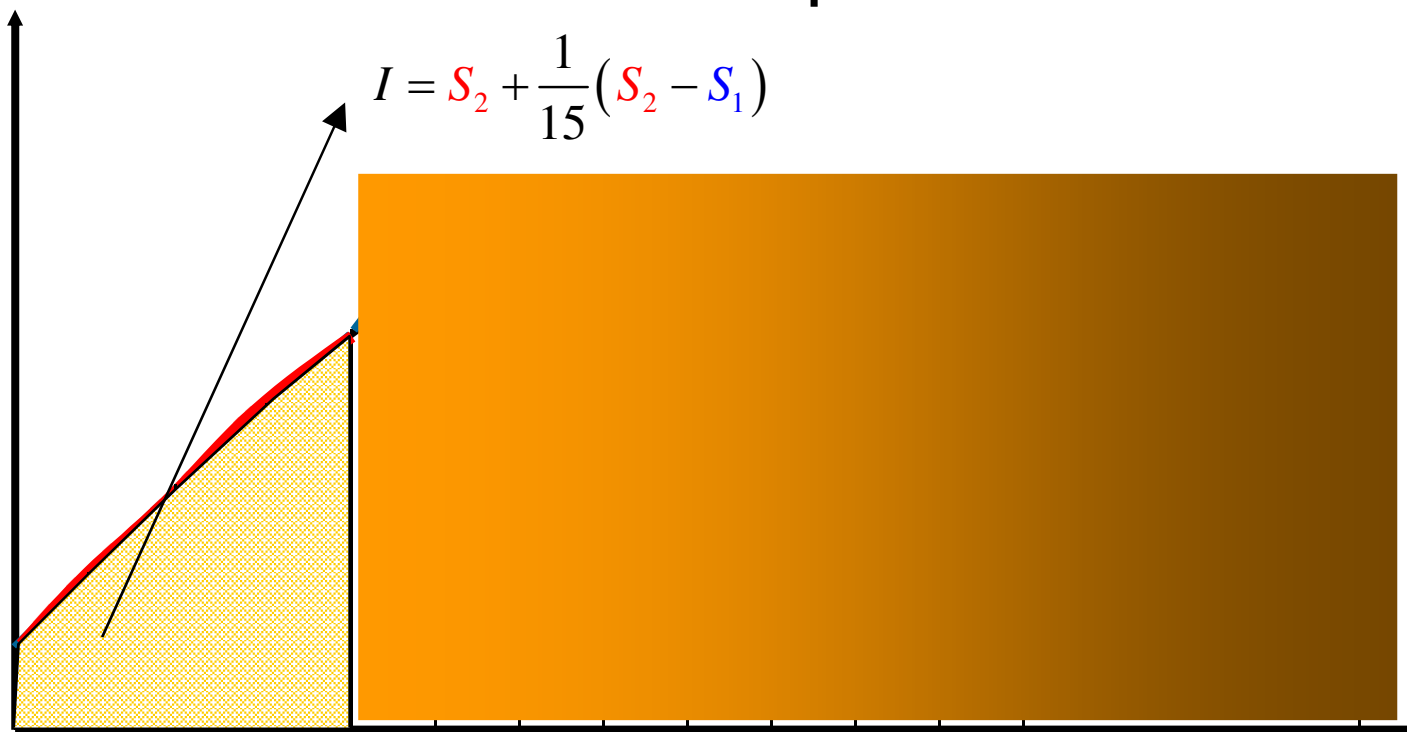




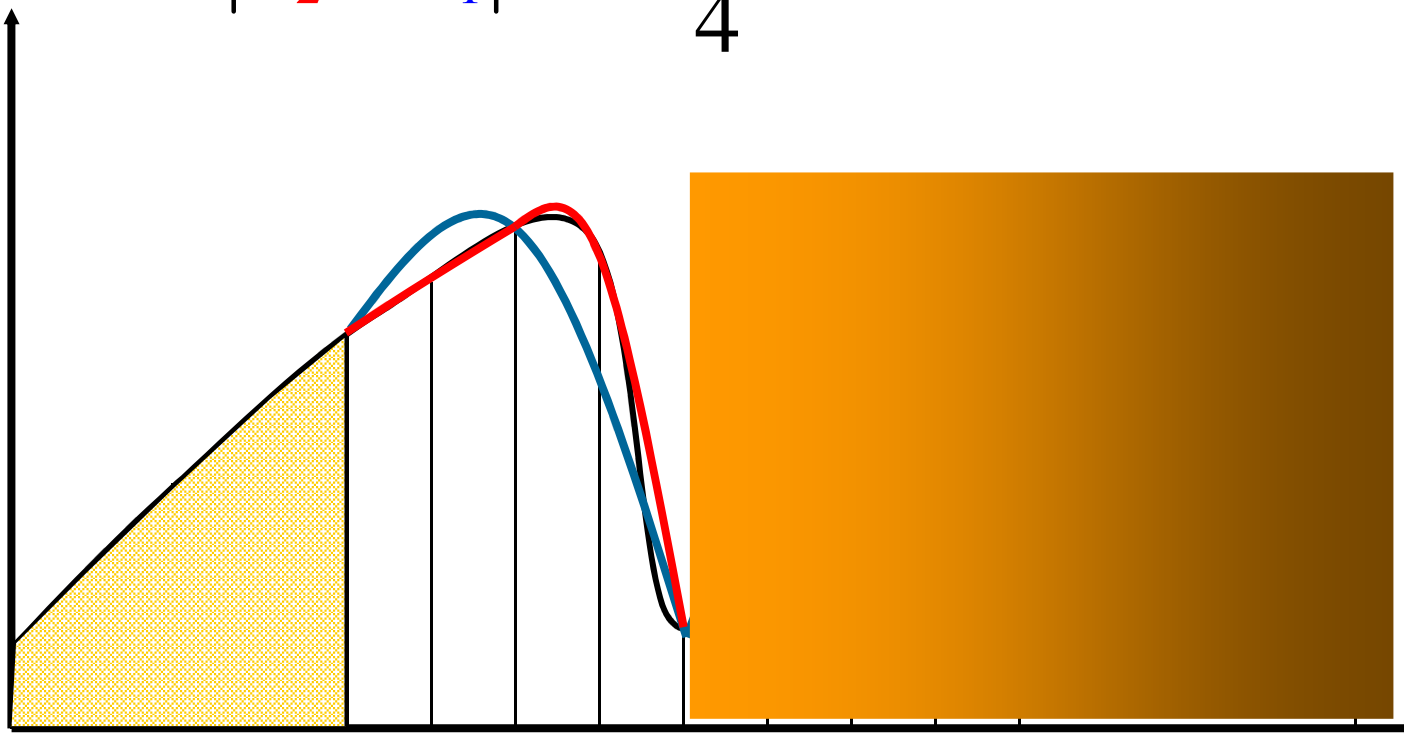
$|S_2 - S_1| \geq 15 \frac{\varepsilon}{2} \rightarrow \textit{subdivide}$

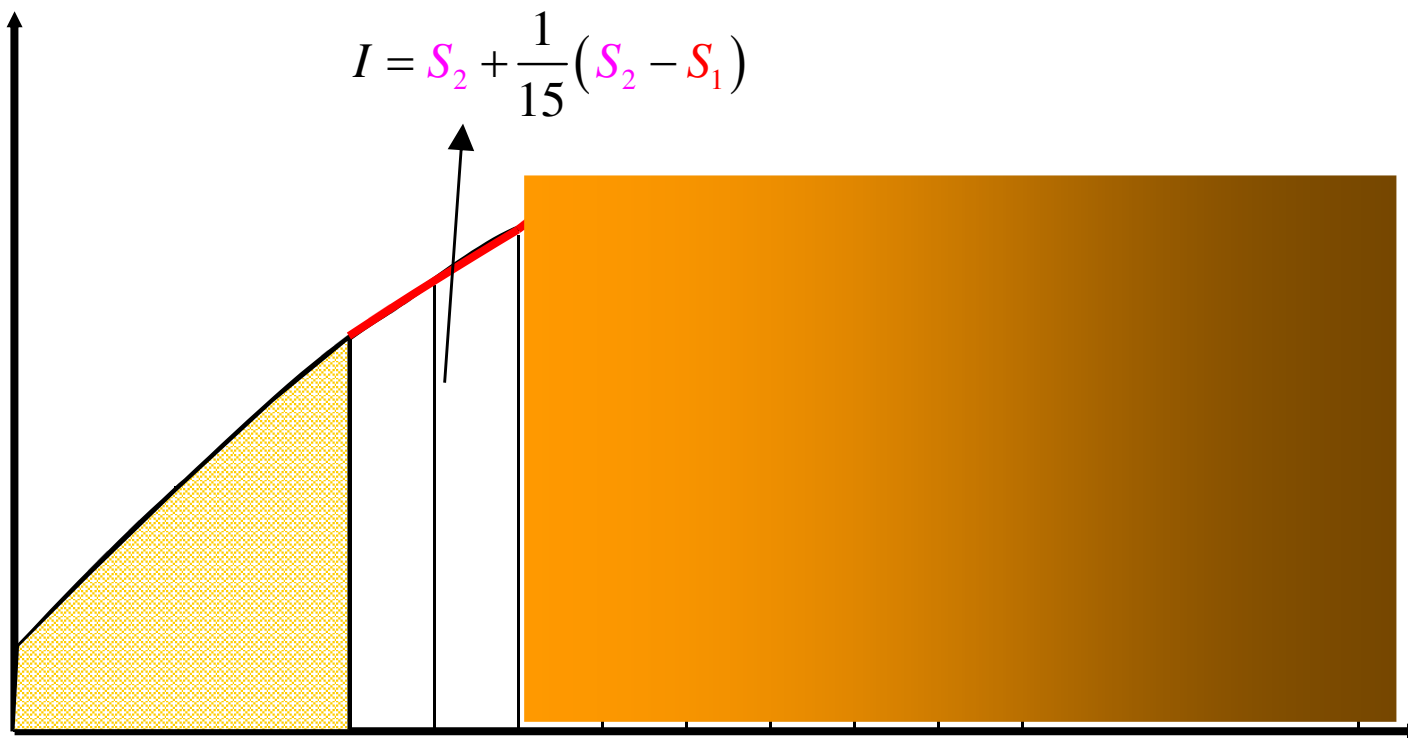


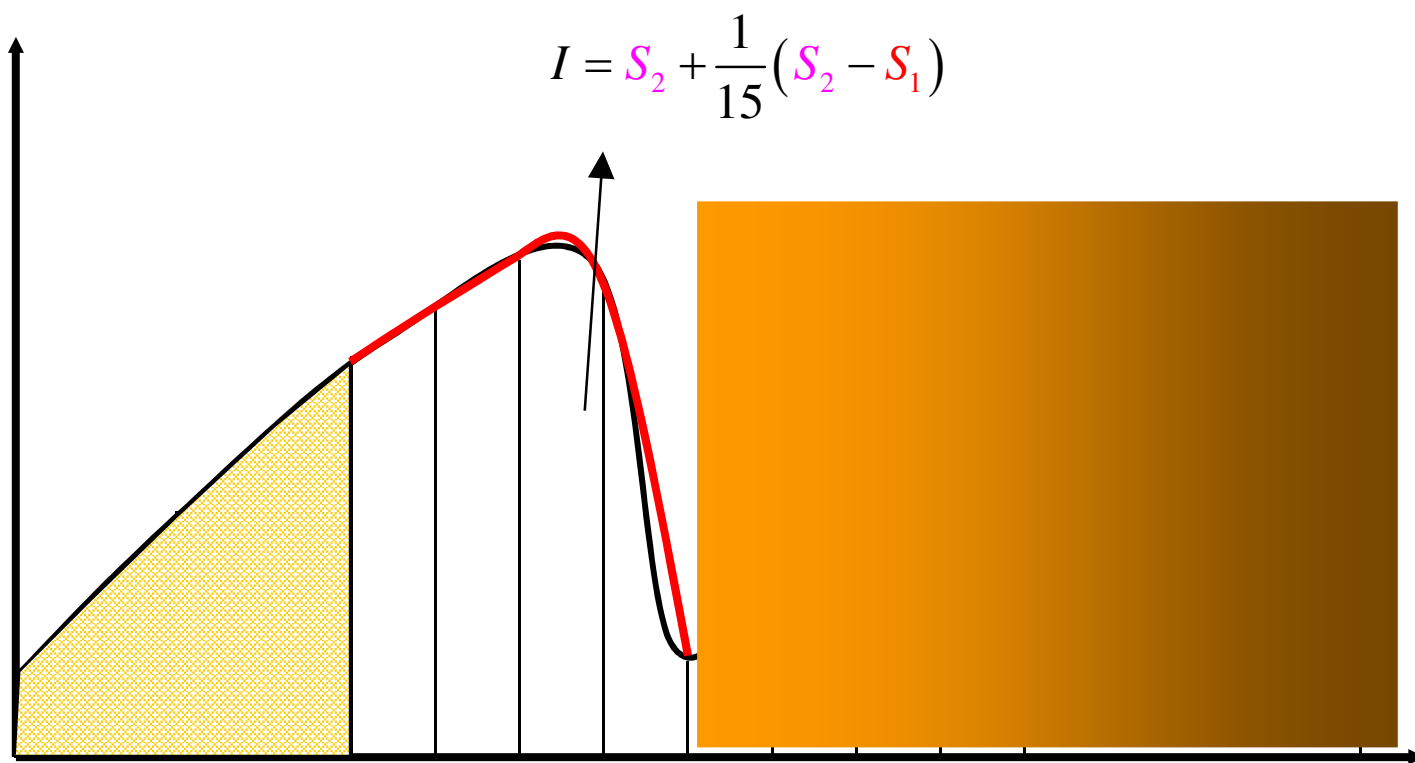
$$|S_2 - S_1| \leq 15 \frac{\varepsilon}{4} \rightarrow \textit{done}$$

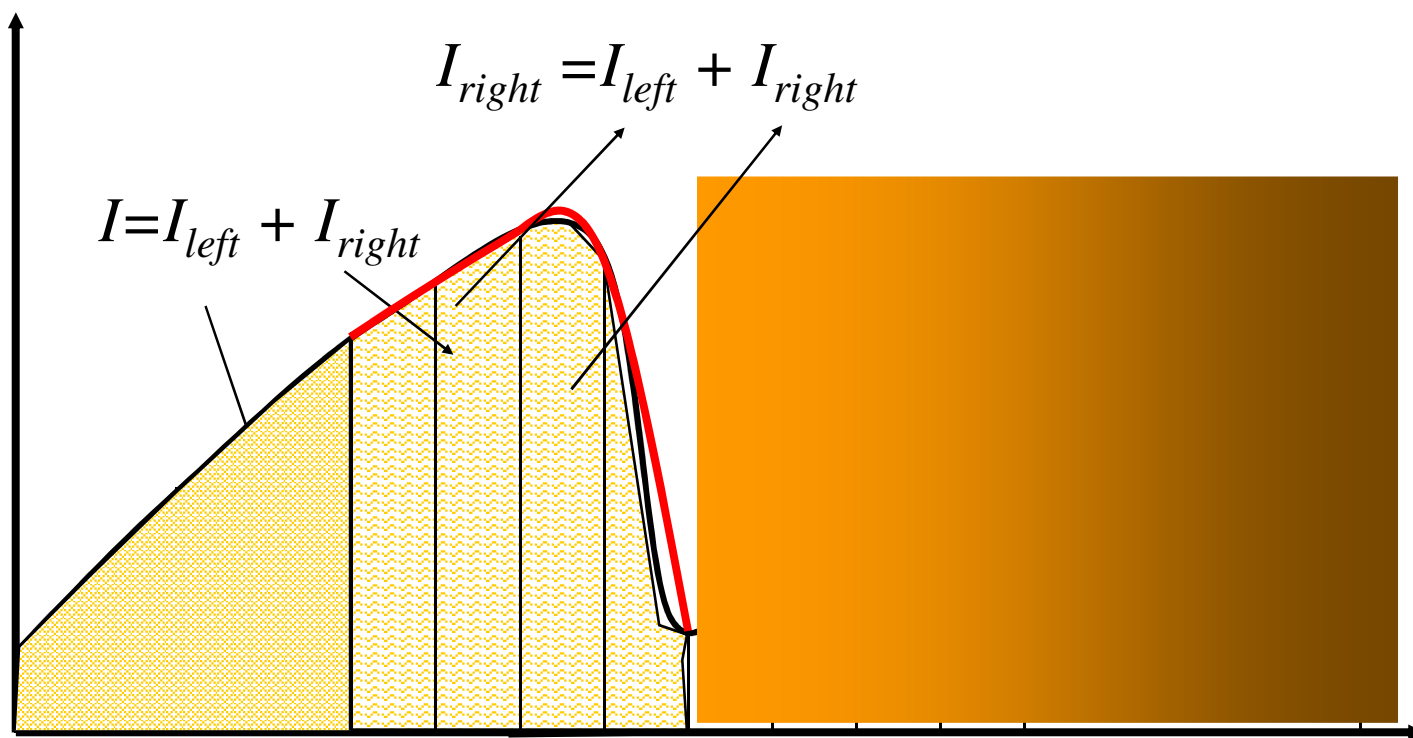


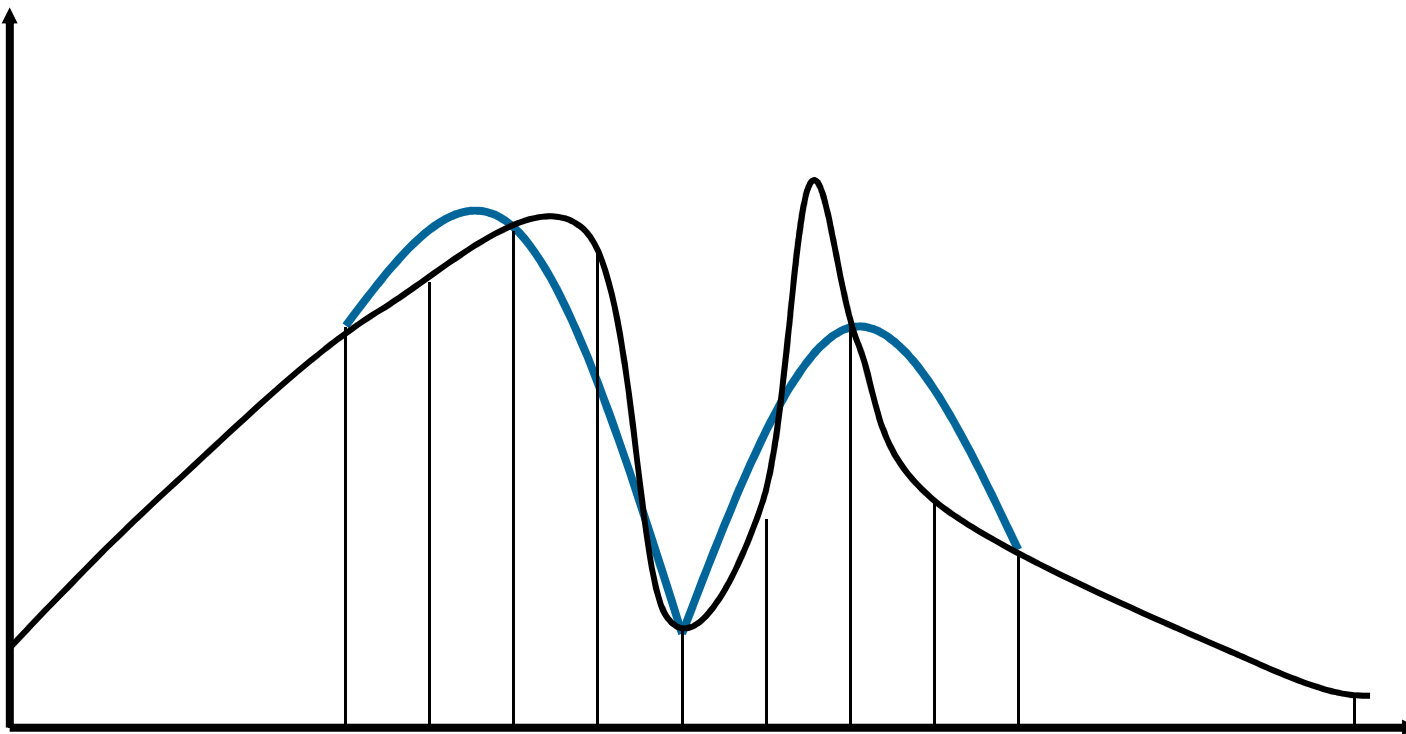
$$|S_2 - S_1| \geq 15 \frac{\varepsilon}{4} \rightarrow \textit{subdivide}$$

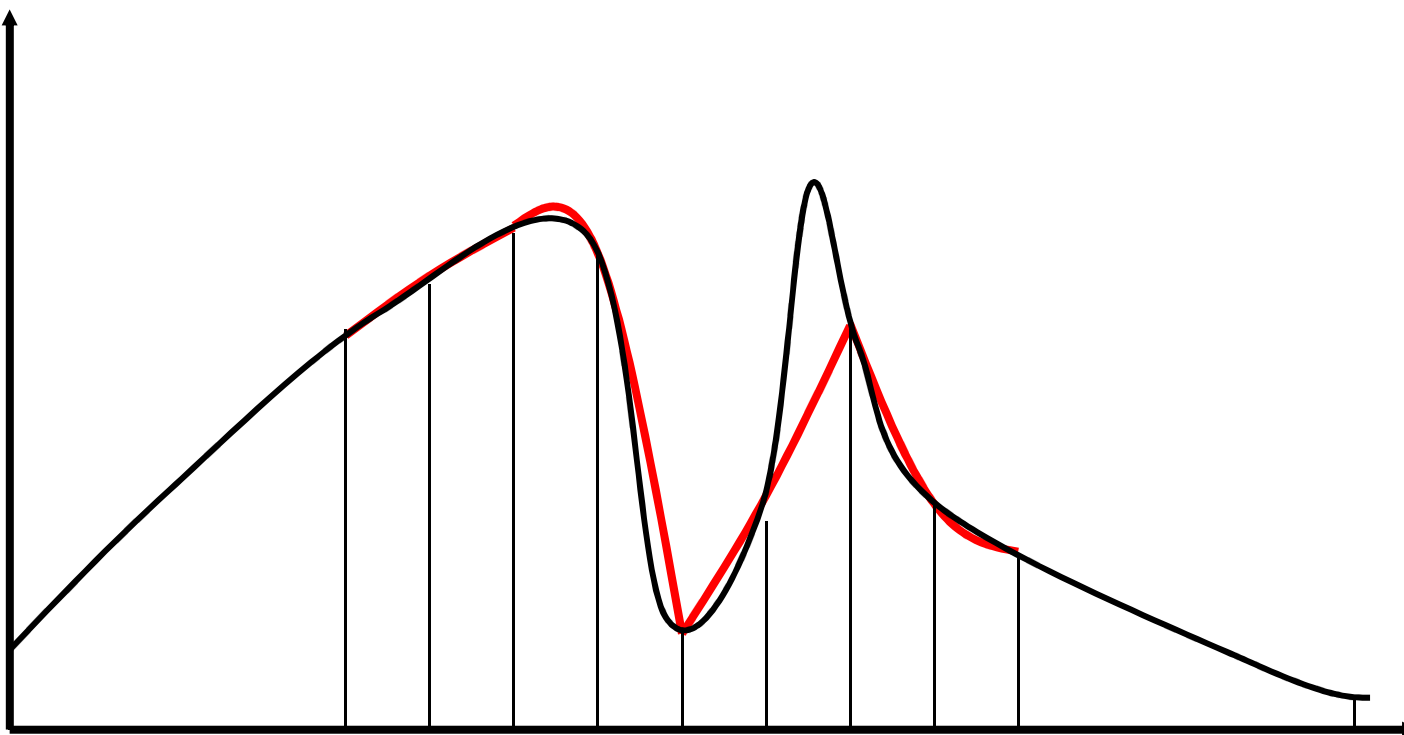






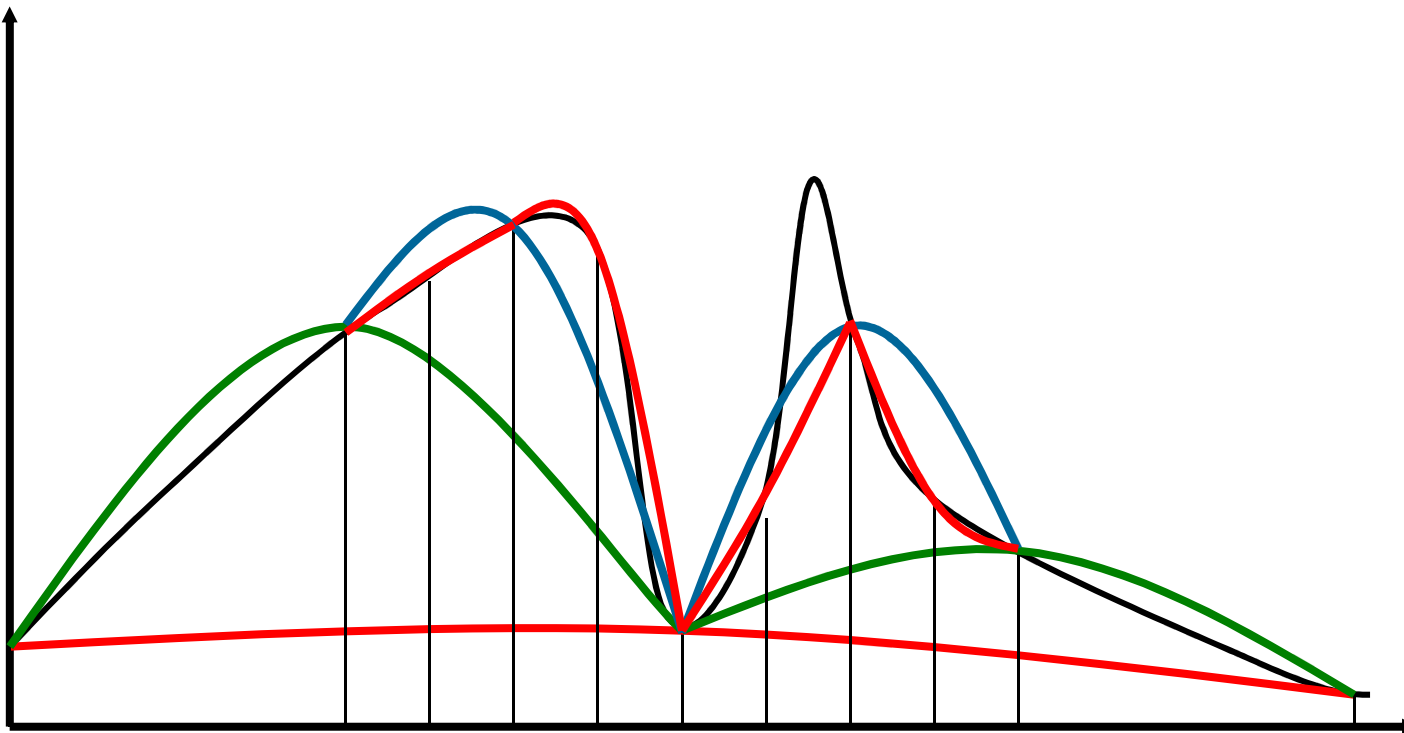






Adaptive Simpson's Scheme

- We gradually capture the difficult spots.



Romberg Method

Motivation

- Trapezoid formula with a sub-interval h gives an error of the order $O(h^2)$.
- *We can combine two Trapezoid estimates with intervals h and $h/2$ to get a better estimate based on Richardson's extrapolation.*

Romberg Method

Estimates using Trapezoid method intervals of size $h, h/2, h/4, h/8 \dots$

are combined to improve the approximation of $\int_a^b f(x) dx$

First column is obtained
using Trapezoid Method

R(0,0)			
R(1,0)	R(1,1)		
R(2,0)	R(2,1)	R(2,2)	
R(3,0)	R(3,1)	R(3,2)	R(3,3)

The other elements
are obtained using
the Romberg Method

First Column

Recursive Trapezoid Method

$$R(0,0) = \frac{b-a}{2} [f(a) + f(b)]$$

$$R(n,0) = \frac{1}{2} R(n-1,0) + h \left[\sum_{k=1}^{2^{(n-1)}} f(a + (2k-1)h) \right]$$

$$h = \frac{b-a}{2^n}$$

Derivation of Romberg Method

$$\int_a^b f(x)dx = R(n-1,0) + O(h^2) \quad \text{Trapezoid method with } h = \frac{b-a}{2^{n-1}}$$

$$\int_a^b f(x)dx = R(n-1,0) + a_2h^2 + a_4h^4 + a_6h^6 + \dots \quad (eq1)$$

More accurate estimate is obtained by $R(n,0)$

$$\int_a^b f(x)dx = R(n,0) + \frac{1}{4}a_2h^2 + \frac{1}{16}a_4h^4 + \frac{1}{64}a_6h^6 + \dots \quad (eq2)$$

$eq1 - 4 * eq2$ gives

$$\int_a^b f(x)dx = \frac{1}{3} [4 \times R(n,0) - R(n-1,0)] + b_4h^4 + b_6h^6 + \dots$$

Romberg Method

$$R(0,0) = \frac{b-a}{2} [f(a) + f(b)]$$

$$h = \frac{b-a}{2^n},$$

R(0,0)			
R(1,0)	R(1,1)		
R(2,0)	R(2,1)	R(2,2)	
R(3,0)	R(3,1)	R(3,2)	R(3,3)

$$R(n,0) = \frac{1}{2} R(n-1,0) + h \left[\sum_{k=1}^{2^{(n-1)}} f(a + (2k-1)h) \right]$$

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

Property of Romberg Method

Theorem

$$\int_a^b f(x)dx = R(n, m) + O(h^{2m+2})$$

R(0,0)			
R(1,0)	R(1,1)		
R(2,0)	R(2,1)	R(2,2)	
R(3,0)	R(3,1)	R(3,2)	R(3,3)

Error Level

$O(h^2)$

$O(h^4)$

$O(h^6)$

$O(h^8)$

Example

Compute $\int_0^1 x^2 dx$

0.5	
3/8	1/3

$$h = 1, \quad R(0,0) = \frac{b-a}{2} [f(a) + f(b)] = \frac{1}{2} [0 + 1] = 0.5$$

$$h = \frac{1}{2}, \quad R(1,0) = \frac{1}{2} R(0,0) + h(f(a+h)) = \frac{1}{2} \left(\frac{1}{2} \right) + \frac{1}{2} \left(\frac{1}{4} \right) = \frac{3}{8}$$

$$R(n,m) = \frac{1}{4^m - 1} \left[4^m \times R(n, m-1) - R(n-1, m-1) \right] \quad \text{for } n \geq 1, \quad m \geq 1$$

$$R(1,1) = \frac{1}{4^1 - 1} \left[4 \times R(1,0) - R(0,0) \right] = \frac{1}{3} \left[4 \times \frac{3}{8} - \frac{1}{2} \right] = \frac{1}{3}$$

Example (cont.)

$$\begin{aligned} h &= \frac{1}{4}, \quad R(2,0) = \frac{1}{2} R(1,0) + h(f(a+h) + f(a+3h)) \\ &= \frac{1}{2} \left(\frac{3}{8} \right) + \frac{1}{4} \left(\frac{1}{16} + \frac{9}{16} \right) = \frac{11}{32} \end{aligned}$$

0.5		
3/8	1/3	
11/32	1/3	1/3

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

$$R(2,1) = \frac{1}{3} \left[4 \times R(2,0) - R(1,0) \right] = \frac{1}{3} \left[4 \times \frac{11}{32} - \frac{3}{8} \right] = \frac{1}{3}$$

$$R(2,2) = \frac{1}{4^2 - 1} \left[4^2 \times R(2,1) - R(1,1) \right] = \frac{1}{15} \left[\frac{16}{3} - \frac{1}{3} \right] = \frac{1}{3}$$

When do we stop?

STOP if

$$|R(n, n) - R(n, n - 1)| \leq \varepsilon$$

or

After a given number of steps,
for example, STOP at $R(4, 4)$

Gauss Quadrature : Motivation

Trapezoid Method :

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

It can be expressed as :

$$\int_a^b f(x)dx \approx \sum_{i=0}^n c_i f(x_i)$$

$$\text{where } c_i = \begin{cases} h & i = 1, 2, \dots, n-1 \\ 0.5h & i = 0 \text{ and } n \end{cases}$$

General Integration Formula

$$\int_a^b f(x)dx \approx \sum_{i=0}^n c_i f(x_i)$$

c_i : *Weights* x_i : *Nodes*

Problem :

How do we select c_i and x_i so that the formula gives a good approximation of the integral?

Lagrange Interpolation

$$\int_a^b f(x)dx \approx \int_a^b P_n(x)dx$$

where $P_n(x)$ is a polynomial that interpolates $f(x)$ at the nodes: $x_0, x_1, \dots, x_n$

$$\int_a^b f(x)dx \approx \int_a^b P_n(x)dx = \int_a^b \left(\sum_{i=0}^n \ell_i(x) f(x_i) \right) dx$$

$$\Rightarrow \int_a^b f(x)dx \approx \sum_{i=0}^n c_i f(x_i) \quad \text{where } c_i = \int_a^b \ell_i(x) dx$$

Weight and Gauss point Derivation

$$\int_{-1}^1 f(x) dx \approx \sum_{i=1}^n c_i f(x_i); n = 2, \text{ Need } c_1, c_2, x_1, x_2$$

$$\text{Case 1: } f(x) = 1 \Rightarrow \int_{-1}^1 (1) dx = 2 = c_1 + c_2$$

$$\text{Case 2: } f(x) = x \Rightarrow \int_{-1}^1 x dx = 0 = c_1 x_1 + c_2 x_2$$

$$\text{Case 3: } f(x) = x^2 \Rightarrow \int_{-1}^1 x^2 dx = \frac{2}{3} = c_1 x_1^2 + c_2 x_2^2$$

$$\text{Case 4: } f(x) = x^3 \Rightarrow \int_{-1}^1 x^3 dx = 0 = c_1 x_1^3 + c_2 x_2^3$$

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Also impose $x_1 = -x_2$, then $c_1 = c_2 = 1$

$$\text{and } x_1^2 + x_2^2 = \frac{2}{3} = 2x_{2,1}^2 \Rightarrow x_{2,1} = \pm \frac{1}{\sqrt{3}}$$

$$\text{Thus } \int_{-1}^1 f(x)dx = f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

Likewise, one can use the same approach to find

c_i, x_i for $n = 3, 4, \dots$

Also, for $\int_a^b f(x)dx$; Use $x = \frac{1}{2}[t(b-a) + a + b]$, then

$$\int_a^b f(x)dx = \int_{-1}^1 f\left(\frac{t(b-a) + a + b}{2}\right) \frac{b-a}{2} dt_{92}$$

Weight and Gauss points

n	Nodes t_j	Coefficients A_j	Degree of Precision
2	-0.57735 02692	1	3
	0.57735 02692	1	
3	-0.77459 66692	0.55555 55556	5
	0	0.88888 88889	
	0.77459 66692	0.55555 55556	
4	-0.86113 63116	0.34785 48451	7
	-0.33998 10436	0.65214 51549	
	0.33998 10436	0.65214 51549	
	0.86113 63116	0.34785 48451	
5	-0.90617 98459	0.23692 68851	9
	-0.53846 93101	0.47862 86705	
	0	0.56888 88889	
	0.53846 93101	0.47862 86705	
	0.90617 98459	0.23692 68851	

Weight and Gauss points

n	Node	Weight	Precision
2	$\pm\sqrt{1/3}$	1	3
3	0	8/9	5
	$\pm\sqrt{3/5}$	5/9	
4	$\pm\sqrt{3/7 - 2/7\sqrt{6/5}}$	$(18 + \sqrt{30})/36$	7
	$\pm\sqrt{3/7 + 2/7\sqrt{6/5}}$	$(18 - \sqrt{30})/36$	
5	0	128/225	9
	$\pm\frac{1}{3}\sqrt{5 - 2\sqrt{10/7}}$	$(322 + 13\sqrt{70})/900$	
	$\pm\frac{1}{3}\sqrt{5 + 2\sqrt{10/7}}$	$(322 - 13\sqrt{70})/900$	

Example

1. Find $\int_{-2}^2 x^2 dx$ (The exact value for $\int_{-2}^2 x^2 dx = \frac{16}{3}$)

$$\int_{-2}^2 x^2 dx \underset{x=2t}{=} \int_{-1}^1 8t^2 dt = 8 \left[f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) \right] = \frac{16}{3}$$

2. Find $\int_0^3 e^{-x} dx$ (The exact value = 0.95021293)

$$\int_0^3 e^{-x} dx \underset{x=(3t+3)/2}{=} \int_{-1}^1 \frac{3}{2} e^{-3(t+1)/2} dt \underset{n=2}{=} \frac{3}{2} \left[f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) \right]$$

$$\underset{n=2}{=} 0.93649827 \underset{n=3}{=} 0.94995372 \underset{n=4}{=} 0.95021032$$

Improper Integrals

Methods discussed earlier cannot be used directly to approximate improper integrals (one of the limits is ∞ or $-\infty$)

$\Rightarrow$ Use a transformation like the following

$$\int_a^b f(x)dx = \int_{\frac{1}{b}}^{\frac{1}{a}} \frac{1}{t^2} f\left(\frac{1}{t}\right)dt, \quad (\text{assuming } ab > 0)$$

and apply the method on the new function.

Example :

$$\int_1^{\infty} \frac{1}{x^2} dx = \int_0^1 \frac{1}{t^2} \left(\frac{1}{\left(\frac{1}{t}\right)^2} \right) dt$$