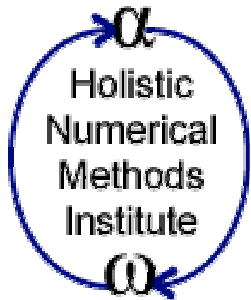




Integration



Topic: Trapezoidal Rule

Major: Chemical Engineering

What is Integration

Integration:

The process of measuring the area under a function plotted on a graph.

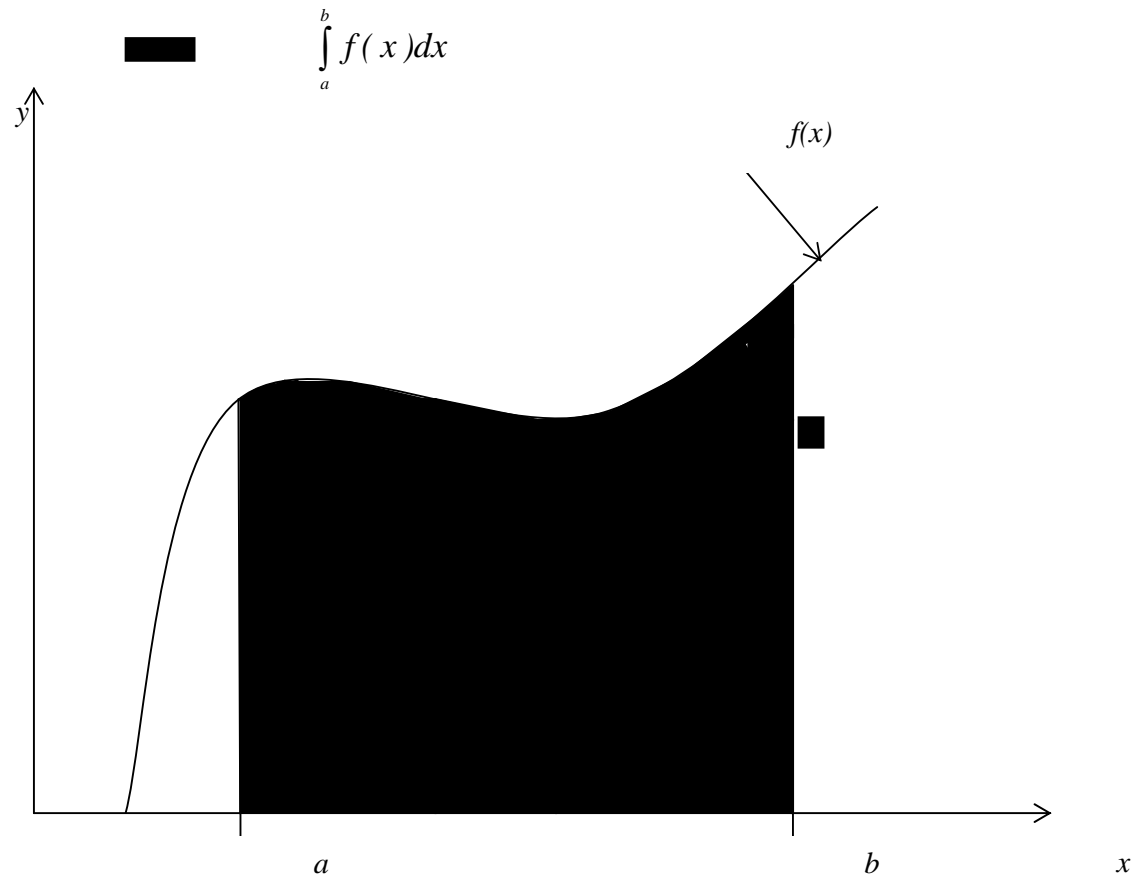
$$I = \int_a^b f(x) dx$$

Where:

$f(x)$ is the integrand

a = lower limit of integration

b = upper limit of integration





Basis of Trapezoidal Rule

Trapezoidal Rule is based on the Newton-Cotes Formula that states if one can approximate the integrand as an n^{th} order polynomial...

$$I = \int_a^b f(x) dx \quad \text{where} \quad f(x) \approx f_n(x)$$

and $f_n(x) = a_0 + a_1x + \dots + a_{n-1}x^{n-1} + a_nx^n$



Basis of Trapezoidal Rule

Then the integral of that function is approximated by the integral of that n^{th} order polynomial.

$$\int_a^b f(x) \approx \int_a^b f_n(x)$$

Trapezoidal Rule assumes $n=1$, that is, the area under the linear polynomial,

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



Derivation of the Trapezoidal Rule

Method Derived From Geometry

The area under the curve is a trapezoid.
The integral

$$\begin{aligned} \int_a^b f(x) dx &\approx \text{Area of trapezoid} \\ &= \frac{1}{2} (\text{Sum of parallel sides}) (\text{height}) \\ &= \frac{1}{2} (f(b) + f(a)) (b - a) \\ &= (b - a) \left[\frac{f(a) + f(b)}{2} \right] \end{aligned}$$

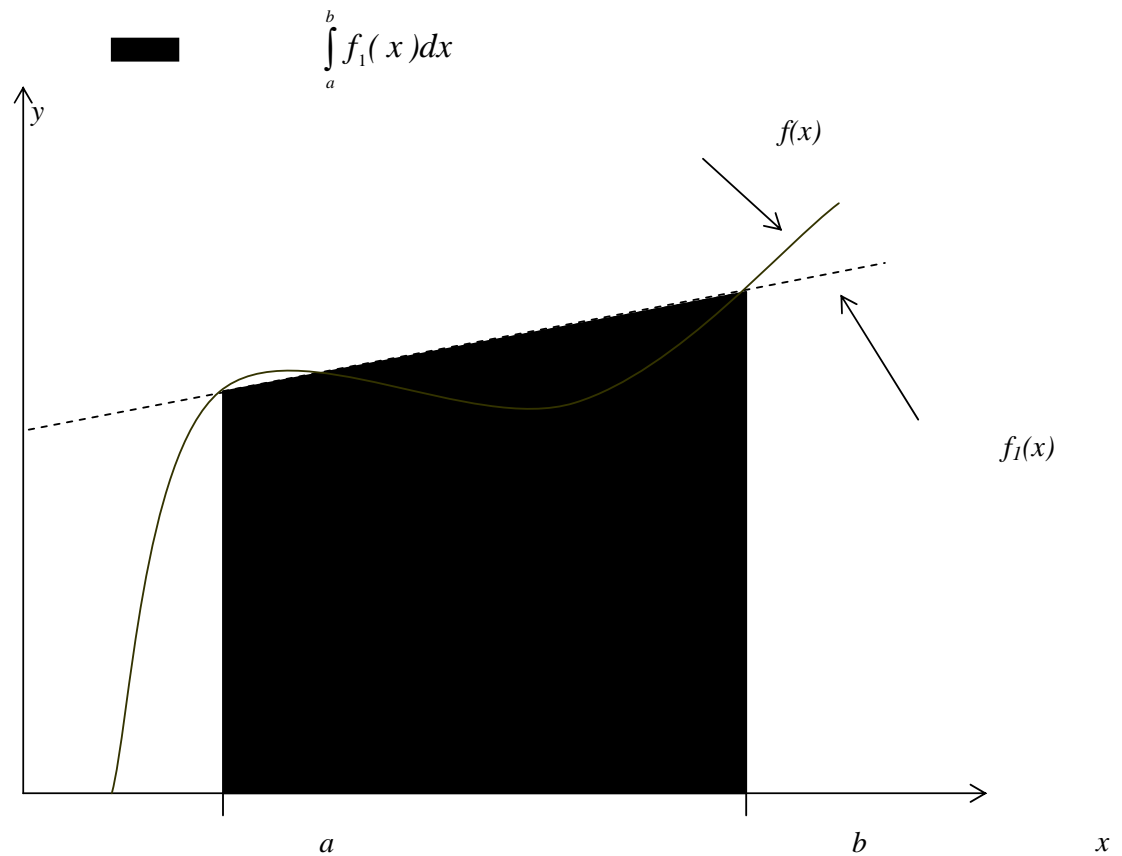


Figure 2: Geometric Representation



Example 1

In an attempt to understand the mechanism of the depolarization process in a fuel cell, an electro-kinetic model for mixed oxygen-methanol current on platinum was developed in the laboratory at FAMU. A very simplified model of the reaction developed suggests a functional relation in an integral form. To find the time required for 50% of the oxygen to be consumed, the time, T (s) is given by

$$T = -\int_{1.22 \times 10^{-6}}^{0.61 \times 10^{-6}} \left(\frac{6.73x + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} x} \right) dx$$

- Use single segment Trapezoidal rule to find the time required for 50% of the oxygen to be consumed.
- Find the true error, E_t for part (a).
- Find the absolute relative true error, $|\epsilon_a|$ for part (a).



Solution

$$a) \quad I \approx (b - a) \left[\frac{f(a) + f(b)}{2} \right]$$

$$f(x) = - \left[\frac{6.73x + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} x} \right] \quad a = 1.22 \times 10^{-6} \quad b = 0.61 \times 10^{-6}$$

$$f(1.22 \times 10^{-6}) = - \left[\frac{6.73(1.22 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} (1.22 \times 10^{-6})} \right] = -3.0582 \times 10^{11}$$

$$f(0.61 \times 10^{-6}) = - \left[\frac{6.73(0.61 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} (0.61 \times 10^{-6})} \right] = -3.2104 \times 10^{11}$$



Solution (cont)

$$\begin{aligned} \text{a)} \quad I &= (0.61 \times 10^{-6} - 1.22 \times 10^{-6}) \left[\frac{-3.0582 \times 10^{11} + (-3.2104 \times 10^{11})}{2} \right] \\ &= 1.9119 \times 10^5 \text{ s} \end{aligned}$$

b) The exact value of the above integral is

$$T = - \int_{1.22 \times 10^{-6}}^{0.61 \times 10^{-6}} \left(\frac{6.73x + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} x} \right) dx = 1.90135 \times 10^5 \text{ s}$$



Solution (cont)

b) $E_t = \text{True Value} - \text{Approximate Value}$

$$= 1.90135 \times 10^5 - 1.9119 \times 10^5$$

$$= -1055.0s$$

c) The absolute relative true error, $|\epsilon_t|$, would be

$$|\epsilon_t| = \left| \frac{\text{True Error}}{\text{True Value}} \right| \times 100 = \left| \frac{-1055.0}{1.90135 \times 10^5} \right| \times 100 = 0.55485\%$$



Multiple Segment Trapezoidal Rule

In Example 1, the true error using single segment trapezoidal rule was large. We can divide the interval $[1.22 \times 10^{-6}, 0.61 \times 10^{-6}]$ into $[1.22 \times 10^{-6}, 0.915 \times 10^{-6}]$ and $[0.915 \times 10^{-6}, 0.61 \times 10^{-6}]$ intervals and apply Trapezoidal rule over each segment.

$$f(x) = - \left[\frac{6.73x + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} x} \right]$$

$$\begin{aligned} \int_{1.22 \times 10^{-6}}^{0.61 \times 10^{-6}} f(x) dx &= \int_{1.22 \times 10^{-6}}^{0.915 \times 10^{-6}} f(x) dx + \int_{0.915 \times 10^{-6}}^{0.61 \times 10^{-6}} f(x) dx \\ &= (0.915 \times 10^{-6} - 1.22 \times 10^{-6}) \left[\frac{f(1.22 \times 10^{-6}) + f(0.915 \times 10^{-6})}{2} \right] \\ &+ (0.61 \times 10^{-6} - 0.915 \times 10^{-6}) \left[\frac{f(0.915 \times 10^{-6}) + f(0.61 \times 10^{-6})}{2} \right] \end{aligned}$$



Multiple Segment Trapezoidal Rule

$$f(1.22 \times 10^{-6}) = - \left[\frac{6.73(1.22 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11}(1.22 \times 10^{-6})} \right] = -3.0582 \times 10^{11}$$

$$f(0.915 \times 10^{-6}) = - \left[\frac{6.73(0.915 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11}(0.915 \times 10^{-6})} \right] = -3.1089 \times 10^{11}$$

Hence

$$f(0.61 \times 10^{-6}) = - \left[\frac{6.73(0.61 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11}(0.61 \times 10^{-6})} \right] = -3.2104 \times 10^{11}$$

$$\begin{aligned} \int_{1.22 \times 10^{-6}}^{0.61 \times 10^{-6}} f(x) dx &= (0.915 \times 10^{-6} - 1.22 \times 10^{-6}) \left[\frac{-3.0582 \times 10^{11} + (-3.1089 \times 10^{11})}{2} \right] \\ &+ (0.61 \times 10^{-6} - 0.915 \times 10^{-6}) \left[\frac{-3.1089 \times 10^{11} + (-3.2104 \times 10^{11})}{2} \right] \\ &= 1.9042 \times 10^5 \text{ s} \end{aligned}$$



Multiple Segment Trapezoidal Rule

The true error is:

$$E_t = 1.90135 \times 10^5 - 1.9042 \times 10^5$$
$$= -282.60s$$

The true error now is reduced from -1055 s to -282.60 s.

Extending this procedure to divide the interval into equal segments to apply the Trapezoidal rule; the sum of the results obtained for each segment is the approximate value of the integral.

Multiple Segment Trapezoidal Rule

Divide into equal segments as shown in Figure 4. Then the width of each segment is:

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

The integral I is:

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

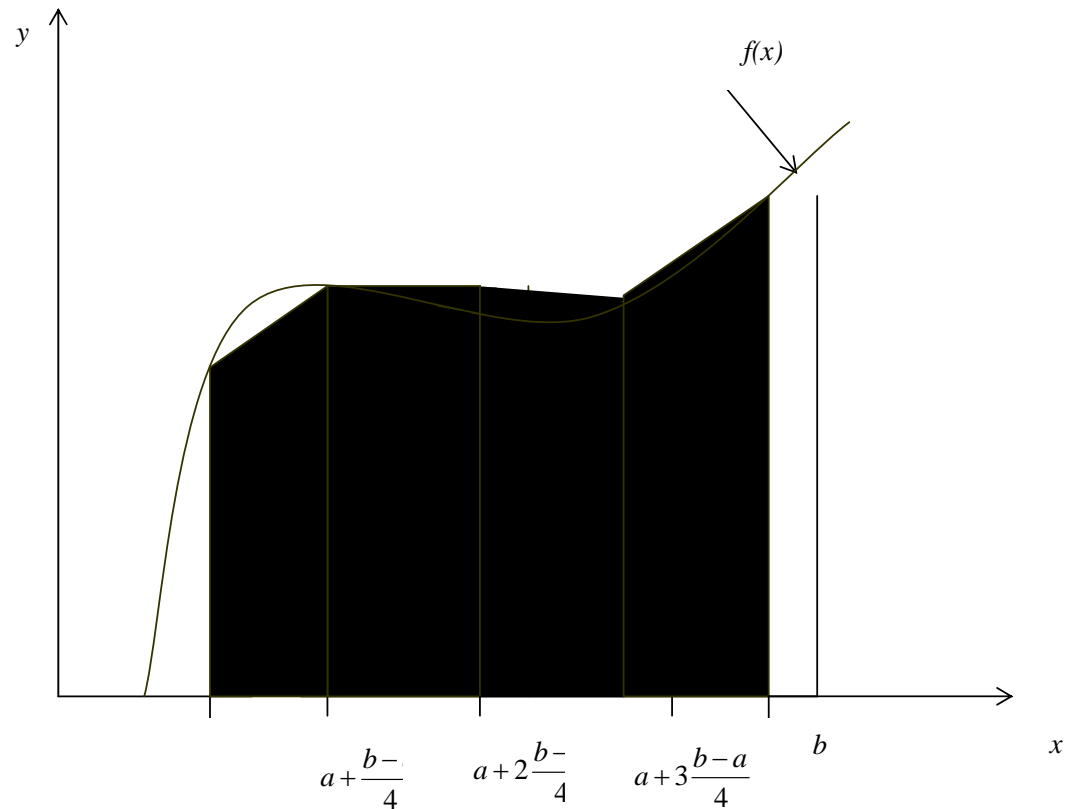


Figure 3: Multiple (n=4) Segment Trapezoidal Rule



Multiple Segment Trapezoidal Rule

The integral I can be broken into n integrals as:

$$\int_a^b f(x) dx = \int_a^{a+h} f(x) dx + \int_{a+h}^{a+2h} f(x) dx + \dots + \int_{a+(n-2)h}^{a+(n-1)h} f(x) dx + \int_{a+(n-1)h}^b f(x) dx$$

Applying Trapezoidal rule on each segment gives:

$$\int_a^b f(x) dx = \frac{b-a}{2n} \left[f(a) + 2 \left\{ \sum_{i=1}^{n-1} f(a+ih) \right\} + f(b) \right]$$



Example 2

In an attempt to understand the mechanism of the depolarization process in a fuel cell, an electro-kinetic model for mixed oxygen-methanol current on platinum was developed in the laboratory at FAMU. A very simplified model of the reaction developed suggests a functional relation in an integral form. To find the time required for 50% of the oxygen to be consumed, the time, T (s) is given by

$$T = - \int_{1.22 \times 10^{-6}}^{0.61 \times 10^{-6}} \left(\frac{6.73x + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} x} \right) dx$$

- Use two-segment Trapezoidal rule to find the time required for 50% of the oxygen to be consumed.
- Find the true error, E_t for part (a).
- Find the absolute relative true error, $|\varepsilon_a|$ for part (a).



Solution

a) The solution using 2-segment Trapezoidal rule is

$$I = \frac{b-a}{2n} \left[f(a) + 2 \left\{ \sum_{i=1}^{n-1} f(a+ih) \right\} + f(b) \right]$$

$$n = 2 \quad a = 1.22 \times 10^{-6} \quad b = 0.61 \times 10^{-6}$$

$$h = \frac{b-a}{n} = \frac{0.61 \times 10^{-6} - 1.22 \times 10^{-6}}{2} = -0.305 \times 10^{-6}$$



Solution (cont)

Then

$$\begin{aligned} I &= \frac{0.61 \times 10^{-6} - 1.22 \times 10^{-6}}{2(2)} \left[f(1.22 \times 10^{-6}) + 2 \left\{ \sum_{i=1}^{2-1} f(a + ih) \right\} + f(0.61 \times 10^{-6}) \right] \\ &= \frac{-0.61 \times 10^{-6}}{4} \left[f(1.22 \times 10^{-6}) + 2f(0.915 \times 10^{-6}) + f(0.61 \times 10^{-6}) \right] \\ &= \frac{-0.61 \times 10^{-6}}{4} \left[-3.0582 \times 10^{11} + 2(-3.1089 \times 10^{11}) - 3.2104 \times 10^{11} \right] \\ &= 1.9042 \times 10^5 \text{ s} \end{aligned}$$



Solution (cont)

b) The exact value of the above integral is

$$T = -\int_{1.22 \times 10^{-6}}^{0.61 \times 10^{-6}} \left(\frac{6.73x + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} x} \right) dx = 1.90135 \times 10^5 s$$

so the true error is

$$E_t = \text{True Value} - \text{Approximate Value}$$

$$= 1.90135 \times 10^5 - 1.9042 \times 10^5$$

$$= -282.60$$



Solution (cont)

c) The absolute relative true error, $|\epsilon_t|$, would be

$$\begin{aligned} |\epsilon_t| &= \left| \frac{\text{True Error}}{\text{True Value}} \right| \times 100 \\ &= \left| \frac{-282.60.0}{1.90135 \times 10^5} \right| \times 100 \\ &= 0.14863\% \end{aligned}$$



Solution (cont)

Table 1 gives the values obtained using multiple segment Trapezoidal rule for:

$$T = -\int_{1.22 \times 10^{-6}}^{0.61 \times 10^{-6}} \left(\frac{6.73x + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} x} \right) dx$$

n	Value	E_t	 ε_t %	 ε_a %
1	191190	-1055.0	0.55485	---
2	190420	-282.60	0.14863	0.40650
3	190260	-127.31	0.067000	0.08140
4	190200	-72.017	0.037900	0.029100
5	190180	-46.216	0.024300	0.013600
6	190170	-32.142	0.016900	0.0074000
7	190160	-23.636	0.012400	0.0045000
8	190150	-18.107	0.0095000	0.0029000

Table 1: Multiple Segment Trapezoidal Rule Values



Example 3

Use Multiple Segment Trapezoidal Rule to find the area under the curve

$$f(x) = \frac{300x}{1+e^x} \quad \text{from } x=0 \quad \text{to} \quad x=10$$

Using two segments, we get $h = \frac{10-0}{2} = 5$ and

$$f(0) = \frac{300(0)}{1+e^0} = 0 \quad f(5) = \frac{300(5)}{1+e^5} = 10.039 \quad f(10) = \frac{300(10)}{1+e^{10}} = 0.136$$



Solution

Then:

$$\begin{aligned} I &= \frac{b-a}{2n} \left[f(a) + 2 \left\{ \sum_{i=1}^{n-1} f(a+ih) \right\} + f(b) \right] \\ &= \frac{10-0}{2(2)} \left[f(0) + 2 \left\{ \sum_{i=1}^{2-1} f(0+5) \right\} + f(10) \right] \\ &= \frac{10}{4} [f(0) + 2f(5) + f(10)] = \frac{10}{4} [0 + 2(10.039) + 0.136] \\ &= 50.535 \end{aligned}$$



Solution (cont)

So what is the true value of this integral?

$$\int_0^{10} \frac{300x}{1+e^x} dx = 246.59$$

Making the absolute relative true error:

$$\begin{aligned} |\epsilon_t| &= \left| \frac{246.59 - 50.535}{246.59} \right| \times 100\% \\ &= 79.506\% \end{aligned}$$



Solution (cont)

Table 2: Values obtained using Multiple Segment Trapezoidal Rule for:

$$\int_0^{10} \frac{300x}{1+e^x} dx$$

n	Approximate Value	E_t	$ \epsilon_t $
1	0.681	245.91	99.724%
2	50.535	196.05	79.505%
4	170.61	75.978	30.812%
8	227.04	19.546	7.927%
16	241.70	4.887	1.982%
32	245.37	1.222	0.495%
64	246.28	0.305	0.124%



Error in Multiple Segment Trapezoidal Rule

The true error for a single segment Trapezoidal rule is given by:

$$E_t = \frac{(b-a)^3}{12} f''(\zeta), \quad a < \zeta < b \quad \text{where } \zeta \text{ is some point in } [a, b]$$

What is the error, then in the multiple segment Trapezoidal rule? It will be simply the sum of the errors from each segment, where the error in each segment is that of the single segment Trapezoidal rule.

The error in each segment is

$$\begin{aligned} E_1 &= \frac{[(a+h)-a]^3}{12} f''(\zeta_1), \quad a < \zeta_1 < a+h \\ &= \frac{h^3}{12} f''(\zeta_1) \end{aligned}$$



Error in Multiple Segment Trapezoidal Rule

Similarly:

$$E_i = \frac{[(a + ih) - (a + (i - 1)h)]^3}{12} f''(\zeta_i), \quad a + (i - 1)h < \zeta_i < a + ih$$

$$= \frac{h^3}{12} f''(\zeta_i)$$

It then follows that:

$$E_n = \frac{[b - \{a + (n - 1)h\}]^3}{12} f''(\zeta_n), \quad a + (n - 1)h < \zeta_n < b$$

$$= \frac{h^3}{12} f''(\zeta_n)$$



Error in Multiple Segment Trapezoidal Rule

Hence the total error in multiple segment Trapezoidal rule is

$$E_t = \sum_{i=1}^n E_i = \frac{h^3}{12} \sum_{i=1}^n f''(\zeta_i) = \frac{(b-a)^3}{12n^2} \frac{\sum_{i=1}^n f''(\zeta_i)}{n}$$

The term $\frac{\sum_{i=1}^n f''(\zeta_i)}{n}$ is an approximate average value of the $f''(x)$, $a < x < b$

Hence:

$$E_t = \frac{(b-a)^3}{12n^2} \frac{\sum_{i=1}^n f''(\zeta_i)}{n}$$



Error in Multiple Segment Trapezoidal Rule

Below is the table for the integral $\int_8^{30} \left(2000 \ln \left[\frac{140000}{140000 - 2100t} \right] - 9.8t \right) dt$

as a function of the number of segments. You can visualize that as the number of segments are doubled, the true error gets approximately quartered.

n	Value	E_t	$ \epsilon_t \%$	$ \epsilon_a \%$
2	11266	-205	1.854	5.343
4	11113	-51.5	0.4655	0.3594
8	11074	-12.9	0.1165	0.03560
16	11065	-3.22	0.02913	0.00401