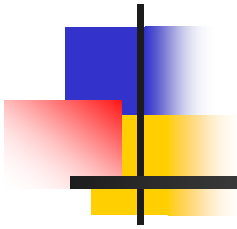


Integration



Topic: Simpson's $1/3^{\text{rd}}$ Rule

Major: Chemical Engineering

What is Integration?

Integration

The process of measuring the area under a curve.

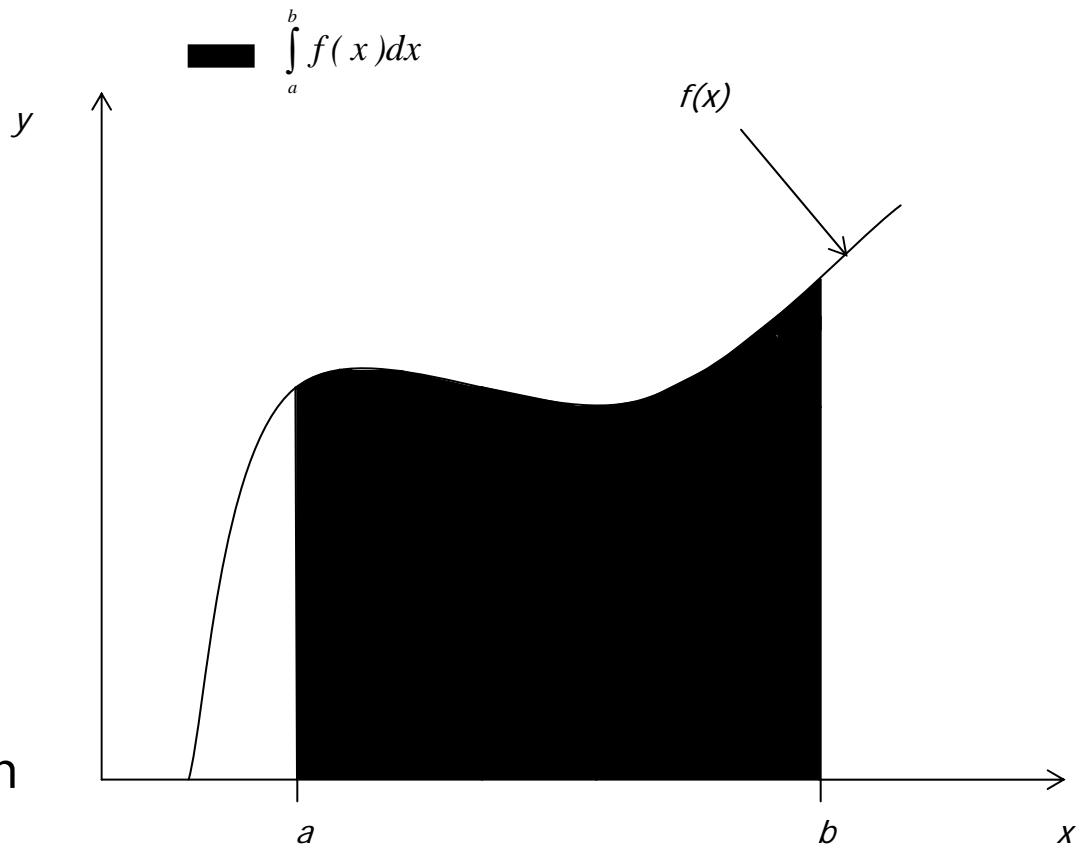
$$I = \int_a^b f(x) dx$$

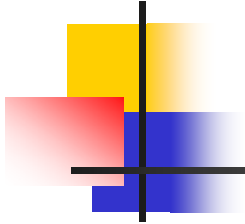
Where:

$f(x)$ is the integrand

a = lower limit of integration

b = upper limit of integration





Simpson's $1/3^{\text{rd}}$ Rule



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

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

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

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

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

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



Basis of Simpson's 1/3rd Rule

Solving the previous equations for a_0 , a_1 and a_2 give

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

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

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



Basis of Simpson's 1/3rd Rule

Then

$$\begin{aligned} I &\approx \int_a^b f_2(x) dx \\ &= \int_a^b (a_0 + a_1 x + a_2 x^2) dx \\ &= \left[a_0 x + a_1 \frac{x^2}{2} + a_2 \frac{x^3}{3} \right]_a^b \\ &= a_0(b-a) + a_1 \frac{b^2 - a^2}{2} + a_2 \frac{b^3 - a^3}{3} \end{aligned}$$



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

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



Basis of Simpson's 1/3rd Rule

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

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 Simpson's 1/3rd 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)

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

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

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

$$= \left(\frac{0.61 \times 10^{-6} - 1.22 \times 10^{-6}}{6} \right) \left[f(1.22 \times 10^{-6}) + 4f(0.915 \times 10^{-6}) + f(0.61 \times 10^{-6}) \right]$$

$$= \left(\frac{-0.61 \times 10^{-6}}{6} \right) \left[-3.0582 \times 10^{11} + 4(-3.1089 \times 10^{11}) - 3.2104 \times 10^{11} \right]$$

$$= 190159s$$



Solution (cont)

b) The exact value of the above integral is

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

$$= 1.90135 \times 10^5 \text{ s}$$

True Error

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

$$= 1.90135 \times 10^5 - 190159$$

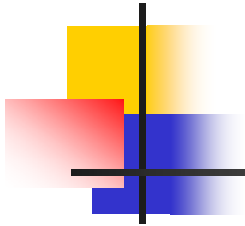
$$= -24.000$$



Solution (cont)

c.) Absolute relative true error,

$$\begin{aligned} |\epsilon_t| &= \left| \frac{\text{True Error}}{\text{True Value}} \right| \times 100 \\ &= \left| \frac{-24}{1.90135 \times 10^5} \right| \times 100 \\ &= 0.012675\% \end{aligned}$$



Multiple Segment Simpson's 1/3rd Rule



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

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

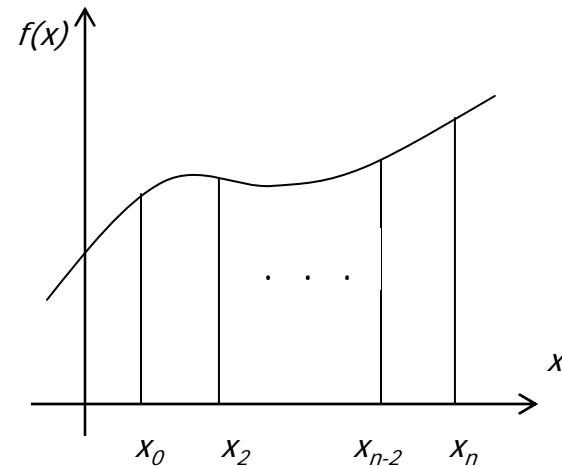
where

$$x_0 = a \qquad x_n = b$$

Multiple Segment Simpson's 1/3rd Rule

$$\int_a^b f(x) dx = \int_{x_0}^{x_2} f(x) dx + \int_{x_2}^{x_4} f(x) dx + \dots$$

$$\dots + \int_{x_{n-4}}^{x_{n-2}} f(x) dx + \int_{x_{n-2}}^{x_n} f(x) dx$$



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

$$\int_a^b f(x) dx = (x_2 - x_0) \left[\frac{f(x_0) + 4f(x_1) + f(x_2)}{6} \right] + \dots$$

$$+ (x_4 - x_2) \left[\frac{f(x_2) + 4f(x_3) + f(x_4)}{6} \right] + \dots$$



Multiple Segment Simpson's 1/3rd Rule

$$\dots + (x_{n-2} - x_{n-4}) \left[\frac{f(x_{n-4}) + 4f(x_{n-3}) + f(x_{n-2})}{6} \right] + \dots$$
$$+ (x_n - x_{n-2}) \left[\frac{f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)}{6} \right]$$

Since

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



Multiple Segment Simpson's 1/3rd Rule

Then

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



Multiple Segment Simpson's 1/3rd Rule

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



Example 2

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

$$h = \frac{b - a}{n} = \frac{0.61 \times 10^{-6} - 1.22 \times 10^{-6}}{4} = -0.15250 \times 10^{-6}$$

So $f(x_0) = f(1.22 \times 10^{-6})$

$$f(x_1) = f(1.22 \times 10^{-6} - 0.15250 \times 10^{-6}) = f(1.0675 \times 10^{-6})$$

$$f(x_2) = f(1.0675 \times 10^{-6} - 0.15250 \times 10^{-6}) = f(0.915 \times 10^{-6})$$

$$f(x_3) = f(0.915 \times 10^{-6} - 0.15250 \times 10^{-6}) = f(0.76250 \times 10^{-6})$$

$$f(x_4) = f(0.61 \times 10^{-6})$$



Solution (cont.)

$$\begin{aligned} T &= \frac{b-a}{3n} \left[f(x_0) + 4 \sum_{\substack{i=1 \\ i=\text{odd}}}^{n-1} f(x_i) + 2 \sum_{\substack{i=2 \\ i=\text{even}}}^{n-2} f(x_i) + f(x_n) \right] \\ &= \frac{0.61 \times 10^{-6} - 1.22 \times 10^{-6}}{3(4)} \left[f(1.22 \times 10^{-6}) + 4 \sum_{\substack{i=1 \\ i=\text{odd}}}^3 f(x_i) + 2 \sum_{\substack{i=2 \\ i=\text{even}}}^2 f(x_i) + f(0.61 \times 10^{-6}) \right] \\ &= \frac{-0.61 \times 10^{-6}}{12} \left[f(1.22 \times 10^{-6}) + 4f(x_1) + 4f(x_3) + 2f(x_2) + f(0.61 \times 10^{-6}) \right] \end{aligned}$$



Solution (cont.)

cont.

$$= \frac{-0.61 \times 10^{-6}}{12} \left[f(1.22 \times 10^{-6}) + 4f(1.0675 \times 10^{-6}) + 4f(0.76250 \times 10^{-6}) + 2f(0.915 \times 10^{-6}) + f(0.61 \times 10^{-6}) \right]$$

$$= \frac{-0.61 \times 10^{-6}}{12} \left[-3.0582 \times 10^{11} + 4(-3.0799 \times 10^{11}) + 4(-3.1495 \times 10^{11}) + 2(-3.1089 \times 10^{11}) - 3.2104 \times 10^{11} \right]$$

$$= 190137s$$



Solution (cont.)

b) In this case, the true error is

$$\begin{aligned}E_t &= \text{True Value} - \text{Approximate Value} \\ &= 1.90135 \times 10^5 - 190137 \\ &= -2.0000\end{aligned}$$

c) The absolute relative true error

$$\begin{aligned}|\epsilon_t| &= \left| \frac{\text{True Error}}{\text{True Value}} \right| \times 100 \\ &= \left| \frac{-2.0000}{1.90135 \times 10^5} \right| \times 100 \\ &= 0.0010434\%\end{aligned}$$



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	190159	-24.000	0.012675%
4	190137	-2.0000	0.0010434%
6	190135	0.0000	0.0000%
8	190135	0.0000	0.0000%
10	190135	0.0000	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

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

⋮

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

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



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

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

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



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

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

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

Hence

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

where

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