Chapter 07.03

Simpson's 1/3 Rule of Integration

After reading this chapter, you should be able to
1. *derive the formula for Simpson's 1/3 rule of integration,*
2. *use Simpson's 1/3 rule it to solve integrals,*
3. *develop the formula for multiple-segment Simpson's 1/3 rule of integration,*
4. *use multiple-segment Simpson's 1/3 rule of integration to solve integrals, and*
5. *derive the true error formula for multiple-segment Simpson's 1/3 rule.*

What is integration?

Integration is the process of measuring the area under a function plotted on a graph. Why would we want to integrate a function? Among the most common examples are finding the velocity of a body from an acceleration function, and displacement of a body from a velocity function. Throughout many engineering fields, there are (what sometimes seems like) countless applications for integral calculus. You can read about some of these applications in Chapters 07.00A-07.00G.

Sometimes, the evaluation of expressions involving these integrals can become daunting, if not indeterminate. For this reason, a wide variety of numerical methods has been developed to simplify the integral. Here, we will discuss Simpson's 1/3 rule of integral approximation, which improves upon the accuracy of the trapezoidal rule.

Here, we will discuss the Simpson's 1/3 rule of approximating integrals of the form

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

where

$f(x)$ is called the integrand,
$a =$ lower limit of integration
$b =$ upper limit of integration

Simpson's 1/3 Rule

The trapezoidal rule was based on approximating the integrand by a first order polynomial, and then integrating the polynomial over interval of integration. Simpson's 1/3 rule is an

extension of Trapezoidal rule where the integrand is approximated by a second order polynomial.
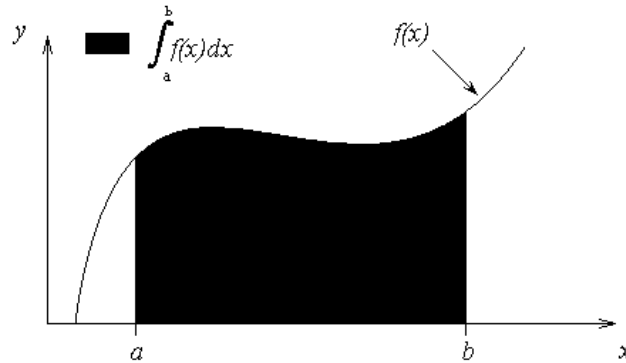
Figure 1 Integration of a function

Method 1:
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 given by

$$f_2(x) = a_0 + a_1 x + a_2 x^2 .$$

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.

$$f(a) = f_2(a) = a_0 + a_1 a + a_2 a^2$$

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

$$f(b) = f_2(b) = a_0 + a_1 b + a_2 b^2$$

Solving the above three equations for unknowns, a_0, a_1 and a_2 give

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

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

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

Then

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

$$= \int_a^b \left(a_0 + a_1 x + a_2 x^2\right)dx$$

$$= \left[a_0 x + a_1 \frac{x^2}{2} + a_2 \frac{x^3}{3} \right]_a^b$$

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

Substituting values of a_0, a_1 and 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 1/3 rule, the interval $[a,b]$ is broken into 2 segments, the segment width

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

Hence the Simpson's 1/3 rule is given by

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

Since the above form has 1/3 in its formula, it is called Simpson's 1/3 rule.

Method 2:
Simpson's 1/3 rule can also be derived by approximating $f(x)$ by a second order polynomial using Newton's divided difference polynomial as

$$f_2(x) = b_0 + b_1(x-a) + b_2(x-a)\left(x - \frac{a+b}{2}\right)$$

where

$$b_0 = f(a)$$

$$b_1 = \frac{f\left(\dfrac{a+b}{2}\right) - f(a)}{\dfrac{a+b}{2} - a}$$

$$b_2 = \cfrac{\cfrac{f(b) - f\left(\dfrac{a+b}{2}\right)}{b - \dfrac{a+b}{2}} - \cfrac{f\left(\dfrac{a+b}{2}\right) - f(a)}{\dfrac{a+b}{2} - a}}{b - a}$$

Integrating Newton's divided difference polynomial gives us

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

$$= \int_a^b \left[b_0 + b_1(x-a) + b_2(x-a)\left(x - \frac{a+b}{2}\right) \right] dx$$

$$= \left[b_0 x + b_1\left(\frac{x^2}{2} - ax\right) + b_2\left(\frac{x^3}{3} - \frac{(3a+b)x^2}{4} + \frac{a(a+b)x}{2}\right) \right]_a^b$$

$$= b_0(b-a) + b_1\left(\frac{b^2 - a^2}{2} - a(b-a)\right)$$

$$+ b_2\left(\frac{b^3 - a^3}{3} - \frac{(3a+b)(b^2 - a^2)}{4} + \frac{a(a+b)(b-a)}{2}\right)$$

Substituting values of b_0, b_1, and b_2 into this equation yields the same result as before

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

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

Method 3:
One could even use the Lagrange polynomial to derive Simpson's formula. Notice any method of three-point quadratic interpolation can be used to accomplish this task. In this case, the interpolating function becomes

$$f_2(x) = \frac{\left(x - \dfrac{a+b}{2}\right)(x-b)}{\left(a - \dfrac{a+b}{2}\right)(a-b)}f(a) + \frac{(x-a)(x-b)}{\left(\dfrac{a+b}{2} - a\right)\left(\dfrac{a+b}{2} - b\right)}f\left(\frac{a+b}{2}\right) + \frac{(x-a)\left(x - \dfrac{a+b}{2}\right)}{(b-a)\left(b - \dfrac{a+b}{2}\right)}f(b)$$

Integrating this function gets

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

$$= \frac{\dfrac{b^3-a^3}{3} - \dfrac{(a+3b)(b^2-a^2)}{4} + \dfrac{b(a+b)(b-a)}{2}}{\left(a - \dfrac{a+b}{2}\right)(a-b)}f(a)$$

$$+ \frac{\dfrac{b^3-a^3}{3} - \dfrac{(a+b)(b^2-a^2)}{2} + ab(b-a)}{\left(\dfrac{a+b}{2}-a\right)\left(\dfrac{a+b}{2}-b\right)}f\left(\dfrac{a+b}{2}\right)$$

$$+ \frac{\dfrac{b^3-a^3}{3} - \dfrac{(3a+b)(b^2-a^2)}{4} + \dfrac{a(a+b)(b-a)}{2}}{(b-a)\left(b - \dfrac{a+b}{2}\right)}f(b)$$

Believe it or not, simplifying and factoring this large expression yields you the same result as before

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

$$= \frac{h}{3}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right].$$

Method 4:
Simpson's 1/3 rule can also be derived by the method of coefficients. Assume

$$\int_a^b f(x)dx \approx c_1 f(a) + c_2 f\left(\frac{a+b}{2}\right) + c_3 f(b)$$

Let the right-hand side be an exact expression for the integrals $\int_a^b 1dx$, $\int_a^b xdx$, and $\int_a^b x^2 dx$. This implies that the right hand side will be exact expressions for integrals of any linear combination of the three integrals for a general second order polynomial. Now

$$\int_a^b 1dx = b - a = c_1 + c_2 + c_3$$

$$\int_a^b x\,dx = \frac{b^2 - a^2}{2} = c_1 a + c_2 \frac{a+b}{2} + c_3 b$$

$$\int_a^b x^2\,dx = \frac{b^3 - a^3}{3} = c_1 a^2 + c_2 \left(\frac{a+b}{2}\right)^2 + c_3 b^2$$

Solving the above three equations for c_0, c_1 and c_2 give

$$c_1 = \frac{b-a}{6}$$

$$c_2 = \frac{2(b-a)}{3}$$

$$c_3 = \frac{b-a}{6}$$

This gives

$$\int_a^b f(x)\,dx \approx \frac{b-a}{6} f(a) + \frac{2(b-a)}{3} f\left(\frac{a+b}{2}\right) + \frac{b-a}{6} f(b)$$

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

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

The integral from the first method

$$\int_a^b f(x)\,dx \approx \int_a^b (a_0 + a_1 x + a_2 x^2)\,dx$$

can be viewed as the area under the second order polynomial, while the equation from Method 4

$$\int_a^b f(x)\,dx \approx \frac{b-a}{6} f(a) + \frac{2(b-a)}{3} f\left(\frac{a+b}{2}\right) + \frac{b-a}{6} f(b)$$

can be viewed as the sum of the areas of three rectangles.

Example 1

The concentration of benzene at a critical location is given by

$$c = 1.75\left[erfc(0.6560) + e^{32.73} erfc(5.758)\right]$$

where

$$erfc(x) = \int_\infty^x e^{-z^2}\,dz$$

So in the above formula

$$erfc(0.6560) = \int_\infty^{0.6560} e^{-z^2}\,dz$$

Since e^{-z^2} decays rapidly as $z \to \infty$, we will approximate

$$erfc(0.6560) = \int_5^{0.6560} e^{-z^2} dz$$

a) Use Simpson's 1/3 Rule to find the value of $erfc(0.6560)$.
b) Find the true error, E_t, for part (a).
c) Find the absolute relative true error for part (a).

Solution

a) $erfc(0.6560) \approx \dfrac{b-a}{6} \left[f(a) + 4f\left(\dfrac{a+b}{2}\right) + f(b) \right]$

$a = 5$
$b = 0.6560$
$\dfrac{a+b}{2} = 2.8280$
$f(z) = e^{-z^2}$
$f(5) = e^{-5^2}$
$\quad = 1.3888 \times 10^{-11}$
$f(0.6560) = e^{-0.6560^2}$
$\quad = 0.65029$

$f(2.8280) = e^{-2.8280^2}$
$\quad = 3.3627 \times 10^{-4}$

$erfc(0.6560) = \left(\dfrac{b-a}{6}\right)\left[f(a) + 4f\left(\dfrac{a+b}{2}\right) + f(b) \right]$

$\quad = \left(\dfrac{0.6560-5}{6}\right)\left[f(5) + 4f(2.8280) + f(0.6560) \right]$

$\quad = \left(\dfrac{-4.3440}{6}\right)\left[1.3888 \times 10^{-11} + 4\left(3.3627 \times 10^{-4}\right) + 0.65029 \right]$

$\quad = -0.47178$

b) The exact value of the above integral cannot be found. For calculating the true error and relative true error, we assume the value obtained by adaptive numerical integration using Maple as the exact value.

$$erfc(0.6560) = \int_5^{0.6560} e^{-z^2} dz$$

$$= -0.31333$$

so the true error is

$\quad E_t = \textit{True Value} - \textit{Approximate Value}$

$$= -0.31333 - (-0.47178)$$
$$= 0.15846$$

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

$$|\epsilon_t| = \left|\frac{\text{True Error}}{\text{True Value}}\right| \times 100$$

$$= \left|\frac{0.15846}{-0.31333}\right| \times 100$$

$$= 50.573\%$$

Multiple-segment Simpson's 1/3 Rule

Just like in multiple-segment trapezoidal rule, one can subdivide the interval $[a,b]$ into n segments and apply Simpson's 1/3 rule repeatedly over every two segments. Note that n needs to be even. Divide interval $[a,b]$ into n equal segments, so that the segment width is given by

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

Now

$$\int_a^b f(x)dx = \int_{x_0}^{x_n} f(x)dx$$

where

$$x_0 = a$$
$$x_n = b$$

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

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

$$\int_a^b f(x)dx \cong (x_2 - x_0)\left[\frac{f(x_0) + 4f(x_1) + f(x_2)}{6}\right] + (x_4 - x_2)\left[\frac{f(x_2) + 4f(x_3) + f(x_4)}{6}\right] + ...$$

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

Since

$$x_i - x_{i-2} = 2h$$
$$i = 2, 4, ..., n$$

then

$$\int_a^b f(x)dx \cong 2h\left[\frac{f(x_0) + 4f(x_1) + f(x_2)}{6}\right] + 2h\left[\frac{f(x_2) + 4f(x_3) + f(x_4)}{6}\right] + ...$$

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

$$= \frac{h}{3}\left[f(x_0)+4\{f(x_1)+f(x_3)+...+f(x_{n-1})\}+2\{f(x_2)+f(x_4)+...+f(x_{n-2})\}+f(x_n)\right]$$

$$= \frac{h}{3}\left[f(x_0)+4\sum_{\substack{i=1\\i=odd}}^{n-1}f(x_i)+2\sum_{\substack{i=2\\i=even}}^{n-2}f(x_i)+f(x_n)\right]$$

$$\boxed{\int_a^b f(x)dx \cong \frac{b-a}{3n}\left[f(x_0)+4\sum_{\substack{i=1\\i=odd}}^{n-1}f(x_i)+2\sum_{\substack{i=2\\i=even}}^{n-2}f(x_i)+f(x_n)\right]}$$

Example 2

The concentration of benzene at a critical location is given by

$$c = 1.75\left[erfc(0.6560)+ e^{32.73}erfc(5.758)\right]$$

where

$$erfc(x) = \int_\infty^x e^{-z^2}dz$$

So in the above formula

$$erfc(0.6560) = \int_\infty^{0.6560} e^{-z^2}dz$$

Since e^{-z^2} decays rapidly as $z \to \infty$, we will approximate

$$erfc(0.6560) = \int_5^{0.6560} e^{-z^2}dz$$

a) Use four segment Simpson's 1/3 Rule to find the value of $erfc(0.6560)$.
b) Find the true error, E_t, for part (a).
c) Find the absolute relative true error for part (a).

Solution

a) $$erfc(0.6560) = \frac{b-a}{3n}\left[f(z_0)+4\sum_{\substack{i=1\\i=odd}}^{n-1}f(z_i)+2\sum_{\substack{i=2\\i=even}}^{n-2}f(z_i)+f(z_n)\right]$$

$n = 4$
$a = 5$
$b = 0.6560$

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

$$= \frac{0.6560 - 5}{4}$$

$$= -1.0860$$

$$f(z) = e^{-z^2}$$

So

$$f(z_0) = f(5)$$

$$f(5) = e^{-5^2}$$

$$= 1.3888 \times 10^{-11}$$

$$f(z_1) = f(5 - 1.0860)$$

$$= f(3.9140)$$

$$f(3.9140) = e^{-3.9140^2}$$

$$= 2.2226 \times 10^{-7}$$

$$f(z_2) = f(3.9140 - 1.0860)$$

$$= f(2.8280)$$

$$f(2.8280) = e^{-2.8280^2}$$

$$= 3.3627 \times 10^{-4}$$

$$f(z_3) = f(2.8280 - 1.0860)$$

$$= f(1.7420)$$

$$f(1.7420) = e^{-1.7420^2}$$

$$= 0.048096$$

$$f(z_4) = f(z_n)$$

$$= f(0.6560)$$

$$f(0.6560) = e^{-0.6560^2}$$

$$= 0.65029$$

$$erfc(0.6560) = \frac{b - a}{3n}\left[f(z_0) + 4 \sum_{\substack{i=1 \\ i=odd}}^{n-1} f(z_i) + 2 \sum_{\substack{i=2 \\ i=even}}^{n-2} f(z_i) + f(z_n) \right]$$

$$= \frac{0.6560 - 5}{3(4)}\left[f(5) + 4 \sum_{\substack{i=1 \\ i=odd}}^{3} f(z_i) + 2 \sum_{\substack{i=2 \\ i=even}}^{2} f(z_i) + f(0.6560) \right]$$

$$= \frac{-4.3440}{12}\left[f(5) + 4f(z_1) + 4f(z_3) + 2f(z_2) + f(0.6560) \right]$$

$$= \frac{-4.3440}{12}\left[\begin{array}{l} f(5)+4f(3.9140)+4f(1.7420) \\ +2f(2.8280)+f(0.6560) \end{array}\right]$$

$$= \frac{-4.3440}{12}\left[\begin{array}{l} 1.3888\times10^{-11}+4(2.2226\times10^{-7})+4(0.048096) \\ +2(3.3627\times10^{-4})+0.65029 \end{array}\right]$$

$$= -0.30529$$

b) The exact value of the above integral cannot be found. For calculating the true error and relative true error, we assume the value obtained by adaptive numerical integration using Maple as the exact value.

$$erfc(0.6560)= \int\limits_{5}^{0.6560} e^{-z^2}\,dz$$

$$= -0.31333$$

so the true error is

$$E_t = True\ Value - Approximate\ Value$$

$$= -0.31333-(-0.30529)$$

$$= -0.0080347$$

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

$$|\epsilon_t| = \left|\frac{True\ Error}{True\ Value}\right|\times100$$

$$= \left|\frac{-0.0080347}{-0.31333}\right|\times100$$

$$= 2.5643\,\%$$

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

n	Approximate Value	E_t	$|\epsilon_t|$ %
2	−0.47178	0.15846	50.573
4	−0.30529	−0.0080347	2.5643
6	−0.30678	−0.0065444	2.0887
8	−0.31110	−0.0022249	0.71009
10	−0.31248	−0.00084868	0.27086

Error in Multiple-segment Simpson's 1/3 rule

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

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

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

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

$$= -\frac{h^5}{90} f^{(4)}(\zeta_1)$$

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

$$= -\frac{h^5}{90} f^{(4)}(\zeta_2)$$

$$\vdots$$

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

$$= -\frac{h^5}{90} f^{(4)}(\zeta_i)$$

$$\vdots$$

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

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

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

Hence, the total error in the multiple-segment Simpson's 1/3 rule is

$$= -\frac{h^5}{90} f^{(4)}\left(\zeta_{\frac{n}{2}}\right)$$

$$E_t = \sum_{i=1}^{\frac{n}{2}} E_i$$

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[1] The $f^{(4)}$ in the true error expression stands for the fourth derivative of the function $f(x)$.

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

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

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

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

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

INTEGRATION	
Topic	Simpson's 1/3 rule
Summary	Textbook notes of Simpson's 1/3 rule
Major	Civil Engineering
Authors	Autar Kaw, Michael Keteltas
Date	November 8, 2012
Web Site	http://numericalmethods.eng.usf.edu