Simpson's Rule

–

Theorem 7.3 (Composite Simpson Rule). Suppose that $[a, b]$ is subdivided into $2M$ subintervals $[x_k, x_{k+1}]$ of equal width $h = (b-a)/(2M)$ by using $x_k = a + kh$ for $k = 0, 1, \ldots, 2M$. The ***composite Simpson rule for 2M subintervals*** can be expressed in any of three equivalent ways:

$$S(f, h) = \frac{h}{3}\sum_{k=1}^{M}(f(x_{2k-2}) + 4f(x_{2k-1}) + f(x_{2k})) \tag{4a}$$

or

$$S(f, h) = \frac{h}{3}(f_0 + 4f_1 + 2f_2 + 4f_3 + \cdots + 2f_{2M-2} + 4f_{2M-1} + f_{2M}) \tag{4b}$$

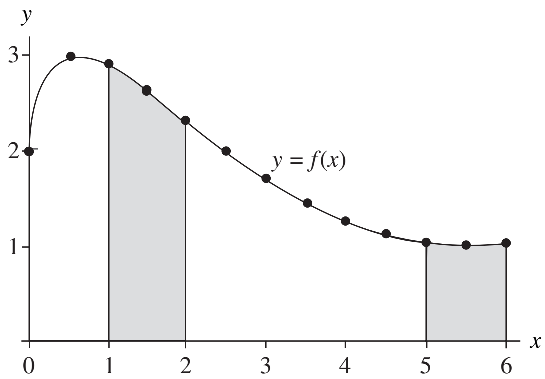

Figure 7.7 Approximating the area under the curve $y = 2 + \sin(2\sqrt{x})$ with the composite Simpson rule.

or

$$S(f, h) = \frac{h}{3}(f(a) + f(b)) + \frac{2h}{3}\sum_{k=1}^{M-1} f(x_{2k}) + \frac{4h}{3}\sum_{k=1}^{M} f(x_{2k-1}). \tag{4c}$$

This is an approximation to the integral of $f(x)$ over $[a, b]$, and we write

$$\int_a^b f(x)\,dx \approx S(f, h). \tag{5}$$

Proof. Apply Simpson's rule over each subinterval $[x_{2k-2}, x_{2k}]$ (see Figure 7.7). Use the additive property of the integral for subintervals:

$$\begin{aligned}\int_a^b f(x)\,dx &= \sum_{k=1}^{M}\int_{x_{2k-2}}^{x_{2k}} f(x)\,dx \\ &\approx \sum_{k=1}^{M}\frac{h}{3}(f(x_{2k-2}) + 4f(x_{2k-1}) + f(x_{2k})).\end{aligned} \tag{6}$$

Since $h/3$ is a constant, the distributive law of addition can be applied to obtain (4a). Formula (4b) is the expanded version of (4a). Formula (4c) groups all the intermediate terms in (4b) that are multiplied by 2 and those that are multiplied by 4. •

Approximating $f(x) = 2 + \sin(2\sqrt{x})$ with piecewise quadratic polynomials produces places where the approximation is close and places where it is not. To achieve accuracy the composite Simpson rule must be applied with several subintervals. In the next example we have chosen to integrate this function numerically over $[1, 6]$ and leave investigation of the integral over $[0, 1]$ as an exercise.

Example 7.6. Consider $f(x) = 2 + \sin(2\sqrt{x})$. Use the composite Simpson rule with 11 sample points to compute an approximation to the integral of $f(x)$ taken over $[1, 6]$.

To generate 11 sample points, we must use $M = 5$ and $h = (6 - 1)/10 = 1/2$. Using formula (4c), the computation is

$$
\begin{aligned}
S(f, \frac{1}{2}) &= \frac{1}{6}(f(1) + f(6)) + \frac{1}{3}(f(2) + f(3) + f(4) + f(5)) \\
&\quad + \frac{2}{3}(f(\tfrac{3}{2}) + f(\tfrac{5}{2}) + f(\tfrac{7}{2}) + f(\tfrac{9}{2}) + f(\tfrac{11}{2})) \\
&= \frac{1}{6}(2.90929743 + 1.01735756) \\
&\quad + \frac{1}{3}(2.30807174 + 1.68305284 + 1.24319750 + 1.02872220) \\
&\quad + \frac{2}{3}(2.63815764 + 1.97931647 + 1.43530410 + 1.10831775 + 1.00024140) \\
&= \frac{1}{6}(3.92665499) + \frac{1}{3}(6.26304429) + \frac{2}{3}(8.16133735) \\
&= 0.65444250 + 2.08768143 + 5.44089157 = 8.18301550.
\end{aligned}
$$

■

Error Analysis

The significance of the next two results is to understand that the error terms $E_T(f, h)$ and $E_S(f, h)$ for the composite trapezoidal rule and composite Simpson rule are of the order $\boldsymbol{O}(h^2)$ and $\boldsymbol{O}(h^4)$, respectively. This shows that the error for Simpson's rule converges to zero faster than the error for the trapezoidal rule as the step size h decreases to zero. In cases where the derivatives of $f(x)$ are known, the formulas

$$
E_T(f, h) = \frac{-(b-a)f^{(2)}(c)h^2}{12} \quad \text{and} \quad E_S(f, h) = \frac{-(b-a)f^{(4)}(c)h^4}{180}
$$

can be used to estimate the number of subintervals required to achieve a specified accuracy.

Corollary 7.3 (Simpson's Rule: Error Analysis). Suppose that $[a, b]$ is subdivided into $2M$ subintervals $[x_k, x_{k+1}]$ of equal width $h = (b - a)/(2M)$. The composite Simpson rule

$$S(f, h) = \frac{h}{3}(f(a) + f(b)) + \frac{2h}{3}\sum_{k=1}^{M-1} f(x_{2k}) + \frac{4h}{3}\sum_{k=1}^{M} f(x_{2k-1}) \tag{14}$$

is an approximation to the integral

$$\int_a^b f(x)\,dx = S(f, h) + E_S(f, h). \tag{15}$$

Furthermore, if $f \in C^4[a, b]$, there exists a value c with $a < c < b$ so that the error term $E_S(f, h)$ has the form

$$E_S(f, h) = \frac{-(b-a)f^{(4)}(c)h^4}{180} = \boldsymbol{O}(h^4). \tag{16}$$

Example 7.7. Consider $f(x) = 2 + \sin(2\sqrt{x})$. Investigate the error when the composite trapezoidal rule is used over $[1, 6]$ and the number of subintervals is 10, 20, 40, 80, and 160.

Table 7.2 shows the approximations $T(f, h)$. The antiderivative of $f(x)$ is

$$F(x) = 2x - \sqrt{x}\cos(2\sqrt{x}) + \frac{\sin(2\sqrt{x})}{2},$$

and the true value of the definite integral is

$$\int_1^6 f(x)\,dx = F(x)\Big|_{x=1}^{x=6} = 8.1834792077.$$

This value was used to compute the values $E_T(f, h) = 8.1834792077 - T(f, h)$ in Table 7.2. It is important to observe that when h is reduced by a factor of $\frac{1}{2}$ the successive errors $E_T(f, h)$ are diminished by approximately $\frac{1}{4}$. This confirms that the order is $\boldsymbol{O}(h^2)$. ■

Example 7.8. Consider $f(x) = 2 + \sin(2\sqrt{x})$. Investigate the error when the composite Simpson rule is used over $[1, 6]$ and the number of subintervals is 10, 20, 40, 80, and 160.

Table 7.3 shows the approximations $S(f, h)$. The true value of the integral is 8.1834792077, which was used to compute the values $E_S(f, h) = 8.1834792077 - S(f, h)$ in Table 7.3. It is important to observe that when h is reduced by a factor of $\frac{1}{2}$, the successive errors $E_S(f, h)$ are diminished by approximately $\frac{1}{16}$. This confirms that the order is $\boldsymbol{O}(h^4)$. ■

Table 7.2 Composite Trapezoidal Rule for $f(x) = 2 + \sin(2\sqrt{x})$ over [1, 6]

M	h	$T(f, h)$	$E_T(f, h) = \boldsymbol{O}(h^2)$
10	0.5	8.19385457	−0.01037540
20	0.25	8.18604926	−0.00257006
40	0.125	8.18412019	−0.00064098
80	0.0625	8.18363936	−0.00016015
160	0.03125	8.18351924	−0.00004003

Table 7.3 Composite Simpson Rule for $f(x) = 2 + \sin(2\sqrt{x})$ over [1, 6]

M	h	$S(f, h)$	$E_S(f, h) = \boldsymbol{O}(h^4)$
5	0.5	8.18301549	0.00046371
10	0.25	8.18344750	0.00003171
20	0.125	8.18347717	0.00000204
40	0.0625	8.18347908	0.00000013
80	0.03125	8.18347920	0.00000001

Example 7.9. Find the number M and the step size h so that the error $E_T(f, h)$ for the composite trapezoidal rule is less than 5×10^{-9} for the approximation $\int_2^7 dx/x \approx T(f, h)$.

The integrand is $f(x) = 1/x$ and its first two derivatives are $f'(x) = -1/x^2$ and $f^{(2)}(x) = 2/x^3$. The maximum value of $|f^{(2)}(x)|$ taken over [2, 7] occurs at the endpoint $x = 2$, and thus we have the bound $|f^{(2)}(c)| \le |f^{(2)}(2)| = \frac{1}{4}$, for $2 \le c \le 7$. This is used with formula (9) to obtain

$$|E_T(f, h)| = \frac{|-(b-a)f^{(2)}(c)h^2|}{12} \le \frac{(7-2)\frac{1}{4}h^2}{12} = \frac{5h^2}{48}. \tag{17}$$

The step size h and number M satisfy the relation $h = 5/M$, and this is used in (17) to get the relation

$$|E_T(f, h)| \le \frac{125}{48M^2} \le 5 \times 10^{-9}. \tag{18}$$

Now rewrite (18) so that it is easier to solve for M:

$$\frac{25}{48} \times 10^9 \le M^2. \tag{19}$$

Solving (19), we find that $22821.77 \le M$. Since M must be an integer, we choose $M = 22{,}822$, and the corresponding step size is $h = 5/22{,}822 = 0.000219086846$. When the composite trapezoidal rule is implemented with this many function evaluations, there is a possibility that the rounded-off function evaluations will produce a significant amount of error. When the computation was performed, the result was

$$T\left(f, \frac{5}{22{,}822}\right) = 1.252762969,$$

which compares favorably with the true value $\int_2^7 dx/x = \ln(x)|_{x=2}^{x=7} = 1.252762968$. The error is smaller than predicted because the bound $\frac{1}{4}$ for $|f^{(2)}(c)|$ was used. Experimentation shows that it takes about 10,001 function evaluations to achieve the desired accuracy of 5×10^{-9}, and when the calculation is performed with $M = 10{,}000$, the result is

$$T\left(f, \frac{5}{10{,}000}\right) = 1.252762973. \quad \blacksquare$$

The composite trapezoidal rule usually requires a large number of function evaluations to achieve an accurate answer. This is contrasted in the next example with Simpson's rule, which will require significantly fewer evaluations.

Example 7.10. Find the number M and the step size h so that the error $E_S(f, h)$ for the composite Simpson rule is less than 5×10^{-9} for the approximation $\int_2^7 dx/x \approx S(f, h)$.

The integrand is $f(x) = 1/x$, and $f^{(4)}(x) = 24/x^5$. The maximum value of $|f^{(4)}(c)|$ taken over [2, 7] occurs at the endpoint $x = 2$, and thus we have the bound $|f^{(4)}(c)| \le |f^{(4)}(2)| = \frac{3}{4}$ for $2 \le c \le 7$. This is used with formula (16) to obtain

$$|E_S(f, h)| = \frac{|-(b-a)f^{(4)}(c)h^4|}{180} \le \frac{(7-2)\frac{3}{4}h^4}{180} = \frac{h^4}{48}. \tag{20}$$

The step size h and number M satisfy the relation $h = 5/(2M)$, and this is used in (20) to get the relation

$$|E_S(f, h)| \le \frac{625}{768M^4} \le 5 \times 10^{-9}. \tag{21}$$

Now rewrite (21) so that it is easier to solve for M:

$$\frac{125}{768} \times 10^9 \le M^4. \tag{22}$$

Solving (22), we find that $112.95 \le M$. Since M must be an integer, we chose $M = 113$, and the corresponding step size is $h = 5/226 = 0.02212389381$. When the composite Simpson rule was performed, the result was

$$S\left(f, \frac{5}{226}\right) = 1.252762969,$$

which agrees with $\int_2^7 dx/x = \ln(x)|_{x=2}^{x=7} = 1.252762968$. Experimentation shows that it takes about 129 function evaluations to achieve the desired accuracy of 5×10^{-9}, and when the calculation is performed with $M = 64$, the result is

$$S\left(f, \frac{5}{128}\right) = 1.252762973. \quad \blacksquare$$

So we see that the composite Simpson rule using 229 evaluations of $f(x)$ and the composite trapezoidal rule using 22,823 evaluations of $f(x)$ achieve the same accuracy. In Example 7.10, Simpson's rule required about $\frac{1}{100}$ the number of function evaluations.

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