n is divisible by 2. Now from basic calculus, we have

$$\int_a^b f(x)\,dx = \sum_{i=1}^{n/2} \int_{a+2(i-1)h}^{a+2ih} f(x)\,dx$$

Using the basic Simpson's Rule, we have, for the right-hand side,

$$\begin{aligned}
&\approx \sum_{i=1}^{n/2} \frac{h}{3}\{f(a+2(i-1)h) + 4f(a+(2i-1)h) + f(a+2ih)\} \\
&= \frac{h}{3}\left\{ f(a) + \sum_{i=1}^{(n/2)-1} f(a+2ih) + 4\sum_{i=1}^{n/2} f(a+(2i-1)h) \right. \\
&\qquad\qquad \left. + \sum_{i=1}^{(n/2)-1} f(a+2ih) + f(b) \right\}
\end{aligned}$$

Thus, we obtain

$$\int_a^b f(x)\,dx \approx \frac{h}{3}\left\{ [f(a)+f(b)] + 4\sum_{i=1}^{n/2} f[a+(2i-1)h] + 2\sum_{i=1}^{(n-2)/2} f(a+2ih) \right\}$$

where $h = (b-a)/n$. The error term is

$$-\frac{1}{180}(b-a)h^4 f^{(4)}(\xi)$$

Many formulas for numerical integration have error estimates that involve derivatives of the function being integrated. An important point that is frequently overlooked is that such error estimates depend on the function having derivatives. So if a piecewise function is being integrated, the numerical integration should be broken up over the region to coincide with the regions of smoothness of the function. Another important point is that no polynomial ever becomes infinite in the finite plane, so any integration technique that uses polynomials to approximate the integrand will fail to give good results without extra work at integrable singularities.

An Adaptive Simpson's Scheme

Now we develop an adaptive scheme based on Simpson's Rule for obtaining a numerical approximation to the integral

$$\int_a^b f(x)\,dx$$

In this adaptive algorithm, the partitioning of the interval $[a, b]$ is not selected beforehand but is automatically determined. The partition is generated adaptively so that more and smaller subintervals are used in some parts of the interval and fewer and larger subintervals are used in other parts.

In the adaptive process, we divide the interval $[a, b]$ into two subintervals and then decide whether each of them is to be divided into more subintervals. This procedure is continued until some specified accuracy is obtained throughout the entire interval $[a, b]$. Since the integrand f may vary in its behavior on the interval $[a, b]$, we do not expect the final partitioning to be uniform but to vary in the density of the partition points.

It is necessary to develop the test for deciding whether subintervals should continue to be divided. One application of Simpson's Rule over the interval $[a, b]$ can be written as

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

where

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

and

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

Letting $h = b - a$, we have

$$I = S^{(1)} + E^{(1)} \tag{4}$$

where

$$S^{(1)} = S(a, b)$$

and

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

Here we assume that $f^{(4)}$ remains a constant value C throughout the interval $[a, b]$. Now two applications of Simpson's Rule over the interval $[a, b]$ give

$$I = S^{(2)} + E^{(2)} \tag{5}$$

where

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

where $c = (a + b)/2$, as in Figure 6.4, and

$$\begin{aligned} E^{(2)} &= -\frac{1}{90}\left(\frac{h/2}{2}\right)^5 f^{(4)}(a) + \cdots - \frac{1}{90}\left(\frac{h/2}{2}\right)^5 f^{(4)}(c) + \cdots \\ &= -\frac{1}{90}\left(\frac{h/2}{2}\right)^5 \left[f^{(4)}(a) + f^{(4)}(c)\right] + \cdots \\ &= -\frac{1}{90}\left(\frac{1}{2^5}\right)\left(\frac{h}{2}\right)^5 (2C) = \frac{1}{16}\left[-\frac{1}{90}\left(\frac{h}{2}\right)^5 C\right] \end{aligned}$$

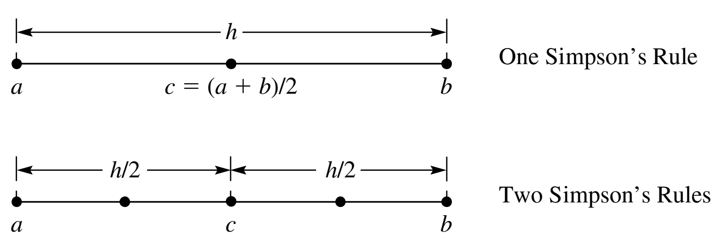

FIGURE 6.4
Simpson's rule

Again, we use the assumption that $f^{(4)}$ remains a constant value C throughout the interval $[a, b]$. We find that

$$16E^{(2)} = E^{(1)}$$

Subtracting Equation (5) from (4), we have

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

From this equation and Equation (4), we have

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

This value of I is the best we have at this step, and we use the inequality

$$\tfrac{1}{15}\left|S^{(2)} - S^{(1)}\right| < \varepsilon \tag{6}$$

to guide the adaptive process.

If Test (6) is not satisfied, the interval $[a, b]$ is split into two subintervals, $[a, c]$ and $[c, b]$, where c is the midpoint $c = (a + b)/2$. On each of these subintervals, we again use Test (6) with ε replaced by $\varepsilon/2$ so that the resulting tolerance will be ε over the entire interval $[a, b]$. A recursive procedure handles this quite nicely.

To see why we take $\varepsilon/2$ on each subinterval, recall that

$$I = \int_a^b f(x)\,dx = \int_a^c f(x)\,dx + \int_c^b f(x)\,dx = I_{\text{left}} + I_{\text{right}}$$

If S is the sum of approximations $S^{(2)}_{\text{left}}$ over $[a, c]$ and $S^{(2)}_{\text{right}}$ over $[c, b]$, we have

$$\begin{aligned}
|I - S| &= \left|I_{\text{left}} + I_{\text{right}} - S^{(2)}_{\text{left}} - S^{(2)}_{\text{right}}\right| \\
&\leqq \left|I_{\text{left}} - S^{(2)}_{\text{left}}\right| + \left|I_{\text{right}} - S^{(2)}_{\text{right}}\right| \\
&= \tfrac{1}{15}\left|S^{(2)}_{\text{left}} - S^{(1)}_{\text{left}}\right| + \tfrac{1}{15}\left|S^{(2)}_{\text{right}} - S^{(1)}_{\text{right}}\right|
\end{aligned}$$

using Equation (6). Hence, if we require

$$\frac{1}{15}\left|S^{(2)}_{\text{left}} - S^{(1)}_{\text{left}}\right| \leqq \frac{\varepsilon}{2} \qquad \text{and} \qquad \frac{1}{15}\left|S^{(2)}_{\text{right}} - S^{(1)}_{\text{right}}\right| \leqq \frac{\varepsilon}{2}$$

then $|I - S| \leqq \varepsilon$ over the entire interval $[a, b]$.

We now describe an adaptive Simpson recursive procedure. The interval $[a, b]$ is partitioned into four subintervals of width $(b-a)/4$. Two Simpson approximations are computed by using two double-width subintervals and four single-width subintervals; that is,

$$\begin{aligned}
\textit{one_simpson} &\leftarrow \frac{h}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] \\
\textit{two_simpson} &\leftarrow \frac{h}{12}\left[f(a) + 4f\left(\frac{a+c}{2}\right) + 2f(c) + 4f\left(\frac{c+b}{2}\right) + f(b)\right]
\end{aligned}$$

where $h = b - a$ and $c = (a + b)/2$.

According to Inequality (6), if *one_simpson* and *two_simpson* agree to within 15ε, then the interval $[a, b]$ does not need to be subdivided further to obtain an accurate approximation to the integral $\int_a^b f(x)\,dx$. In this case, the value of $[16\,(\textit{two\_simpson}) - (\textit{one\_simpson})]/15$ is used as the approximate value of the integral over the interval $[a, b]$. If the desired accuracy for the integral has not been obtained, then the interval $[a, b]$ is divided in half. The