derivative over the interval can be computed by differentiating the original function twice to give

$$f''(x) = -400 + 4050x - 10{,}800x^2 + 8000x^3$$

The average value of the second derivative can be computed using Eq. (PT6.4):

$$\bar{f}''(x) = \frac{\int_0^{0.8} (-400 + 4050x - 10{,}800x^2 + 8000x^3)\, dx}{0.8 - 0} = -60$$

which can be substituted into Eq. (21.6) to yield

$$E_a = -\frac{1}{12}(-60)(0.8)^3 = 2.56$$

which is of the same order of magnitude and sign as the true error. A discrepancy does exist, however, because of the fact that for an interval of this size, the average second derivative is not necessarily an accurate approximation of $f''(\xi)$. Thus, we denote that the error is approximate by using the notation E_a, rather than exact by using E_t.

21.1.2 The Multiple-Application Trapezoidal Rule

One way to improve the accuracy of the trapezoidal rule is to divide the integration interval from a to b into a number of segments and apply the method to each segment (Fig. 21.7). The areas of individual segments can then be added to yield the integral for the entire interval. The resulting equations are called *multiple-application*, or *composite, integration formulas*.

Figure 21.8 shows the general format and nomenclature we will use to characterize multiple-application integrals. There are $n + 1$ equally spaced base points $(x_0, x_1, x_2, \ldots, x_n)$. Consequently, there are n segments of equal width:

$$h = \frac{b - a}{n} \tag{21.7}$$

If a and b are designated as x_0 and x_n, respectively, the total integral can be represented as

$$I = \int_{x_0}^{x_1} f(x)\, dx + \int_{x_1}^{x_2} f(x)\, dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)\, dx$$

Substituting the trapezoidal rule for each integral yields

$$I = h\frac{f(x_0) + f(x_1)}{2} + h\frac{f(x_1) + f(x_2)}{2} + \cdots + h\frac{f(x_{n-1}) + f(x_n)}{2} \tag{21.8}$$

or, grouping terms,

$$I = \frac{h}{2}\left[f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)\right] \tag{21.9}$$

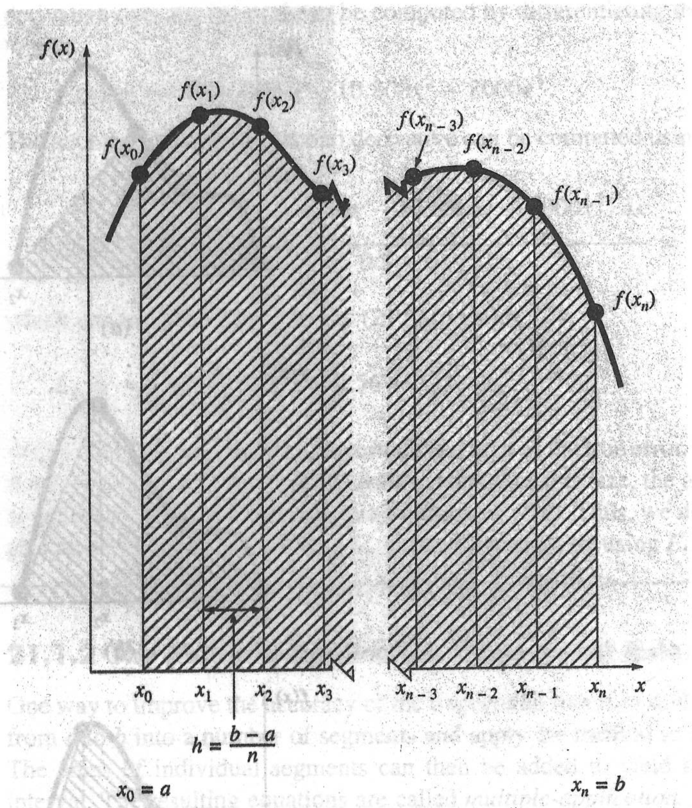

FIGURE 21.8
The general format and nomenclature for multiple-application integrals.

or, using Eq. (21.7) to express Eq. (21.9) in the general form of Eq. (21.5),

$$I = \underbrace{(b-a)}_{\text{Width}} \underbrace{\frac{f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)}{2n}}_{\text{Average height}} \tag{21.10}$$

Because the summation of the coefficients of $f(x)$ in the numerator divided by $2n$ is equal to 1, the average height represents a weighted average of the function values. According to Eq. (21.10), the interior points are given twice the weight of the two end points $f(x_0)$ and $f(x_n)$.

An error for the multiple-application trapezoidal rule can be obtained by summing the individual errors for each segment to give

$$E_t = -\frac{(b-a)^3}{12n^3} \sum_{i=1}^{n} f''(\xi_i) \tag{21.11}$$

where $f''(\xi_i)$ is the second derivative at a point ξ_i located in segment i. This result can be simplified by estimating the mean or average value of the second derivative for the entire interval as [Eq. (PT6.3)]

$$\bar{f}'' \cong \frac{\sum_{i=1}^{n} f''(\xi_i)}{n} \tag{21.12}$$

Therefore $\Sigma f''(\xi_i) \cong n\bar{f}''$ and Eq. (21.11) can be rewritten as

$$E_a = -\frac{(b-a)^3}{12n^2}\bar{f}'' \tag{21.13}$$

Thus, if the number of segments is doubled, the truncation error will be quartered. Note that Eq. (21.13) is an approximate error because of the approximate nature of Eq. (21.12).

EXAMPLE 21.2 Multiple-Application Trapezoidal Rule

Problem Statement. Use the two-segment trapezoidal rule to estimate the integral of

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from $a = 0$ to $b = 0.8$. Employ Eq. (21.13) to estimate the error. Recall that the correct value for the integral is 1.640533.

Solution. $n = 2$ $(h = 0.4)$:

$$f(0) = 0.2 \qquad f(0.4) = 2.456 \qquad f(0.8) = 0.232$$

$$I = 0.8\frac{0.2 + 2(2.456) + 0.232}{4} = 1.0688$$

$$E_t = 1.640533 - 1.0688 = 0.57173 \qquad \varepsilon_t = 34.9\%$$

$$E_a = -\frac{0.8^3}{12(2)^2}(-60) = 0.64$$

where -60 is the average second derivative determined previously in Example 21.1.

The results of the previous example, along with three- through ten-segment applications of the trapezoidal rule, are summarized in Table 21.1. Notice how the error decreases as the number of segments increases. However, also notice that the rate of decrease is gradual. This is because the error is inversely related to the square of n [Eq. (21.13)]. Therefore, doubling the number of segments quarters the error. In subsequent sections we develop higher-order formulas that are more accurate and that converge more quickly on the true integral as the segments are increased. However, before investigating these formulas, we will first discuss computer algorithms to implement the trapezoidal rule.

21.1.3 Computer Algorithms for the Trapezoidal Rule

Two simple algorithms for the trapezoidal rule are listed in Fig. 21.9. The first (Fig. 21.9*a*) is for the single-segment version. The second (Fig. 21.9*b*) is for the multiple-segment

Finally, round-off errors can limit our ability to determine integrals. This is due both to the machine precision as well as to the numerous computations involved in simple techniques like the multiple-segment trapezoidal rule.

We now turn to one way in which efficiency is improved. That is, by using higher-order polynomials to approximate the integral.

21.2 SIMPSON'S RULES

Aside from applying the trapezoidal rule with finer segmentation, another way to obtain a more accurate estimate of an integral is to use higher-order polynomials to connect the points. For example, if there is an extra point midway between $f(a)$ and $f(b)$, the three points can be connected with a parabola (Fig. 21.10*a*). If there are two points equally spaced between $f(a)$ and $f(b)$, the four points can be connected with a third-order polynomial (Fig. 21.10*b*). The formulas that result from taking the integrals under these polynomials are called *Simpson's rules.*

21.2.1 Simpson's 1/3 Rule

Simpson's 1/3 rule results when a second-order interpolating polynomial is substituted into Eq. (21.1):

$$I = \int_a^b f(x)\,dx \cong \int_a^b f_2(x)\,dx$$

If a and b are designated as x_0 and x_2 and $f_2(x)$ is represented by a second-order Lagrange polynomial [Eq. (18.23)], the integral becomes

$$I = \int_{x_0}^{x_2} \left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \right] dx$$

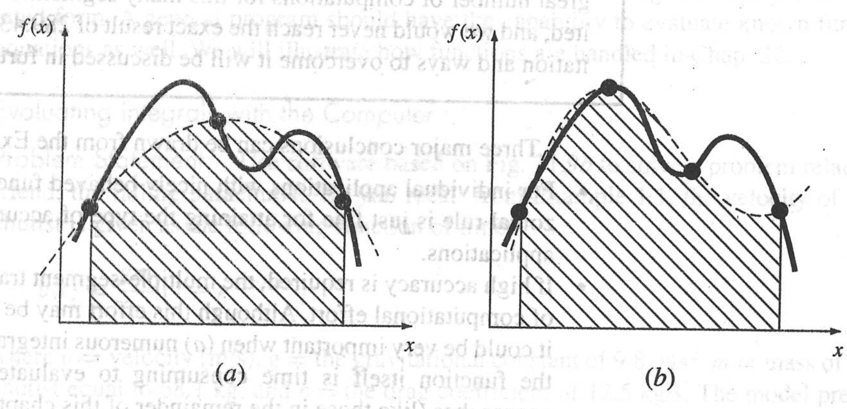

FIGURE 21.10
(*a*) Graphical depiction of Simpson's 1/3 rule: It consists of taking the area under a parabola connecting three points. (*b*) Graphical depiction of Simpson's 3/8 rule: It consists of taking the area under a cubic equation connecting four points.

After integration and algebraic manipulation, the following formula results:

$$I \cong \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] \tag{21.14}$$

where, for this case, $h = (b - a)/2$. This equation is known as *Simpson's 1/3 rule*. It is the second Newton-Cotes closed integration formula. The label "1/3" stems from the fact that h is divided by 3 in Eq. (21.14). An alternative derivation is shown in Box 21.3 where the Newton-Gregory polynomial is integrated to obtain the same formula.

Simpson's 1/3 rule can also be expressed using the format of Eq. (21.5):

$$I \cong \underbrace{(b - a)}_{\text{Width}} \underbrace{\frac{f(x_0) + 4f(x_1) + f(x_2)}{6}}_{\text{Average height}} \tag{21.15}$$

Box 21.3 Derivation and Error Estimate of Simpson's 1/3 Rule

As was done in Box 21.2 for the trapezoidal rule, Simpson's 1/3 rule can be derived by integrating the forward Newton-Gregory interpolating polynomial (Box 18.2):

$$I = \int_{x_0}^{x_2} \left[f(x_0) + \Delta f(x_0)\alpha + \frac{\Delta^2 f(x_0)}{2}\alpha(\alpha - 1) + \frac{\Delta^3 f(x_0)}{6}\alpha(\alpha - 1)(\alpha - 2) + \frac{f^{(4)}(\xi)}{24}\alpha(\alpha - 1)(\alpha - 2)(\alpha - 3)h^4 \right] dx$$

Notice that we have written the polynomial up to the fourth-order term rather than the third-order term as would be expected. The reason for this will be apparent shortly. Also notice that the limits of integration are from x_0 to x_2. Therefore, when the simplifying substitutions are made (recall Box 21.2), the integral is from $\alpha = 0$ to 2:

$$I = h\int_{0}^{2} \left[f(x_0) + \Delta f(x_0)\alpha + \frac{\Delta^2 f(x_0)}{2}\alpha(\alpha - 1) + \frac{\Delta^3 f(x_0)}{6}\alpha(\alpha - 1)(\alpha - 2) + \frac{f^{(4)}(\xi)}{24}\alpha(\alpha - 1)(\alpha - 2)(\alpha - 3)h^4 \right] d\alpha$$

which can be integrated to yield

$$I = h\left[\alpha f(x_0) + \frac{\alpha^2}{2}\Delta f(x_0) + \left(\frac{\alpha^3}{6} - \frac{\alpha^2}{4}\right)\Delta^2 f(x_0) + \left(\frac{\alpha^4}{24} - \frac{\alpha^3}{6} + \frac{\alpha^2}{6}\right)\Delta^3 f(x_0) + \left(\frac{\alpha^5}{120} - \frac{\alpha^4}{16} + \frac{11\alpha^3}{72} - \frac{\alpha^2}{8}\right) f^{(4)}(\xi)h^4 \right]_0^2$$

and evaluated for the limits to give

$$I = h\left[2f(x_0) + 2\Delta f(x_0) + \frac{\Delta^2 f(x_0)}{3} + (0)\Delta^3 f(x_0) - \frac{1}{90}f^{(4)}(\xi)h^4 \right] \tag{B21.3.1}$$

Notice the significant result that the coefficient of the third divided difference is zero. Because $\Delta f(x_0) = f(x_1) - f(x_0)$ and $\Delta^2 f(x_0) = f(x_2) - 2f(x_1) + f(x_0)$, Eq. (B21.3.1) can be rewritten as

$$I = \underbrace{\frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)]}_{\text{Simpson's 1/3 rule}} - \underbrace{\frac{1}{90}f^{(4)}(\xi)h^5}_{\text{Truncation error}}$$

Thus, the first term is Simpson's 1/3 rule and the second is the truncation error. Because the third divided difference dropped out, we obtain the significant result that the formula is third-order accurate.

where $a = x_0$, $b = x_2$, and x_1 = the point midway between a and b, which is given by $(b + a)/2$. Notice that, according to Eq. (21.15), the middle point is weighted by two-thirds and the two end points by one-sixth.

It can be shown that a single-segment application of Simpson's 1/3 rule has a truncation error of (Box 21.3)

$$E_t = -\frac{1}{90}h^5 f^{(4)}(\xi)$$

or, because $h = (b - a)/2$,

$$E_t = -\frac{(b-a)^5}{2880} f^{(4)}(\xi) \tag{21.16}$$

where ξ lies somewhere in the interval from a to b. Thus, Simpson's 1/3 rule is more accurate than the trapezoidal rule. However, comparison with Eq. (21.6) indicates that it is more accurate than expected. Rather than being proportional to the third derivative, the error is proportional to the fourth derivative. This is because, as shown in Box 21.3, the coefficient of the third-order term goes to zero during the integration of the interpolating polynomial. Consequently, Simpson's 1/3 rule is third-order accurate even though it is based on only three points. In other words, it yields exact results for cubic polynomials even though it is derived from a parabola!

EXAMPLE 21.4 Single Application of Simpson's 1/3 Rule

Problem Statement. Use Eq. (21.15) to integrate

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from $a = 0$ to $b = 0.8$. Recall that the exact integral is 1.640533.

Solution.

$$f(0) = 0.2 \qquad f(0.4) = 2.456 \qquad f(0.8) = 0.232$$

Therefore, Eq. (21.15) can be used to compute

$$I \cong 0.8\frac{0.2 + 4(2.456) + 0.232}{6} = 1.367467$$

which represents an exact error of

$$E_t = 1.640533 - 1.367467 = 0.2730667 \qquad \varepsilon_t = 16.6\%$$

which is approximately 5 times more accurate than for a single application of the trapezoidal rule (Example 21.1).

The estimated error is [Eq. (21.16)]

$$E_a = -\frac{(0.8)^5}{2880}(-2400) = 0.2730667$$

where −2400 is the average fourth derivative for the interval as obtained using Eq. (PT6.4). As was the case in Example 21.1, the error is approximate (E_a) because the average fourth derivative is not an exact estimate of $f^{(4)}(\xi)$. However, because this case deals with a fifth-order polynomial, the result matches.

21.2.2 The Multiple-Application Simpson's 1/3 Rule

Just as with the trapezoidal rule, Simpson's rule can be improved by dividing the integration interval into a number of segments of equal width (Fig. 21.11):

$$h = \frac{b-a}{n} \tag{21.17}$$

The total integral can be represented as

$$I = \int_{x_0}^{x_2} f(x)\,dx + \int_{x_2}^{x_4} f(x)\,dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)\,dx$$

Substituting Simpson's 1/3 rule for the individual integral yields

$$I \cong 2h\frac{f(x_0)+4f(x_1)+f(x_2)}{6} + 2h\frac{f(x_2)+4f(x_3)+f(x_4)}{6} + \cdots + 2h\frac{f(x_{n-2})+4f(x_{n-1})+f(x_n)}{6}$$

or, combining terms and using Eq. (21.17),

$$I \cong \underbrace{(b-a)}_{\text{Width}}\ \underbrace{\frac{f(x_0)+4\sum_{i=1,3,5}^{n-1} f(x_i) + 2\sum_{j=2,4,6}^{n-2} f(x_j) + f(x_n)}{3n}}_{\text{Average height}} \tag{21.18}$$

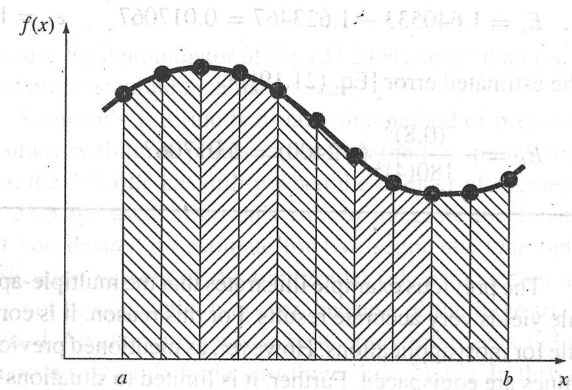

FIGURE 21.11
Graphical representation of the multiple application of Simpson's 1/3 rule. Note that the method can be employed only if the number of segments is even.

Notice that, as illustrated in Fig. 21.11, an even number of segments must be utilized to implement the method. In addition, the coefficients "4" and "2" in Eq. (21.18) might seem peculiar at first glance. However, they follow naturally from Simpson's 1/3 rule. The odd points represent the middle term for each application and hence carry the weight of 4 from Eq. (21.15). The even points are common to adjacent applications and hence are counted twice.

An error estimate for the multiple-application Simpson's rule is obtained in the same fashion as for the trapezoidal rule by summing the individual errors for the segments and averaging the derivative to yield

$$E_a = -\frac{(b-a)^5}{180n^4}\bar{f}^{(4)} \tag{21.19}$$

where $\bar{f}^{(4)}$ is the average fourth derivative for the interval.

EXAMPLE 21.5 Multiple-Application Version of Simpson's 1/3 Rule

Problem Statement. Use Eq. (21.18) with $n = 4$ to estimate the integral of

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from $a = 0$ to $b = 0.8$. Recall that the exact integral is 1.640533.

Solution. $n = 4$ $(h = 0.2)$:

$$f(0) = 0.2 \qquad f(0.2) = 1.288$$
$$f(0.4) = 2.456 \qquad f(0.6) = 3.464$$
$$f(0.8) = 0.232$$

From Eq. (21.18),

$$I = 0.8\,\frac{0.2 + 4(1.288 + 3.464) + 2(2.456) + 0.232}{12} = 1.623467$$

$$E_t = 1.640533 - 1.623467 = 0.017067 \qquad \varepsilon_t = 1.04\%$$

The estimated error [Eq. (21.19)] is

$$E_a = -\frac{(0.8)^5}{180(4)^4}(-2400) = 0.017067$$

The previous example illustrates that the multiple-application version of Simpson's 1/3 rule yields very accurate results. For this reason, it is considered superior to the trapezoidal rule for most applications. However, as mentioned previously, it is limited to cases where the values are equispaced. Further, it is limited to situations where there are an even number of segments and an odd number of points. Consequently, as discussed in the next section, an