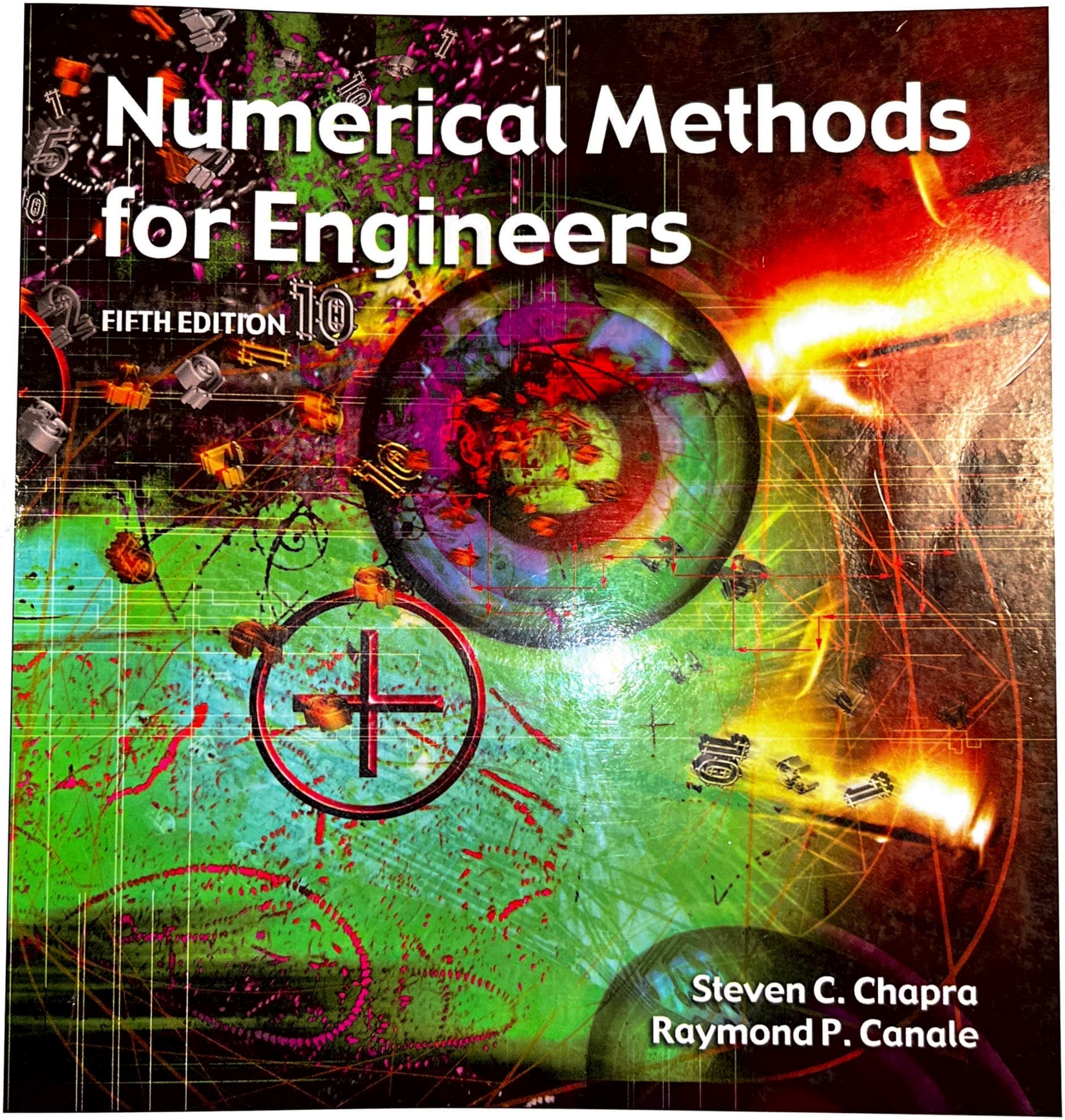

Numerical Methods for Engineers

FIFTH EDITION

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McGRAW-HILL INTERNATIONAL EDITION

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CHAPTER 21

Newton-Cotes Integration Formulas

The *Newton-Cotes formulas* are the most common numerical integration schemes. They are based on the strategy of replacing a complicated function or tabulated data with an approximating function that is easy to integrate:

$$I = \int_a^b f(x)\,dx \cong \int_a^b f_n(x)\,dx \tag{21.1}$$

where $f_n(x) =$ a polynomial of the form

$$f_n(x) = a_0 + a_1 x + \cdots + a_{n-1}x^{n-1} + a_n x^n$$

where n is the order of the polynomial. For example, in Fig. 21.1*a*, a first-order polynomial (a straight line) is used as an approximation. In Fig. 21.1*b*, a parabola is employed for the same purpose.

The integral can also be approximated using a series of polynomials applied piecewise to the function or data over segments of constant length. For example, in Fig. 21.2, three

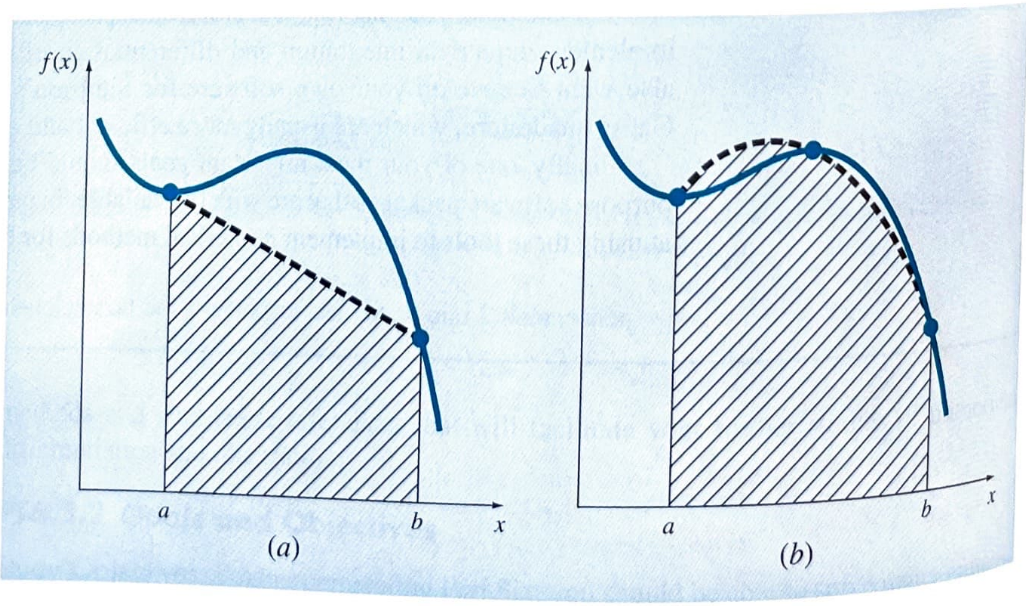


FIGURE 21.1
The approximation of an integral by the area under (*a*) a single straight line and (*b*) a single parabola.

straight-line segments are used to approximate the integral. Higher-order polynomials can be utilized for the same purpose. With this background, we now recognize that the "strip method" in Fig. PT6.6 employed a series of zero-order polynomials (that is, constants) to approximate the integral.

Closed and open forms of the Newton-Cotes formulas are available. The *closed forms* are those where the data points at the beginning and end of the limits of integration are known (Fig. 21.3*a*). The *open forms* have integration limits that extend beyond the range of the data (Fig. 21.3*b*). In this sense, they are akin to extrapolation as discussed in Sec. 18.5. Open Newton-Cotes formulas are not generally used for definite integration.

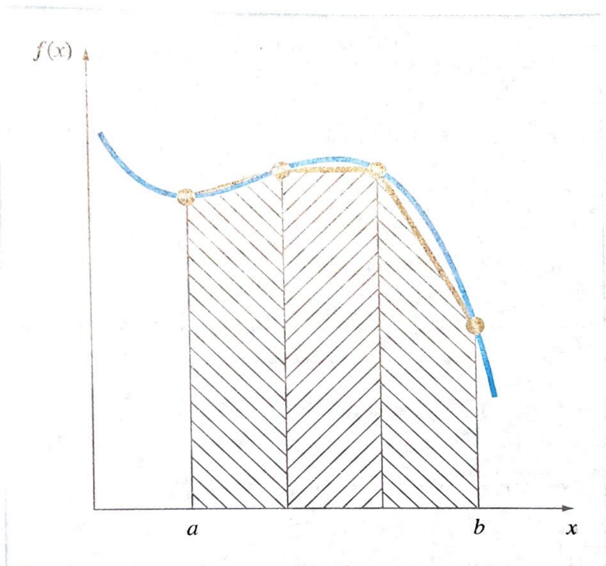


FIGURE 21.2
The approximation of an integral by the area under three straight-line segments.

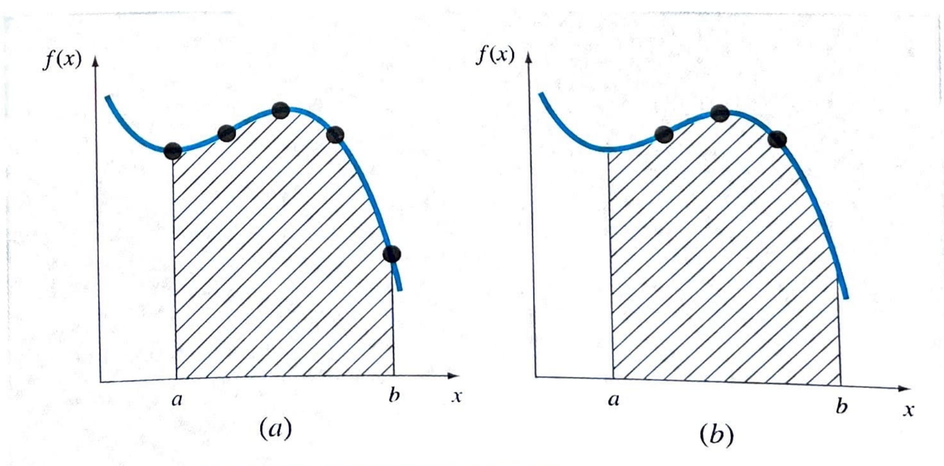


FIGURE 21.3
The difference between (*a*) closed and (*b*) open integration formulas.

However, they are utilized for evaluating improper integrals and for the solution of ordinary differential equations. This chapter emphasizes the closed forms. However, material on open Newton-Cotes formulas is briefly introduced at the end of this chapter.

21.1 THE TRAPEZOIDAL RULE

The *trapezoidal rule* is the first of the Newton-Cotes closed integration formulas. It corresponds to the case where the polynomial in Eq. (21.1) is first-order:

$$I = \int_a^b f(x)\,dx \cong \int_a^b f_1(x)\,dx$$

Recall from Chap. 18 that a straight line can be represented as [Eq. (18.2)]

$$f_1(x) = f(a) + \frac{f(b) - f(a)}{b - a}(x - a) \tag{21.2}$$

The area under this straight line is an estimate of the integral of $f(x)$ between the limits a and b:

$$I = \int_a^b \left[f(a) + \frac{f(b) - f(a)}{b - a}(x - a) \right] dx$$

The result of the integration (see Box 21.1 for details) is

$$\boxed{I = (b - a)\frac{f(a) + f(b)}{2}} \tag{21.3}$$

which is called the *trapezoidal rule.*

Box 21.1 Derivation of Trapezoidal Rule

Before integration, Eq. (21.2) can be expressed as

$$f_1(x) = \frac{f(b) - f(a)}{b - a}x + f(a) - \frac{af(b) - af(a)}{b - a}$$

Grouping the last two terms gives

$$f_1(x) = \frac{f(b) - f(a)}{b - a}x + \frac{bf(a) - af(a) - af(b) + af(a)}{b - a}$$

or

$$f_1(x) = \frac{f(b) - f(a)}{b - a}x + \frac{bf(a) - af(b)}{b - a}$$

which can be integrated between $x = a$ and $x = b$ to yield

$$I = \left. \frac{f(b) - f(a)}{b - a}\frac{x^2}{2} + \frac{bf(a) - af(b)}{b - a}x \right|_a^b$$

This result can be evaluated to give

$$I = \frac{f(b) - f(a)}{b - a}\frac{(b^2 - a^2)}{2} + \frac{bf(a) - af(b)}{b - a}(b - a)$$

Now, since $b^2 - a^2 = (b - a)(b + a)$,

$$I = [f(b) - f(a)]\frac{b + a}{2} + bf(a) - af(b)$$

Multiplying and collecting terms yields

$$I = (b - a)\frac{f(a) + f(b)}{2}$$

which is the formula for the trapezoidal rule.

Geometrically, the trapezoidal rule is equivalent to approximating the area of the trapezoid under the straight line connecting $f(a)$ and $f(b)$ in Fig. 21.4. Recall from geometry that the formula for computing the area of a trapezoid is the height times the average of the bases (Fig. 21.5*a*). In our case, the concept is the same but the trapezoid is on its side (Fig. 21.5*b*). Therefore, the integral estimate can be represented as

$$I \cong \text{width} \times \text{average height} \tag{21.4}$$

FIGURE 21.4
Graphical depiction of the trapezoidal rule.

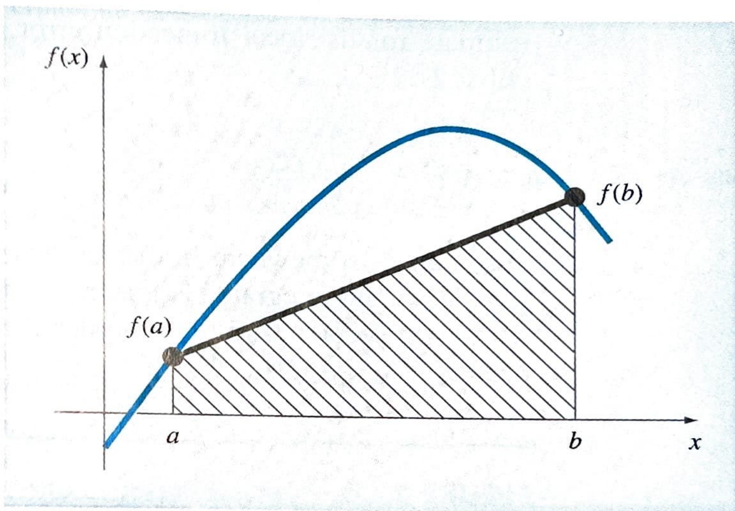
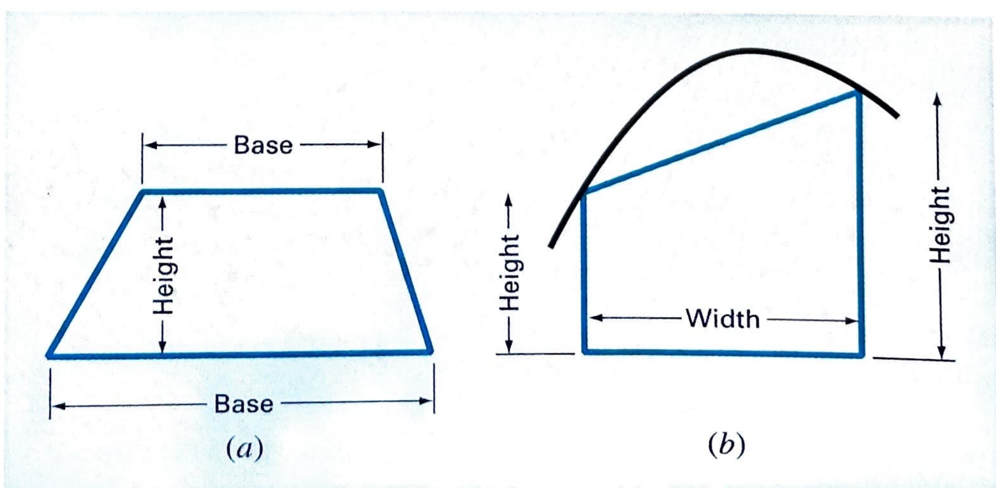


FIGURE 21.5
(*a*) The formula for computing the area of a trapezoid: height times the average of the bases. (*b*) For the trapezoidal rule, the concept is the same but the trapezoid is on its side.



or

$$I \cong (b - a) \times \text{average height} \tag{21.5}$$

where, for the trapezoidal rule, the average height is the average of the function values at the end points, or $[f(a) + f(b)]/2$.

All the Newton-Cotes closed formulas can be expressed in the general format of Eq. (21.5). In fact, they differ only with respect to the formulation of the average height.

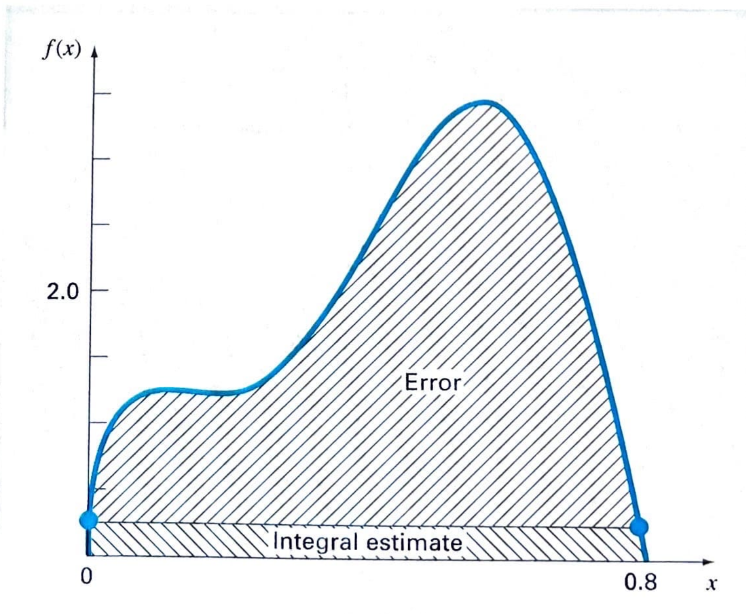
21.1.1 Error of the Trapezoidal Rule

When we employ the integral under a straight-line segment to approximate the integral under a curve, we obviously can incur an error that may be substantial (Fig. 21.6). An estimate for the local truncation error of a single application of the trapezoidal rule is (Box. 21.2)

$$E_t = -\frac{1}{12} f''(\xi)(b - a)^3 \tag{21.6}$$

where ξ lies somewhere in the interval from a to b. Equation (21.6) indicates that if the function being integrated is linear, the trapezoidal rule will be exact. Otherwise, for functions with second- and higher-order derivatives (that is, with curvature), some error can occur.

FIGURE 21.6
Graphical depiction of the use of a single application of the trapezoidal rule to approximate the integral of $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$ from $x = 0$ to 0.8.



Box 21.2 Derivation and Error Estimate of the Trapezoidal Rule

An alternative derivation of the trapezoidal rule is possible by integrating the forward Newton-Gregory interpolating polynomial. Recall that for the first-order version with error term, the integral would be (Box 18.2)

$$I = \int_a^b \left[f(a) + \Delta f(a)\alpha + \frac{f''(\xi)}{2}\alpha(\alpha-1)h^2 \right] dx \tag{B21.2.1}$$

To simplify the analysis, realize that because $\alpha = (x-a)/h$,

$$dx = h\,d\alpha$$

Inasmuch as $h = b - a$ (for the one-segment trapezoidal rule), the limits of integration a and b correspond to 0 and 1, respectively. Therefore, Eq. (B21.2.1) can be expressed as

$$I = h\int_0^1 \left[f(a) + \Delta f(a)\alpha + \frac{f''(\xi)}{2}\alpha(\alpha-1)h^2 \right] d\alpha$$

If it is assumed that, for small h, the term $f''(\xi)$ is approximately constant, this equation can be integrated:

$$I = h\left[\alpha f(a) + \frac{\alpha^2}{2}\Delta f(a) + \left(\frac{\alpha^3}{6} - \frac{\alpha^2}{4}\right) f''(\xi)h^2 \right]_0^1$$

and evaluated as

$$I = h\left[f(a) + \frac{\Delta f(a)}{2} \right] - \frac{1}{12} f''(\xi)h^3$$

Because $\Delta f(a) = f(b) - f(a)$, the result can be written as

$$I = \underbrace{h\frac{f(a)+f(b)}{2}}_{\text{Trapezoidal rule}} \underbrace{- \frac{1}{12} f''(\xi)h^3}_{\text{Truncation error}}$$

Thus, the first term is the trapezoidal rule and the second is an approximation for the error.

EXAMPLE 21.1 Single Application of the Trapezoidal Rule

Problem Statement. Use Eq. (21.3) to numerically integrate

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

from $a = 0$ to $b = 0.8$. Recall from Sec. PT6.2 that the exact value of the integral can be determined analytically to be 1.640533.

Solution. The function values

$$f(0) = 0.2$$
$$f(0.8) = 0.232$$

can be substituted into Eq. (21.3) to yield

$$I \cong 0.8\frac{0.2 + 0.232}{2} = 0.1728$$

which represents an error of

$$E_t = 1.640533 - 0.1728 = 1.467733$$

which corresponds to a percent relative error of $\varepsilon_t = 89.5\%$. The reason for this large error is evident from the graphical depiction in Fig. 21.6. Notice that the area under the straight line neglects a significant portion of the integral lying above the line.

In actual situations, we would have no foreknowledge of the true value. Therefore, an approximate error estimate is required. To obtain this estimate, the function's second 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,

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

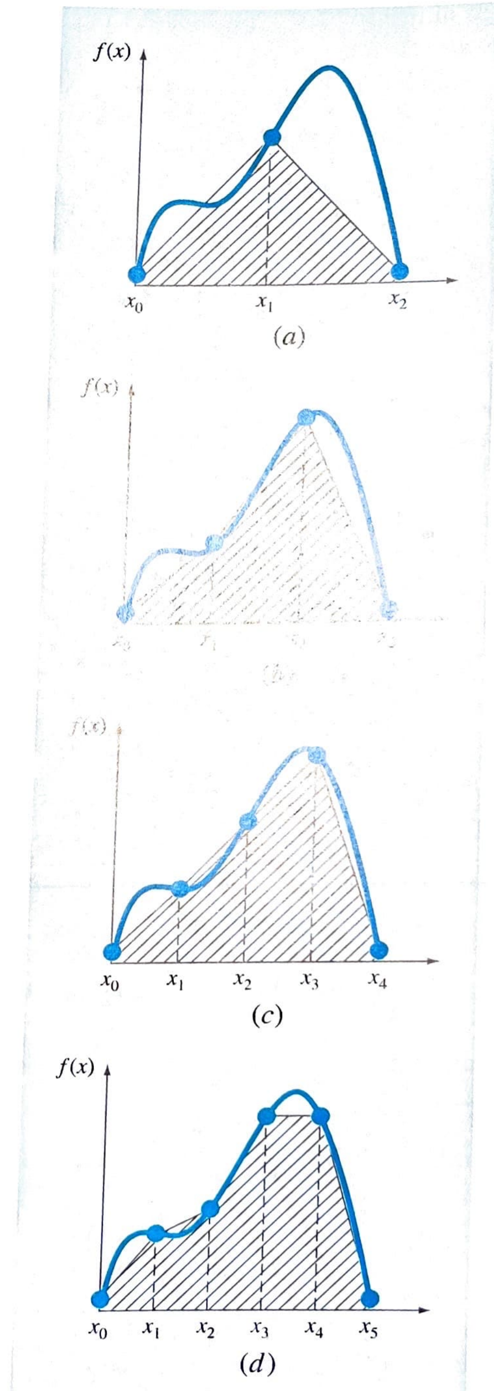


FIGURE 21.7
Illustration of the multiple-application trapezoidal rule. (*a*) Two segments, (*b*) three segments, (*c*) four segments, and (*d*) five segments.

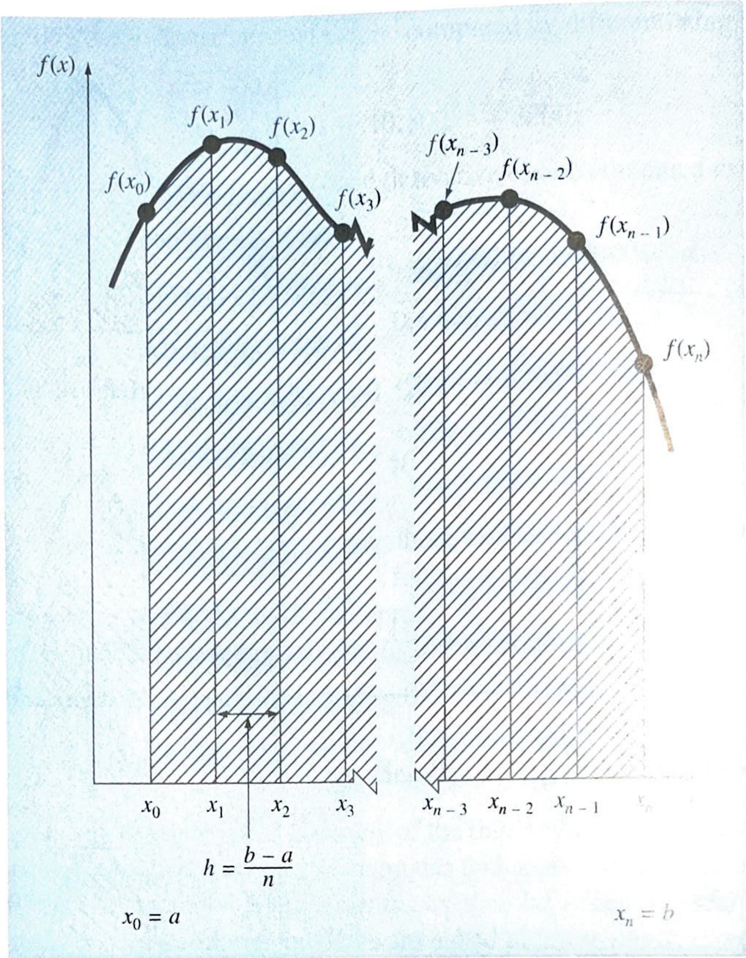


FIGURE 21.8
The general format and nomenclature for multiple-application integrals.

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. 21.9a) is for the single-segment version. The second (Fig. 21.9b) is for the multiple-segment

TABLE 21.1 Results for multiple-application trapezoidal rule to estimate the integral of $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$ from $x = 0$ to 0.8. The exact value is 1.640533.

n	h	I	ε_t (%)
2	0.4	1.0688	34.9
3	0.2667	1.3695	16.5
4	0.2	1.4848	9.5
5	0.16	1.5399	6.1
6	0.1333	1.5703	4.3
7	0.1143	1.5887	3.2
8	0.1	1.6008	2.4
9	0.0889	1.6091	1.9
10	0.08	1.6150	1.6

(a) Single-segment

```
FUNCTION Trap (h, f0, f1)
  Trap = h * (f0 + f1)/2
END Trap
```

(b) Multiple-segment

```
FUNCTION Trapm (h, n, f)
  sum = f0
  DOFOR i = 1, n - 1
    sum = sum + 2 * fi
  END DO
  sum = sum + fn
  Trapm = h * sum / 2
END Trapm
```

FIGURE 21.9
Algorithms for the (*a*) single-segment and (*b*) multiple-segment trapezoidal rule.

version with a constant segment width. Note that both are designed for data that is in tabulated form. A general program should have the capability to evaluate known functions or equations as well. We will illustrate how functions are handled in Chap. 22.

EXAMPLE 21.3 Evaluating Integrals with the Computer

Problem Statement. Use software based on Fig. 21.9*b* to solve a problem related to our friend, the falling parachutist. As you recall from Example 1.1, the velocity of the parachutist is given as the following function of time:

$$v(t) = \frac{gm}{c}\left(1 - e^{-(c/m)t}\right) \tag{E21.3.1}$$

where v = velocity (m/s), g = the gravitational constant of 9.8 m/s^2, m = mass of the parachutist equal to 68.1 kg, and c = the drag coefficient of 12.5 kg/s. The model predicts the velocity of the parachutist as a function of time as described in Example 1.1.

Suppose we would like to know how far the parachutist has fallen after a certain time t. This distance is given by [Eq. (PT6.5)]

$$d = \int_0^t v(t)\, dt$$

where d is the distance in meters. Substituting Eq. (E21.3.1),

$$d = \frac{gm}{c} \int_0^t \left(1 - e^{-(c/m)t}\right) dt$$

Use your software to determine this integral with the multiple-segment trapezoidal rule using different numbers of segments. Note that performing the integration analytically and substituting known parameter values results in an exact value of $d = 289.43515$ m.

Solution. For the case where $n = 10$ segments, a calculated integral of 288.7491 is obtained. Thus, we have attained the integral to three significant digits of accuracy. Results for other numbers of segments can be readily generated.

Segments	Segment Size	Estimated d, m	ε_t (%)
10	1.0	288.7491	0.237
20	0.5	289.2636	0.0593
50	0.2	289.4076	9.5×10^{-3}
100	0.1	289.4282	2.4×10^{-3}
200	0.05	289.4336	5.4×10^{-4}
500	0.02	289.4348	1.2×10^{-4}
1,000	0.01	289.4360	-3.0×10^{-4}
2,000	0.005	289.4369	-5.9×10^{-4}
5,000	0.002	289.4337	5.2×10^{-4}
10,000	0.001	289.4317	1.2×10^{-3}

Up to about 500 segments, the multiple-application trapezoidal rule attains excellent accuracy. However, notice how the error changes sign and begins to increase in absolute value beyond the 500-segment case. The 10,000-segment case actually seems to be diverging from the true value. This is due to the intrusion of round-off error because of the great number of computations for this many segments. Thus, the level of precision is limited, and we would never reach the exact result of 289.4351 obtained analytically. This limitation and ways to overcome it will be discussed in further detail in Chap. 22.

Three major conclusions can be drawn from the Example 21.3:

- For individual applications with nicely behaved functions, the multiple-segment trapezoidal rule is just fine for attaining the type of accuracy required in many engineering applications.
- If high accuracy is required, the multiple-segment trapezoidal rule demands a great deal of computational effort. Although this effort may be negligible for a single application, it could be very important when (*a*) numerous integrals are being evaluated or (*b*) where the function itself is time consuming to evaluate. For such cases, more efficient approaches (like those in the remainder of this chapter and the next) may be necessary.

- 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

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

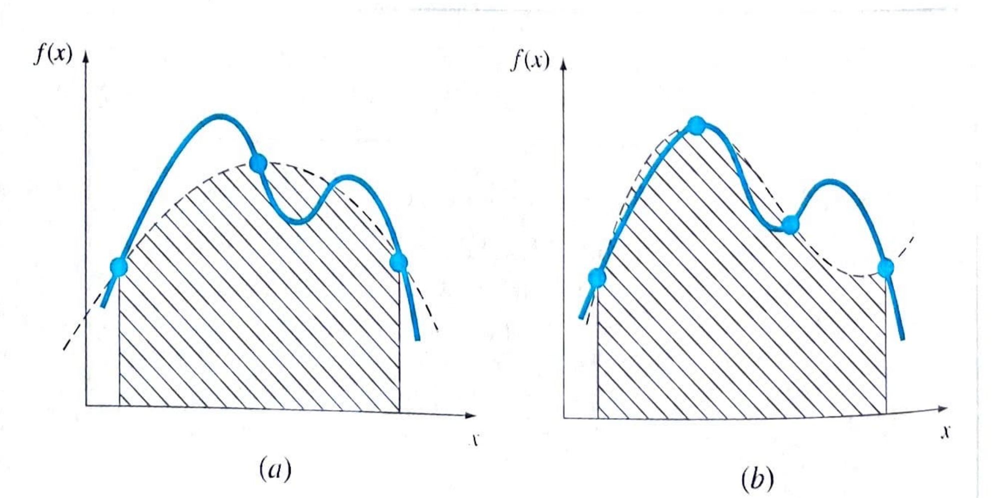


FIGURE 21.10
(*a*) Graphical depiction of Simpson's 1/3 rule: It consists of taking the area under a parabola connecting three points. (*b*) Graphical depiction of Simpson's 3/8 rule: It consists of taking the area under a cubic equation connecting four points.

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),

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

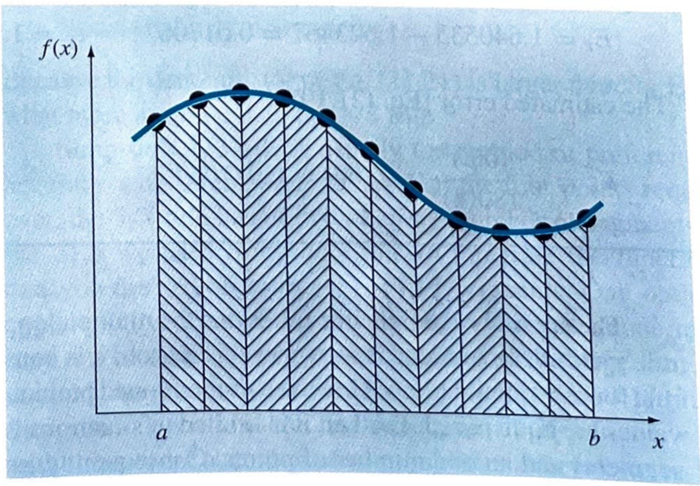


FIGURE 21.11
Graphical representation of the multiple application of Simpson's 1/3 rule. Note that the method can be employed only if the number of segments is even.

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 odd-segment–even-point formula known as Simpson's 3/8 rule is used in conjunction with the 1/3 rule to permit evaluation of both even and odd numbers of segments.

21.2.3 Simpson's 3/8 Rule

In a similar manner to the derivation of the trapezoidal and Simpson's 1/3 rule, a third-order Lagrange polynomial can be fit to four points and integrated:

$$I = \int_a^b f(x)\,dx \cong \int_a^b f_3(x)\,dx$$

to yield

$$I \cong \frac{3h}{8}[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)]$$

where $h = (b - a)/3$. This equation is called *Simpson's 3/8 rule* because h is multiplied by 3/8. It is the third Newton-Cotes closed integration formula. The 3/8 rule can also be expressed in the form of Eq. (21.5):

$$I \cong \underbrace{(b-a)}_{\text{Width}} \underbrace{\frac{f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)}{8}}_{\text{Average height}} \tag{21.20}$$

Thus, the two interior points are given weights of three-eighths, whereas the end points are weighted with one-eighth. Simpson's 3/8 rule has an error of

$$E_t = -\frac{3}{80}h^5 f^{(4)}(\xi)$$

or, because $h = (b - a)/3$,

$$E_t = -\frac{(b-a)^5}{6480} f^{(4)}(\xi) \tag{21.21}$$

Because the denominator of Eq. (21.21) is larger than for Eq. (21.16), the 3/8 rule is somewhat more accurate than the 1/3 rule.

Simpson's 1/3 rule is usually the method of preference because it attains third-order accuracy with three points rather than the four points required for the 3/8 version. However, the 3/8 rule has utility when the number of segments is odd. For instance, in Example 21.5 we used Simpson's rule to integrate the function for four segments. Suppose that you desired an estimate for five segments. One option would be to use a multiple-application version of the trapezoidal rule as was done in Examples 21.2 and 21.3. This may not be advisable, however, because of the large truncation error associated with this method. An alternative would be to apply Simpson's 1/3 rule to the first two segments and Simpson's 3/8 rule to the last three (Fig. 21.12). In this way, we could obtain an estimate with third-order accuracy across the entire interval.

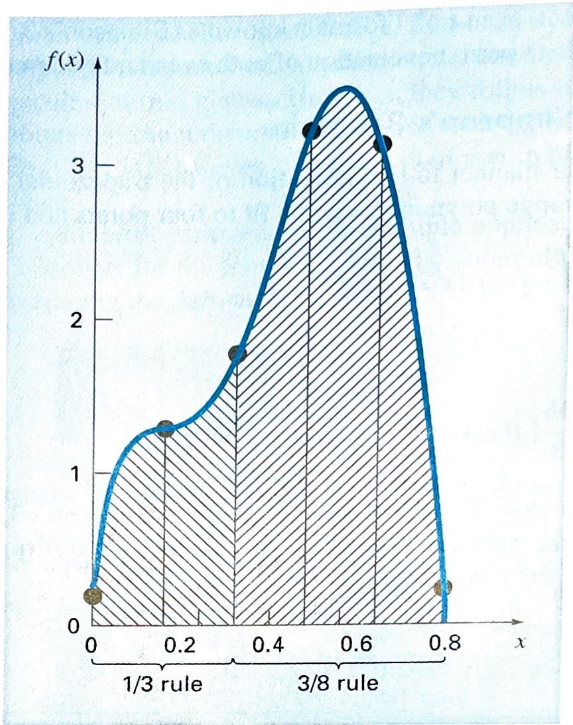


FIGURE 21.12
Illustration of how Simpson's 1/3 and 3/8 rules can be applied in tandem to handle multiple applications with odd numbers of intervals.

EXAMPLE 21.6 **Simpson's 3/8 Rule**

Problem Statement.

(a) Use Simpson's 3/8 rule to integrate

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

from $a = 0$ to $b = 0.8$.

(b) Use it in conjunction with Simpson's 1/3 rule to integrate the same function for five segments.

Solution.

(a) A single application of Simpson's 3/8 rule requires four equally spaced points:

$$f(0) = 0.2 \qquad f(0.2667) = 1.432724$$
$$f(0.5333) = 3.487177 \qquad f(0.8) = 0.232$$

Using Eq. (21.20),

$$I \cong 0.8\,\frac{0.2 + 3(1.432724 + 3.487177) + 0.232}{8} = 1.519170$$

$$E_t = 1.640533 - 1.519170 = 0.1213630 \qquad \varepsilon_t = 7.4\%$$

$$E_a = -\frac{(0.8)^5}{6480}(-2400) = 0.1213630$$

(b) The data needed for a five-segment application ($h = 0.16$) is

$$f(0) = 0.2 \qquad f(0.16) = 1.296919$$
$$f(0.32) = 1.743393 \qquad f(0.48) = 3.186015$$
$$f(0.64) = 3.181929 \qquad f(0.80) = 0.232$$

The integral for the first two segments is obtained using Simpson's 1/3 rule:

$$I \cong 0.32\,\frac{0.2 + 4(1.296919) + 1.743393}{6} = 0.3803237$$

For the last three segments, the 3/8 rule can be used to obtain

$$I \cong 0.48\,\frac{1.743393 + 3(3.186015 + 3.181929) + 0.232}{8} = 1.264754$$

The total integral is computed by summing the two results:

$$I = 0.3803237 + 1.264753 = 1.645077$$
$$E_t = 1.640533 - 1.645077 = -0.00454383 \qquad \varepsilon_t = -0.28\%$$

21.2.4 Computer Algorithms for Simpson's Rules

Pseudocodes for a number of forms of Simpson's rule are outlined in Fig. 21.13. Note that all are designed for data that is in tabulated form. A general program should have the capability to evaluate known functions or equations as well. We will illustrate how functions are handled in Chap. 22.

Notice that the program in Fig. 21.13*d* is set up so that either an even or odd number of segments may be used. For the even case, Simpson's 1/3 rule is applied to each pair of segments, and the results are summed to compute the total integral. For the odd case, Simpson's 3/8 rule is applied to the last three segments, and the 1/3 rule is applied to all the previous segments.

21.2.5 Higher-Order Newton-Cotes Closed Formulas

As noted previously, the trapezoidal rule and both of Simpson's rules are members of a family of integrating equations known as the Newton-Cotes closed integration formulas. Some of the formulas are summarized in Table 21.2 along with their truncation-error estimates.

Notice that, as was the case with Simpson's 1/3 and 3/8 rules, the five- and six-point formulas have the same order error. This general characteristic holds for the higher-point formulas and leads to the result that the even-segment–odd-point formulas (for example, 1/3 rule and Boole's rule) are usually the methods of preference.

However, it must also be stressed that, in engineering practice, the higher-order (that is, greater than four-point) formulas are rarely used. Simpson's rules are sufficient for most applications. Accuracy can be improved by using the multiple-application version. Furthermore, when the function is known and high accuracy is required, methods such as

(a)

```
FUNCTION Simp13 (h, f0, f1, f2)
  Simp13 = 2*h* (f0+4*f1+f2) / 6
END Simp13
```

(b)

```
FUNCTION Simp38 (h, f0, f1, f2, f3)
  Simp38 = 3*h* (f0+3*(f1+f2)+f3) / 8
END Simp38
```

(c)

```
FUNCTION Simp13m (h, n, f)
  sum = f(0)
  DOFOR i = 1, n - 2, 2
    sum = sum + 4 * f_i + 2 * f_i+1
  END DO
  sum = sum + 4 * f_n-1 + f_n
  Simp13m = h * sum / 3
END Simp13m
```

(d)

```
FUNCTION SimpInt(a,b,n,f)
  h = (b - a) / n
  IF n = 1 THEN
    sum = Trap(h, f_n-1, f_n)
  ELSE
    m = n
    odd = n / 2 - INT(n / 2)
    IF odd > 0 AND n > 1 THEN
      sum = sum+Simp38(h, f_n-3, f_n-2, f_n-1, f_n)
      m = n - 3
    END IF
    IF m > 1 THEN
      sum = sum + Simp13m(h,m,f)
    END IF
  END IF
  SimpInt = sum
END SimpInt
```

FIGURE 21.13
Pseudocode for Simpson's rules. (*a*) Single-application Simpson's 1/3 rule, (*b*) single-application Simpson's 3/8 rule, (*c*) multiple-application Simpson's 1/3 rule, and (*d*) multiple-application Simpson's rule for both odd and even number of segments. Note that for all cases, n must be ≥ 1.

TABLE 21.2 Newton-Cotes closed integration formulas. The formulas are presented in the format of Eq. (21.5) so that the weighting of the data points to estimate the average height is apparent. The step size is given by $h = (b - a)/n$.

Segments (n)	Points	Name	Formula	Truncation Error
1	2	Trapezoidal rule	$(b-a)\dfrac{f(x_0)+f(x_1)}{2}$	$-(1/12)h^3f''(\xi)$
2	3	Simpson's 1/3 rule	$(b-a)\dfrac{f(x_0)+4f(x_1)+f(x_2)}{6}$	$-(1/90)h^5f^{(4)}(\xi)$
3	4	Simpson's 3/8 rule	$(b-a)\dfrac{f(x_0)+3f(x_1)+3f(x_2)+f(x_3)}{8}$	$-(3/80)h^5f^{(4)}(\xi)$
4	5	Boole's rule	$(b-a)\dfrac{7f(x_0)+32f(x_1)+12f(x_2)+32f(x_3)+7f(x_4)}{90}$	$-(8/945)h^7f^{(6)}(\xi)$
5	6		$(b-a)\dfrac{19f(x_0)+75f(x_1)+50f(x_2)+50f(x_3)+75f(x_4)+19f(x_5)}{288}$	$-(275/12{,}096)h^7f^{(6)}(\xi)$

Romberg integration or Gauss quadrature, described in Chap. 22, offer viable and attractive alternatives.

21.3 INTEGRATION WITH UNEQUAL SEGMENTS

To this point, all formulas for numerical integration have been based on equally spaced data points. In practice, there are many situations where this assumption does not hold and we must deal with unequal-sized segments. For example, experimentally derived data is often of this type. For these cases, one method is to apply the trapezoidal rule to each segment and sum the results:

$$I = h_1 \frac{f(x_0) + f(x_1)}{2} + h_2 \frac{f(x_1) + f(x_2)}{2} + \cdots + h_n \frac{f(x_{n-1}) + f(x_n)}{2} \tag{21.22}$$

where h_i = the width of segment i. Note that this was the same approach used for the multiple-application trapezoidal rule. The only difference between Eqs. (21.8) and (21.22) is that the h's in the former are constant. Consequently, Eq. (21.8) could be simplified by grouping terms to yield Eq. (21.9). Although this simplification cannot be applied to Eq. (21.22), a computer program can be easily developed to accommodate unequal-sized segments. Before describing such an algorithm, we will illustrate in the following example how Eq. (21.22) is applied to evaluate an integral.

EXAMPLE 21.7 Trapezoidal Rule with Unequal Segments

Problem Statement. The information in Table 21.3 was generated using the same polynomial employed in Example 21.1. Use Eq. (21.22) to determine the integral for this data. Recall that the correct answer is 1.640533.

Solution. Applying Eq. (21.22) to the data in Table 21.3 yields

$$I = 0.12 \frac{1.309729 + 0.2}{2} + 0.10 \frac{1.305241 + 1.309729}{2} + \cdots + 0.10 \frac{0.232 + 2.363}{2}$$

$$= 0.090584 + 0.130749 + \cdots + 0.12975 = 1.594801$$

which represents an absolute percent relative error of $\varepsilon_t = 2.8\%$.

TABLE 21.3 Data for $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$, with unequally spaced values of x.

x	f(x)	x	f(x)
0.0	0.200000	0.44	2.842985
0.12	1.309729	0.54	3.507297
0.22	1.305241	0.64	3.181929
0.32	1.743393	0.70	2.363000
0.36	2.074903	0.80	0.232000
0.40	2.456000		