CHAPTER 22
Integration of Equations

In the introduction to Part Six, we noted that functions to be integrated numerically will typically be of two forms: a table of values or a function. The form of the data has an important influence on the approaches that can be used to evaluate the integral. For tabulated information, you are limited by the number of points that are given. In contrast, if the function is available, you can generate as many values of \( f(x) \) as are required to attain acceptable accuracy (recall Fig. PT6.7).

This chapter is devoted to two techniques that are expressly designed to analyze cases where the function is given. Both capitalize on the ability to generate function values to develop efficient schemes for numerical integration. The first is based on Richardson's extrapolation, which is a method for combining two numerical integral estimates to obtain a third, more accurate value. The computational algorithm for implementing Richardson's extrapolation in a highly efficient manner is called Romberg integration. This technique is recursive and can be used to generate an integral estimate within a prespecified error tolerance.

The second method is called Gauss quadrature. Recall that, in the last chapter, values of \( f(x) \) for the Newton-Cotes formulas were determined at specified values of \( x \). For example, if we used the trapezoidal rule to determine an integral, we were constrained to take the weighted average of \( f(x) \) at the ends of the interval. Gauss-quadrature formulas employ \( x \) values that are positioned between \( a \) and \( b \) in such a manner that a much more accurate integral estimate results.

In addition to these two standard techniques, we devote a final section to the evaluation of improper integrals. In this discussion, we focus on integrals with infinite limits and show how a change of variable and open integration formulas prove useful for such cases.

22.1 NEWTON-COTES ALGORITHMS FOR EQUATIONS

In Chap. 21, we presented algorithms for multiple-application versions of the trapezoidal rule and Simpson's rules. Although these pseudocodes can certainly be used to analyze equations, in our effort to make them compatible with either data or functions, they could not exploit the convenience of the latter.

Figure 22.1 shows pseudocodes that are expressly designed for cases where the function is analytical. In particular, notice that neither the independent nor the dependent
**FIGURE 22.1**
Algorithms for multiple applications of (a) trapezoidal and (b) Simpson’s 1/3 rules, where the function is available.

(a)  
```plaintext
FUNCTION TrapEq (n, a, b)  
  h = (b - a) / n  
  x = a  
  sum = f(x)  
  DO i = 1, n - 1  
    x = x + h  
    sum = sum + 2 * f(x)  
  END DO  
  sum = sum + f(b)  
  TrapEq = (b - a) * sum / (2 * n)  
END TrapEq
```

(b)  
```plaintext
FUNCTION SImpEq (n, a, b)  
  h = (b - a) / n  
  x = a  
  sum = f(x)  
  DO i = 1, n - 2, 2  
    x = x + h  
    sum = sum + 4 * f(x)  
    x = x + h  
    sum = sum + 2 * f(x)  
  END DO  
  x = x + h  
  sum = sum + 4 * f(x)  
  sum = sum + f(b)  
  SImpEq = (b - a) * sum / (3 * n)  
END SImpEq
```

**FIGURE 22.2**
Absolute value of the true percent relative error versus number of segments for the determination of the integral of \( f(x) = 0.2 + 2.5x - 200x^2 + 675x^3 - 9000x^4 + 4000x^5 \), evaluated from \( a = 0 \) to \( b = 0.8 \) using the multiple-application trapezoidal rule and the multiple-application Simpson’s 1/3 rule. Note that both results indicate that for a large number of segments, roundoff errors limit precision.
variable values are passed into the function via its argument as was the case for the codes in Chap. 21. For the independent variable \( x \), the integration interval \((a, b)\) and the number of segments are passed. This information is then employed to generate equispaced values of \( x \) within the function. For the dependent variable, the function values in Fig. 22.1 are computed using calls to the function being analyzed, \( f(x) \).

We developed single-precision programs based on these pseudocodes to analyze the effort involved and the errors incurred as we progressively used more segments to estimate the integral of a simple function. For an analytical function, the error equations [Eqs. (21.13) and (21.19)] indicate that increasing the number of segments \( n \) will result in more accurate integral estimates. This observation is borne out by Fig. 22.2, which is a plot of true error versus \( n \) for the integral of \( f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5 \). Notice how the error drops as \( n \) increases. However, also notice that at large values of \( n \), the error starts to increase as round-off errors begin to dominate. Also observe that a very large number of function evaluations (and, hence, computational effort) is required to attain high levels of accuracy. As a consequence of these shortcomings, the multiple-application trapezoidal rule and Simpson's rules are sometimes inadequate for problem contexts where high efficiency and low errors are needed.

## 22.2 ROMBERG INTEGRATION

**Romberg integration** is one technique that is designed to attain efficient numerical integrals of functions. It is quite similar to the techniques discussed in Chap. 21 in the sense that it is based on successive application of the trapezoidal rule. However, through mathematical manipulations, superior results are attained for less effort.

### 22.2.1 Richardson's Extrapolation

Recall that, in Sec. 10.3.3, we used iterative refinement to improve the solution of a set of simultaneous linear equations. Error-correction techniques are also available to improve the results of numerical integration on the basis of the integral estimates themselves. Generally called Richardson's extrapolation, these methods use two estimates of an integral to compute a third, more accurate approximation.

The estimate and error associated with a multiple-application trapezoidal rule can be represented generally as

\[
I = I(h) + E(h)
\]

where \( I \) is the exact value of the integral, \( I(h) \) is the approximation from an \( n \)-segment application of the trapezoidal rule with step size \( h = (b - a)/n \), and \( E(h) \) is the truncation error. If we make two separate estimates using step sizes of \( h_1 \) and \( h_2 \) and have exact values for the error,

\[
I(h_1) + E(h_1) = I(h_2) + E(h_2)
\]

Now recall that the error of the multiple-application trapezoidal rule can be represented approximately by Eq. (21.13) [with \( n = (b - a)/h \)]:

\[
E \approx \frac{b - a}{12} h^2 \int_a^b f'(x) dx
\]

\[
(22.2)
\]
If it is assumed that \( f'' \) is constant regardless of step size, Eq. (22.2) can be used to determine that the ratio of the two errors will be

\[
\frac{E(h_1)}{E(h_2)} \approx h_1^2 \frac{h_1}{h_2^2} \tag{22.3}
\]

This calculation has the important effect of removing the term \( f'' \) from the computation. In so doing, we have made it possible to utilize the information embodied by Eq. (22.2) without prior knowledge of the function’s second derivative. To do this, we rearrange Eq. (22.3) to give

\[
E(h_1) \approx E(h_2) \left( \frac{h_1}{h_2} \right)^2
\]

which can be substituted into Eq. (22.1):

\[
I(h_1) + E(h_2) \left( \frac{h_1}{h_2} \right)^2 \approx I(h_2) + E(h_2)
\]

which can be solved for

\[
E(h_2) \approx \frac{I(h_1) - I(h_2)}{1 - \left( \frac{h_1}{h_2} \right)^2}
\]

Thus, we have developed an estimate of the truncation error in terms of the integral estimates and their step sizes. This estimate can then be substituted into

\[
I = I(h_2) + E(h_2)
\]

to yield an improved estimate of the integral:

\[
I \equiv I(h_2) + \frac{1}{(h_1/h_2)^2 - 1} \left[ I(h_2) - I(h_1) \right] \tag{22.4}
\]

It can be shown (Ralston and Rabinowitz, 1978) that the error of this estimate is \( O(h^4) \). Thus, we have combined two trapezoidal rule estimates of \( O(h^5) \) to yield a new estimate of \( O(h^4) \). For the special case where the interval is halved \( (h_2 = h_1/2) \), this equation becomes

\[
I \equiv I(h_2) + \frac{1}{2^2 - 1} \left[ I(h_2) - I(h_1) \right]
\]

or, collecting terms,

\[
I \equiv \frac{4}{3} I(h_2) - \frac{1}{3} I(h_1) \tag{22.5}
\]

**EXAMPLE 22.1  Error Corrections of the Trapezoidal Rule**

**Problem Statement.** In the previous chapter (Example 21.1 and Table 21.1), we used a variety of numerical integration methods to evaluate the integral of \( f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5 \) from \( a = 0 \) to \( b = 0.8 \). For example, single and multiple
applications of the trapezoidal rule yielded the following results:

<table>
<thead>
<tr>
<th>Segments</th>
<th>$h$</th>
<th>Integral</th>
<th>$%$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.8</td>
<td>0.1728</td>
<td>89.5</td>
</tr>
<tr>
<td>2</td>
<td>0.4</td>
<td>1.0686</td>
<td>34.9</td>
</tr>
<tr>
<td>4</td>
<td>0.2</td>
<td>1.4848</td>
<td>9.5</td>
</tr>
</tbody>
</table>

Use this information along with Eq. (22.5) to compute improved estimates of the integral.

**Solution.** The estimates for one and two segments can be combined to yield

$$I \approx \frac{4}{3}(1.0688) - \frac{1}{3}(0.1728) = 1.367467$$

The error of the improved integral is $E_i = 1.640533 - 1.367467 = 0.273067 (e_i = 16.6 \%)$, which is superior to the estimates upon which it was based.

In the same manner, the estimates for two and four segments can be combined to give

$$I \approx \frac{4}{3}(1.4848) - \frac{1}{3}(1.0688) = 1.623467$$

which represents an error of $E_i = 1.640533 - 1.623467 = 0.017067 (e_i = 1.0 \%)$.

Equation (22.4) provides a way to combine two applications of the trapezoidal rule with error $O(h^2)$ to compute a third estimate with error $O(h^4)$. This approach is a subset of a more general method for combining integrals to obtain improved estimates. For instance, in Example 22.1, we computed two improved integrals of $O(h^4)$ on the basis of three trapezoidal rule estimates. These two improved estimates can, in turn, be combined to yield an even better value with $O(h^6)$. For the special case where the original trapezoidal estimates are based on successive halving of the step size, the equation used for $O(h^6)$ accuracy is

$$I \approx \frac{16}{15} I_n - \frac{1}{15} I_i \tag{22.6}$$

where $I_n$ and $I_i$ are the more and less accurate estimates, respectively. Similarly, two $O(h^6)$ results can be combined to compute an integral that is $O(h^8)$ using

$$I \approx \frac{64}{63} I_n - \frac{1}{63} I_i \tag{22.7}$$

**EXAMPLE 22.2 Higher-Order Error Correction of Integral Estimates**

**Problem Statement.** In Example 22.1, we used Richardson’s extrapolation to compute two integral estimates of $O(h^4)$. Utilize Eq. (22.6) to combine these estimates to compute an integral with $O(h^6)$.
Solution. The two integral estimates of $O(h^4)$ obtained in Example 22.1 were 1.367467 and 1.623467. These values can be substituted into Eq. (22.6) to yield

$$I = \frac{16}{15}(1.623467) - \frac{1}{15}(1.367467) = 1.640533$$

which is the correct answer to the seven significant figures that are carried in this example.

22.2.2 The Romberg Integration Algorithm

Notice that the coefficients in each of the extrapolation equations [Eqs. (22.5), (22.6), and (22.7)] add up to 1. Thus, they represent weighting factors that, as accuracy increases, place relatively greater weight on the superior integral estimate. These formulations can be expressed in a general form that is well-suited for computer implementation:

$$I_{j,k} \approx \frac{4^k - 1}{4^k - 1} I_{j+1,k-1} - I_{j,k-1}$$

(22.8)

where $I_{j+1,k-1}$ and $I_{j,k-1}$ = the more and less accurate integrals, respectively, and $I_{j,k}$ = the improved integral. The index $k$ signifies the level of the integration, where $k = 1$ corresponds to the original trapezoidal rule estimates, $k = 2$ corresponds to $O(h^4)$, $k = 3$ to $O(h^6)$, and so forth. The index $j$ is used to distinguish between the more $(j + 1)$ and the less $(j)$ accurate estimates. For example, for $k = 2$ and $j = 1$, Eq. (22.8) becomes

$$I_{1,2} \approx \frac{4I_{2,1} - I_{1,1}}{3}$$

which is equivalent to Eq. (22.5).

The general form represented by Eq. (22.8) is attributed to Romberg, and its systematic application to evaluate integrals is known as Romberg integration. Figure 22.3 is a

<table>
<thead>
<tr>
<th>$O(h^2)$</th>
<th>$O(h^4)$</th>
<th>$O(h^6)$</th>
<th>$O(h^8)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.172800</td>
<td>1.367467</td>
<td>1.640533</td>
<td>1.640533</td>
</tr>
<tr>
<td>1.068800</td>
<td>1.623467</td>
<td>1.640533</td>
<td>1.640533</td>
</tr>
<tr>
<td>1.484800</td>
<td>1.639467</td>
<td>1.640533</td>
<td>1.640533</td>
</tr>
<tr>
<td>1.600800</td>
<td>1.639467</td>
<td>1.640533</td>
<td>1.640533</td>
</tr>
</tbody>
</table>
22.2 ROMBERG INTEGRATION

A graphical depiction of the sequence of integral estimates generated using this approach. Each matrix corresponds to a single iteration. The first column contains the trapezoidal rule evaluations that are designated \( I_{1,1} \), where \( j = 1 \) is for a single-segment application (step size is \( b - a \)), \( j = 2 \) is for a two-segment application (step size is \( (b - a)/2 \)), \( j = 3 \) is for a four-segment application (step size is \( (b - a)/4 \)), and so forth. The other columns of the matrix are generated by systematically applying Eq. (22.8) to obtain successively better estimates of the integral.

For example, the first iteration (Fig. 22.3a) involves computing the one- and two-segment trapezoidal rule estimates \( (I_{1,1} \text{ and } I_{2,1}) \). Equation (22.8) is then used to compute the element \( I_{1,2} = 1.367467 \), which has an error of \( O(h^4) \).

Now, we must check to determine whether this result is adequate for our needs. As in other approximate methods in this book, a termination, or stopping, criterion is required to assess the accuracy of the results. One method that can be employed for the present purposes is [Eq. (3.5)]

\[
|\varepsilon_a| = \left| \frac{I_{1,k} - I_{1,k-1}}{I_{1,k}} \right| \times 100\% \tag{22.9}
\]

where \( \varepsilon_a \) is an estimate of the percent relative error. Thus, as was done previously in other iterative processes, we compare the new estimate with a previous value. When the change between the old and new values as represented by \( \varepsilon_a \) is below a prespecified error criterion \( \varepsilon_a \), the computation is terminated. For Fig. 22.3a, this evaluation indicates an 87.4 percent change over the course of the first iteration.

The object of the second iteration (Fig. 22.3b) is to obtain the \( O(h^6) \) estimate — \( I_{1,3} \). To do this, an additional trapezoidal rule estimate, \( I_{1,1} = 1.4848 \), is determined. Then it is combined with \( I_{2,1} \) using Eq. (22.8) to generate \( I_{2,2} = 1.623467 \). The result is, in turn, combined with \( I_{1,2} \) to yield \( I_{1,3} = 1.640533 \). Equation (22.9) can be applied to determine that this result represents a change of 22.6 percent when compared with the previous result \( I_{1,2} \).

The third iteration (Fig. 22.3c) continues the process in the same fashion. In this case, a trapezoidal estimate is added to the first column, and then Eq. (22.8) is applied to compute successively more accurate integrals along the lower diagonal. After only three iterations, because we are evaluating a fifth-order polynomial, the result \( (I_{1,4} = 1.640533) \) is exact.

Romberg integration is more efficient than the trapezoidal rule and Simpson’s rules discussed in Chap. 21. For example, for determination of the integral as shown in Fig. 22.1, Simpson’s 1/3 rule would require a 256-segment application to yield an estimate of 1.640533. Finer approximations would not be possible because of round-off error. In contrast, Romberg integration yields an exact result (to seven significant figures) based on combining one-, two-, four-, and eight-segment trapezoidal rules; that is, with only 15 function evaluations!

Figure 22.4 presents pseudocode for Romberg integration. By using loops, this algorithm implements the method in an efficient manner. Romberg integration is designed for cases where the function to be integrated is known. This is because knowledge of the function permits the evaluations required for the initial implementations of the trapezoidal rule. Tabulated data is rarely in the form needed to make the necessary successive halvings.
FUNCTION Rhomberg (a, b, maxit, es)
    LOCAL n(10, 10)
    n = 1
    $I_{1,1} = \text{TrapEq}(n, a, b)$
    iter = 0
    DO
        $n = 2^{\text{iter}}$
        $I_{n+1,1} = \text{TrapEq}(n, a, b)$
        DO k = 2, iter + 1
            f = $2 + \text{iter} - k$
            $I_{j,k} = (f^{-1} - I_{j-1,k-1} - I_{j,k-1}) / (f^{-1} - 1)$
        ENDDO
        $e_n = \text{ABS}((I_{1,\text{iter}+1} - I_{1,\text{iter}}) / I_{1,\text{iter}+1}) \times 100$
        IF (iter = maxit OR $e_n \leq es$) EXIT
    ENDDO
    Rhomberg = $I_{1,\text{iter}+1}$
END Rhomberg

22.3 GAUSS QUADRATURE

In Chap. 21, we studied the group of numerical integration or quadrature formulas known as the Newton-Cotes equations. A characteristic of these formulas (with the exception of the special case of Sec. 21.3) was that the integral estimate was based on evenly spaced function values. Consequently, the location of the base points used in these equations was predetermined or fixed.

For example, as depicted in Fig. 22.5a, the trapezoidal rule is based on taking the area under the straight line connecting the function values at the ends of the integration interval. The formula that is used to compute this area is

$$ I \equiv (b - a) \frac{f(a) + f(b)}{2} \quad (22.10) $$

where $a$ and $b$ = the limits of integration and $b - a$ = the width of the integration interval. Because the trapezoidal rule must pass through the end points, there are cases such as Fig. 22.5a where the formula results in a large error.

Now, suppose that the constraint of fixed base points was removed and we were free to evaluate the area under a straight line joining any two points on the curve. By positioning these points wisely, we could define a straight line that would balance the positive and negative errors. Hence, as in Fig. 22.5b, we would arrive at an improved estimate of the integral.

Gauss quadrature is the name for one class of techniques to implement such a strategy. The particular Gauss quadrature formulas described in this section are called Gauss-Legendre formulas. Before describing the approach, we will show how numerical integration formulas such as the trapezoidal rule can be derived using the method of undetermined coefficients. This method will then be employed to develop the Gauss-Legendre formulas.
22.3 GAUSS QUADRATURE

**FIGURE 22.5**
(a) Graphical depiction of the trapezoidal rule as the area under the straight line joining fixed end points. (b) An improved integral estimate obtained by taking the area under the straight line passing through two intermediate points. By positioning these points wisely, the positive and negative errors are balanced, and an improved integral estimate results.

22.3.1 Method of Undetermined Coefficients

In Chap. 21, we derived the trapezoidal rule by integrating a linear interpolating polynomial and by geometrical reasoning. The method of undetermined coefficients offers a third approach that also has utility in deriving other integration techniques such as Gauss quadrature.

To illustrate the approach, Eq. (22.10) is expressed as

\[ I = c_0 f(a) + c_1 f(b) \]  

(22.11)

where the \( c \)'s = constants. Now realize that the trapezoidal rule should yield exact results when the function being integrated is a constant or a straight line. Two simple equations that represent these cases are \( y = 1 \) and \( y = x \). Both are illustrated in Fig. 22.6. Thus, the following equalities should hold:

\[ c_0 + c_1 = \int_{-(b-a)/2}^{(b-a)/2} 1 \, dx \]

and

\[-c_0 \frac{b-a}{2} + c_1 \frac{b-a}{2} = \int_{-(b-a)/2}^{(b-a)/2} x \, dx \]
or, evaluating the integrals,
\[ c_0 + c_1 = b - a \]
and
\[ -c_0 \frac{b - a}{2} + c_1 \frac{b - a}{2} = 0 \]
These are two equations with two unknowns that can be solved for
\[ c_0 = c_1 = \frac{b - a}{2} \]
which, when substituted back into Eq. (22.11), gives
\[ I = \frac{b - a}{2} f(a) + \frac{b - a}{2} f(b) \]
which is equivalent to the trapezoidal rule.
22.3.2 Derivation of the Two-Point Gauss-Legendre Formula

Just as was the case for the above derivation of the trapezoidal rule, the object of Gauss quadrature is to determine the coefficients of an equation of the form

$$I \cong c_0 f(x_0) + c_1 f(x_1)$$  \hspace{1cm} (22.12)

where the \(c's\) = the unknown coefficients. However, in contrast to the trapezoidal rule that used fixed end points \(a\) and \(b\), the function arguments \(x_0\) and \(x_1\) are not fixed at the end points, but are unknowns (Fig. 22.7). Thus, we now have a total of four unknowns that must be evaluated, and consequently, we require four conditions to determine them exactly.

Just as for the trapezoidal rule, we can obtain two of these conditions by assuming that Eq. (22.12) fits the integral of a constant and a linear function exactly. Then, to arrive at the other two conditions, we merely extend this reasoning by assuming that it also fits the integral of a parabolic \((y = x^2)\) and a cubic \((y = x^3)\) function. By doing this, we determine all four unknowns and in the bargain derive a linear two-point integration formula that is exact for cubics. The four equations to be solved are

$$c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} 1 \, dx = 2 \hspace{1cm} (22.13)$$

$$c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} x \, dx = 0 \hspace{1cm} (22.14)$$

$$c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} x^2 \, dx = \frac{2}{3} \hspace{1cm} (22.15)$$

$$c_0 f(x_0) + c_1 f(x_1) = \int_{-1}^{1} x^3 \, dx = 0 \hspace{1cm} (22.16)$$

FIGURE 22.7

Graphical depiction of the unknown variables \(x_0\) and \(x_1\) for integration by Gauss quadrature.
Equations (22.13) through (22.16) can be solved simultaneously for
\[
c_0 = c_1 = 1
\]
\[
x_0 = -\frac{1}{\sqrt{3}} = -0.5773503\ldots
\]
\[
x_1 = \frac{1}{\sqrt{3}} = 0.5773503\ldots
\]
which can be substituted into Eq. (22.12) to yield the two-point Gauss-Legendre formula
\[
I \approx f \left( -\frac{1}{\sqrt{3}} \right) + f \left( \frac{1}{\sqrt{3}} \right)
\]  
(22.17)

Thus, we arrive at the interesting result that the simple addition of the function values at \( x = 1/\sqrt{3} \) and \(-1/\sqrt{3}\) yields an integral estimate that is third-order accurate.

Notice that the integration limits in Eqs. (22.13) through (22.16) are from \(-1\) to \(1\). This was done to simplify the mathematics and to make the formulation as general as possible. A simple change of variable can be used to translate other limits of integration into this form. This is accomplished by assuming that a new variable \( x_d \) is related to the original variable \( x \) in a linear fashion, as in
\[
x = a_0 + a_1 x_d
\]  
(22.18)
If the lower limit, \( x = a \), corresponds to \( x_d = -1 \), these values can be substituted into Eq. (22.18) to yield
\[
a = a_0 + a_1 (-1)
\]  
(22.19)
Similarly, the upper limit, \( x = b \), corresponds to \( x_d = 1 \), to give
\[
b = a_0 + a_1 (1)
\]  
(22.20)
Equations (22.19) and (22.20) can be solved simultaneously for
\[
a_0 = \frac{b + a}{2}
\]  
(22.21)
and
\[
a_1 = \frac{b - a}{2}
\]  
(22.22)
which can be substituted into Eq. (22.18) to yield
\[
x = \frac{(b + a) + (b - a)x_d}{2}
\]  
(22.23)
This equation can be differentiated to give
\[
dx = \frac{b - a}{2} dx_d
\]  
(22.24)
Equations (22.23) and (22.24) can be substituted for \( x \) and \( dx \), respectively, in the equation to be integrated. These substitutions effectively transform the integration interval without
changing the value of the integral. The following example illustrates how this is done in practice.

**Example 22.3** Two-Point Gauss-Legendre Formula

**Problem Statement.** Use Eq. (22.17) to evaluate the integral of

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

between the limits \( x = 0 \) to \( 0.8 \). Recall that this was the same problem that we solved in Chap. 21 using a variety of Newton-Cotes formulations. The exact value of the integral is 1.640533.

**Solution.** Before integrating the function, we must perform a change of variable so that the limits are from \(-1\) to \(1\). To do this, we substitute \( a = 0 \) and \( b = 0.8 \) into Eq. (22.23) to yield

\[ x = 0.4 + 0.4x_d \]

The derivative of this relationship is [Eq. (22.24)]

\[ dx = 0.4 \, dx_d \]

Both of these can be substituted into the original equation to yield

\[ \int_{0}^{0.8} (0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5) \, dx \]

\[ = \int_{-1}^{1} [0.2 + 25(0.4 + 0.4x_d) - 200(0.4 + 0.4x_d)^2 + 675(0.4 + 0.4x_d)^3 \]

\[ - 900(0.4 + 0.4x_d)^4 + 400(0.4 + 0.4x_d)^5]0.4 \, dx_d \]

Therefore, the right-hand side is in the form that is suitable for evaluation using Gauss quadrature. The transformed function can be evaluated at \(-1/\sqrt{3}\) to be equal to 0.516741 and at \(1/\sqrt{3}\) to be equal to 1.305837. Therefore, the integral according to Eq. (22.17) is

\[ I \approx 0.516741 + 1.305837 = 1.822578 \]

which represents a percent relative error of \(-11.1\) percent. This result is comparable in magnitude to a four-segment application of the trapezoidal rule (Table 21.1) or a single application of Simpson’s 1/3 and 3/8 rules (Examples 21.4 and 21.6). This latter result is to be expected because Simpson’s rules are also third-order accurate. However, because of the clever choice of base points, Gauss quadrature attains this accuracy on the basis of only two function evaluations.

**22.3.3 Higher-Point Formulas**

Beyond the two-point formula described in the previous section, higher-point versions can be developed in the general form

\[ I \approx c_0 f(x_0) + c_1 f(x_1) + \cdots + c_{n-1} f(x_{n-1}) \]

\[ (22.25) \]
### Table 22.1

<table>
<thead>
<tr>
<th>Points</th>
<th>Weighting Factors</th>
<th>Function Arguments</th>
<th>Truncation Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>$c_0 = 1.0000000$</td>
<td>$x_0 = -0.577350269$</td>
<td>$\approx f^{[8]}[g]$</td>
</tr>
<tr>
<td></td>
<td>$c_1 = 1.0000000$</td>
<td>$x_1 = 0.577350269$</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>$c_0 = 0.5555556$</td>
<td>$x_0 = -0.774596669$</td>
<td>$\approx f^{[10]}[g]$</td>
</tr>
<tr>
<td></td>
<td>$c_1 = 0.8888889$</td>
<td>$x_1 = 0.0$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$c_2 = 0.5555556$</td>
<td>$x_2 = 0.774596669$</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>$c_0 = 0.3478548$</td>
<td>$x_0 = -0.861135312$</td>
<td>$\approx f^{[10]}[g]$</td>
</tr>
<tr>
<td></td>
<td>$c_1 = 0.6521452$</td>
<td>$x_1 = -0.339981044$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$c_2 = 0.6521452$</td>
<td>$x_2 = 0.339981044$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$c_3 = 0.3478548$</td>
<td>$x_3 = 0.861135312$</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>$c_0 = 0.2369269$</td>
<td>$x_0 = -0.906179846$</td>
<td>$\approx f^{[12]}[g]$</td>
</tr>
<tr>
<td></td>
<td>$c_1 = 0.4786287$</td>
<td>$x_1 = -0.538469310$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$c_2 = 0.5688889$</td>
<td>$x_2 = 0.0$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$c_3 = 0.4786287$</td>
<td>$x_3 = 0.538469310$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$c_4 = 0.2369269$</td>
<td>$x_4 = 0.906179846$</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>$c_0 = 0.1713245$</td>
<td>$x_0 = -0.932459514$</td>
<td>$\approx f^{[12]}[g]$</td>
</tr>
<tr>
<td></td>
<td>$c_1 = 0.3607616$</td>
<td>$x_1 = -0.661209336$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$c_2 = 0.4679139$</td>
<td>$x_2 = -0.238619136$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$c_3 = 0.4679139$</td>
<td>$x_3 = 0.238619136$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$c_4 = 0.3607616$</td>
<td>$x_4 = 0.661209336$</td>
<td></td>
</tr>
<tr>
<td></td>
<td>$c_5 = 0.1713245$</td>
<td>$x_5 = 0.932459514$</td>
<td></td>
</tr>
</tbody>
</table>

where $n$ is the number of points. Values for $c$’s and $x$’s for up to and including the six-point formula are summarized in Table 22.1.

### Example 22.4

**Three-Point Gauss-Legendre Formula**

**Problem Statement.** Use the three-point formula from Table 22.1 to estimate the integral for the same function as in Example 22.3.

**Solution.** According to Table 22.1, the three-point formula is

$$ I = 0.5555556 f(-0.7745967) + 0.8888889 f(0) + 0.5555556 f(0.7745967) $$

which is equal to

$$ I = 0.2813013 + 0.8732444 + 0.4859876 = 1.640533 $$

which is exact.

Because Gauss quadrature requires function evaluations at nonuniformly spaced points within the integration interval, it is not appropriate for cases where the function is unknown. Thus, it is not suited for engineering problems that deal with tabulated data. However, where the function is known, its efficiency can be a decided advantage. This is particularly true when numerous integral evaluations must be performed.
EXAMPLE 22.5  Applying Gauss Quadrature to the Falling Parachutist Problem

Problem Statement. In Example 21.3, we used the multiple-application trapezoidal rule to evaluate

\[ d = \frac{gm}{c} \int_0^{10} \left[ 1 - e^{-(c/m)t} \right] dt \]

where \( g = 9.8 \), \( c = 12.5 \), and \( m = 68.1 \). The exact value of the integral was determined by calculus to be 289.4351. Recall that the best estimate obtained using a 500-segment trapezoidal rule was 289.4348 with an \( |\varepsilon| \cong 1.15 \times 10^{-4} \) percent. Repeat this computation using Gauss quadrature.

Solution. After modifying the function, the following results are obtained:

Two-point estimate = 290.0145
Three-point estimate = 289.4393
Four-point estimate = 289.4352
Five-point estimate = 289.4351
Six-point estimate = 289.4351

Thus, the five- and six-point estimates yield results that are exact to seven significant figures.

22.3.4 Error Analysis for Gauss Quadrature

The error for the Gauss-Legendre formulas is specified generally by (Carnahan et al., 1969)

\[ E_t = \frac{2^{2n+3}[(n+1)]!4}{(2n+3)(2n+2)!} f^{(2n+2)}(\xi) \]  \hspace{1cm} (22.26)

where \( n \) = the number of points minus one and \( f^{(2n+2)}(\xi) \) = the \((2n+2)\)th derivative of the function after the change of variable \( \xi \), located somewhere on the interval from \(-1\) to \(1\).

Comparison of Eq. (22.26) with Table 21.2 indicates the superiority of Gauss quadrature to Newton-Cotes formulas, provided the higher-order derivatives do not increase substantially with increasing \( n \). Problem 22.8 at the end of this chapter illustrates a case where the Gauss-Legendre formulas perform poorly. In these situations, the multiple-application Simpson’s rule or Romberg integration would be preferable. However, for many functions confronted in engineering practice, Gauss quadrature provides an efficient means for evaluating integrals.

22.4 IMPROPER INTEGRALS

To this point, we have dealt exclusively with integrals having finite limits and bounded integrands. Although these types are commonplace in engineering, there will be times when improper integrals must be evaluated. In this section, we will focus on one type of improper integral—that is, one with a lower limit of \(-\infty\) or an upper limit of \(+\infty\).

Such integrals usually can be evaluated by making a change of variable that transforms the infinite range of one that is finite. The following identity serves this purpose and works
for any function that decreases toward zero at least as fast as \(1/x^2\) as \(x\) approaches infinity:

\[
\int_a^b f(x) \, dx = \int_{1/a}^{1/b} \frac{1}{t^2} f \left( \frac{1}{t} \right) \, dt
\]

(22.27)

for \(ab > 0\). Therefore, it can be used only when \(a\) is positive and \(b\) is \(\infty\) or when \(a\) is \(-\infty\) and \(b\) is negative. For cases where the limits are from \(-\infty\) to a positive value or from a negative value to \(\infty\), the integral can be implemented in two steps. For example,

\[
\int_{-\infty}^b f(x) \, dx = \int_{-\infty}^{-A} f(x) \, dx + \int_{-A}^b f(x) \, dx
\]

(22.28)

where \(-A\) is chosen as a sufficiently large negative value so that the function has begun to approach zero asymptotically at least as fast as \(1/x^2\). After the integral has been divided into two parts, the first can be evaluated with Eq. (22.27) and the second with a Newton-Cotes closed formula such as Simpson’s 1/3 rule.

One problem with using Eq. (22.27) to evaluate an integral is that the transformed function will be singular at one of the limits. The open integration formulas can be used to circumvent this dilemma as they allow evaluation of the integral without employing data at the end points of the integration interval. To allow the maximum flexibility, a multiple-application version of one of the open formulas from Table 21.4 is required.

Multiple-application versions of the open formulas can be concocted by using closed formulas for the interior segments and open formulas for the ends. For example, the multiple-segment trapezoidal rule and the midpoint rule can be combined to give

\[
\int_{x_0}^{x_n} f(x) \, dx = h \left[ \frac{3}{2} f(x_1) + \sum_{i=2}^{n-2} f(x_i) + \frac{3}{2} f(x_{n-1}) \right]
\]

In addition, semihopen formulas can be developed for cases where one or the other end of the interval is closed. For example, a formula that is open at the lower limit and closed at the upper limit is given as

\[
\int_{x_0}^{x_n} f(x) \, dx = h \left[ \frac{3}{2} f(x_1) + \sum_{i=2}^{n-1} f(x_i) + \frac{1}{2} f(x_n) \right]
\]

Although these relationships can be used, a preferred formula is (Press et al., 1992)

\[
\int_{x_0}^{x_n} f(x) \, dx = h [ f(x_{1/2}) + f(x_{3/2}) + \cdots + f(x_{n-3/2}) + f(x_{n-1/2}) ]
\]

(22.29)

which is called the extended midpoint rule. Notice that this formula is based on limits of integration that are \(h/2\) after and before the first and last data points (Fig. 22.8).

---

**FIGURE 22.8**
Placement of data points relative to integration limits for the extended midpoint rule.
22.4 IMPROPER INTEGRALS

EXAMPLE 22.6 Evaluation of an Improper Integral

Problem Statement. The cumulative normal distribution is an important formula in statistics (see Fig. 22.9):

\[ N(x) = \int_{-\infty}^{x} \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \, dx \]  \hspace{1cm} (E22.6.1)

FIGURE 22.9
(a) The normal distribution, (b) the transformed abscissa in terms of the standardized normal deviate, and (c) the cumulative normal distribution. The shaded area in (a) and the point in (c) represent the probability that a random event will be less than the mean plus one standard deviation.
where \( x = (y - \bar{y}) / s_y \) is called the *normalized standard deviate*. It represents a change of variable to scale the normal distribution so that it is centered on zero and the distance along the abscissa is measured in multiples of the standard deviation (Fig. 22.9b).

Equation (E22.6.1) represents the probability that an event will be less than \( x \). For example, if \( x = 1 \), Eq. (E22.6.1) can be used to determine that the probability that an event will occur that is less than one standard deviation above the mean is \( N(1) = 0.8413 \). In other words, if 100 events occur, approximately 84 will be less than the mean plus one standard deviation. Because Eq. (E22.6.1) cannot be evaluated in a simple functional form, it is solved numerically and listed in statistical tables. Use Eq. (22.28) in conjunction with Simpson's 1/3 rule and the extended midpoint rule to determine \( N(1) \) numerically.

**Solution.** Equation (E22.6.1) can be reexpressed in terms of Eq. (22.28) as

\[
N(x) = \frac{1}{\sqrt{2\pi}} \left( \int_{-\infty}^0 e^{-x^2/2} \, dx + \int_0^1 e^{-x^2/2} \, dx \right)
\]

The first integral can be evaluated by applying Eq. (22.27) to give

\[
\int_{-\infty}^0 e^{-x^2/2} \, dx = \int_{-1/2}^0 \frac{1}{t^2} e^{-1/(2t^2)} \, dt
\]

Then the extended midpoint rule with \( h = 1/8 \) can be employed to estimate

\[
\int_{-1/2}^0 \frac{1}{t^2} e^{-1/(2t^2)} \, dt \approx \frac{1}{8} \left[ f(x_{-7/16}) + f(x_{-5/16}) + f(x_{-3/16}) + f(x_{-1/16}) \right]
\]

\[
= \frac{1}{8} [0.3833 + 0.0612 + 0 + 0] = 0.0556
\]

Simpson's 1/3 rule with \( h = 0.5 \) can be used to estimate the second integral as

\[
\int_{-1/2}^1 e^{-x^2/2} \, dx
\]

\[
= \left[ 1 - (-2) \right] \frac{0.1353 + 4(0.3247 + 0.8825 + 0.8825) + 2(0.6065 + 1) + 0.6065}{3(6)}
\]

\[
= 2.0523
\]

Therefore, the final result can be computed as

\[
N(1) \approx \frac{1}{\sqrt{2\pi}} (0.0556 + 2.0523) = 0.8409
\]

which represents an error of \( \varepsilon_t = 0.046 \) percent.

The foregoing computation can be improved in a number of ways. First, higher-order formulas could be used. For example, a Romberg integration could be employed. Second, more points could be used. Press et al. (1986) explore both options in depth.

Aside from infinite limits, there are other ways in which an integral can be improper. Common examples include cases where the integral is singular at either the limits or at a point within the integral. Press et al. (1986) provide a nice discussion of ways to handle these situations.
PROBLEMS

22.1 Use Romberg integration to evaluate
\[ \int_1^2 (x + 1/x)^2 \, dx \]
to an accuracy of \( \varepsilon_i = 0.5\% \). Your results should be presented in the form of Fig. 22.3. Use the true value of 4.8333 to determine the true error \( \varepsilon_t \) of the result obtained with Romberg integration. Check that \( \varepsilon_t \) is less than the stopping criterion \( \varepsilon_i \).

22.2 Use order of \( h^3 \) Romberg integration to evaluate
\[ \int_0^3 xe^{x^2} \, dx \]
Compare \( \varepsilon_t \) and \( \varepsilon_i \).

22.3 Use Romberg integration to evaluate
\[ \int_0^1 \frac{\sin x}{1 + x^2} \, dx \]
to an accuracy of the order of \( h^3 \). Your results should be presented in the form of Fig. 22.3.

22.4 Obtain an estimate of the integral from Prob. 22.1, but using two-, three-, and four-point Gauss-Legendre formulas. Compute \( \varepsilon_t \) for each case on the basis of the analytical solution.

22.5 Obtain an estimate of the integral from Prob. 22.2, but using two-, three-, and four-point Gauss-Legendre formulas. Compute \( \varepsilon_t \) for each case on the basis of the analytical solution.

22.6 Obtain an estimate of the integral from Prob. 22.3 using six-point Gauss-Legendre formulas.

22.7 Perform the computation in Examples 22.3 and 22.5 for the falling parachutist, but use Romberg integration (\( \varepsilon_i = 0.01\% \)).

22.8 Employ two- through six-point Gauss-Legendre formulas to solve
\[ \int_{-1}^1 \frac{2}{1 + 2x^2} \, dx \]
Interpret your results in light of Eq. (22.26).

22.9 Use numerical integration to evaluate the following:

(a) \[ \int_1^\infty \frac{dx}{x(x + 2)} \]

(b) \[ \int_0^\infty e^{-y} \sin y \, dy \]

(c) \[ \int_0^\infty \frac{1}{(1 + y^2)(1 + y^2/2)} \, dy \]

(d) \[ \int_{-2}^2 ye^{-y} \, dy \]

(e) \[ \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi}} e^{-x^2} \, dx \]

Note that (d) is the normal distribution (recall Fig. 22.9).

22.10 Develop a user-friendly computer program for the multiple-segment trapezoidal and Simpson’s 1/3 rule based on Fig. 22.1. Test it by integrating
\[ \int_0^1 x^{6/3} \left( (1 - x) \left( 1 - e^{2(x-1)} \right) \right) \, dx \]
Use the true value of 0.602297 to compute \( \varepsilon_t \) for \( n = 4 \).

22.11 Develop a user-friendly computer program for Romberg integration based on Fig. 22.4. Test it by duplicating the results of Examples 22.3 and 22.4 and the function in Prob. 22.10.

22.12 Develop a user-friendly computer program for Gauss quadrature. Test it by duplicating the results of Examples 22.3 and 22.4 and the function in Prob. 22.10.

22.13 Use the program developed in Prob. 22.11 to solve Probs. (a) 22.1, (b) 22.2, and (c) 22.3.

22.14 Use the program developed in Prob. 22.12 to solve Probs. (a) 22.4, (b) 22.5, and (c) 22.6.

22.15 Develop a program to implement the extended midpoint rule iteratively. Start the iterations with an initial estimate based on a single point and the midpoint rule from Table 21.4. Then successively apply Eq. (22.29) with the interval divided by 3 at each stage, that is, \( h = (b - a)/3, (b - a)/9, (b - a)/27, \) etc. Note that this means that one-third of the function estimates will have been determined in the previous iteration. Develop your algorithm so that it capitalizes on this property. Perform iterations until an approximate error estimate \( \varepsilon_t \) falls below a prespecified stopping criteria \( \varepsilon_i \). Test the program by evaluating Example 22.6.