

Chapter 4

Numerical Integration

Numerical integration is a primary tool used by engineers and scientists to obtain approximate answers for definite integrals that cannot be solved analytically. In the area of statistical thermodynamics, the Debye model for calculating the heat capacity of a solid involves the following function;

$$\Phi(x) = \int_0^x \frac{t^3}{e^t - 1} dt.$$

Since there is no analytic expression for $\Phi(x)$, numerical integration must be used to obtain approximate values. For example, the value $\Phi(5)$ is the area under the curve

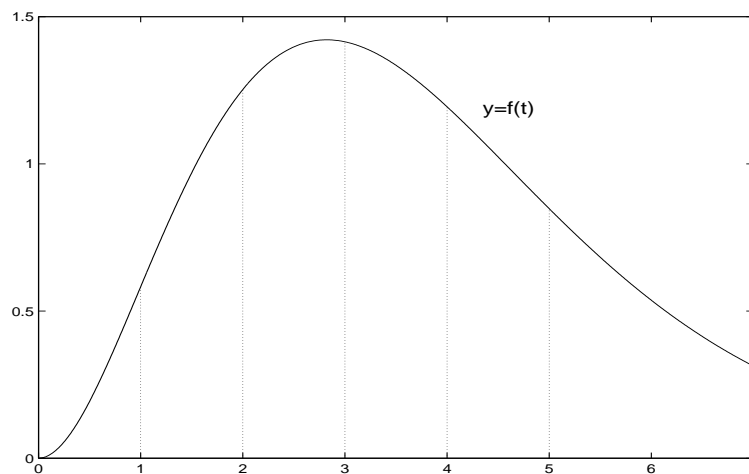


Figure 4.1 The area under the curve $y = f(t)$ for $0 \leq t \leq 5$.

Figure 4.1 Values of $\Phi(x)$

x	$\Phi(x)$
1.0	0.2248052
2.0	1.1763426
3.0	2.5522185
4.0	3.8770542
5.0	4.8998922
6.0	5.5858554
7.0	6.0031690
8.0	6.2396238
9.0	6.3665739
10.0	6.4319219

$y = f(t) = t^3/(e^t - 1)$ for $0 \leq t \leq 5$ (see Figure 4.1). The numerical approximation for $\Phi(5)$ is

$$\Phi(5) = \int_0^5 \frac{t^3}{e^t - 1} dt \approx 4.8998922.$$

Each additional value of $\Phi(x)$ must be determined by another numerical integration. Table 4.1 lists several of these approximations over the interval $[1, 10]$.

The purpose of this chapter is to develop the basic principles of numerical integration. In Chapter 9, numerical integration formulas are used to derive the predictor-corrector methods for solving differential equations.

4.1 Introduction to Quadrature

We now approach the subject of numerical integration. The goal is to approximate the definite integral of $f(x)$ over the interval $[a, b]$ by evaluating $f(x)$ at a finite number of sample points.

Definition 4.1 Suppose that $a = x_0 < x_1 < \cdots < x_M = b$. A formula of the form

$$Q[f] = \sum_{k=0}^M w_k f(x_k) = w_0 f(x_0) + w_1 f(x_1) + \cdots + w_M f(x_M) \quad (4.1)$$

with the property that

$$\int_a^b f(x) dx = Q[f] + E[f] \quad (4.2)$$

is called a numerical integration or **quadrature** formula. The term $E(f)$ is called the truncation error for integration. The values $\{x_k\}_{k=0}^M$ are called the **quadrature nodes**, and $\{w_k\}_{k=0}^M$ are called the **weights**.

Depending on the application, the nodes $\{x_k\}$ are chosen in various ways. For the trapezoidal rule, Simpson's rule, and Boole's rule, the nodes are chosen to be equally spaced. For Gauss-Legendre quadrature, the nodes are chosen to be zeros of certain Legendre polynomials. When the integration formula is used to develop a predictor formula for differential equations, all the nodes are chosen less than b . For all application, it is necessary to know something about the accuracy of the numerical solution.

Definition 4.2. The **degree of precision** of a quadrature formula is the positive integer n such that $E[P_i] = 0$ for all polynomials $P_i(x)$ of degree $i \leq n$, but for which $E[P_{n+1}] \neq 0$ for some polynomial $P_{n+1}(x)$ of degree $n + 1$.

The form of $E[P_i]$ can be anticipated by studying what happens when $f(x)$ is a polynomial. Consider the arbitrary polynomial

$$P_i(x) = a_i x^i + x_{i-1} x^{i-1} + \cdots + a_1 x + a_0$$

of degree i . If $i \leq n$, then $P_i^{(n+1)}(x) \equiv 0$ for all x , and $P_{n+1}^{(n+1)}(x) = (n+1)! a_{n-1}$ for all x . Thus it is not surprising that the general form for the truncation error term is

$$E[f] = K f^{(n+1)}(c), \tag{4.3}$$

where K is a suitably chosen constant and n is the degree of precision. The proof of this general result can be found in advanced books on numerical integration.

The derivation of quadrature formulas is sometimes based on polynomial interpolation. Recall that there exists a unique polynomial $P_M(x)$ of degree $\leq M$ passing through the $M + 1$ equally spaced points $\{(x_k, y_k)\}_{k=0}^M$. When this polynomial is used to approximate $f(x)$, over $[a, b]$, and then the integral of $f(x)$ is approximated by the integral of $P_M(x)$, the resulting formula is called a **Newton-Cotes quadrature formula** (see Figure 2.2). When the sample points $x_0 = a$ and $x_M = b$ are used, it is called a **closed** Newton-Cotes formula. The next result gives the formulas when approximating polynomials of degree $M = 1, 2, 3$, and 4 are used.

Theorem 4.1 (Closed Newton-Cotes Quadrature Formula). Assume that $x_k = x_0 + kh$ are equally spaced nodes and $f_k = f(x_k)$. The first four closed Newton-Cotes

quadrature formulas are

$$\int_{x_0}^{x_1} f(x)dx \approx \frac{h}{2}(f_0 + f_1) \quad (\text{the trapezoidal rule}), \quad (4.4)$$

$$\int_{x_0}^{x_2} f(x)dx \approx \frac{h}{3}(f_0 + 4f_1 + f_2) \quad (\text{Simpson's rule}), \quad (4.5)$$

$$\int_{x_0}^{x_3} f(x)dx \approx \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3) \quad (\text{Simpson's } \frac{3}{8}\text{rule}), \quad (4.6)$$

$$\int_{x_0}^{x_4} f(x)dx \approx \frac{2h}{45}(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4) \quad (\text{Boole's rule}). \quad (4.7)$$

Figure 2.2 (a) The trapezoidal rule integrates (b) Simpson's rule integrates (c) Simpson's rule integrates (d) Boole's rule integrates

Corollary 4.1 (Newton-Cotes Precision). Assume that $f(x)$ is sufficiently differentiable; then $E[f]$ for Newton-Cotes quadrature involves an appropriate higher derivative. The trapezoidal rule has degree of precision $n = 1$. If $f \in C^2[a, b]$, then

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f_0 + f_1) - \frac{h^3}{12}f^{(2)}(c). \quad (4.8)$$

Simpson's rule has degree of precision $n = 3$. If $f \in C^4[a, b]$, then

$$\int_{x_0}^{x_2} f(x) dx = \frac{h}{3}(f_0 + 4f_1 + f_2) - \frac{h^5}{90}f^{(4)}(c). \quad (4.9)$$

Simpson's $\frac{3}{8}$ rule has degree of precision $n = 3$. If $f \in C^4[a, b]$, then

$$\int_{x_0}^{x_3} f(x) dx = \frac{3h}{8}(f_0 + 3f_1 + 3f_2 + f_3) - \frac{3h^5}{80}f^{(4)}(c). \quad (4.10)$$

Boole's rule has degree of precision $n = 5$, If $f \in C^6[a, b]$, then

$$\int_{x_0}^{x_4} f(x) dx = \frac{2h}{45}(7f_0 + 32f_1 + 12f_2 + 32f_3 + 7f_4) - \frac{8h^7}{945}f^{(6)}(c). \quad (4.11)$$

Proof of Theorem 4.1. Start with the Lagrange polynomial $P_M(x)$ based on x_0, x_1, \dots, x_M that can be used to approximate $f(x)$:

$$f(x) \approx P_M(x) = \sum_{k=0}^M f_k L_{M,k}(x), \quad (4.12)$$

where $f_k = f(x_k)$ for $k = 0, 1, \dots, M$. An approximation for the integral is obtained by replacing the integrand $f(x)$ with the polynomial $P_M(x)$. This is the general method for obtaining a Newton-Cotes integration formula:

$$\begin{aligned} \int_{x_0}^{x_M} f(x) dx &\approx \int_{x_0}^{x_M} P_M(x) dx \\ &= \int_{x_0}^{x_M} \left(\sum_{k=0}^M f_k L_{M,k}(x) \right) dx = \sum_{k=0}^M \left(\int_{x_0}^{x_M} f_k L_{M,k}(x) dx \right) \\ &= \sum_{k=0}^M \left(\int_{x_0}^{x_M} L_{M,k}(x) dx \right) f_k = \sum_{k=0}^M w_k f_k. \end{aligned} \quad (4.13)$$

The details for the general computations of coefficients of w_k in (4.13) are tedious. We shall give a sample proof of Simpson's rule, which is the case $M = 2$. This case involves the approximating polynomial

$$P_2(x) = f_0 \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} + f_1 \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} + f_2 \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)}. \quad (4.14)$$

Since f_0, f_1 , and f_2 are constants with respect to integration, the relations in (4.13) lead to

$$\begin{aligned} \int_{x_0}^{x_2} f(x)dx &\approx f_0 \int_{x_0}^{x_2} \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} dx \\ &+ f_1 \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} dx + f_2 \int_{x_0}^{x_2} \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} dx \end{aligned} \quad (4.15)$$

We introduce the change of variable $x = x_0 + ht$ with $dx = hdt$ to assist with the evaluation of the integrals in (4.15). The new limits of integration are from $t = 0$ to $t = 2$. The equal spacing of the nodes $x_k = x_0 + kh$ leads to $x_k - x_j = (k - j)h$ and $x - x_k = h(t - k)$, which are used to simplify (4.15) and get

$$\begin{aligned} \int_{x_0}^{x_2} f(x)dx &\approx f_0 \int_0^2 \frac{h(t-1)h(t-2)}{(-h)(-2h)} hdt + f_1 \int_0^2 \frac{h(t-0)h(t-2)}{(h)(-h)} hdt \\ &+ f_2 \int_0^2 \frac{h(t-0)h(t-1)}{(2h)(h)} hdt \\ &= f_0 \frac{h}{2} \int_0^2 (t^2 - 3t + 2)dt - f_1 h \int_0^2 (t^2 - 2t)dt + f_2 \frac{h}{2} \int_0^2 (t^2 - t)dt \\ &= f_0 \frac{h}{2} \left(\frac{t^3}{3} - \frac{3t^2}{2} + 2t \right) \Big|_{t=0}^{t=2} - f_1 h \left(\frac{t^3}{3} - t^2 \right) \Big|_{t=0}^{t=2} \\ &+ f_2 \frac{h}{2} \left(\frac{t^3}{3} - \frac{t^2}{2} \right) \Big|_{t=0}^{t=2} \\ &= f_0 \frac{h}{2} \left(\frac{2}{3} \right) - f_1 h \left(\frac{-4}{3} \right) + f_2 \frac{h}{2} \left(\frac{2}{3} \right) \\ &= \frac{h}{3} (f_0 + 4f_1 + f_2). \end{aligned} \quad (4.16)$$

and the proof is complete. We postpone a sample proof of Corollary 4.1 until Section 4.2.

Example 2.1. Consider the function $f(x) = 1 + e^{-x} \sin(4x)$, the equally spaced spaced quadrature nodes $x_0 = 0.0, x_1 = 0.5, x_2 = 1.0, x_3 = 1.5$, and $x_4 = 2.0$, and the corresponding function values $f_0 = 1.00000, f_2 = 0.72159, f_3 = 0.93765$, and $f_4 = 1.13390$. Apply the various quadrature formulas (2.4) through (2.7).

The step size is $h = 0.5$, and the computations are

$$\begin{aligned}\int_0^{0.5} f(x)dx &\approx \frac{0.5}{2}(1.00000 + 1.55152) = 0.63788 \\ \int_0^{1.0} f(x)dx &\approx \frac{0.5}{3}(1.00000 + 4(1.55152) + 0.72159) = 1.32128 \\ \int_0^{1.5} f(x)dx &\approx \frac{3(0.5)}{8}(1.00000 + 3(1.55152) + 3(0.72159) + 0.93765) \\ &= 1.64193 \\ \int_0^{2.0} f(x)dx &\approx \frac{2(0.5)}{45}(7(1.00000) + 32(1.55152) + 12(0.72159) \\ &\quad + 32(0.93765) + 7(1.13390)) = 1.29444.\end{aligned}$$

It is important to realize that the quadrature formulas (4.4) through (4.7) applied in the above illustration give approximations for definite integrals over different intervals. The graph of the curve $y = f(x)$ and the areas under the Lagrange polynomials $y = P_1(x)$, $y = P_2(x)$, $y = P_3(x)$, and $P_4(x)$ are shown in Figure 4.2 (a) through (d), respectively.

In Example 4.1 we applied the quadrature rules with $h = 0.5$. If the endpoints of the interval $[a, b]$ are held fixed, the step size must be adjusted for each rule. The step sizes are $h = b - a$, $h = (b - a)/2$, $h = (b - a)/3$, and $h = (b - a)/4$ for the trapezoidal rule, Simpson's rule, Simpson's $\frac{3}{8}$ rule, and Boole's rule, respectively. The next example illustrates this point.

Example 2.2 Consider the integration of the function $f(x) = 1 + e^{-x} \sin(4x)$ over the fixed interval $[a, b] = [0, 1]$. Apply the various formulas (4.4) through (4.7).

For the trapezoidal rule, $h = 1$ and

$$\begin{aligned}\int_0^1 f(x)dx &\approx \frac{1}{2}(f(0) + f(1)) \\ &= \frac{1}{2}(1.00000 + 0.72159) = 0.86079.\end{aligned}$$

For Simpson's rule, $h = 1/2$, we get

$$\begin{aligned}\int_0^1 f(x)dx &\approx \frac{1/2}{3}(f(0) + 4f(1/2) + f(1)) \\ &= \frac{1}{6}(1.00000 + 4(1.55152) + 0.72159) = 1.32128.\end{aligned}$$

For Simpson's $\frac{3}{8}$ rule, $h = 1/3$, and we obtain

$$\int_0^1 f(x)dx \approx \frac{3(1/3)}{8}(f(0) + 3f(\frac{1}{3}) + 3f(\frac{2}{3}) + f(1))$$

$$= \frac{1}{8}(1.00000 + 3(1.69642) + 3(1.23447) + 0.72159) = 1.31440.$$

For Boole's rule, $h = 1/4$, and the result is

$$\begin{aligned} \int_0^1 f(x)dx &\approx \frac{2(1/4)}{45}(7f(0) + 32f(\frac{1}{4}) + 12f(\frac{1}{2}) + 32f(\frac{3}{4}) + 7f(1)) \\ &= \frac{1}{90}(7(1.00000) + 32(1.65534) + 12(1.55152) \\ &\quad + 32(1.06666) + 7(0.72159)) = 1.30859. \end{aligned}$$

The true value of the definite integral is

$$\int_0^1 f(x)dx = \frac{21e - 4 \cos(4) - \sin(4)}{17e} = 1.3082506046426 \dots,$$

and the approximation 1.30859 from Boole's rule is best, the area under each of the Lagrange polynomials $P_1(x)$, $P_2(x)$, $P_3(x)$, and $P_4(x)$ is shown in Figure 2.3(a) through (d), respectively.

Figure 2.3 (a) the trapezoidal rule used over $[0,1]$ yields the approximation 0.86079 (b) simpson's rule used over $[0,1]$ yields the approximation 1.32128. (c) simpson's rule used over $[0,1]$ yields the approximation 1.31440. [d] boole's rule used over $[0,1]$ yields the approximation 1.30859.

To make a fair comparison of quadrature methods, we must use the same number of function evaluations in each method. Our final example is concerned with comparing integration over a fixed interval $[a, b]$ using exactly five function evaluations $f_k = f(x_k)$, for $k = 0, 1, \dots, 4$ for each method. When the trapezoidal rule is applied on the four subintervals $[x_0, x_1]$, $[x_1, x_2]$, $[x_2, x_3]$, and $[x_3, x_4]$, it is called a **composite trapezoidal rule**:

$$\begin{aligned} \int_{x_0}^{x_4} f(x)dx &= \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \int_{x_2}^{x_3} f(x)dx + \int_{x_3}^{x_4} f(x)dx \\ &\approx \frac{h}{2}(f_0 + f_1) + \frac{h}{2}(f_1 + f_2) + \frac{h}{2}(f_2 + f_3) + \frac{h}{2}(f_3 + f_4) \\ &= \frac{h}{2}(f_0 + 2f_1 + 2f_2 + 2f_3 + f_4). \end{aligned} \tag{4.17}$$

Simpson's rule can also be used in this manner. When Simpson's rule is applied on the two subintervals $[x_0, x_2]$ and $[x_2, x_4]$, it is called a **composite Simpson's rule**:

$$\begin{aligned} \int_{x_0}^{x_4} f(x)dx &= \int_{x_0}^{x_2} f(x)dx + \int_{x_2}^{x_4} f(x)dx \\ &\approx \frac{h}{3}(f_0 + 4f_1 + f_2) + \frac{h}{3}(f_2 + 4f_3 + f_4) \end{aligned} \tag{4.18}$$

$$= \frac{h}{3}(f_0 + 4f_1 + 2f_2 + 4f_3 + f_4)$$

The next example compares the values obtained with (2.17), (2.18), and (2.7).

Example 2.3. Consider the integration of the function $f(x) = 1 + e^{-x} \sin(4x)$ over $[a, b] = [0, 1]$. Use exactly five function evaluations and compare the results from the composite trapezoidal rule, composite Simpson rule, and Boole's rule.

The uniform step size is $h = 1/4$. The composite trapezoidal rule (2.17) produces

$$\begin{aligned} \int_0^1 f(x)dx &\approx \frac{1/4}{2}(f(0) + 2f(\frac{1}{4}) + 2f(\frac{1}{2}) + 2f(\frac{3}{4}) + f(1)) \\ &= \frac{1}{8}(1.00000 + 2(1.65534) + 2(1.55152) + 2(1.06666) + 0.72159) \\ &= 1.28358 \end{aligned}$$

Using the composite Simpson's rule (2.18), we get

$$\begin{aligned} \int_0^1 f(x)dx &\approx \frac{1/4}{3}(f(0) + 4f(\frac{1}{4}) + 2f(\frac{1}{2}) + 4f(\frac{3}{4}) + f(1)) \\ &= \frac{1}{12}(1.00000 + 4(1.65534) + 2(1.55152) + 4(1.06666) + 0.72159) \\ &= 1.30938 \end{aligned}$$

We have already seen the result of Boole's rule in Example 7.2:

$$\begin{aligned} \int_0^1 f(x)dx &\approx \frac{2(1/4)}{45}(7f(0) + 32f(\frac{1}{4}) + 12f(\frac{1}{2}) + 32f(\frac{3}{4}) + 7f(1)) \\ &= 1.30859. \end{aligned}$$

Figure 2.4 (a) the composite trapezoidal rule yields the approximation 1.28358. (b) the composite Simpson rule yields the approximation 1.30938.

The true value of the integral is

$$\int_0^1 f(x)dx = \frac{21e - 4 \cos(4) - \sin(4)}{17e} = 1.30825046426 \dots,$$

and the approximation 1.30938 from Simpson's rule is much better than the value 1.28358 obtained from the trapezoidal rule. Again, the approximation 1.30859 from Boole's rule is closest. Graphs for the areas under the trapezoids and parabolas are shown in Figure 2.4(a) and (b), respectively.

Example 2.4 determine the degree of precision of Simpson's $\frac{3}{8}$ rule.

It will suffice to apply Simpson's $\frac{3}{8}$ rule over the interval $[0, 3]$ with the five test functions $f(x) = 1, x, x^2, x^3$ and x^4 . For the first four functions, Simpson's $\frac{3}{8}$ rule is exact.

$$\begin{aligned}\int_0^3 1 dx &= 3 = \frac{3}{8}(1 + 3(1) + 3(1) + 1) \\ \int_0^3 x dx &= \frac{9}{2} = \frac{3}{8}(0 + 3(1) + 3(2) + 3) \\ \int_0^3 x^2 dx &= 9 = \frac{3}{8}(0 + 3(1) + 3(4) + 9) \\ \int_0^3 x^3 dx &= \frac{81}{4} = \frac{3}{8}(0 + 3(1) + 3(8) + 27).\end{aligned}$$

The function $f(x) = x^4$ is the lowest power of x for which the rule is not exact.

$$\int_0^3 x^4 dx = \frac{243}{5} \approx \frac{99}{2} = \frac{3}{8}(0 + 3(1) + 3(16) + 81).$$

Therefore, the degree of precision of Simpson's $\frac{3}{8}$ rule is $n = 3$.

4.1.1 Exercises for introduction to quadrature

1. Consider integration of $f(x)$ over the fixed interval $[a, b] = [0, 1]$. Apply the various quadrature formulas (4) through (7). The step sizes are $h = 1, h = \frac{1}{2}, h = \frac{1}{3}$, and $h = \frac{1}{4}$ for the trapezoidal rule, Simpson's rule, Simpson's $\frac{3}{8}$ rule, and Boole's rule, respectively.

- (a) $f(x) = \sin(\pi x)$
- (b) $f(x) = 1 + e^{-x} \cos(4x)$
- (c) $f(x) = \sin(\sqrt{x})$

Remark. The true values of the definite integrals are (a) $2/\pi = 0.636619772367\dots$, (b) $18e - \cos(4) + 4 \sin(4)/(17e) = -1.007459631397\dots$, and (c) $2(\sin(1) - \cos(1)) = 0.602337357879\dots$. Graphs of the functions are shown in Figures 2.5(a) through (c), respectively.

2. Consider integration of over the fixed interval $[a, b]=[0, 1]$. Apply the various quadrature formulas; the composite trapezoidal rule (2.17), the composite Simpson rule (2.18), and Boole's rule (2.7). Use five function evaluations at equally spaced nodes. The uniform step size is $h = \frac{1}{4}$.

- (a) $f(x) = \sin(\pi x)$
- (b) $f(x) = 1 + e^{-x} \cos(4x)$
- (c) $f(x) = \sin(\sqrt{x})$

3. Consider a general interval $[a, b]$. Show that Simpson's rule produces exact results for the functions $f(x) = x^2$ and $f(x) = x^3$; that is,

$$\text{(a)} \int_a^b x^2 dx = \frac{b^3}{3} - \frac{a^3}{3} \quad \text{(b)} \int_a^b x^3 dx = \frac{b^4}{4} - \frac{a^4}{4}$$

4. Integrate the Lagrange interpolation polynomial

$$P_1(x) = f_0 \frac{x - x_1}{x_0 - x_1} + f_1 \frac{x - x_0}{x_1 - x_0}$$

over the interval $[x_0, x_1]$ and establish the trapezoidal rule.

Figure 7.5

5. Determine the degree of precision of the trapezoidal rule. It will suffice to apply the trapezoidal rule over $[0, 1]$ with the three test functions $f(x) = 1, x,$ and x^2 .

6. Determine the degree of precision of Simpson's rule. It will suffice to apply Simpson's rule over $[0, 2]$ with the five test functions $f(x) = 1, x, x^2, x^3,$ and x^4 . Contrast your result with the degree of precision of Simpson's $\frac{3}{8}$ rule.

7. Determine the degree of precision of Boole's rule. It will suffice to apply Boole's rule over $[0, 4]$ with the seven test functions $f(x) = 1, x, x^2, x^3, x^4, x^5,$ and x^6 .

8. The intervals in exercises 5, 6, and 7 and Example 2.4 were selected to simplify the calculation of the quadrature nodes. But, on any closed interval $[a, b]$ over which the function f is integrable, each of the four quadrature rules (2.4) through (2.7) has the degree of precision determined in Exercises 5, 6, and 7 and Example 2.4, respectively. A quadrature formula on the interval $[a, b]$ can be obtained from a quadrature formula on the interval $[c, d]$ by making a change of variables with the linear function

$$x = g(t) = \frac{b - a}{d - c}t + \frac{ad - bc}{d - c}.$$

where $dx = \frac{b-a}{d-c}dt$.

(a) Verify that $x = g(t)$ is the line passing through the points (c, a) and (d, b) .

(b) Verify that the trapezoidal rule has the same degree of precision on the interval $[a, b]$ as on the interval $[0, 1]$.

(c) Verify that Simpson's rule has the same degree of precision on the interval $[a, b]$ as on the interval $[0, 2]$.

(d) Verify that Simpson's rule has the same degree of precision on the interval $[a, b]$ as on the interval $[0, 4]$.

9. Derive Simpson's rule using Lagrange polynomial interpolation. *Hint.* After changing the variable, integrals similar to those in (2.16) are obtained:

$$\begin{aligned} \int_{x_0}^{x_3} f(x)dx &\approx -f_0 \frac{h}{6} \int_0^3 (t-1)(t-2)(t-3)dt + f_1 \frac{h}{2} \int_0^3 (t-0)(t-2)(t-3)dt \\ &\quad - f_2 \frac{h}{2} \int_0^3 (t-0)(t-1)(t-3)dt + f_3 \frac{h}{6} \int_0^3 (t-0)(t-1)(t-2)dt \\ &= f_0 \frac{h}{2} \left(\frac{t^4}{4} + 2t^3 - \frac{11t^2}{2} + 6t \right) \Big|_{t=0}^{t=3} + f_1 \frac{h}{2} \left(\frac{t^4}{4} - \frac{5t^3}{3} + 3t^2 \right) \Big|_{t=0}^{t=3} \end{aligned}$$

$$+ f_2 \frac{h}{2} \left(\frac{-t^4}{4} + \frac{4t^3}{3} - \frac{3t^2}{2} \right) \Big|_{t=0}^{t=3} + f_3 \frac{h}{6} \left(\frac{t^4}{4} - t^3 + t^2 \right) \Big|_{t=0}^{t=3}$$

10. Derive the closed Newton-Cotes quadrature formula, based on a Lagrange approximating polynomial of degree 5, using the 6 equally spaced nodes $x_k = x_0 + kh$, where $k = 0, 1, \dots, 5$.

11. In the proof of Theorem 2.1. Simpson's rule was derived by integrating the second-degree Lagrange polynomial based on the three equally spaced nodes x_0, x_1 , and x_2 . Derive Simpson's rule by integrating the second-degree Newton polynomial based on the three equally spaced nodes x_0, x_1 , and x_2 .

4.2 Composite Trapezoidal and Simpson's Rule

An intuitive method of finding the area under the curve $y = f(x)$ over $[a, b]$ is by approximating that area with a series of trapezoids that lie above the intervals $\{[x_k, x_{k+1}]\}$.

Theorem 2.2 (Composite Trapezoidal Rule). Suppose that the interval $[a, b]$ is subdivided into M subintervals $[x_k, x_{k+1}]$ of width $h = (b - a)/M$ by using the equally spaced nodes $x_k = a + kh$, for $k = 0, 1, \dots, M$. The **composite trapezoidal rule for M subintervals** can be expressed in any of three equivalent ways:

$$T(f, h) = \frac{h}{2} \sum_{k=1}^M (f(x_{k-1}) + f(x_k)) \quad (4.19)$$

or

$$T(f, h) = \frac{h}{2} (f_0 + 2f_1 + 2f_2 + 2f_3 + \dots + 2f_{M-2} + 2f_{M-1} + f_M) \quad (4.20)$$

or

$$T(f, h) = \frac{h}{2} (f(a) + f(b)) + h \sum_{k=1}^{M-1} f(x_k). \quad (4.21)$$

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

$$\int_a^b f(x) dx \approx T(f, h). \quad (4.22)$$

Proof. Apply the trapezoidal rule over each subinterval $[x_{k-1}, x_k]$ (see Figure 2.6). Use the additive property of the integral for subintervals:

$$\int_a^b f(x) dx = \sum_{k=1}^M \int_{x_{k-1}}^{x_k} f(x) dx \approx \sum_{k=1}^M \frac{h}{2} (f(x_{k-1}) + f(x_k)). \quad (4.23)$$

Since $h/2$ is a constant, the distributive law of addition can be applied to obtain (2.19). Formula (2.20) is the expanded version of (2.19). Formula (2.21) shows how to group all the intermediate terms in (2.20) that are multiplied by 2.

Approximating $f(x) = 2 + \sin(2\sqrt{x})$ with piecewise linear polynomials results in places where the approximating is close and places where it is not. To achieve accuracy the composite trapezoidal rule must be applied with many subintervals. In the next example we have chosen to numerically integrate this function over the interval $[1, 6]$. Investigation of the integral over $[0, 1]$ is left as an exercise.

Example 2.5. Consider $f(x) = 2 + \sin(2\sqrt{x})$. Use the composite trapezoidal rule with 11 sample points to compute an approximation to the integral of $f(x)$ taken over $[1, 6]$.

To generate 11 sample points, we use $M = 10$ and $h = (6 - 1)/10 = 1/2$. Using formula (2.21), the computation is

$$\begin{aligned} T(f, \frac{1}{2}) &= \frac{1/2}{2}(f(1) + f(6)) \\ &+ \frac{1}{2} \left(f(\frac{3}{2}) + f(2) + f(\frac{5}{2}) + f(3) + f(\frac{7}{2}) + f(4) + f(\frac{9}{2}) + f(5) + f(\frac{11}{2}) \right) \\ &= \frac{1}{4}(2.90929743 + 1.01735756) \\ &+ \frac{1}{2}(2.63815764 + 2.30807174 + 1.97931647 + 1.68305284 + 1.43530410 \\ &+ 1.24319750 + 1.10831775 + 1.02872220 + 1.00024140) \\ &= \frac{1}{4}(3.92665499) + \frac{1}{2}(14.42438165) \\ &= 0.98166375 + 7.21219083 = 8.19385457. \end{aligned}$$

Theorem 2.3 (Composite Simpson Rule). Suppose that $[a, b]$ is subdivided into $2M$ subintervals $[x_k, x_{k+1}]$ of equal width $h = (b - a)/(2M)$ by using $x_k = a + kh$ for $k = 0, 1, \dots, 2M$. The *composite Simpson rule for $2M$ subintervals* can be expressed in any of three equivalent ways:

$$S(f, h) = \frac{h}{3} \sum_{k=1}^M (f(x_{2k-2}) + 4f(x_{2k-1}) + f(x_{2k})) \quad (4.24)$$

or

$$S(f, h) = \frac{h}{3}(f_0 + 4f_1 + 2f_2 + 4f_3 + \dots + 2f_{2M-2} + 4f_{2M-1} + f_{2M}) \quad (4.25)$$

or

$$S(f, h) = \frac{h}{3}(f(a) + f(b)) + \frac{2h}{3} \sum_{k=1}^{M-1} f(x_{2k}) + \frac{4h}{3} \sum_{k=1}^M f(x_{2k-1}). \quad (4.26)$$

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

$$\int_a^b f(x)dx \approx S(f, h). \quad (4.27)$$

Proof. Apply Simpson's rule over each subinterval $[x_{2k-2}, x_{2k}]$ (see Figure 2.7). Use the additive property of the integral for subintervals:

$$\begin{aligned} \int_a^b f(x)dx &= \sum_{k=1}^M \int_{x_{2k-2}}^{x_{2k}} f(x)dx \\ &\approx \sum_{k=1}^M \frac{h}{3} (f(x_{2k-2}) + 4f(x_{2k-1}) + f(x_{2k})). \end{aligned} \quad (4.28)$$

Since $h/3$ is a constant, the distributive law of addition can be applied to obtain (2.24). Formula (2.25) is the expanded version of (2.24). Formula (2.26) groups all the intermediate terms in (2.25) that are multiplied by 2 and those that are multiplied by 4.

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

Example 2.6. Consider $f(x) = 2 + \sin(2\sqrt{x})$. Use the composite Simpson rule with 11 sample points to compute an approximation to the integral of $f(x)$ taken over $[1, 6]$.

To generate 11 sample points, we must use $M = 5$ and $h = (6 - 1)/10 = 1/2$. Using formula (2.26), the computation is

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

4.2.1 Error Analysis

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

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

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

Corollary 2.2 (Trapezoidal Rule: Error Analysis). Suppose that $[a, b]$ is subdivided into M subintervals $[x_k, x_{k+1}]$ of width $h = (b-a)/M$. The composite trapezoidal rule

$$T(f, h) = \frac{h}{2}(f(a) + f(b)) + h \sum_{k=1}^{M-1} f(x_k) \quad (4.29)$$

is an approximation to the integral

$$\int_a^b f(x)dx = T(f, h) + E_T(f, h). \quad (4.30)$$

Furthermore, if $f \in C^2[a, b]$, there exists a value c with $a < c < b$ so that the error term $E_T(f, h)$ has the form

$$E_T(f, h) = \frac{(b-a)f^{(2)}(c)h^2}{12} = O(h^2). \quad (4.31)$$

Proof. We first determine the error term when the rule is applied over $[x_0, x_1]$. Integrating the Lagrange polynomial $P_1(x)$ and its remainder yields

$$\int_{x_0}^{x_1} f(x)dx = \int_{x_0}^{x_1} P_1(x)dx + \int_{x_0}^{x_1} \frac{(x-x_0)(x-x_1)f^{(2)}(c(x))}{2!}dx. \quad (4.32)$$

The term $(x-x_0)(x-x_1)$ does not change sign on $[x_0, x_1]$, and $f^{(2)}(c(x))$ is continuous. Hence the second Mean Value Theorem for integrals implies that there exists a value c_1 so that

$$\int_{x_0}^{x_1} f(x)dx = \frac{h}{2}(f_0 + f_1) + f^{(2)}(c_1) \int_{x_0}^{x_1} \frac{(x-x_0)(x-x_1)}{2!}dx. \quad (4.33)$$

Use the change of variable $x = x_0 + ht$ in the integral on the right side of (2.33):

$$\begin{aligned} \int_{x_0}^{x_1} f(x)dx &= \frac{h}{2}(f_0 + f_1) + \frac{f^{(2)}(c_1)}{2} \int_0^1 h(t-0)h(t-1)hdt \\ &= \frac{h}{2}(f_0 + f_1) + \frac{f^{(2)}(c_1)h^3}{2} \int_0^1 (t^2 - t)dt \\ &= \frac{h}{2}(f_0 + f_1) - \frac{f^{(2)}(c_1)h^3}{12}. \end{aligned} \quad (4.34)$$

Now we are ready to add up the error terms for all of the intervals $[x_k, x_{k+1}]$:

$$\int_a^b f(x)dx = \sum_{k=1}^M \int_{x_{k-1}}^{x_k} f(x)dx$$

$$= \sum_{k=1}^M \frac{h}{2}(f(x_{k-1}) + f(x_k)) - \frac{h^3}{12} \sum_{k=1}^M f^{(2)}(c_k). \quad (4.35)$$

The first sum is the composite trapezoidal rule $T(f, h)$. In the second term, one factor of h is replaced with its equivalent $h = (b - a)/M$, and the result is

$$\int_a^b f(x)dx = T(f, h) - \frac{(b - a)h^2}{12} \left(\frac{1}{M} \sum_{k=1}^M f^{(2)}(c_k) \right).$$

The term in parentheses can be recognized as an average of values for the second derivative and hence is replaced by $f^{(2)}(c)$. Therefore, we have established that

$$\int_a^b f(x)dx = T(f, h) - \frac{(b - a)f^{(2)}(c)h^2}{12},$$

and the proof of Corollary 2.2 is complete.

Corollary 2.3 (Simpson's Rule: Error Analysis). Suppose that $[a, b]$ is subdivided into $2M$ subintervals $[x_k, x_{k+1}]$ of equal width $h = (b - a)/(2M)$. The composite Simpson rule

$$S(f, h) = \frac{h}{3}(f(a) + f(b)) + \frac{2h}{3} \sum_{k=1}^{M-1} f(x_{2k}) + \frac{4h}{3} \sum_{k=1}^M f(x_{2k-1}) \quad (4.36)$$

is an approximation to the integral

$$\int_a^b f(x)dx = S(f, h) + E_S(f, h). \quad (4.37)$$

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

$$E_S(f, h) = \frac{(b - a)f^{(4)}(c)h^4}{180} = O(h^4) \quad (4.38)$$

Example 2.7. Consider $f(x) = 2 + \sin(2\sqrt{x})$. Investigate the error then the composite trapezoidal rule is used over $[1, 6]$ and the number of subintervals is 10, 20, 40, 80, and 160.

Table 2.2. The Composite Trapezoidal Rule for $f(x) = 2 + \sin(2\sqrt{x})$ over $[1, 6]$

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

Table 2.2 shows the approximations $T(f, h)$. The antiderivative of $f(x)$ is

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

and the true value of the definite integral is

$$\int_0^6 f(x) dx = F(x) \Big|_{x=1}^{x=6} = 8.1834792077.$$

This value was used to compute the values $E_T(f, h) = 8.1834792077 - T(f, h)$ in Table 2.2. It is important to observe that when h is reduced by a factor of $\frac{1}{2}$ the successive errors $E_T(f, h)$ are diminished by approximately $\frac{1}{4}$. This confirms that the order is $O(h^2)$.

Example 2.8. Consider $f(x) = 2 + \sin(2\sqrt{x})$. Investigate the error when the composite Simpson rule is used over $[1, 6]$ and the number of subintervals is 10, 20, 40, 80, and 160.

Table 2.3 shows the approximations $S(f, h)$. The true value of the integral is 8.1834792077, which was used to compute the values $E_S(f, h) = 8.1834792077 - S(f, h)$ in Table 2.3. It is important to observe that when h is reduced by a factor of $\frac{1}{2}$ the successive errors $E_S(f, h)$ are diminished by approximately $\frac{1}{16}$. This confirms that the order is $O(h^4)$.

Table 2.3 The Composite Simpson Rule for $f(x) = 2 + \sin(2\sqrt{x})$ over $[1, 6]$

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

Example 2.9. Find the number M and the step size h so that the error $E_T(f, h)$ for the composite trapezoidal rule is less than 5×10^{-9} for the approximation $\int_2^7 dx/x \approx T(f, h)$.

The integrand is $f(x) = 1/x$ and its first two derivatives are $f'(x) = -1/x^2$ and $f''(x) = 2/x^3$. The maximum value of $|f''(x)|$ taken over $[2, 7]$ occurs at the end point, $x = 2$ and thus we have the bound $|f''(c)| \leq |f''(2)| = \frac{1}{4}$, for $2 \leq c \leq 7$. This is used with formula (2.31) to obtain

$$|E_T(f, h)| = \frac{|-(b-a)f''(c)h^2|}{12} \leq \frac{(7-2)\frac{1}{4}h^2}{12} = \frac{5h^2}{48}. \quad (4.39)$$

The step size h and number M satisfy the relation $h = 5/M$, and this is used in (2.39) to get the relation

$$|E_T(f, h)| \leq \frac{125}{48M^2} \leq 5 \times 10^{-9}. \quad (4.40)$$

Now rewrite (2.40) so that it is easier to solve for M :

$$\frac{25}{48} \times 10^9 \leq M^2 \quad (4.41)$$

Solving (2.41), we find that $22821.77 \leq M$. Since M must be an integer, we choose $M = 22,822$ and the corresponding step size is $h = 5/22,822 = 0.000219086846$. When the composite trapezoidal rule is implemented with this many function evaluations, there is a possibility that the rounded-off function evaluations will produce a significant amount of error. When the computation was performed, the result was

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

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

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

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

Example 2.10. Find the number M and the step size h so that the error $E_S(f, h)$ for the composite Simpson rule is less than 5×10^{-9} for the approximation $\int_2^7 dx/x \approx S(f, h)$.

The integrand is $f(x) = 1/x$, and $f^{(4)}(x) = 24/x^5$. The maximum value of $|f^{(4)}(c)|$ taken over $[2, 7]$ occurs at the end point $x = 2$, and thus we have the bound $|f^{(4)}(c)| \leq |f^{(4)}(2)| = \frac{3}{4}$ for $2 \leq c \leq 7$. This is used with formula (2.38) to obtain

$$|E_S(f, h)| = \frac{|-(b-a)f^{(4)}(c)h^4|}{180} \leq \frac{(7-2)\frac{3}{4}h^4}{180} = \frac{h^4}{48}. \quad (4.42)$$

The step size h and number M satisfy the relation $h = 5/(2M)$, and this is used in (2.42) to get the relation

$$|E_S(f, h)| \leq \frac{625}{768M^4} \leq 5 \times 10^{-9}. \quad (4.43)$$

Now rewrite (2.43) so that it is easier to solve for M :

$$\frac{125}{768} \times 10^{-9} \leq M^4. \quad (4.44)$$

Solving (2.44), we find that $112.95 \leq M$. Since M must be an integer, we chose $M = 113$, and the corresponding step size is $h = 5/226 = 0.02212389381$. When the composite Simpson rule was performed, the result was

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

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

$$S(f, \frac{5}{128}) = 1.252762973.$$

So we see that the composite Simpson rule using 229 evaluations of and the composite trapezoidal rule using 22,823 evaluations of $f(x)$ achieve the same accuracy. In Example 2,10, Simpson's rule required about 1/100 the number of function evaluations.

Program 2.1 (Composite Trapezoidal Rule). To approximate the integral

$$\int_a^b f(x)dx = \frac{h}{2}(f(a) + f(b)) + h \sum_{k=1}^{M-1} f(x_k)$$

by sample $f(x)$ at the $M + 1$ equally spaced points $x_k = a + kh$, for $k = 0, 1, 2, \dots, M$. Notice that $x_0 = a$ and $x_M = b$.

```
Function s=trapr(f,a,b,M)
%Input   - f is the integrand input as a string 'f'
%         - a and b are upper and lower limits of integration
%         - M is the number of subintervals
%Output  - s is the trapezoidal rule sum
h=(b-a)/M;
s=0;
for k=1:(M-1)
    x=a+h*k;
    s=s+feval(f,x);
end
s=h*(feval(f,a)+feval(f,b))/2+h*s;
```

Program 7.2 (Composite Simpson Rule). To approximate the integral

$$\int_a^b f(x)dx = \frac{h}{3}(f(a) + f(b)) + \frac{2h}{3} \sum_{k=1}^{M-1} f(x_{2k}) + \frac{4h}{3} \sum_{k=1}^M f(x_{2k-1})$$

by sample $f(x)$ at the $2M + 1$ equally spaced points $x_k = a + kh$, for $k = 0, 1, 2, \dots, 2M$. Notice that $x_0 = a$ and $x_{2M} = b$.

```

Function s=simprl(f,a,b,M)
%Input   - f is the integrand input as a string 'f'
%         - a and b are upper and lower limits of integration
%         - M is the number of subintervals
%Output  - s is the simpson rule sum
h=(b-a)/(2*M);
s1=0
s2=0;
for k=1:M
    x=a+h*(2k-1);
    s1=s1+feval(f,x);
end
for k=1:(M-1)
    x=a+h+2*k;
    s2=s2+feval(f,x);
end
s=h*(feval(f,a)+feval(f,b)+4*s1+2*s2)/3;

```

4.3 Exercises For Composite Trapezoidal and Simpson's Rule

- Approximate each integral using the composite trapezoidal rule with $M = 10$.
 - Approximate each integral using the composite Simpson rule with $M = 5$.
 - $\int_{-1}^1 (1+x^2)^{-1} dx$
 - $\int_0^1 (2+\sin(2\sqrt{x})) dx$
 - $\int_{0.25}^4 dx/\sqrt{x}$
 - $\int_0^4 x^2 e^{-x} dx$
 - $\int_0^2 2x \cos(x) dx$
 - $\int_0^\pi \sin(2x) e^{-x} dx$
- Length of a curve.* The arc length of the curve $y = f(x)$ over the interval $a \leq x \leq b$ is

$$\text{length} = \int_a^b \sqrt{1 + (f'(x))^2} dx$$

- Approximate the arc length of each function using the composite trapezoidal rule with $M = 10$.
- Approximate the arc length of each function using the composite Simpson rule with $M = 5$.
- Approximate the surface area using the composite Simpson rule with $M = 5$.
 - $f(x) = x^3$ for $0 \leq x \leq 1$
 - $f(x) = \sin(x)$ for $0 \leq x \leq \pi/4$

- (c) $f(x) = e^{-x}$ for $0 \leq x \leq 1$
4. (a) Verify that the trapezoidal rule ($M = 1, h = 1$) is exact for polynomials of degree ≤ 1 of the form $f(x) = c_1x + c_0$ over $[0, 1]$.
- (b) Use the integrand $f(x) = c_2x^2$ and verify that the error term for the trapezoidal rule $M = 1, h = 1$ over the interval $[0, 1]$ is

$$E_T(f, h) = \frac{(b-a)f^{(2)}h^2}{12}.$$

5. (a) Verify that Simpson's rule ($M = 1, h = 1$) is exact for polynomials of degree ≤ 3 of form $f(x) = c_3x^3 + c_2x^2 + c_1x + c_0$ over $[0, 2]$.
- (b) Use the integrand $f(x) = c_4x^4$ and verify that the error term for Simpson's rule ($M = 1, h = 1$) over the interval $[0, 2]$ is

$$E_S(f, h) = \frac{(b-a)f^{(4)}(c)h^4}{180}$$

6. Derive the trapezoidal rule ($M = 1, h = 1$) by using the method of undetermined coefficients.

(a) Find the constants w_0 and w_1 so that $\int_0^1 g(t)dt = w_0g(0) + w_1g(1)$ is exact for the two functions $g(t) = 1$ and $g(t) = t$.

(b) Use the relation $f(x_0 + ht) = g(t)$ and the change of variable $x = x_0 + ht$ and $dx = hdt$ to translate the trapezoidal rule over $[0, 1]$ to the interval $[x_0, x_1]$.

Hint for part (a). You will get a linear system involving the two unknowns w_0 , and w_1 .

7. Derive Simpson's rule ($M = 1, h = 1$) by using the method of undetermined coefficients.

(a) Find the constants w_0, w_1 , and w_2 so that $\int_0^2 g(t)dt = w_0g(0) + w_1g(1) + w_2g(2)$ is exact for the three functions $g(t) = 1, g(t) = t$, and $g(t) = t^2$.

(b) Use the relation $f(x_0 + ht) = g(t)$ and the change of variable $x = x_0 + ht$ and $dx = hdt$ to translate the trapezoidal rule over $[0, 2]$ to the interval $[x_0, x_2]$.

Hint for part (a) You will get a linear system involving the three unknowns w_0, w_1 , and w_2 .

8. Determine the number M and the interval width h so that the composite trapezoidal rule for M subintervals can be used to compute the given integral with an accuracy of 5×10^{-9} .

$$(a) \int_{-\pi/6}^{\pi/6} \cos(x)dx \quad (b) \int_2^3 \frac{1}{5-x}dx \quad (c) \int_0^2 xe^{-x}dx$$

Hint for part (c) $f^{(2)}(x) = (x-2)e^{-x}$.

9. Determine the number M and the interval width h so that the composite Simpson rule for $2M$ subintervals can be used to compute the given integral with an accuracy

of 5×10^{-9} .

$$(a) \int_{-\pi/6}^{\pi/6} \cos(x) dx \quad (b) \int_2^3 \frac{1}{5-x} dx \quad (c) \int_0^2 x e^{-x} dx$$

Hint for part (c) $f^{(4)}(x) = (x-4)e^{-x}$.

CHQP .7NUMERICAL INTEGRATION 10.consider the definite integral .The following table gives approximations using the composite trapezoidal rule .Calculate and confirm that the order is 11.Consider the definite integral .The following table gives approximations using the composite Simpson rule .Calculate and confirm that the order is 12.Midpoint rule .The midpoint rule on is (a) Expand ,the ant antiderivative of, in a Taylor series about and establish the midpoint rule on (b) Use part (a) and shoe that the composite midpoint rule for approximating the integral of is This is an approximation to the integral of over and we write (c) Show that the error term for part is 13.Use the midpoint rule with to approximate the integrals in Exercise 1. 14.Prove Corollary 7.3. SEC.7.2 COMPOSITE TRAPEZOIDAL AND SIMPSON'S RULE Algorithms and Programs 1.(a) For each integral in Exercise 1,compute Mand the interval width h so that the composite trapezoidal rule can be used to compute the given integral with an accuracy of nine decimal places .Use Program 7.1 to approximate each integral. (b)For each integral in Exercise 1, compute M and the interval width h so that the composite Simpson's rule can be used to compute the given integral with an accuracy of nine4 decimal places .Use Program 7.2 to approximate each integral 2.Use Program 7.2 to approximate the definite integrals in Exercise 2 with an accuracy of 11 decimal places. 3.The composite trapezoidal rule can adapted to integrate a function known only at a set of points .Adapt Program 7.1 to approximate the integral of a function over an interval that passes through M given points (Note. The nodes need not be equally spaced .)Use this program to approximate the integral of a function that passes through the points 5.Modify Program 7.1 so that it uses the composite midpoint rule (Exercise 12)to approximate the integral of .Use this program to approximate the definite integrals in Exercise 1 with an accuracy of 11decimal places. 6.Obtain approximations to each of the following definite integrals with an accuracy of ten decimal places.Use any of the programs from this section 7.The following example shows how Simpson's rule can be used to approximate the solution of an integral equation .The equation be solved using Simpson's rule with; then let Substituting into equation (1) yields the system of Linear equations: Subsuming the solution of system into equation and simplifying yields the approximation (a) As a check, substitute the solution right-hand side of the integral equation, integrate and simplify the right-hand side, and compare the result with the approximation in (3) (b) Use the composite Simpson rule with to approximate the solution of the integral equation Use the procedure outlined in part (a)to check your solution.

4.4 Recursive Rules and Romberg Integration

In this section we show how to compute Simpson approximations with a special linear combination of trapezoidal rules. The approximation will have greater accuracy if one uses a larger number of subintervals. How many should we choose? The sequential process helps answer this question by trying two subintervals, four subintervals, and so on, until the desired accuracy is obtained. First, a sequence $\{T(J)\}$ of trapezoidal rule approximations must be generated. As the number of subintervals is doubled, the number of function values is roughly doubled, because the function must be evaluated at all the previous points and at the midpoints of the previous subintervals (see Figure 2.8). Theorem 2.4 explains how to eliminate redundant function evaluations and additions.

Theorem 7.4 (Successive Trapezoidal Rules). Suppose that $J \geq 1$ and the points $\{x_k = a + kh\}$ subdivide $[a, b]$ into $2^J = 2M$ subintervals of equal width $h = (b - a)/2^J$. The trapezoidal rules $T(f, h)$ and $T(f, 2h)$ obey the relationship

$$T(f, h) = \frac{T(f, 2h)}{2} + h \sum_{k=1}^M f(x_{2k-1}). \quad (4.45)$$

Definition 2.3 (Sequence of Trapezoidal Rules). Define $T(0) = (h/2)(f(a) + f(b))$, which is the trapezoidal rule with step size $h = b - a$. Then for each $J \geq 1$ define $T(J) = T(f, h)$, where $T(f, h)$ is the trapezoidal rule with step size $h = (b - a)/2^J$.

Corollary 7.4 (Recursive Trapezoidal Rule). Start with $T(0) = (h/2)(f(a) + f(b))$. Then a sequence of trapezoidal rules $\{T(J)\}$ is generated by the recursive formula

$$T(J) = \frac{T(J-1)}{2} + h \sum_{k=1}^M f(x_{2k-1}) \quad \text{for } J = 1, 2, \dots, \quad (4.46)$$

where $h = (b - a)/2^J$ and $\{x_k = a + kh\}$.

Proof. For the even nodes $x_0 < x_2 < \dots < x_{2M-2} < x_{2M}$, we use the trapezoidal rule with step size $2h$:

$$T(J-1) = \frac{2h}{2}(f_0 + 2f_2 + 2f_4 + \dots + 2f_{2M-4} + 2f_{2M-2} + f_{2M}). \quad (4.47)$$

For all of the nodes $x_0 < x_1 < x_2 < \dots < x_{2M-1} < x_{2M}$, we use the trapezoidal rule with step size h :

$$T(J) = \frac{h}{2}(f_0 + 2f_1 + 2f_2 + \dots + 2f_{2M-2} + 2f_{2M-1} + f_{2M}). \quad (4.48)$$

Collecting the even and odd subscripts in (2.48) yields

$$T(J) = \frac{h}{2}(f_0 + 2f_2 + \dots + 2f_{2M-2} + f_{2M}) + h \sum_{k=1}^M f_{2k-1}. \quad (4.49)$$

Substituting (2.47) into (2.49) results in $T(J) = T(J - 1)/2 + h \sum_{k=1}^M f_{2k-1}$, and the proof of the theorem is complete.

Example 2.11. Use the sequential trapezoidal rule to compute the approximations $T(0)$, $T(1)$, $T(2)$, and $T(3)$ for the integral $\int_1^5 dx/x = \ln(5) - \ln(1) = 1.609437912$.

Table 2.4 show the nine values required to compute $T(3)$ and the midpoints required to compute $T(1)$, $T(2)$, and $T(3)$. Details for obtaining the results are as follows:

Table 2.4 The Nine Points Used to Compute $T(3)$ and the Midpoints Required to Compute $T(1)$, $T(2)$, and $T(3)$

x	$f(x) = \frac{1}{x}$	$T(0)$	$T(1)$	$T(2)$	$T(3)$
1.0	1.000000	1.000000			
1.5	0.666667				0.666667
2.0	0.500000			0.500000	
2.5	0.400000				0.400000
3.0	0.333333		0.333333		
3.5	0.285714				0.285714
4.0	0.250000			0.250000	
4.5	0.222222				0.222222
5.0	0.200000	0.200000			

$$\text{When } h = 4 : \quad T(0) = \frac{4}{2}(1.000000 + 0.200000) = 2.400000.$$

$$\begin{aligned} \text{When } h = 2 : \quad T(1) &= \frac{T(0)}{2} + 2(0.333333) \\ &= 1.200000 + 0.666666 = 1.866666. \end{aligned}$$

$$\begin{aligned} \text{When } h = 1 : \quad T(2) &= \frac{T(1)}{2} + 1(0.500000 + 0.250000) \\ &= 0.933333 + 0.750000 = 1.683333. \end{aligned}$$

$$\begin{aligned} \text{When } h = \frac{1}{2} : \quad T(3) &= \frac{T(2)}{2} + \frac{1}{2}(0.666667 + 0.400000 \\ &\quad + 0.285714 + 0.222222) \\ &= 0.8416667 + 0.787302 = 1.628968. \end{aligned}$$

Our next result shows an important relationship between the trapezoidal rule and Simpson's rule. When the trapezoidal rule is computed using step sizes $2h$ and h , the result is $T(f, 2h)$ and $T(f, h)$, respectively. These values are combined to obtain Simpson's rule:

$$S(f, h) = \frac{4T(f, h) - T(f, 2h)}{3}. \tag{4.50}$$

Theorem 2.5 (Recursive Simpson Rules). Suppose that $\{T(J)\}$ is the sequence of trapezoidal rules generated by Corollary 2.4. If $J \geq 1$ and $S(J)$ is Simpson's rule for 2^J subintervals of $[a, b]$, then $S(J)$ and the trapezoidal rules $T(J - 1)$ and $T(J)$ obey the relationship

$$S(J) = \frac{4T(J) - T(J - 1)}{3} \quad \text{for } J = 1, 2, \dots \quad (4.51)$$

Proof. The trapezoidal rule $T(J)$ with step size h yields the approximation

$$\int_a^b f(x)dx \approx \frac{h}{2}(f_0 + 2f_1 + 2f_2 + \dots + 2f_{2M-2} + 2f_{2M-1} + f_{2M}) = T(J). \quad (4.52)$$

The trapezoidal rule $T(J - 1)$ with step size $2h$ produces

$$\int_a^b f(x)dx \approx h(f_0 + 2f_2 + \dots + 2f_{2M-2} + f_{2M}) = T(J - 1). \quad (4.53)$$

Multiplying relation (2.52) by 4 yields

$$4 \int_a^b f(x)dx \approx h(2f_0 + 4f_1 + 4f_2 + \dots + 4f_{2M-2} + 4f_{2M-1} + 2f_{2M}) = 4T(J). \quad (4.54)$$

Now subtract (2.53) from (2.54) and the result is

$$3 \int_a^b f(x)dx \approx h(f_0 + 4f_1 + 2f_2 + \dots + 2f_{2M-2} + 4f_{2M-1} + f_{2M}) = 4T(J) - T(J - 1). \quad (4.55)$$

This can be rearranged to obtain

$$\int_a^b f(x)dx \approx \frac{h}{3}(f_0 + 4f_1 + 2f_2 + \dots + 2f_{2M-2} + 4f_{2M-1} + f_{2M}) = \frac{4T(J) - T(J - 1)}{3}. \quad (4.56)$$

The middle term in (2.57) is Simpson's rule $S(J) = S(f, h)$ and hence the theorem is proved.

Example 2.12. Use the sequential Simpson rule to compute the approximations $S(1)$, $S(2)$, and $S(3)$ for the integral of Example 2.11.

Using the results of Example 2.11 and formula (2.50) with $J = 1, 2$, and 3, we compute

$$S(1) = \frac{4T(1) - T(0)}{3} = \frac{4(1.866666) - 2.400000}{3} = 1.688888.$$

$$S(2) = \frac{4T(2) - T(1)}{3} = \frac{4(1.683333) - 1.866666}{3} = 1.622222$$

$$S(3) = \frac{4T(3) - T(2)}{3} = \frac{4(1.628968) - 1.683333}{3} = 1.610846.$$

In Section 2.1 the formula for Boole's rule was given in Theorem 2.1. It was obtained by integrating the Lagrange polynomial of degree 4 based on the nodes x_0, x_1, x_2, x_3 , and x_4 . An alternative method for establishing Boole's rule is mentioned in the exercises. When it is applied M times over $4M$ equally spaced subintervals of $[a, b]$ of step size $h = (b - a)/(4M)$, we call it the **composite Boole rule**:

$$B(f, h) = \frac{2h}{45} \sum_{k=1}^M (7f_{4k-4} + 32f_{4k-3} + 12f_{4k-2} + 32f_{4k-1} + 7f_{4k}). \quad (4.57)$$

The next result gives the relationship between the sequential Boole and Simpson rules.

Theorem 2.6 (Recursive Boole Rules). Suppose that $\{S(J)\}$ is the sequence of Simpson's rules generated by Theorem 2.5. If $J \geq 2$ and $B(J)$ is Boole's rule for 2^J subintervals of $[a, b]$, then $B(J)$ and Simpson's rules $S(J - 1)$ and $S(J)$ obey the relationship

$$B(J) = \frac{16S(J) - S(J - 1)}{15} \quad \text{for } J = 2, 3, \dots \quad (4.58)$$

Proof. The proof is left as an exercise for reader.

Example 2.13. Use the sequential Boole rule to compute the approximations $B(2)$ and $B(3)$ for the integral of Example 2.11.

Using the results of Example 2.12 and formula (2.59) with $J = 2$ and 3, we compute

$$B(2) = \frac{16S(2) - S(1)}{15} + \frac{16(1.622222) - 1.688888}{15} = 1.617778.$$

$$B(3) = \frac{16S(3) - S(2)}{15} = \frac{16(1.610846) - 1.622222}{15} = 1.610088.$$

The reader may wonder what we are leading up to. We will now show that formulas (2.50) and (2.59) are special cases of the process of Romberg integration. Let us announce that the next level of approximation for the integral of Example 2.11 is

$$\frac{64B(3) - B(2)}{63} = \frac{64(1.610088) - 1.617778}{63} = 1.609490,$$

and this answer gives an accuracy of five decimal places.

4.5 Romberg Integration

In Section 2.2 we saw that the error terms $E_T(f, h)$ and $E_S(f, h)$ for the composite trapezoidal rule and composite Simpson rule are of order $O(h^2)$ and $O(h^4)$, respectively.

It is not difficult to show that the error term $E_B(f, h)$ for the composite Boole rule is of the order $O(h^6)$. Thus we have the pattern

$$\int_a^b f(x)dx = T(f, h) + O(h^2). \quad (4.59)$$

$$\int_a^b f(x)dx = S(f, h) + O(h^4). \quad (4.60)$$

$$\int_a^b f(x)dx = B(f, h) + O(h^6). \quad (4.61)$$

The pattern for the remainders in (2.60) through (2.62) is extended in the following sense. Suppose that an approximation rule is used with step sizes h and $2h$; then an algebraic manipulation of the two answers is used to produce an improved answer. Each successive level of improvement increases the order of the error term from $O(h^{2N})$ to $O(h^{2N+2})$. This process, called **Romberg integration**, has its strengths and weaknesses.

The Newton-Cotes rules are seldom used past Boole's rule. This is because the nine-point Newton-Cotes quadrature rule involves negative weights, and all the rules past the ten-point rule involve negative weights. This could introduce loss of significance error due to round off. The Romberg method has the advantages that all the weights are positive and the equally spaced abscissas are easy to compute.

A computational weakness of Romberg integration is that twice as many function evaluations are needed to decrease the error from $O(h^{2N})$ to $O(h^{2N+2})$. The use of the sequential rules will help keep the number of computations down. The development of Romberg integration relies on the theoretical assumption that, if $f \in C^N[a, b]$ for all N , then the error term for the trapezoidal rule can be represented a series involving only even powers of h ; that is,

$$\int_a^b f(x)dx = T(f, h) + E_T(f, h), \quad (4.62)$$

where

$$E_T(f, h) = a_1h^2 + a_2h^4 + a_3h^6 + \dots, \quad (4.63)$$

A derivation of formula (2.64) can be found in Reference [153].

Since only even powers of h can occur in (1.64), the Richardson improvement process is used successively first to eliminate a_1 , next to eliminate a_2 , then to eliminate a_3 . and so on. This process generates quadrature formulas whose error terms have even orders $O(h^4), O(h^6), O(h^8)$, and so on. We shall show that the first improvement is Simpson's rule for $2M$ intervals. Start with $T(f, 2h)$ and $T(f, h)$ and the equations

$$\int_a^b f(x)dx = T(f, 2h) + a_14h^2 + a_216h^4 + a_364h^6 + \dots \quad (4.64)$$

and

$$\int_a^b f(x)dx = T(f, h) + a_1h^2 + a_2h^4 + a_3h^6 + \dots \quad (4.65)$$

Multiply equation (2.66) by 4 and obtain

$$4 \int_a^b f(x)dx = 4T(f, h) + a_14h^2 + a_24h^4 + a_34h^6 + \dots \quad (4.66)$$

Eliminate a_1 by subtracting (2.65) from (2.67). The result is

$$3 \int_a^b f(x)dx = 4T(f, h) - T(f, 2h) - a_212h^4 - a_360h^6 + \dots \quad (4.67)$$

Now divide equation (2.68) by 3 and rename the coefficients in the series:

$$\int_a^b f(x)dx = \frac{4T(f, h) - T(f, 2h)}{3} + b_1h^4 + b_2h^6 + \dots \quad (4.68)$$

As noted in (2.49), the first quantity on the right side of (2.69) is Simpson's rule $S(f, h)$. This shows that $E_S(f, h)$ involves only even powers of h :

$$\int_a^b f(x)dx = S(f, h) + b_1h^4 + b_2h^6 + b_3h^8 + \dots \quad (4.69)$$

To show that the second improvement is Boole's rule, start with (2.70) and write down the formula involving $S(f, 2h)$:

$$\int_a^b f(x)dx = S(f, 2h) + b_116h^4 + b_264h^6 + b_3256h^8 + \dots \quad (4.70)$$

When b_1 is eliminated from (2.70) and (2.71), the result involves Boole's rule:

$$\begin{aligned} \int_a^b f(x)dx &= \frac{16S(f, h) - S(f, 2h)}{15} - \frac{b_248h^6}{15} - \frac{b_3240h^8}{15} \dots \\ &= B(f, h) - \frac{b_248h^6}{15} - \frac{b_3240h^8}{15} \dots \end{aligned} \quad (4.71)$$

The general pattern for romberg integration relies on lemma 2.1.

Lemma 2.1 (Richardson's Improvement for Romberg integration). Given two approximations $R(2h, K - 1)$ and $R(h, K - 1)$ for the quantity Q that satisfy

$$Q = R(h, K - 1) + c_1h^{2K} + c_2h^{2K+2} + \dots \quad (4.72)$$

and

$$Q = R(2h, K - 1) + c_14^K h^{2K} + c_24^{K+1} h^{2K+2} + \dots, \quad (4.73)$$

an improved approximation has the form

$$Q = \frac{4^K R(h, K-1) - R(2h, K-1)}{4^K - 1} + O(h^{2K+2}). \quad (4.74)$$

The proof is straightforward and is left for the reader.

Definition 2.4. Define the sequence $\{R(J, K) : J \geq K\}_{J=0}^\infty$ of quadrature formulas for $f(x)$ over $[a, b]$ as follows

$$\begin{aligned} R(J, 0) &= T(J) \quad \text{for } J \geq 0, \text{ is the sequential trapezoidal rule.} \\ R(J, 1) &= S(J) \quad \text{for } J \geq 1, \text{ is the sequential Simpson rule.} \\ R(J, 2) &= B(J) \quad \text{for } J \geq 2, \text{ is the sequential Boole's rule.} \end{aligned} \quad (4.75)$$

The starting rules, $\{R(J, 0)\}$, are used to generate the first improvement, $\{R(J, 1)\}$, which in turn is used to generate the second improvement, $\{R(J, 2)\}$. We have already seen the patterns

$$\begin{aligned} R(J, 1) &= \frac{4^1 R(J, 0) - R(J-1, 0)}{4^1 - 1} \quad \text{for } J \geq 1 \\ R(J, 2) &= \frac{4^2 R(J, 1) - R(J-1, 1)}{4^2 - 1} \quad \text{for } J \geq 2, \end{aligned} \quad (4.76)$$

which are rules in (2.69) and (2.72) stated using the notation in (2.71). The general rule for constructing improvements is

$$R(J, K) = \frac{4^K R(J, K-1) - R(J-1, K-1)}{4^K - 1} \quad \text{for } J \geq K. \quad (4.77)$$

Table 2.5 Romberg Integration Tableau

J	R(J,0)	R(J,1)	R(J,2)	R(J,3)	R(J,4)
0	R(0,0)				
1					

Table 7.6 Romberg Integration Tableau for example 7.14

For computational purposes, the values are arranged in the romberg integration tableau given in table 7.5. Example 7.14. Use Romberg integration to find approximations for the definite integral The computations are given in table 7.6. In each column the numbers are converging to the value 2.038197427067 the values in the simpson's rule column converge faster than the values in the trapezoidal rule column. For this example, convergence in columns to the right is faster than the adjacent column to the left. Convergence of the Romberg values in table 7.6 is easier to see if we lood at the error terms . suppose that the interval width is a and that the higher derivatives of

are of the same magnitude. The error in column of the romberg table diminishes by about a factor of as one progresses down its rows. The errors diminish by a factor of , the errors diminish by a factor of 1/16, and so on. This can be observed by inspecting the entries in Table 7.7

SEC. 7.3 RECURSIVE RULES AND ROMBERG INTEGRATION 377 Table 7.7 Romberg Error Tobleau for Example 7.14 Theorem 7.7 (Precision of Romberg Integration). Assume that Then the truncation error term for Romberg approximation is given in the formula Where = , is a constant that depends on, and ;see Reference [153], page 126. Example 7.15. Apply Theorem 7.7 and show that The integrand is ,and . Thus the value = will make the error term identically zero. A numerical computation will produce =1024. Program 7.3 (recursive Trapezoidal Rule). To approximate By using the trapezoidal rule and successively increasing the number of subintervals of .The iteration samples +1 equally spaced points. Function T = rctrap (f, a, b,n)

378 CHAP. 7 NUMERICAL INTEGRATION M=1; H=b-a; T=zeros (1, n+1); T(1) =h*(feval (f,a)+feval(f,b))/2; For j=1:n M=2*M; h=h/2; s=0; for k=1:M/2 x=a+h*(2*k-1); s=s+feval(f,x); end T(j+1)=T(j)/2+h*s; End Program 7.4 (Romberg Integration). To approximate the integral by generating a table of approximations for and using as the final answer. The approximations are stored in a special lower-triangular matrix. The elements of column 0 are computed using the sequential trapezoidal rule based on 2 subintervals of [a, b]; then is computed using Romberg's rule. The elements of row are The program is terminated in the st row when. Function [R, quad, err, h]=romber(f, a, b, n, tol)

SEC. 7.3 RECURSIVE RULES AND ROMBERG INTEGRATION 379 M=1; h=b-a; err=1; J=0; R=zeros (4, 4); R(1,1) =h*(feval(f,a)+feval(f,b))/2; While J=J+1; h=h/2; s=0; for p=1:M x=a+h*(2*p-1); s=s+feval(f,x); end R(J+1, 1)=R(J, 1)/2+h*s; M=2*M; for K=1:J R(J+1, K+1)=R(J+1, K)+(R(J+1, K)-R(J, K))/(4^K - 1); end err=abs(R(J, J)-R(J+1, K+1)); end quad=R(J+1, J+1); Exercises for Recursive Rules and Romberg Integration 1.For each of the following definite integrals, construct (by hand) a Romberg table (Table 7.5) with three rows.

380 CHAP. 7 NUMERICAL INTEGRATION 2.Assume that the sequential trapezoidal rule converges to . (a) Show that the sequential Simpson rule converges to. (b) Show that the sequential Boole rule converges to 3.(a) Verify that Boole's rule is exact for polynomials of degree of the form. (c) Use the integrand and verify that the error term for Boole's rule over the interval is 4.Derive Boole's rule by using the method of undetermined coefficients: Find the constants and so that is exact for the five functions and you will get the linear system. 5.Establish the relation for the case .Use the following information: and 6.Simpson's . Consider the trapezoidal rules over the closed interval: with step size 3h,and with step size . Show that the linear combination produces Simpson' rule. 7.Use equations (25) and (26) to establish equatio (27). 8.Use equations (28) and (29) to establish equation (30).

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mine the smallest integer K for which 10. Romberg integration was used to approximate the integrals, and the results are given in the following table: (a) Use the change of variable and show that the two integrals have the same numerical value. (ii). 11. Romberg integration based on the midpoint rule. The composite midpoint rule is competitive with the composite trapezoidal rule with respect to efficiency and the speed of convergence. Use the following facts about the midpoint rule: The rule and the error term are given by and (a) Start with Develop the sequential midpoint rule for computing (b) Show how the sequential midpoint rule can be used in place of the sequential trapezoidal rule in Romberg integration.

382 CHAP. 7 NUMERICAL INTEGRATION Algorithms and Programs

1. Use Program 7.4 to approximate the definite integrals in Exercise 1 with an accuracy of 11 decimal places.
2. Use Program 7.4 to approximate the following two definite integrals with an accuracy of 10 decimal places. The exact value of each definite integral is . Explain any apparent differences in the rates of convergence of the two Romberg sequences.
3. The normal probability density function is , and the cumulative distribution is a function defined by the integral Compute values for , and that have eight digits of accuracy.
4. Modify Program 7.3 so that it will also compute values for the sequential Simpson and Boole rules.
5. Modify Program 7.3 so that it will also compute values for the sequential Simpson and Boole rules.
6. Modify Program 7.4 so that it uses the sequential midpoint rule to perform Romberg integration (use the results of Exercise 11). Use your program to approximate the following integrals with an accuracy of 10 decimal places.
7. In Program 7.4 the approximations to a given definite integral are stored on the main diagonal of a lower-triangular matrix. Modify Program 7.4 so that the rows of the Romberg integration tableau are sequentially computed and stored in matrix R ; hence it saves space. Test your program on the integrals in Exercise 1.

Adaptive Quadrature The composite quadrature rules necessitate the use of equally spaced points. Typically, a small step size h was used uniformly across the entire interval of integration to ensure the overall accuracy. This does not take into account that some portions of the curve may have large functional variations that require more attention than other portions of the curve. It is useful to introduce a method that adjusts the step size to be smaller over portions of the curve where a larger functional variation occurs. This technique is called adaptive quadrature. The method is based on Simpson's rule. Simpson's rule uses two subintervals over:

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where ξ is the center of $[\xi - h/6, \xi + h/6]$ = furthermore, if so that Refinement A composite Simpson rule using four subintervals of $h/6$ can be performed by bisecting this interval into two equal subintervals and applying formula (1) recursively over each piece. Only two additional evaluations of f are needed, and the result is $\frac{1}{3} [f(\xi - h/6) + 4f(\xi) + f(\xi + h/6)]$ where ξ is the midpoint of $[\xi - h/6, \xi + h/6]$, and ξ is the midpoint of $[\xi - h/3, \xi + h/3]$. In formula (3) the step size is $h/2$, which accounts for the factors $h/6$ on the right side of the equation. Furthermore, if there exists a value ξ so that Assume that $f'(\xi) = 0$; then the right sides of equations (2) and (4) are used to obtain the relation Which can be written as Then (6) is substituted in (4) to obtain the error estimate: Because of the assumption $f'(\xi) = 0$, the fraction is replaced

with on the right side of (7) when implementing the method. This justifies the following test.

384 CHAP. 7 NUMERICAL INTEGRATION Accuracy Test Assume that the tolerance is specified for the interval. If we infer that thus the composite simpson rule (3) is used to approximate the integral and the error bound for this approximation over is. Adaptive quadrature is implemented by applying simpson's rules (1) and (3). Start with, where is the tolerance for numerical quadrature over. The interval is refined into subintervals labeled and . if the accuracy test (8) is passed, quadrature formula (3) is applied to and we are done. If the test in (8) fails, the two subintervals are relabeled and , over which we use the tolerances and , respectively. Thus we have two intervals with their associated tolerances to consider for further refinement and testing: and , where ,if adaptive quadrature must be continued, the smaller intervals must be refined and tested, each with its own associated tolerance. In the second step we first consider and refine the interval into and . if they pass the accuracy test (8) with the tolerance, quadrature formula (3) is applied to and accuracy has been achieved over this interval. If they fail the test in (8) with the tolerance, each subinterval and must be refined and tested in the third step with the reduced tolerance Moreover, the second step involves looking at and refining into and . if they pass the accuracy test (8) with tolerance , quadrature formula (3) is applied to and accuracy is achieved over this interval. If they fail the test in (8) with the tolerance, each subinterval and must be refined and tested in the third step with the reduced tolerancee. Therefore, the second step produces either three or four intervals, which we relabel consecutively. The three intervals would be relabeled to produce. Where . in the case of four intervals, we would obtain , where. If adaptive quadrature must be continued, the smaller intervals must be tested, each with its own associated tolerance. The error term in (4) shows that each time a refinement is made over a smaller subinterval there is a reduction of error by about

SEC. 7.4 ADAPTIVE QUADRATURE 385 Table 7.8 Adaptive Quadrature Computations for A factor of . Thus the process will terminate after a finite number of steps. The booddeeping for implementing the metheod includes a sentinel variable which indicates if a particular subinterval has passed its accuracy test. To avoid unnecessary additional evaluations of, the function values can be included in a data list corresponding to each subinterval. The details are shown in program 7.6. Example 7.16. Use adaptive quadrature to numerically approximate the value of the definite integral with the starting tolerance =0.00001. Implementation of the method revealed that 20 subintervals are needed. Table 7.8 lists each interval, composite simpson rule , the error bound for this approximation, and the associated tolerance . the approximate value of the integral is obtained by summing the simpson rule approximations to get

386 CHAP. 7 NUMERICAL INTEGRATION The true value of the integral is Therefore, the error for adaptive quadrature is Which is smaller than the specified tolerance =0.00001. the adaptive methoe involves 20 subintervals of [0.4]. and 81 function evaluations were used. Figure 7.9 shows the graph of and these 20 subintervals.

The intervals are smaller where a larger functional variation occurs near the origin. In the refinement and testing process in the adaptive method, the first four intervals were bisected into eight subintervals of width 0.03125. If this uniform spacing is continued throughout the interval [0,4], $M = 128$ subintervals are required for the composite Simpson rule, which yields the approximation 1.54878844029, which is in error by the amount 0.00000006776. Although the composite Simpson method contains half the error of the adaptive quadrature method, 176 more function evaluations are required. This gain of accuracy is negligible; hence there is a considerable saving of computing effort with the adaptive method. Program 7.5, `srule`, is a modification of Simpson's rule from section 7.1. The output is a vector `Z` that contains the results of Simpson's rule on the interval. Program 7.6 calls `srule` as a subroutine to carry out Simpson's rule on each of the subintervals generated by the adaptive quadrature process.

SEC. 7.4 ADAPTIVE QUADRATURE 387 Program 7.5 (Simpson's rule). To approximate the integral by using Simpson's rule, where Function `Z = srule(f, a0, b0, tol)`
`h = C=zeros(1,3); C=feval S= S2=S; Toll=tol; Err=tol; Z=[a0 b0 S S2 err toll];`
 Program 7.6 produces a matrix `srmat`, `quad` (adaptive quadrature approximation to definite integral) and `err` (the error bound for the approximation). The rows of `srmat` consist of the end points, the Simpson's rule approximation, and the error bound on each subinterval generated by the adaptive quadrature process. Program 7.6 (adaptive quadrature using Simpson's rule). To approximate the integral The composite Simpson rule is applied to the $4M$ subintervals, where and function [`srmat`, `quad`, `err`] = `adapt(f, a, b, tol)`

388 CHAP. 7 NUMERICAL INTEGRATION `srmat = zeros(30,6); iterating = 0; done = 1 srvec = zeros(1,6); srvec = srule(f, a, b, tol); srmat(1,1:6) = srvec m=1 state=iterating; while(state==iterating) n=m; for j=n:-1:1 p=j srovec=srmat(p,:) err=srovec(5) tol=srovec(6) if state=done; srvec=srovec; sr2vec=srovec; a=srovec(1) b=srovec(2) c=(a+b)/2 err=srovec(5) tol=srovec(6) tol2=tol/2 srvec=srule(f, a, c, tol2) sr2vec=srule(f, c, b, tol2) err=abs(srovec(3)-sr1vec(3)-sr2vec(3))/10 if srmat(p,:)=srovec; srmat(p,4)=srvec(3)+sr2vec(3) srmat(p,5)=err; else srmat(p+1:m+1,:)=srmat(p:m,:) m=m+1 srmat(p+1,:)=sr2vec; state=iterating; end`

SEC. 7.5 GAUSS-LEGENDRE INTEGRATION (OPTIONAL) 389 `end end end quad=sum(srmat(:,4)) err=sum(abs(srmat(:,5))) srmat=srmat(1:m,1:6)` Algorithms and programs 1. Use program 7.6 to approximate the value of the definite integral. Use the starting tolerance 2. For each of the definite integrals in problem 1 construct a graph analogous to figure 7.9. hint. The first column of `srmat` contains the end points (except for `b`) of the subintervals from the adaptive quadrature process. If `t=srmat(:,1)` and `z=zeros(length(T))'`, then `plot(T,Z, '.')` will produce the subintervals (except for the right end point `b`). 3. Modify Program 7.6 so that Boole's rule is used in each subinterval 4. Use the modified program in problem 3 to compute approximations and construct graphs analogous to figure 7.9 for the definite integrals in problem 1.

4.6 Gauss-Legendre Integration (Optional)

We wish to find the area under the curve

$$y = f(x), \quad -1 \leq x \leq 1.$$

What method gives the best answer if only two function evaluations are to be made? We have already seen that the trapezoidal rule is a method for finding the area under the curve and that it uses two function evaluations at the end points $(-1, f(-1))$, and $(1, f(1))$. But if the graph of $y = f(x)$ is concave down, the error in approximation is the entire region that lies between the curve and the line segment joining the points (see Figure 2.10(a)).

If we can use nodes x_1 and x_2 that lie inside the interval $[-1, 1]$, the line through the two points $(x_1, f(x_1))$ and $(x_2, f(x_2))$ crosses the curve, and the area under the line more closely approximates the area under the curve (see Figure 2.10(b)). The equation of the line is

$$y = f(x_1) + \frac{(x - x_1)(f(x_2) - f(x_1))}{x_2 - x_1} \quad (4.78)$$

and the area of the trapezoid under the line is

$$A_{\text{trap}} = \frac{2x_2}{x_2 - x_1} f(x_1) - \frac{2x_1}{x_2 - x_1} f(x_2). \quad (4.79)$$

Notice that the trapezoidal rule is a special case of (2.79). When we choose $x_1 = -1, x_2 = 1$, and $h = 2$, then

$$T(f, h) = \frac{2}{2} f(x_1) - \frac{-2}{2} f(x_2) = f(x_1) + f(x_2).$$

We shall use the method of undetermined coefficients to find the abscissas x_1, x_2 and weights w_1, w_2 so that the formula

$$\int_{-1}^1 f(x) dx \approx w_1 f(x_1) + w_2 f(x_2) \quad (4.80)$$

is exact for cubic polynomials (i.e., $f(x) = a_3 x^3 + a_2 x^2 + a_1 x + a_0$). Since four coefficients w_1, w_2, x_1 , and x_2 need to be determined in equation (2.80), we can select four conditions to be satisfied. Using the fact that integration is additive, it will suffice to require that (2.80) be exact for the four functions $f(x) = 1, x, x^2, x^3$. The four integral conditions are

$$\begin{aligned} f(x) = 1 : \quad & \int_{-1}^1 1 dx = 2 = w_1 + w_2 \\ f(x) = x : \quad & \int_{-1}^1 x dx = 0 = w_1 x_1 + w_2 x_2 \end{aligned}$$

$$f(x) = x^2 \quad \int_{-1}^1 x^2 = \frac{2}{3} = w_1 x_1^2 + w_2 x_2^2 \quad (4.81)$$

$$f(x) = x^3 \quad \int_{-1}^1 x^3 dx = 0 = w_1 x_1^3 + w_2 x_2^3.$$

Now solve the system of nonlinear equations

$$w_1 + w_2 = 2 \quad (4.82)$$

$$w_1 x_1 = -w_2 x_2 \quad (4.83)$$

$$w_1 x_1^2 + w_2 x_2^2 = \frac{2}{3} \quad (4.84)$$

$$w_1 x_1^3 = -w_2 x_2^3 \quad (4.85)$$

We can divide (2.85) by (2.83) and the result is

$$x_1^2 = x_2^2 \quad \text{or} \quad x_1 = -x_2. \quad (4.86)$$

Use (2.86) and divide (2.83) by x_1 on the left and $-x_2$ on the right to get

$$w_1 = w_2. \quad (4.87)$$

Substituting (2.87) into (2.82) results in $w_1 + w_2 = 2$. Hence

$$w_1 = w_2 = 1. \quad (4.88)$$

Now using (2.88) and (2.86) in (2.84), we write

$$w_1 x_1^2 + w_2 x_2^2 = x_2^2 + x_2^2 = \frac{2}{3} \quad \text{for} \quad x_2^2 = \frac{1}{3} \quad (4.89)$$

Finally, from (2.89) and (2.86) we see that the nodes are

$$x_1 = x_2 = 1/3^{1/2} \approx 0.5773502692.$$

We have found the nodes and weights that make up the two-point Gauss-Legendre rule. Since the formula is exact for cubic equations, the error term will involve the fourth derivative. A discussion of the error term can be found in Reference [41].

Theorem 2.8 (Gauss-Legendre Two-Point Rule). If f is continuous on $[-1, 1]$, then

$$\int_{-1}^1 f(x) dx \approx G_2(f) = f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right). \quad (4.90)$$

The Gauss-legendre rule $G_2(f)$ has degree of precision $n = 3$. If $f \in C^4[-1, 1]$, then

$$\int_{-1}^1 f(x) dx \approx G_2(f) = f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) + E_2(f). \quad (4.91)$$

where

$$E_2(f) = \frac{f^{(4)}(c)}{135}. \quad (4.92)$$

Example 2.17. Use the two-point Gauss-Legendre rule to approximate

$$\int_{-1}^1 \frac{dx}{x+2} = \ln(3) - \ln(1) \approx 1.09861$$

and compare the result with the trapezoidal rule $T(f, h)$ with $h = 2$ and Simpson's rule $S(f, h)$ with $h = 1$.

Let $G_2(f)$ denote the two-point Gauss-Legendre rule; then

$$G_2(f) = f(-0.57735) + f(0.57735) = 0.70291 + 0.38800 = 1.09091,$$

$$T(f, 2) = f(-1.00000) + f(1.00000) = 1.00000 + 0.33333 = 1.33333,$$

$$S(f, 1) = \frac{f(-1) + 4f(0) + f(1)}{3} = \frac{1 + 2 + \frac{1}{3}}{3} = 1.11111.$$

The errors are 0.00770, 0.23472, and 0.01250, respectively, so the Gauss-Legendre rule is seen to be best. Notice that the Gauss-Legendre rule required only two function evaluations and Simpson's rule required three. In this example the size of the error for $G_2(f)$ is about 61% of the size of the error for $S(f, 1)$

The general N -point Gauss-Legendre rule is exact for polynomial functions of degree $\leq 2N - 1$, and the numerical integration formula is

$$G_N(f) = w_{N,1}f(x_{N,1}) + w_{N,2}f(x_{N,2}) + \cdots + w_{N,N}f(x_{N,N}). \quad (4.93)$$

Table 2.9 Gauss-Legendre Abscissas and Weights

$$\int_{-1}^1 f(x)dx = \sum_{k=1}^N w_{N,k}f(x_{N,k}) + E_N(f)$$

N	abscissas, $x_{N,k}$	Weights, $w_{N,k}$	Truncation error, $E_N(f)$
2	0.5773502692 -0.5773502692	1.0000000000 1.0000000000	$\frac{f^{(4)}(c)}{135}$
3	± 0.7745966692 0.0000000000	0.5555555556 0.8888888888	$\frac{f^{(6)}(c)}{15,750}$
4	± 0.8611363116 ± 0.3399810436	0.3478548451 0.6521451549	$\frac{f^{(8)}(c)}{3,472,875}$
5	± 0.9061798459 ± 0.5384693101 0.0000000000	0.2369268851 0.4786286705 0.5688888888	$\frac{f^{(10)}(c)}{1,237,732,650}$
6	± 0.9324695142 ± 0.6612093865 ± 0.2386191861	0.1713244924 0.3607615730 0.4679139346	$\frac{f^{(12)}(c)2^{13}(6!)^4}{(12!)^3 13!}$
7	± 0.9491079123 ± 0.7415311856 ± 0.4058451514 0.0000000000	0.1294849662 0.2797053915 0.3818300505 0.4179591837	$\frac{f^{(14)}2^{15}(8!)^4(c)}{(14!)^3 15!}$
8	± 0.9602898565 ± 0.7966664774 ± 0.5255324099 ± 0.1834346425	0.1012285363 0.2223810345 0.3137066459 0.3626837834	$\frac{f^{(16)}(c)2^{17}(8!)^4}{(16!)^3 17!}$

The abscissas $x_{N,k}$ and weights $w_{N,k}$ to be used have been tabulated and are easily available; Table 2.9 gives the values up to eight points. Also included in the table is the form of the error term $E_N(f)$ that corresponds to $G_N(f)$, and it can be used to determine the accuracy of the Gauss-Legendre integration formula.

The values in table 2.9 in general have no easy representation. This fact makes the method less attractive for humans to use when hand calculations are required. But once the values are stored in a computer it is easy to call them up when needed. The nodes are actually roots of the Legendre polynomials, and the corresponding weights must be obtained by solving a system of equations. For the three-point Gauss-Legendre rule the nodes are $(0.6)^{1/2}$, and the corresponding weights are $5/9$, $8/9$, and $5/9$.

Theorem 2.9 (Gauss-Legendre three-point rule). If f is continuous on $[-1, 1]$, then

$$\int_{-1}^1 f(x)dx \approx G_3(f) = \frac{5f(-\sqrt{3/5}) + 8f(0) + 5f(\sqrt{3/5})}{9}. \quad (4.94)$$

The Gauss-Legendre rule $G_3(f)$ has degree of precision $n = 5$. If $f \in C^6[-1, 1]$, then

$$\int_{-1}^1 f(x)dx = \frac{5f(-\sqrt{3/5}) + 8f(0) + 5f(\sqrt{3/5})}{9} + E_3(f), \quad (4.95)$$

where

$$E_3(f) = \frac{f^{(6)}(c)}{15,750}. \quad (4.96)$$

Example 2.18. Show that the three-point Gauss-Legendre rule is exact for

$$\int_{-1}^1 5x^4 dx = 2 = G_3(f).$$

Since the integrand is $f(x) = 5x^4$ and $f^{(6)}(x) = 0$, we can use (2.96) to see that $E_3(f) = 0$. But it is instructive to use (2.94) and do the calculations in this case.

$$G_3(f) = \frac{5(5)(0.6)^2 + 0 + 5(5)(0.6)^2}{9} = \frac{18}{9} = 2.$$

The next result shows how to change the variable of integration so that the Gauss-Legendre rules can be used on the interval $[a, b]$.

Theorem 2.10 (The Gauss-Legendre Translation). Suppose that the abscissas $\{x_{N,k}\}_{k=1}^N$ and weights $\{w_{N,k}\}_{k=1}^N$ are given for the N -point Gauss-Legendre rule over $[-1, 1]$. To apply the rule over the interval $[a, b]$, use the change of variable

$$t = \frac{a+b}{2} + \frac{b-a}{2}x \quad \text{and} \quad dt = \frac{b-a}{2}dx \quad (4.97)$$

Then the relationship

$$\int_a^b f(t)dt = \int_{-1}^1 f\left(\frac{a+b}{2} + \frac{b-a}{2}x\right) \frac{b-a}{2}dx \quad (4.98)$$

is used to obtain the quadrature formula

$$\int_a^b f(t)dt = \frac{b-a}{2} \sum_{k=1}^N w_{N,k} f\left(\frac{a+b}{2} + \frac{b-a}{2}x_{N,k}\right). \quad (4.99)$$

Example 2.19 Use the three-point Gauss-Legendre rule to approximate

$$\int_1^5 \frac{dt}{t} = \ln(5) - \ln(1) = 1.609438$$

and compare the result with Boole's rule $B(2)$ with $h = 1$.

Here $a = 1$ and $b = 5$, so the rule in (2.99) yields

$$\begin{aligned} G_3(f) &= (2) \frac{5f(3 - 2(0.6)^{1/2}) + 8f(3 + 0) + 5f(3 + 2(0.6)^{1/2})}{9} \\ &= (2) \frac{3.446359 + 2.666667 + 1.099096}{9} = 1.602694. \end{aligned}$$

In Example 4.13 we saw that Boole's rule gave $B(2) = 1.617778$. The errors are 0.006744 and -0.008340 , respectively, so that the Gauss-Legendre rule is slightly better in this case. Notice that the Gauss-Legendre rule requires three function evaluations and Boole's rule requires five. In this example the size of the two errors is about the same.

Gauss-Legendre integration formulas are extremely accurate, and they should be considered seriously when many integrals of a similar nature are to be evaluated. In this case, proceed as follows. Pick a few representative integrals, including some with the worst behavior that is likely to occur. Determine the number of sample points N that is needed to obtain the required accuracy. Then fix the value N , and use the Gauss-Legendre rule with N sample points for all the integrals.

For a given value of N , Program 2.7 requires that the abscissas and weights from Table 2.9 be saved in $1 \times N$ matrices A and W , respectively. This can be done in the MATLAB command window or the matrices can be saved as M-files. It would be expedient to save Table 2.9 in a 35×2 matrix G . The first column of G would contain the abscissas and the second column the corresponding weights. Then, for a given value of N , the matrices A and W would be submatrices of G . For example, if $N = 3$ then $A = G(3:5,1)'$ and $W = G(3:5,2)'$.

Program 4.7 (Gauss-Legendre Quadrature). To approximate the integral

$$\int_a^b f(x) dx \approx \frac{b-a}{2} \sum_{k=1}^N w_{N,k} f(t_{N,k})$$

By sampling $f(x)$ at the N unequally spaced points $\{t_{N,k}\}_{k=1}^N$, the changes of variable

$$t = \frac{a+b}{2} + \frac{b-a}{2}x \quad \text{and} \quad dt = \frac{b-a}{2}dx$$

are used. The abscissas $\{x_{N,k}\}_{k=1}^N$ and the corresponding weights $\{w_{N,k}\}_{k=1}^N$ must be obtained from a table of known values.

Function quad=gauss(f, a, b, A, W)

4.6.1 Exercises for Gauss-Legendre integration

In Exercises 1 through 4, (a) show that the two integrals are equivalent and (b) calculate $G_2(f)$.

$$1. \int_0^2 6t^5 dt = \int_{-1}^1 6(x+1)^5 dx \qquad 2. \int_0^2 \sin(t) dt = \int_{-1}^1 \sin(x+1) dx$$

$$3. \int_0^1 \frac{\sin(t)}{t} dt = \int_{-1}^1 \frac{\sin((x+1)/2)}{x+1} dx \qquad 4. \frac{1}{\sqrt{2\pi}} \int_{-1}^1 \frac{e^{-(x+1)^2/8}}{2} dx$$

$$5. \frac{1}{\pi} \int_0^\pi \cos(0.6 \sin(t)) dt = 0.5 \int_{-1}^1 \cos\left(0.6 \sin\left((x+1)\frac{\pi}{2}\right)\right) dx$$

6. Use $E_N(f)$ in Table 7.9 and the change of variable given in Theorem 4.10 to find the smallest integer N so that $E_N(f) = 0$ for

(a) $\int_0^2 8x^7 dx = 256 = G_N(f)$.

(b) $\int_0^2 11x^{10} dx = 2048 = G_N(f)$.

7. Find the roots of the following Legendre polynomials and compare them with the abscissa in Table 7.9.

(a) $P_2(x) = (3x^2 - 1)/2$

(b) $P_3(x) = (5x^3 - 3x)/2$

(c) $P_4(x) = (35x^4 - 30x^2 + 3)/8$

8. The truncation error term for the two-point Gauss-Legendre rule on the closed interval $[-1, 1]$ is $f(4)(c_1)/135$. The truncation error for Simpson's rule on $[a, b]$ is $-h^5 f^4(c_2)/90$. Compare the truncation error terms when $[a, b] = [-1, 1]$. Which method do you think is best? Why?

9. The three-point Gauss-Legendre rule is

$$\int_{-1}^1 f(x) dx \approx \frac{5f(-(0.6)^{1/2}) + 8f(0) + 5f((0.6)^{1/2})}{9}.$$

Show that the formula is exact for $f(x) = 1, x, x^2, x^3, x^4, x^5$. Hint. If f is an odd function (i.e., $f(-x) = -f(x)$), the integral of f over $[-1, 1]$ is zero.

10. The truncation error term for the three-point Gauss-Legendre rule on the interval $[-1, 1]$ is $f^6(c_1)/15,750$. The truncation error term for Boole's rule on $[a, b]$ is $-8h^7 f^6(c^2)/945$. Compare the error terms when $[a, b] = [-1, 1]$. Which method is better? Why?

11. Derive the three-point Gauss-Legendre rule using the following steps. Use the fact that the abscissas are the roots of the Legendre polynomial of degree 3.

$$x_1 = -(0.6)^{1/2}, \quad x_2 = 0, \quad x_3 = (0.6)^{1/2}.$$

Find the weights w_1, w_2, w_3 so that the relation

$$\int_{-1}^1 f(x) dx \approx w_1 f(-(0.6)^{1/2}) + w_2 f(0) + w_3 f((0.6)^{1/2})$$

is exact for the functions $f(x) = 1, x,$ and x^2 . *Hint.* First obtain and then solve the linear system of equations

$$\begin{aligned}w_1 + w_2 + w_3 &= 2 \\-(0.6)^{1/2}w_1 + (0.6)^{1/2}w_3 &= 0 \\0.6w_1 + 0.6w_3 &= \frac{2}{3}.\end{aligned}$$

12. In practice, if many integrals of a similar type are evaluated, a preliminary analysis is made to determine the number of function evaluations required to obtain the desired accuracy. Suppose that 17 function evaluations are to be made. Compare the Romberg $R(4, 4)$ with the Gauss-Legendre answer $G_{17}(f)$.

4.6.2 Algorithms and Programs

- For each of the integrals in exercises 1 through 5, use Program 7.7 to find $G_6(f)$, $G_7(f)$, and $G_8(f)$.
- (a) Modify Program 7.7 so that it will compute $G_1(f), G_2(f), \dots, G_8(f)$ and stop when the relative error in the approximations $G_{N-1}(f)$ and $G_N(f)$ is less than the preassigned value `tol`, that is,

$$\frac{2|G_{N-1}(f) - G_N(f)|}{|G_{N-1}(f) + G_N(f)|} < \text{tol}.$$

Hint. As discussed at the end of the section, save Table 4.9 in an M-file `G` as a 35×2 matrix `G`.

- (b) Use your program from part (a) to approximate the integrals in Exercises 1 through 5 with an accuracy of five decimal places.
- (a) Use the six-point Gauss-Legendre rule to approximate the solution of the integral equation

$$v(x) = x^2 + 0.1 \int_0^3 (x^2 + t)v(t)dt.$$

Substitute your approximate solution into the right-hand side of the integral equation and simplify.

- (b) Repeat part (a) using an eight-point Gauss-Legendre rule.