d.   Use Taylor Series to show that

$$\pi = p_k + \frac{\pi^3}{3!}\left(\frac{1}{k}\right)^2 - \frac{\pi^5}{5!}\left(\frac{1}{k}\right)^4 + \cdots$$

and

$$\pi = P_k - \frac{\pi^3}{3}\left(\frac{1}{k}\right)^2 + \frac{2\pi^5}{15}\left(\frac{1}{k}\right)^4 - \cdots .$$

e.   Use extrapolation with $h = 1/k$ to better approximate π.

4.3   Elements of Numerical Integration

The need often arises for evaluating the definite integral of a function that has no explicit antiderivative or whose antiderivative is not easy to obtain. The basic method involved in approximating $\int_a^b f(x)\,dx$ is called **numerical quadrature**. It uses a sum $\sum_{i=0}^n a_i f(x_i)$ to approximate $\int_a^b f(x)\,dx$.

The methods of quadrature in this section are based on the interpolation polynomials given in Chapter 3. The basic idea is to select a set of distinct nodes $\{x_0, \ldots, x_n\}$ from the interval $[a, b]$. Then integrate the Lagrange interpolating polynomial

$$P_n(x) = \sum_{i=0}^n f(x_i)L_i(x)$$

and its truncation error term over $[a, b]$ to obtain

$$\int_a^b f(x)\,dx = \int_a^b \sum_{i=0}^n f(x_i)L_i(x)\,dx + \int_a^b \prod_{i=0}^n (x - x_i)\frac{f^{(n+1)}(\xi(x))}{(n+1)!}\,dx$$

$$= \sum_{i=0}^n a_i f(x_i) + \frac{1}{(n+1)!}\int_a^b \prod_{i=0}^n (x - x_i)f^{(n+1)}(\xi(x))\,dx,$$

where $\xi(x)$ is in $[a, b]$ for each x and

$$a_i = \int_a^b L_i(x)\,dx, \quad \text{for each } i = 0, 1, \ldots, n.$$

The quadrature formula is, therefore,

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^n a_i f(x_i),$$

with error given by

$$E(f) = \frac{1}{(n+1)!}\int_a^b \prod_{i=0}^n (x - x_i)f^{(n+1)}(\xi(x))\,dx.$$

Before discussing the general situation of quadrature formulas, let us consider formulas produced by using first and second Lagrange polynomials with equally-spaced nodes. This gives the **Trapezoidal rule** and **Simpson's rule**, which are commonly introduced in calculus courses.

The Trapezoidal Rule

To derive the Trapezoidal rule for approximating $\int_a^b f(x)\, dx$, let $x_0 = a$, $x_1 = b$, $h = b - a$ and use the linear Lagrange polynomial:

$$P_1(x) = \frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1).$$

Then

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

$$+ \frac{1}{2} \int_{x_0}^{x_1} f''(\xi(x))(x - x_0)(x - x_1)\, dx. \qquad (4.23)$$

The product $(x - x_0)(x - x_1)$ does not change sign on $[x_0, x_1]$, so the Weighted Mean Value Theorem for Integrals 1.13 can be applied to the error term to give, for some ξ in (x_0, x_1),

$$\int_{x_0}^{x_1} f''(\xi(x))(x - x_0)(x - x_1)\, dx = f''(\xi) \int_{x_0}^{x_1} (x - x_0)(x - x_1)\, dx$$

$$= f''(\xi) \left[\frac{x^3}{3} - \frac{(x_1 + x_0)}{2} x^2 + x_0 x_1 x \right]_{x_0}^{x_1}$$

$$= -\frac{h^3}{6} f''(\xi).$$

Consequently, Eq. (4.23) implies that

$$\int_a^b f(x)\, dx = \left[\frac{(x - x_1)^2}{2(x_0 - x_1)} f(x_0) + \frac{(x - x_0)^2}{2(x_1 - x_0)} f(x_1) \right]_{x_0}^{x_1} - \frac{h^3}{12} f''(\xi)$$

$$= \frac{(x_1 - x_0)}{2} [f(x_0) + f(x_1)] - \frac{h^3}{12} f''(\xi).$$
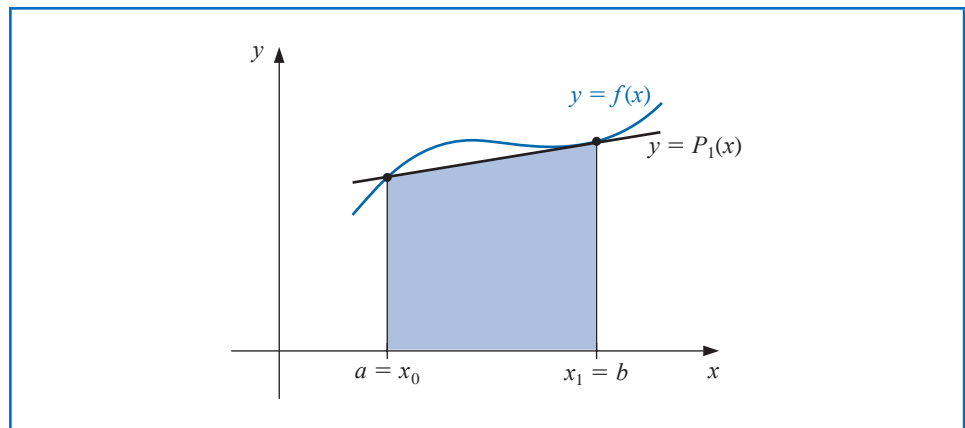
Using the notation $h = x_1 - x_0$ gives the following rule:

Trapezoidal Rule:

$$\int_a^b f(x)\, dx = \frac{h}{2} [f(x_0) + f(x_1)] - \frac{h^3}{12} f''(\xi).$$

This is called the Trapezoidal rule because when f is a function with positive values, $\int_a^b f(x)\, dx$ is approximated by the area in a trapezoid, as shown in Figure 4.3.

Figure 4.3

The error term for the Trapezoidal rule involves f'', so the rule gives the exact result when applied to any function whose second derivative is identically zero, that is, any polynomial of degree one or less.

Simpson's Rule

Simpson's rule results from integrating over $[a, b]$ the second Lagrange polynomial with equally-spaced nodes $x_0 = a$, $x_2 = b$, and $x_1 = a + h$, where $h = (b - a)/2$. (See Figure 4.4.)

Figure 4.4
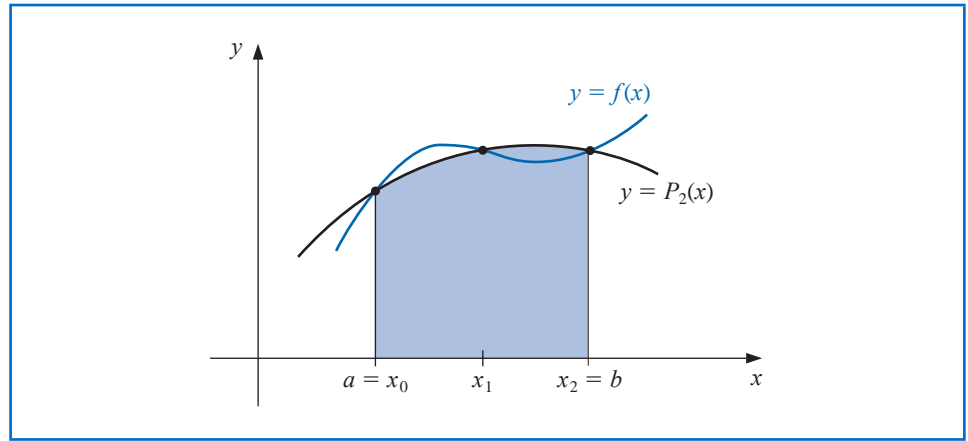
Therefore

$$\int_a^b f(x)\, dx = \int_{x_0}^{x_2} \left[\frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} f(x_0) + \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} f(x_1) \right.$$

$$\left. + \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)} f(x_2) \right] dx$$

$$+ \int_{x_0}^{x_2} \frac{(x - x_0)(x - x_1)(x - x_2)}{6} f^{(3)}(\xi(x))\, dx.$$

Deriving Simpson's rule in this manner, however, provides only an $O(h^4)$ error term involving $f^{(3)}$. By approaching the problem in another way, a higher-order term involving $f^{(4)}$ can be derived.

To illustrate this alternative method, suppose that f is expanded in the third Taylor polynomial about x_1. Then for each x in $[x_0, x_2]$, a number $\xi(x)$ in (x_0, x_2) exists with

$$f(x) = f(x_1) + f'(x_1)(x - x_1) + \frac{f''(x_1)}{2}(x - x_1)^2 + \frac{f'''(x_1)}{6}(x - x_1)^3 + \frac{f^{(4)}(\xi(x))}{24}(x - x_1)^4$$

and

$$\int_{x_0}^{x_2} f(x)\, dx = \left[f(x_1)(x - x_1) + \frac{f'(x_1)}{2}(x - x_1)^2 + \frac{f''(x_1)}{6}(x - x_1)^3 \right.$$

$$\left. + \frac{f'''(x_1)}{24}(x - x_1)^4 \right]_{x_0}^{x_2} + \frac{1}{24} \int_{x_0}^{x_2} f^{(4)}(\xi(x))(x - x_1)^4\, dx. \quad (4.24)$$

Because $(x - x_1)^4$ is never negative on $[x_0, x_2]$, the Weighted Mean Value Theorem for Integrals 1.13 implies that

$$\frac{1}{24} \int_{x_0}^{x_2} f^{(4)}(\xi(x))(x - x_1)^4 \, dx = \frac{f^{(4)}(\xi_1)}{24} \int_{x_0}^{x_2} (x - x_1)^4 \, dx = \frac{f^{(4)}(\xi_1)}{120} (x - x_1)^5 \Big]_{x_0}^{x_2},$$

for some number ξ_1 in (x_0, x_2).

However, $h = x_2 - x_1 = x_1 - x_0$, so

$$(x_2 - x_1)^2 - (x_0 - x_1)^2 = (x_2 - x_1)^4 - (x_0 - x_1)^4 = 0,$$

whereas

$$(x_2 - x_1)^3 - (x_0 - x_1)^3 = 2h^3 \quad \text{and} \quad (x_2 - x_1)^5 - (x_0 - x_1)^5 = 2h^5.$$

Consequently, Eq. (4.24) can be rewritten as

$$\int_{x_0}^{x_2} f(x) \, dx = 2hf(x_1) + \frac{h^3}{3} f''(x_1) + \frac{f^{(4)}(\xi_1)}{60} h^5.$$

If we now replace $f''(x_1)$ by the approximation given in Eq. (4.9) of Section 4.1, we have

$$\int_{x_0}^{x_2} f(x) \, dx = 2hf(x_1) + \frac{h^3}{3} \left\{ \frac{1}{h^2} [f(x_0) - 2f(x_1) + f(x_2)] - \frac{h^2}{12} f^{(4)}(\xi_2) \right\} + \frac{f^{(4)}(\xi_1)}{60} h^5$$

$$= \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{12} \left[\frac{1}{3} f^{(4)}(\xi_2) - \frac{1}{5} f^{(4)}(\xi_1) \right].$$

It can be shown by alternative methods (see Exercise 24) that the values ξ_1 and ξ_2 in this expression can be replaced by a common value ξ in (x_0, x_2). This gives Simpson's rule.

Thomas Simpson (1710–1761) was a self-taught mathematician who supported himself during his early years as a weaver. His primary interest was probability theory, although in 1750 he published a two-volume calculus book entitled *The Doctrine and Application of Fluxions.*

Simpson's Rule:

$$\int_{x_0}^{x_2} f(x) \, dx = \frac{h}{3} [f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90} f^{(4)}(\xi).$$

The error term in Simpson's rule involves the fourth derivative of f, so it gives exact results when applied to any polynomial of degree three or less.

Example 1   Compare the Trapezoidal rule and Simpson's rule approximations to $\int_0^2 f(x) \, dx$ when $f(x)$ is

(a) x^2 (b) x^4 (c) $(x + 1)^{-1}$
(d) $\sqrt{1 + x^2}$ (e) $\sin x$ (f) e^x

Solution   On $[0, 2]$ the Trapezoidal and Simpson's rule have the forms

$$\text{Trapezoid:} \quad \int_0^2 f(x) \, dx \approx f(0) + f(2) \quad \text{and}$$

$$\text{Simpson's:} \quad \int_0^2 f(x) \, dx \approx \frac{1}{3} [f(0) + 4f(1) + f(2)].$$

When $f(x) = x^2$ they give

$$\text{Trapezoid:} \quad \int_0^2 f(x)\, dx \approx 0^2 + 2^2 = 4 \quad \text{and}$$

$$\text{Simpson's:} \quad \int_0^2 f(x)\, dx \approx \frac{1}{3}[(0^2) + 4 \cdot 1^2 + 2^2] = \frac{8}{3}.$$

The approximation from Simpson's rule is exact because its truncation error involves $f^{(4)}$, which is identically 0 when $f(x) = x^2$.

The results to three places for the functions are summarized in Table 4.7. Notice that in each instance Simpson's Rule is significantly superior. ∎

Table 4.7

$f(x)$	(a) x^2	(b) x^4	(c) $(x+1)^{-1}$	(d) $\sqrt{1+x^2}$	(e) $\sin x$	(f) e^x
Exact value	2.667	6.400	1.099	2.958	1.416	6.389
Trapezoidal	4.000	16.000	1.333	3.326	0.909	8.389
Simpson's	2.667	6.667	1.111	2.964	1.425	6.421

Measuring Precision

The standard derivation of quadrature error formulas is based on determining the class of polynomials for which these formulas produce exact results. The next definition is used to facilitate the discussion of this derivation.

Definition 4.1   The **degree of accuracy**, or **precision**, of a quadrature formula is the largest positive integer n such that the formula is exact for x^k, for each $k = 0, 1, \ldots, n$. ∎

The improved accuracy of Simpson's rule over the Trapezoidal rule is intuitively explained by the fact that Simpson's rule includes a midpoint evaluation that provides better balance to the approximation.

Definition 4.1 implies that the Trapezoidal and Simpson's rules have degrees of precision one and three, respectively.

Integration and summation are linear operations; that is,

$$\int_a^b (\alpha f(x) + \beta g(x))\, dx = \alpha \int_a^b f(x)\, dx + \beta \int_a^b g(x)\, dx$$

and

$$\sum_{i=0}^n (\alpha f(x_i) + \beta g(x_i)) = \alpha \sum_{i=0}^n f(x_i) + \beta \sum_{i=0}^n g(x_i),$$

for each pair of integrable functions f and g and each pair of real constants α and β. This implies (see Exercise 25) that:

The open and closed terminology for methods implies that the open methods use as nodes only points in the open interval, (a, b) to approximate $\int_a^b f(x)\, dx$. The closed methods include the points a and b of the closed interval $[a, b]$ as nodes.

- The degree of precision of a quadrature formula is n if and only if the error is zero for all polynomials of degree $k = 0, 1, \ldots, n$, but is not zero for some polynomial of degree $n + 1$.

The Trapezoidal and Simpson's rules are examples of a class of methods known as Newton-Cotes formulas. There are two types of Newton-Cotes formulas, open and closed.

Closed Newton-Cotes Formulas

The $(n+1)$-*point closed Newton-Cotes formula* uses nodes $x_i = x_0 + ih$, for $i = 0, 1, \ldots, n$, where $x_0 = a$, $x_n = b$ and $h = (b-a)/n$. (See Figure 4.5.) It is called closed because the endpoints of the closed interval $[a, b]$ are included as nodes.

Figure 4.5
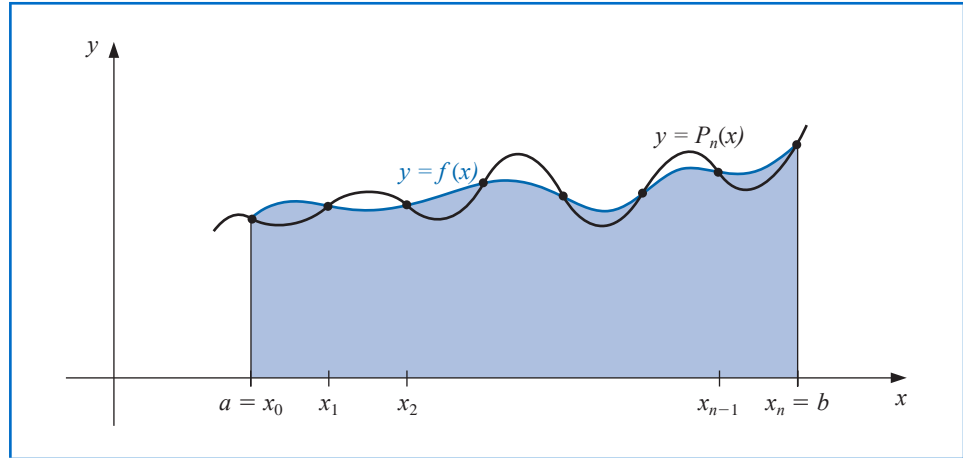
The formula assumes the form

$$\int_a^b f(x) \, dx \approx \sum_{i=0}^n a_i f(x_i),$$

where

$$a_i = \int_{x_0}^{x_n} L_i(x) \, dx = \int_{x_0}^{x_n} \prod_{\substack{j=0 \\ j \neq i}}^n \frac{(x - x_j)}{(x_i - x_j)} \, dx.$$

The following theorem details the error analysis associated with the closed Newton-Cotes formulas. For a proof of this theorem, see [IK], p. 313.

Theorem 4.2   Suppose that $\sum_{i=0}^n a_i f(x_i)$ denotes the $(n+1)$-point closed Newton-Cotes formula with $x_0 = a$, $x_n = b$, and $h = (b-a)/n$. There exists $\xi \in (a, b)$ for which

$$\int_a^b f(x) \, dx = \sum_{i=0}^n a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_0^n t^2(t-1) \cdots (t-n) \, dt,$$

if n is even and $f \in C^{n+2}[a, b]$, and

$$\int_a^b f(x) \, dx = \sum_{i=0}^n a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_0^n t(t-1) \cdots (t-n) \, dt,$$

if n is odd and $f \in C^{n+1}[a, b]$.   ▪

Note that when n is an even integer, the degree of precision is $n + 1$, although the interpolation polynomial is of degree at most n. When n is odd, the degree of precision is only n.

Some of the common **closed Newton-Cotes formulas** with their error terms are listed. Note that in each case the unknown value ξ lies in (a, b).

$n = 1$: Trapezoidal rule

$$\int_{x_0}^{x_1} f(x)\, dx = \frac{h}{2}[f(x_0) + f(x_1)] - \frac{h^3}{12} f''(\xi), \quad \text{where} \quad x_0 < \xi < x_1. \tag{4.25}$$

$n = 2$: Simpson's rule

$$\int_{x_0}^{x_2} f(x)\, dx = \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)] - \frac{h^5}{90} f^{(4)}(\xi), \quad \text{where} \quad x_0 < \xi < x_2. \tag{4.26}$$

$n = 3$: Simpson's Three-Eighths rule

$$\int_{x_0}^{x_3} f(x)\, dx = \frac{3h}{8}[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)] - \frac{3h^5}{80} f^{(4)}(\xi), \tag{4.27}$$

$$\text{where} \quad x_0 < \xi < x_3.$$

$n = 4$:

$$\int_{x_0}^{x_4} f(x)\, dx = \frac{2h}{45}[7f(x_0) + 32f(x_1) + 12f(x_2) + 32f(x_3) + 7f(x_4)] - \frac{8h^7}{945} f^{(6)}(\xi),$$

$$\text{where} \quad x_0 < \xi < x_4. \tag{4.28}$$

Open Newton-Cotes Formulas

The *open Newton-Cotes formulas* do not include the endpoints of $[a, b]$ as nodes. They use the nodes $x_i = x_0 + ih$, for each $i = 0, 1, \ldots, n$, where $h = (b - a)/(n + 2)$ and $x_0 = a + h$. This implies that $x_n = b - h$, so we label the endpoints by setting $x_{-1} = a$ and $x_{n+1} = b$, as shown in Figure 4.6 on page 200. Open formulas contain all the nodes used for the approximation within the open interval (a, b). The formulas become

$$\int_a^b f(x)\, dx = \int_{x_{-1}}^{x_{n+1}} f(x)\, dx \approx \sum_{i=0}^n a_i f(x_i),$$

where

$$a_i = \int_a^b L_i(x)\, dx.$$

Figure 4.6
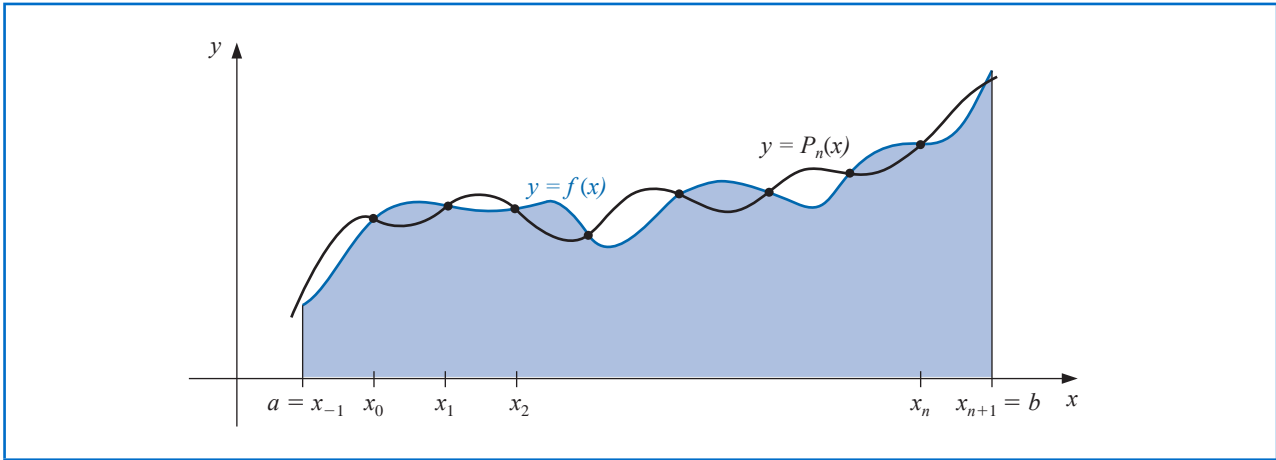
The following theorem is analogous to Theorem 4.2; its proof is contained in [IK], p. 314.

Theorem 4.3 Suppose that $\sum_{i=0}^{n} a_i f(x_i)$ denotes the $(n+1)$-point open Newton-Cotes formula with $x_{-1} = a$, $x_{n+1} = b$, and $h = (b-a)/(n+2)$. There exists $\xi \in (a, b)$ for which

$$\int_a^b f(x)\, dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+3} f^{(n+2)}(\xi)}{(n+2)!} \int_{-1}^{n+1} t^2(t-1)\cdots(t-n)\, dt,$$

if n is even and $f \in C^{n+2}[a, b]$, and

$$\int_a^b f(x)\, dx = \sum_{i=0}^{n} a_i f(x_i) + \frac{h^{n+2} f^{(n+1)}(\xi)}{(n+1)!} \int_{-1}^{n+1} t(t-1)\cdots(t-n)\, dt,$$

if n is odd and $f \in C^{n+1}[a, b]$.   ▪

Notice, as in the case of the closed methods, we have the degree of precision comparatively higher for the even methods than for the odd methods.

Some of the common **open Newton-Cotes** formulas with their error terms are as follows:

$n = 0$: Midpoint rule

$$\int_{x_{-1}}^{x_1} f(x)\, dx = 2hf(x_0) + \frac{h^3}{3} f''(\xi), \quad \text{where} \quad x_{-1} < \xi < x_1. \tag{4.29}$$

$n = 1$:

$$\int_{x_{-1}}^{x_2} f(x)\, dx = \frac{3h}{2}[f(x_0) + f(x_1)] + \frac{3h^3}{4} f''(\xi), \quad \text{where} \quad x_{-1} < \xi < x_2. \tag{4.30}$$

n = 2:

$$\int_{x_{-1}}^{x_3} f(x)\, dx = \frac{4h}{3}[2f(x_0) - f(x_1) + 2f(x_2)] + \frac{14h^5}{45} f^{(4)}(\xi), \tag{4.31}$$

where $x_{-1} < \xi < x_3$.

n = 3:

$$\int_{x_{-1}}^{x_4} f(x)\, dx = \frac{5h}{24}[11f(x_0) + f(x_1) + f(x_2) + 11f(x_3)] + \frac{95}{144} h^5 f^{(4)}(\xi), \tag{4.32}$$

where $x_{-1} < \xi < x_4$.

Example 2 Compare the results of the closed and open Newton-Cotes formulas listed as (4.25)–(4.28) and (4.29)–(4.32) when approximating

$$\int_0^{\pi/4} \sin x\, dx = 1 - \sqrt{2}/2 \approx 0.29289322.$$

Solution For the closed formulas we have

$$n = 1: \quad \frac{(\pi/4)}{2}\left[\sin 0 + \sin \frac{\pi}{4}\right] \approx 0.27768018$$

$$n = 2: \quad \frac{(\pi/8)}{3}\left[\sin 0 + 4\sin \frac{\pi}{8} + \sin \frac{\pi}{4}\right] \approx 0.29293264$$

$$n = 3: \quad \frac{3(\pi/12)}{8}\left[\sin 0 + 3\sin \frac{\pi}{12} + 3\sin \frac{\pi}{6} + \sin \frac{\pi}{4}\right] \approx 0.29291070$$

$$n = 4: \quad \frac{2(\pi/16)}{45}\left[7\sin 0 + 32\sin \frac{\pi}{16} + 12\sin \frac{\pi}{8} + 32\sin \frac{3\pi}{16} + 7\sin \frac{\pi}{4}\right] \approx 0.29289318$$

and for the open formulas we have

$$n = 0: \quad 2(\pi/8)\left[\sin \frac{\pi}{8}\right] \approx 0.30055887$$

$$n = 1: \quad \frac{3(\pi/12)}{2}\left[\sin \frac{\pi}{12} + \sin \frac{\pi}{6}\right] \approx 0.29798754$$

$$n = 2: \quad \frac{4(\pi/16)}{3}\left[2\sin \frac{\pi}{16} - \sin \frac{\pi}{8} + 2\sin \frac{3\pi}{16}\right] \approx 0.29285866$$

$$n = 3: \quad \frac{5(\pi/20)}{24}\left[11\sin \frac{\pi}{20} + \sin \frac{\pi}{10} + \sin \frac{3\pi}{20} + 11\sin \frac{\pi}{5}\right] \approx 0.29286923$$

Table 4.8 summarizes these results and shows the approximation errors. ∎

Table 4.8

n	0	1	2	3	4
Closed formulas		0.27768018	0.29293264	0.29291070	0.29289318
Error		0.01521303	0.00003942	0.00001748	0.00000004
Open formulas	0.30055887	0.29798754	0.29285866	0.29286923	
Error	0.00766565	0.00509432	0.00003456	0.00002399	

EXERCISE SET 4.3

1. Approximate the following integrals using the Trapezoidal rule.

   a. $\int_{0.5}^{1} x^4 \, dx$

   b. $\int_{0}^{0.5} \frac{2}{x-4} \, dx$

   c. $\int_{1}^{1.5} x^2 \ln x \, dx$

   d. $\int_{0}^{1} x^2 e^{-x} \, dx$

   e. $\int_{1}^{1.6} \frac{2x}{x^2-4} \, dx$

   f. $\int_{0}^{0.35} \frac{2}{x^2-4} \, dx$

   g. $\int_{0}^{\pi/4} x \sin x \, dx$

   h. $\int_{0}^{\pi/4} e^{3x} \sin 2x \, dx$

2. Approximate the following integrals using the Trapezoidal rule.

   a. $\int_{-0.25}^{0.25} (\cos x)^2 \, dx$

   b. $\int_{-0.5}^{0} x \ln(x+1) \, dx$

   c. $\int_{0.75}^{1.3} \left((\sin x)^2 - 2x \sin x + 1\right) \, dx$

   d. $\int_{e}^{e+1} \frac{1}{x \ln x} \, dx$

3. Find a bound for the error in Exercise 1 using the error formula, and compare this to the actual error.

4. Find a bound for the error in Exercise 2 using the error formula, and compare this to the actual error.

5. Repeat Exercise 1 using Simpson's rule.

6. Repeat Exercise 2 using Simpson's rule.

7. Repeat Exercise 3 using Simpson's rule and the results of Exercise 5.

8. Repeat Exercise 4 using Simpson's rule and the results of Exercise 6.

9. Repeat Exercise 1 using the Midpoint rule.

10. Repeat Exercise 2 using the Midpoint rule.

11. Repeat Exercise 3 using the Midpoint rule and the results of Exercise 9.

12. Repeat Exercise 4 using the Midpoint rule and the results of Exercise 10.

13. The Trapezoidal rule applied to $\int_0^2 f(x) \, dx$ gives the value 4, and Simpson's rule gives the value 2. What is $f(1)$?

14. The Trapezoidal rule applied to $\int_0^2 f(x) \, dx$ gives the value 5, and the Midpoint rule gives the value 4. What value does Simpson's rule give?

15. Find the degree of precision of the quadrature formula
$$\int_{-1}^{1} f(x) \, dx = f\left(-\frac{\sqrt{3}}{3}\right) + f\left(\frac{\sqrt{3}}{3}\right).$$

16. Let $h = (b-a)/3$, $x_0 = a$, $x_1 = a+h$, and $x_2 = b$. Find the degree of precision of the quadrature formula
$$\int_a^b f(x) \, dx = \frac{9}{4} h f(x_1) + \frac{3}{4} h f(x_2).$$

17. The quadrature formula $\int_{-1}^{1} f(x) \, dx = c_0 f(-1) + c_1 f(0) + c_2 f(1)$ is exact for all polynomials of degree less than or equal to 2. Determine c_0, c_1, and c_2.

18. The quadrature formula $\int_0^2 f(x) \, dx = c_0 f(0) + c_1 f(1) + c_2 f(2)$ is exact for all polynomials of degree less than or equal to 2. Determine c_0, c_1, and c_2.

19. Find the constants c_0, c_1, and x_1 so that the quadrature formula
$$\int_0^1 f(x) \, dx = c_0 f(0) + c_1 f(x_1)$$
has the highest possible degree of precision.

20. Find the constants x_0, x_1, and c_1 so that the quadrature formula
$$\int_0^1 f(x) \, dx = \frac{1}{2} f(x_0) + c_1 f(x_1)$$
has the highest possible degree of precision.

21. Approximate the following integrals using formulas (4.25) through (4.32). Are the accuracies of the approximations consistent with the error formulas? Which of parts (d) and (e) give the better approximation?

    a. $\int_0^{0.1} \sqrt{1+x}\,dx$ **b.** $\int_0^{\pi/2} (\sin x)^2\,dx$

    c. $\int_{1.1}^{1.5} e^x\,dx$ **d.** $\int_1^{10} \frac{1}{x}\,dx$

    e. $\int_1^{5.5} \frac{1}{x}\,dx + \int_{5.5}^{10} \frac{1}{x}\,dx$ **f.** $\int_0^1 x^{1/3}\,dx$

22. Given the function f at the following values,

x	1.8	2.0	2.2	2.4	2.6
$f(x)$	3.12014	4.42569	6.04241	8.03014	10.46675

    approximate $\int_{1.8}^{2.6} f(x)\,dx$ using all the appropriate quadrature formulas of this section.

23. Suppose that the data of Exercise 22 have round-off errors given by the following table.

x	1.8	2.0	2.2	2.4	2.6
Error in $f(x)$	2×10^{-6}	-2×10^{-6}	-0.9×10^{-6}	-0.9×10^{-6}	2×10^{-6}

    Calculate the errors due to round-off in Exercise 22.

24. Derive Simpson's rule with error term by using

    $$\int_{x_0}^{x_2} f(x)\,dx = a_0 f(x_0) + a_1 f(x_1) + a_2 f(x_2) + k f^{(4)}(\xi).$$

    Find a_0, a_1, and a_2 from the fact that Simpson's rule is exact for $f(x) = x^n$ when $n = 1, 2$, and 3. Then find k by applying the integration formula with $f(x) = x^4$.

25. Prove the statement following Definition 4.1; that is, show that a quadrature formula has degree of precision n if and only if the error $E(P(x)) = 0$ for all polynomials $P(x)$ of degree $k = 0, 1, \ldots, n$, but $E(P(x)) \neq 0$ for some polynomial $P(x)$ of degree $n + 1$.

26. Derive Simpson's three-eighths rule (the closed rule with $n = 3$) with error term by using Theorem 4.2.

27. Derive the open rule with $n = 1$ with error term by using Theorem 4.3.

4.4 Composite Numerical Integration

The Newton-Cotes formulas are generally unsuitable for use over large integration intervals. High-degree formulas would be required, and the values of the coefficients in these formulas are difficult to obtain. Also, the Newton-Cotes formulas are based on interpolatory polynomials that use equally-spaced nodes, a procedure that is inaccurate over large intervals because of the oscillatory nature of high-degree polynomials.

Piecewise approximation is often effective. Recall that this was used for spline interpolation.

    In this section, we discuss a *piecewise* approach to numerical integration that uses the low-order Newton-Cotes formulas. These are the techniques most often applied.

Example 1   Use Simpson's rule to approximate $\int_0^4 e^x\,dx$ and compare this to the results obtained by adding the Simpson's rule approximations for $\int_0^2 e^x\,dx$ and $\int_2^4 e^x\,dx$. Compare these approximations to the sum of Simpson's rule for $\int_0^1 e^x\,dx$, $\int_1^2 e^x\,dx$, $\int_2^3 e^x\,dx$, and $\int_3^4 e^x\,dx$.

Solution Simpson's rule on $[0, 4]$ uses $h = 2$ and gives

$$\int_0^4 e^x \, dx \approx \frac{2}{3}(e^0 + 4e^2 + e^4) = 56.76958.$$

The exact answer in this case is $e^4 - e^0 = 53.59815$, and the error -3.17143 is far larger than we would normally accept.

Applying Simpson's rule on each of the intervals $[0, 2]$ and $[2, 4]$ uses $h = 1$ and gives

$$\int_0^4 e^x \, dx = \int_0^2 e^x \, dx + \int_2^4 e^x \, dx$$

$$\approx \frac{1}{3}\left(e^0 + 4e + e^2\right) + \frac{1}{3}\left(e^2 + 4e^3 + e^4\right)$$

$$= \frac{1}{3}\left(e^0 + 4e + 2e^2 + 4e^3 + e^4\right)$$

$$= 53.86385.$$

The error has been reduced to -0.26570.

For the integrals on $[0, 1], [1, 2], [3, 4]$, and $[3, 4]$ we use Simpson's rule four times with $h = \frac{1}{2}$ giving

$$\int_0^4 e^x \, dx = \int_0^1 e^x \, dx + \int_1^2 e^x \, dx + \int_2^3 e^x \, dx + \int_3^4 e^x \, dx$$

$$\approx \frac{1}{6}\left(e_0 + 4e^{1/2} + e\right) + \frac{1}{6}\left(e + 4e^{3/2} + e^2\right)$$

$$+ \frac{1}{6}\left(e^2 + 4e^{5/2} + e^3\right) + \frac{1}{6}\left(e^3 + 4e^{7/2} + e^4\right)$$

$$= \frac{1}{6}\left(e^0 + 4e^{1/2} + 2e + 4e^{3/2} + 2e^2 + 4e^{5/2} + 2e^3 + 4e^{7/2} + e^4\right)$$

$$= 53.61622.$$

The error for this approximation has been reduced to -0.01807. ∎

To generalize this procedure for an arbitrary integral $\int_a^b f(x)\, dx$, choose an even integer n. Subdivide the interval $[a, b]$ into n subintervals, and apply Simpson's rule on each consecutive pair of subintervals. (See Figure 4.7.)

Figure 4.7
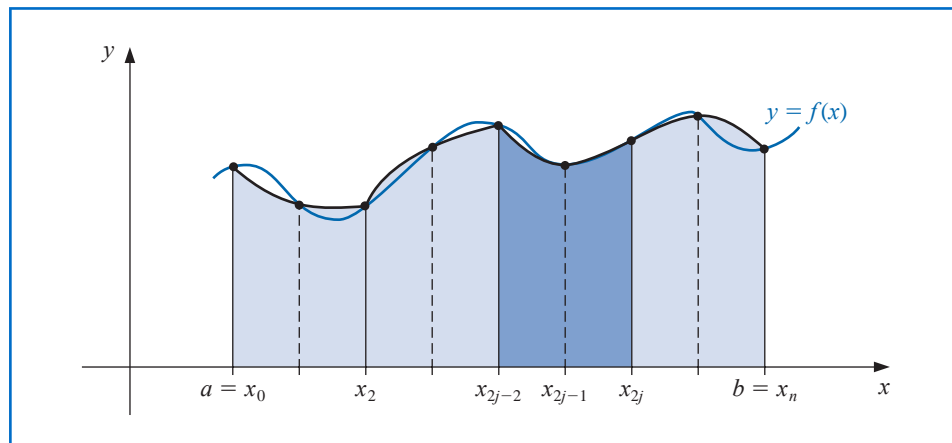
With $h = (b - a)/n$ and $x_j = a + jh$, for each $j = 0, 1, \ldots, n$, we have

$$\int_a^b f(x)\, dx = \sum_{j=1}^{n/2} \int_{x_{2j-2}}^{x_{2j}} f(x)\, dx$$

$$= \sum_{j=1}^{n/2} \left\{ \frac{h}{3}[f(x_{2j-2}) + 4f(x_{2j-1}) + f(x_{2j})] - \frac{h^5}{90} f^{(4)}(\xi_j) \right\},$$

for some ξ_j with $x_{2j-2} < \xi_j < x_{2j}$, provided that $f \in C^4[a, b]$. Using the fact that for each $j = 1, 2, \ldots, (n/2) - 1$ we have $f(x_{2j})$ appearing in the term corresponding to the interval $[x_{2j-2}, x_{2j}]$ and also in the term corresponding to the interval $[x_{2j}, x_{2j+2}]$, we can reduce this sum to

$$\int_a^b f(x)\, dx = \frac{h}{3}\left[f(x_0) + 2\sum_{j=1}^{(n/2)-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(x_n) \right] - \frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j).$$

The error associated with this approximation is

$$E(f) = -\frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j),$$

where $x_{2j-2} < \xi_j < x_{2j}$, for each $j = 1, 2, \ldots, n/2$.

If $f \in C^4[a, b]$, the Extreme Value Theorem 1.9 implies that $f^{(4)}$ assumes its maximum and minimum in $[a, b]$. Since

$$\min_{x \in [a,b]} f^{(4)}(x) \le f^{(4)}(\xi_j) \le \max_{x \in [a,b]} f^{(4)}(x),$$

we have

$$\frac{n}{2} \min_{x \in [a,b]} f^{(4)}(x) \le \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \le \frac{n}{2} \max_{x \in [a,b]} f^{(4)}(x)$$

and

$$\min_{x \in [a,b]} f^{(4)}(x) \le \frac{2}{n} \sum_{j=1}^{n/2} f^{(4)}(\xi_j) \le \max_{x \in [a,b]} f^{(4)}(x).$$

By the Intermediate Value Theorem 1.11, there is a $\mu \in (a, b)$ such that

$$f^{(4)}(\mu) = \frac{2}{n} \sum_{j=1}^{n/2} f^{(4)}(\xi_j).$$

Thus

$$E(f) = -\frac{h^5}{90} \sum_{j=1}^{n/2} f^{(4)}(\xi_j) = -\frac{h^5}{180} n f^{(4)}(\mu),$$

or, since $h = (b - a)/n$,

$$E(f) = -\frac{(b - a)}{180} h^4 f^{(4)}(\mu).$$

These observations produce the following result.

Theorem 4.4   Let $f \in C^4[a, b]$, n be even, $h = (b - a)/n$, and $x_j = a + jh$, for each $j = 0, 1, \ldots, n$. There exists a $\mu \in (a, b)$ for which the **Composite Simpson's rule** for n subintervals can be written with its error term as

$$\int_a^b f(x)\, dx = \frac{h}{3}\left[f(a) + 2\sum_{j=1}^{(n/2)-1} f(x_{2j}) + 4\sum_{j=1}^{n/2} f(x_{2j-1}) + f(b) \right] - \frac{b - a}{180} h^4 f^{(4)}(\mu).$$

■

Notice that the error term for the Composite Simpson's rule is $O(h^4)$, whereas it was $O(h^5)$ for the standard Simpson's rule. However, these rates are not comparable because for standard Simpson's rule we have h fixed at $h = (b - a)/2$, but for Composite Simpson's rule we have $h = (b - a)/n$, for n an even integer. This permits us to considerably reduce the value of h when the Composite Simpson's rule is used.

Algorithm 4.1 uses the Composite Simpson's rule on n subintervals. This is the most frequently used general-purpose quadrature algorithm.

ALGORITHM 4.1

Composite Simpson's Rule

To approximate the integral $I = \int_a^b f(x)\, dx$:

INPUT   endpoints a, b; even positive integer n.

OUTPUT   approximation XI to I.

Step 1   Set $h = (b - a)/n$.

Step 2   Set $XI0 = f(a) + f(b)$;
                $XI1 = 0$;   (*Summation of $f(x_{2i-1})$.*)
                $XI2 = 0$.   (*Summation of $f(x_{2i})$.*)

Step 3   For $i = 1, \ldots, n - 1$ do Steps 4 and 5.

   Step 4   Set $X = a + ih$.

   Step 5   If i is even then set $XI2 = XI2 + f(X)$
                        else set $XI1 = XI1 + f(X)$.

*Step 6*   Set $XI = h(XI0 + 2 \cdot XI2 + 4 \cdot XI1)/3$.

Step 7   OUTPUT (XI);
           STOP.

■

The subdivision approach can be applied to any of the Newton-Cotes formulas. The extensions of the Trapezoidal (see Figure 4.8) and Midpoint rules are given without proof. The Trapezoidal rule requires only one interval for each application, so the integer n can be either odd or even.

Theorem 4.5   Let $f \in C^2[a, b]$, $h = (b - a)/n$, and $x_j = a + jh$, for each $j = 0, 1, \ldots, n$. There exists a $\mu \in (a, b)$ for which the **Composite Trapezoidal rule** for n subintervals can be written with its error term as
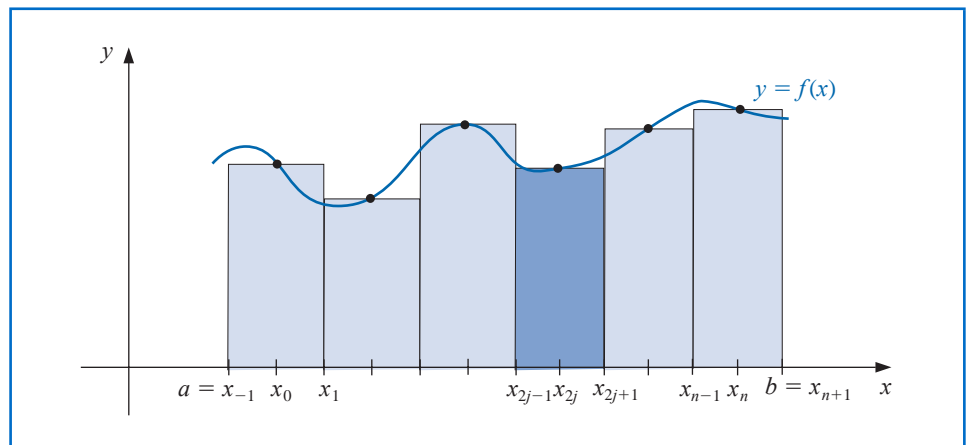
$$\int_a^b f(x)\, dx = \frac{h}{2}\left[f(a) + 2\sum_{j=1}^{n-1} f(x_j) + f(b) \right] - \frac{b - a}{12} h^2 f''(\mu).$$

■

Figure 4.8
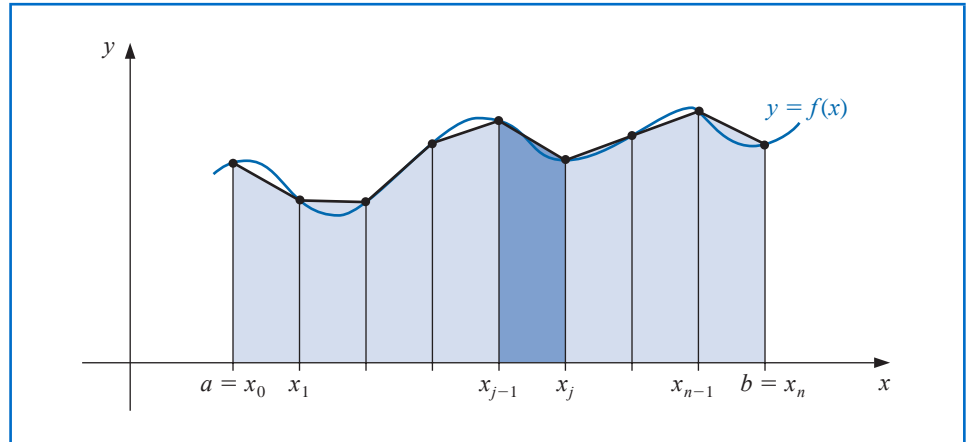
For the Composite Midpoint rule, n must again be even. (See Figure 4.9.)

Figure 4.9

Theorem 4.6   Let $f \in C^2[a,b]$, n be even, $h = (b-a)/(n+2)$, and $x_j = a + (j+1)h$ for each $j = -1, 0, \ldots, n+1$. There exists a $\mu \in (a,b)$ for which the **Composite Midpoint rule** for $n + 2$ subintervals can be written with its error term as

$$\int_a^b f(x)\,dx = 2h \sum_{j=0}^{n/2} f(x_{2j}) + \frac{b-a}{6}h^2 f''(\mu). \qquad \blacksquare$$

Example 2   Determine values of h that will ensure an approximation error of less than 0.00002 when approximating $\int_0^\pi \sin x\,dx$ and employing
(a) Composite Trapezoidal rule and **(b)** Composite Simpson's rule.

Solution   **(a)** The error form for the Composite Trapezoidal rule for $f(x) = \sin x$ on $[0, \pi]$ is

$$\left| \frac{\pi h^2}{12} f''(\mu) \right| = \left| \frac{\pi h^2}{12}(-\sin \mu) \right| = \frac{\pi h^2}{12}|\sin \mu|.$$

To ensure sufficient accuracy with this technique we need to have

$$\frac{\pi h^2}{12}|\sin\mu| \le \frac{\pi h^2}{12} < 0.00002.$$

Since $h = \pi/n$ implies that $n = \pi/h$, we need

$$\frac{\pi^3}{12n^2} < 0.00002 \quad \text{which implies that} \quad n > \left(\frac{\pi^3}{12(0.00002)}\right)^{1/2} \approx 359.44.$$

and the Composite Trapezoidal rule requires $n \ge 360$.

(b) The error form for the Composite Simpson's rule for $f(x) = \sin x$ on $[0, \pi]$ is

$$\left|\frac{\pi h^4}{180} f^{(4)}(\mu)\right| = \left|\frac{\pi h^4}{180} \sin\mu\right| = \frac{\pi h^4}{180}|\sin\mu|.$$

To ensure sufficient accuracy with this technique we need to have

$$\frac{\pi h^4}{180}|\sin\mu| \le \frac{\pi h^4}{180} < 0.00002.$$

Using again the fact that $n = \pi/h$ gives

$$\frac{\pi^5}{180n^4} < 0.00002 \quad \text{which implies that} \quad n > \left(\frac{\pi^5}{180(0.00002)}\right)^{1/4} \approx 17.07.$$

So Composite Simpson's rule requires only $n \ge 18$.
Composite Simpson's rule with $n = 18$ gives

$$\int_0^\pi \sin x \, dx \approx \frac{\pi}{54}\left[2\sum_{j=1}^{8}\sin\left(\frac{j\pi}{9}\right) + 4\sum_{j=1}^{9}\sin\left(\frac{(2j-1)\pi}{18}\right)\right] = 2.0000104.$$

This is accurate to within about 10^{-5} because the true value is $-\cos(\pi) - (-\cos(0)) = 2$. ▪

Composite Simpson's rule is the clear choice if you wish to minimize computation. For comparison purposes, consider the Composite Trapezoidal rule using $h = \pi/18$ for the integral in Example 2. This approximation uses the same function evaluations as Composite Simpson's rule but the approximation in this case

$$\int_0^\pi \sin x \, dx \approx \frac{\pi}{36}\left[2\sum_{j=1}^{17}\sin\left(\frac{j\pi}{18}\right) + \sin 0 + \sin\pi\right] = \frac{\pi}{36}\left[2\sum_{j=1}^{17}\sin\left(\frac{j\pi}{18}\right)\right] = 1.9949205.$$

is accurate only to about 5×10^{-3}.

Maple contains numerous procedures for numerical integration in the *NumericalAnalysis* subpackage of the *Student* package. First access the library as usual with

with(*Student*[*NumericalAnalysis*])

The command for all methods is *Quadrature* with the options in the call specifying the method to be used. We will use the Trapezoidal method to illustrate the procedure. First define the function and the interval of integration with

$f := x \to \sin(x); \ a := 0.0; \ b := \pi$

After Maple responds with the function and the interval, enter the command

$Quadrature(f(x), x = a..b, method = trapezoid, partition = 20, output = value)$

$$1.995885973$$

The value of the step size h in this instance is the width of the interval $b - a$ divided by the number specified by $partition = 20$.

Simpson's method can be called in a similar manner, except that the step size h is determined by $b - a$ divided by twice the value of $partition$. Hence, the Simpson's rule approximation using the same nodes as those in the Trapezoidal rule is called with

$Quadrature(f(x), x = a..b, method = simpson, partition = 10, output = value)$

$$2.000006785$$

Any of the Newton-Cotes methods can be called using the option

$$method = newtoncotes[open, n] \quad \text{or} \quad method = newtoncotes[closed, n]$$

Be careful to correctly specify the number in $partition$ when an even number of divisions is required, and when an open method is employed.

Round-Off Error Stability

In Example 2 we saw that ensuring an accuracy of 2×10^{-5} for approximating $\int_0^\pi \sin x \, dx$ required 360 subdivisions of $[0, \pi]$ for the Composite Trapezoidal rule and only 18 for Composite Simpson's rule. In addition to the fact that less computation is needed for the Simpson's technique, you might suspect that because of fewer computations this method would also involve less round-off error. However, an important property shared by all the composite integration techniques is a stability with respect to round-off error. That is, the round-off error does not depend on the number of calculations performed.

Numerical integration is expected to be stable, whereas numerical differentiation is unstable.

To demonstrate this rather amazing fact, suppose we apply the Composite Simpson's rule with n subintervals to a function f on $[a, b]$ and determine the maximum bound for the round-off error. Assume that $f(x_i)$ is approximated by $\tilde{f}(x_i)$ and that

$$f(x_i) = \tilde{f}(x_i) + e_i, \quad \text{for each} \quad i = 0, 1, \ldots, n,$$

where e_i denotes the round-off error associated with using $\tilde{f}(x_i)$ to approximate $f(x_i)$. Then the accumulated error, $e(h)$, in the Composite Simpson's rule is

$$e(h) = \left| \frac{h}{3} \left[e_0 + 2 \sum_{j=1}^{(n/2)-1} e_{2j} + 4 \sum_{j=1}^{n/2} e_{2j-1} + e_n \right] \right|$$

$$\leq \frac{h}{3} \left[|e_0| + 2 \sum_{j=1}^{(n/2)-1} |e_{2j}| + 4 \sum_{j=1}^{n/2} |e_{2j-1}| + |e_n| \right].$$

If the round-off errors are uniformly bounded by ε, then

$$e(h) \leq \frac{h}{3} \left[\varepsilon + 2 \left(\frac{n}{2} - 1 \right) \varepsilon + 4 \left(\frac{n}{2} \right) \varepsilon + \varepsilon \right] = \frac{h}{3} 3n\varepsilon = nh\varepsilon.$$

But $nh = b - a$, so

$$e(h) \leq (b - a)\varepsilon,$$

a bound independent of h (and n). This means that, even though we may need to divide an interval into more parts to ensure accuracy, the increased computation that is required does not increase the round-off error. This result implies that the procedure is stable as h approaches zero. Recall that this was not true of the numerical differentiation procedures considered at the beginning of this chapter.

EXERCISE SET 4.4

1. Use the Composite Trapezoidal rule with the indicated values of n to approximate the following integrals.

    a. $\int_1^2 x \ln x \, dx, \quad n = 4$

    b. $\int_{-2}^2 x^3 e^x \, dx, \quad n = 4$

    c. $\int_0^2 \frac{2}{x^2 + 4} \, dx, \quad n = 6$

    d. $\int_0^\pi x^2 \cos x \, dx, \quad n = 6$

    e. $\int_0^2 e^{2x} \sin 3x \, dx, \quad n = 8$

    f. $\int_1^3 \frac{x}{x^2 + 4} \, dx, \quad n = 8$

    g. $\int_3^5 \frac{1}{\sqrt{x^2 - 4}} \, dx, \quad n = 8$

    h. $\int_0^{3\pi/8} \tan x \, dx, \quad n = 8$

2. Use the Composite Trapezoidal rule with the indicated values of n to approximate the following integrals.

    a. $\int_{-0.5}^{0.5} \cos^2 x \, dx, \quad n = 4$

    b. $\int_{-0.5}^{0.5} x \ln(x + 1) \, dx, \quad n = 6$

    c. $\int_{.75}^{1.75} (\sin^2 x - 2x \sin x + 1) \, dx, \quad n = 8$

    d. $\int_e^{e+2} \frac{1}{x \ln x} \, dx, \quad n = 8$

3. Use the Composite Simpson's rule to approximate the integrals in Exercise 1.

4. Use the Composite Simpson's rule to approximate the integrals in Exercise 2.

5. Use the Composite Midpoint rule with $n + 2$ subintervals to approximate the integrals in Exercise 1.

6. Use the Composite Midpoint rule with $n + 2$ subintervals to approximate the integrals in Exercise 2.

7. Approximate $\int_0^2 x^2 \ln(x^2 + 1) \, dx$ using $h = 0.25$. Use

    a. Composite Trapezoidal rule.

    b. Composite Simpson's rule.

    c. Composite Midpoint rule.

8. Approximate $\int_0^2 x^2 e^{-x^2} \, dx$ using $h = 0.25$. Use

    a. Composite Trapezoidal rule.

    b. Composite Simpson's rule.

    c. Composite Midpoint rule.

9. Suppose that $f(0) = 1$, $f(0.5) = 2.5$, $f(1) = 2$, and $f(0.25) = f(0.75) = \alpha$. Find α if the Composite Trapezoidal rule with $n = 4$ gives the value 1.75 for $\int_0^1 f(x) \, dx$.

10. The Midpoint rule for approximating $\int_{-1}^1 f(x) \, dx$ gives the value 12, the Composite Midpoint rule with $n = 2$ gives 5, and Composite Simpson's rule gives 6. Use the fact that $f(-1) = f(1)$ and $f(-0.5) = f(0.5) - 1$ to determine $f(-1)$, $f(-0.5)$, $f(0)$, $f(0.5)$, and $f(1)$.

11. Determine the values of n and h required to approximate

$$\int_0^2 e^{2x} \sin 3x \, dx$$

    to within 10^{-4}. Use

    a. Composite Trapezoidal rule.

    b. Composite Simpson's rule.

    c. Composite Midpoint rule.