2. Divide $[a, b]$ into several subintervals of small length, use a simple quadrature of fairly low precision on each, and add the results to obtain an approximation for $I(f)$.

The methods generated by (2) above are called *composite* quadratures, and we shall study them in this section. First we consider $(N + 1)$ points $\{x_j\}_{j=0}^{N}$ such that $a = x_0 < x_1 < \cdots < x_N = b$. From calculus we know that

$$I(f) = \int_a^b f(x)w(x)\,dx = \sum_{j=0}^{N-1} \int_{x_j}^{x_{j+1}} f(x)w(x)\,dx.$$

Thus approximating $I(f)$ by composite quadrature amounts to approximating each $\int_{x_j}^{x_{j+1}} f(x)w(x)\,dx$ by a low order quadrature, $Q_k^{(j)}(f)$, and adding the resulting approximations. The three rules (trapezoidal, Simpson, and corrected trapezoidal) specifically studied in Section 6.2.2 are very well suited for our purposes here, and we shall concentrate on their use. We shall see that their form is especially simple if we take the points $\{x_j\}_{j=0}^{N}$ to be equally spaced; that is, $x_j = a + jh$ for $h = (b - a)/N$ and $0 \le j \le N$. [Using these rules, of course, we take $w(x) \equiv 1$ in $I(f)$.]

First we consider the composite trapezoidal rule. From (6.5) and the error formula (6.9), we see that for any j

$$\int_{x_j}^{x_{j+1}} f(x)\,dx = \frac{h}{2}\,(f(x_j) + f(x_{j+1})) - \frac{f''(\eta_j)}{12}\,h^3, \qquad x_j < \eta_j < x_{j+1}.$$

Thus we define the composite trapezoidal rule, $T_N(f)$, as

$$T_N(f) = \sum_{j=0}^{N-1} \frac{h}{2}\,(f(x_j) + f(x_{j+1})) = h \sum_{j=1}^{N-1} f(x_j) + \frac{h}{2}\,(f(x_0) + f(x_N)). \tag{6.12a}$$

The error, $I(f) - T_N(f) \equiv e_N^{\mathrm{T}}$, is the sum of the errors on each interval and so

$$e_N^{\mathrm{T}} = \sum_{j=0}^{N-1} f''(\eta_j)(-h^3/12).$$

We pause here to give a lemma that will significantly simplify e_N^{T} above, and can also be used when investigating the errors of other composite rules.

Lemma 6.1

Let $g(x) \in C[a, b]$; and let $\{a_j\}_{j=0}^{N-1}$ be any set of constants, all of which have the same sign. If $t_j \in [a, b]$ for $0 \le j \le N - 1$, then for some $\eta \in [a, b]$

$$\sum_{j=0}^{N-1} a_j g(t_j) = g(\eta) \sum_{j=0}^{N-1} a_j.$$

Proof. Let $m = \min_{a \le x \le b} (g(x)) = g(y_m)$ and $M = \max_{a \le x \le b} (g(x)) = g(y_M)$. Then if the a_j's are nonnegative,

$$m \sum_{j=0}^{N-1} a_j \le \sum_{j=0}^{N-1} a_j g(t_j) \le M \sum_{j=0}^{N-1} a_j.$$

Define r by $r = \sum_{j=0}^{N-1} a_j g(t_j)$ and let $G(x) \equiv g(x) \sum_{j=0}^{N-1} a_j$. Then $G(x) \in C[a, b]$; and by the above inequalities, $G(y_m) \le r \le G(y_M)$. By the intermediate-value theorem, there exists an $\eta \in [a, b]$ such that $G(\eta) = r$, or

$$g(\eta) \sum_{j=0}^{N-1} a_j = \sum_{j=0}^{N-1} a_j g(t_j).$$

The case in which the a_j's are all negative is similar and left to the reader. ∎

If $f''(x) = g(x)$ and $a_j = -h^3/12$ are used in Lemma 6.1, the expression for e_N^T becomes

$$e_N^T = f''(\eta) \sum_{j=0}^{N-1} \left(\frac{-h^3}{12}\right) = -f''(\eta)\frac{Nh^3}{12} = -\frac{f''(\eta)h^2(b-a)}{12}. \quad (6.12b)$$

Continuing in the same fashion, from Simpson's rule, (6.6), and its error, we see that for any j

$$\int_{x_j}^{x_{j+1}} f(x)\, dx = \frac{h}{6}\left(f(x_j) + 4f((x_j + x_{j+1})/2) + f(x_{j+1})\right) - \frac{f^{(iv)}(\eta_j)}{90}\left(\frac{h}{2}\right)^5,$$

$$x_j < \eta_j < x_{j+1}.$$

Summing the approximations for each interval, we have the composite Simpson's rule:

$$S_N(f) = \frac{h}{6}\left\{f(x_0) + f(x_N) + 2\sum_{j=1}^{N-1} f(x_j) + 4\sum_{j=0}^{N-1} f((x_j + x_{j+1})/2)\right\}. \quad (6.13a)$$

Summing the individual errors for $0 \le j \le N-1$ and using Lemma 6.1, we obtain the error, $e_N^S \equiv I(f) - S_N(f)$:

$$\begin{aligned} e_N^S &= -\sum_{j=0}^{N-1} \frac{f^{(iv)}(\eta_j)}{90}\left(\frac{h}{2}\right)^5 = -\frac{f^{(iv)}(\eta)}{90} N \left(\frac{h}{2}\right)^5 \\ &= -\frac{f^{(iv)}(\eta)}{180}\left(\frac{h}{2}\right)^4 (b-a). \end{aligned} \quad (6.13b)$$

We note that Simpson's rule in the form (6.13a) actually requires the evaluation of $f(x)$ at $(2N+1)$ equally spaced points, $\{x_j\}_{j=0}^{N}$ and $\{(x_j + x_{j+1})/2\}_{j=0}^{N-1}$. For a fair comparison with the accuracy of the composite trapezoidal rule, we should actually display a form of the composite Simpson's rule using only $(N + 1)$ points, $\{x_j\}_{j=0}^{N}$. From above we see immediately that we must restrict N to be even and investigate the formulas

$$\int_{x_j}^{x_{j+2}} f(x)\,dx = \frac{2h}{6}\,(f(x_j) + 4f(x_{j+1}) + f(x_{j+2})) - \frac{f^{(iv)}(\eta_j)}{90}\,h^5, \qquad x_j < \eta_j < x_{j+2},$$

for $j = 0, 2, 4, \ldots, N - 2$. Doing this and summing, we obtain

$$S_N'(f) = \frac{h}{3}\left(f(x_0) + f(x_N) + 2\sum_{j=1}^{(N-2)/2} f(x_{2j}) + 4\sum_{j=0}^{(N-2)/2} f(x_{2j+1})\right) \tag{6.14a}$$

and

$$e_N^{S'} = -\frac{f^{(iv)}(\eta)}{180}\,h^4(b - a). \tag{6.14b}$$

We leave to the reader to verify in the manner above that from the corrected trapezoidal rule, (6.7), and its error, (6.10), the composite corrected trapezoidal rule and its error are given by

$$\begin{aligned} CT_N(f) &= h\sum_{j=1}^{N-1} f(x_j) + \frac{h}{2}\,(f(x_0) + f(x_N)) + \frac{h^2}{12}\,(f'(a) - f'(b)) \\ &= T_N(f) + \frac{h^2}{12}\,(f'(a) - f'(b)) \end{aligned} \tag{6.15a}$$

$$e_N^{\mathrm{CT}} = \frac{f^{(iv)}(\eta)}{720}\,h^4(b - a). \tag{6.15b}$$

The reader will note in the derivation of (6.15a) that the derivative evaluations of $f(x)$ at the interior nodes cancel out, and the only two required derivative evaluations are $f'(a)$ and $f'(b)$. This observation, plus the fact that the method has precision 3 and has an h^4 term in the error, makes this rule computationally attractive.

Since the precision of a composite quadrature formula is not increased by taking N larger and larger, we cannot use Theorem 6.1 to guarantee convergence. However, it is fairly easy to show that $\lim_{N\to\infty} T_N(f) = \lim_{N\to\infty} S_N(f) = I(f)$ for any $f \in C[a, b]$. To see this, we merely recall that $T_N(f) = \sum_{j=0}^{N-1} [f(x_j) + f(x_{j+1})](h/2)$. Since $[f(x_j) + f(x_{j+1})]/2$ is just an average, we have by the intermediate-value theorem that there is a point $z_j \in [x_j, x_{j+1}]$ such that $f(z_j) = [f(x_j) + f(x_{j+1})]/2$. Thus $T_N(f) = \sum_{j=0}^{N-1} f(z_j)h$ is a Riemann sum; so from the definition of the definite integral it follows that $T_N(f) \to I(f)$ as $N \to \infty$. A similar analysis can be carried out for Simpson's rule. (See Problem 11 for a general result on the convergence of composite quadratures.)

Because Simpson's rule is derived from quadratic interpolation on the subintervals whereas the trapezoidal rule comes from linear interpolation, we might jump to the conclusion that Simpson's rule is always preferable. This is often true, but in certain instances the trapezoidal rule yields surprisingly good results. For example if $f(x)$ has the property that $f'(a) = f'(b)$, then the trapezoidal rule is equivalent to the corrected trapezoidal rule. [See (6.15a) and compare the error (6.15b) to the Simpson error (6.14b) for application of both rules to $(N + 1)$ points.] Davis and Rabinowitz (1975) is rich with comparative numerical examples from the literature using both rules.

EXAMPLE 6.4. As an example showing how the error bounds of this section can be used, we consider again (as in Example 6.3), the problem of computing $Si(1)$. Suppose we want accuracy on the order of 10^{-8}. How large must N be in order that $|I(f) - T_N(f)| \le 10^{-8}$ and how large must N be in order that $|I(f) - S'_N(f)| \le 10^{-8}$ where

$$I(f) = Si(1) = \int_0^1 \frac{\sin(t)}{t}\,dt?$$

Using the information derived in Example 6.3, we know that $|f''(x)| \le \frac{1}{3}$ and $|f^{(iv)}(x)| \le \frac{1}{5}$ for $0 \le x \le 1$. From (6.12b) and (6.14b) with $b - a = 1$ and $h = 1/N$, we have

$$|e_N^{\mathrm{T}}| \le \frac{1}{36N^2}, \qquad |e_N^{S'}| \le \frac{1}{900N^4}.$$

A quick computation then shows that $N \ge 1667$ is required to make $|e_N^{\mathrm{T}}| \le 10^{-8}$, and $N \ge 19$ is necessary to ensure that $|e_N^{S'}| \le 10^{-8}$.

PROBLEMS, SECTION 6.2.4

1. Write a subroutine that uses the composite trapezoid rule T_N. Test your routine on

   a) $\displaystyle\int_1^2 \frac{1}{x}\,dx$ b) $\displaystyle\int_{-1}^1 \frac{1}{1 + x^2}\,dx$ c) $\displaystyle\int_0^2 \cos(x)dx$

   with $N = 2^k$, $k = 3, 4, \ldots, 10$. Print all your estimates and compare them with the exact result.
2. Apply (6.12b) to each of the integrals in Problem 1 and determine a value of N so that $|e_N^{\mathrm{T}}| \le 10^{-3}$. Compare this value with the actual errors.
3. Repeat Problem 1 with the Simpson's rule S'_N and the corrected trapezoid rule CT_N. Also repeat the analysis in Problem 2 for the integrals (1a) and (1c).
4. This problem and Problem 5 describe how one might construct an elementary "adaptive quadrature", using T_N. The idea is to design a subroutine that accepts an interval $[a, b]$, a function $f(x)$, and an input tolerance TOL. The routine should

return an estimate EST to the integral, and there should be a reasonable expectation that

$$\left|\int_a^b f(x)dx - \text{EST}\right| \le \text{TOL}.$$

The estimate EST is given by $T_N(f)$; so the subroutine somehow has to select an appropriate value for N so that $T_N(f)$ meets the input accuracy request. The subroutine will select N by using an error monitor that is based on the theoretical form of the error in (6.12b); however, the subroutine will *not* calculate $f''(x)$.

To begin, consider the form of the error for (6.12a):

$$I(f) - T_N(f) = \frac{-h^3}{12} \sum_{j=0}^{N-1} f''(\eta_j) \tag{P.1}$$

where $x_1 \le \eta_j \le x_{i+1}$. Now, $T_{2N}(f)$ uses knots $y_0, y_1, \ldots, y_{2N}$ where $y_{2i} = x_i$ and $y_{2i+1} = (x_i + x_{i+1})/2$. Assume that h is small enough so that $f''(x)$ is approximately constant in $[x_i, x_{i+1}]$. Write the expression for $I(f) - T_{2N}(f)$ and show that

$$I(f) - T_{2N}(f) \simeq \frac{1}{4}(I(f) - T_N(f)). \tag{P.2}$$

[Note: In (P.1), h is replaced by $h/2$ to obtain (P.2).] Next, show that the approximation (P.2) is the same as

$$I(f) - T_{2N}(f) \simeq \frac{1}{3}\,[T_{2N}(f) - T_N(f)]. \tag{P.3}$$

5. By Problem 4 (to the extent that h is small enough so that $f''(x)$ is nearly constant over intervals of length h) we see that the error $I(f) - T_{2N}(f)$ can be estimated by a quantity we can monitor; $[T_{2N}(f) - T_N(f)]/3$. Write a subroutine that calculates $T_K(f), T_{2K}(f), T_{4K}(f), \ldots$ and that accepts $T_{2N}(f)$ as an estimate to the integral when

$$|T_{2N}(f) - T_N(f)| \le \text{TOL} \tag{P.4}$$

where TOL is an input accuracy request. [Note that the termination test (P.4) is three times more severe than is required by (P.3); this excess severity is a safety factor.] To ensure that the smoothness assumption on $f''(x)$ has a chance of holding, also insist that K be chosen so that $K \ge 8$ and $h \le .125$. If (P.4) cannot be satisfied with $N \le 1024$, set an error flag to signal failure of the method, and return. Code the subroutine so that only M evaluations of $f(x)$ are necessary in going from $T_M(f)$ to $T_{2M}(f)$. (Note: This formulation of an adaptive quadrature based on T_N is quite inefficient but is simple enough to serve as an introduction to Section 6.3.) Test your routine on the integrals in Problem 1; use TOL $= 10^{-2}$, TOL $= 10^{-3}$, TOL $= 10^{-4}$. Also test your routine on $\int_0^3 f(x)\,dx$ where $f(x) = 1/(x - \sqrt{2})$; the integral does not exist and the routine should signal a failure.

6. Once the construction of any adaptive quadrature is known, it is easy to devise a function that will fool the routine. Try to estimate $\int_0^{\frac{1}{2}} \cos(64\pi x)dx$ with the routine in Problem 5; use TOL $= 10^{-2}$. Why did the routine fail to get a good estimate?

7. Given x_0 and $h > 0$, let $x_1 = x_0 + h$, $x_2 = x_0 + 2h$. Suppose $f \in C^1[x_0, x_2]$. Using the method of undetermined coefficients, show that there is a cubic polynomial $p(x)$ such that $p(x_i) = f(x_i)$, $i = 0, 1, 2$ and $p'(x_1) = f'(x_1)$.
8. Verify the error formula (6.15b) for the corrected trapezoidal rule.
9. How small must h be in order that $|I(f) - S_N(f)| \leq 10^{-6}$ for $f(x) = \sin(10x)$ and $[a, b] = [0, \pi]$? How small must h be in order that $|I(f) - T_N(f)| \leq 10^{-6}$?
10. Show that $\lim_{N\to\infty} S_N(f) = I(f)$ for any $f \in C[a, b]$ where $S_N(f)$ denotes the composite Simpson's rule for $[a, b]$.
11. Suppose $Q(f) = \Sigma_{j=0}^{n} A_j f(x_j)$ is a quadrature formula to approximate $I(f) = \int_{-1}^{1} f(x)dx$ where $\Sigma_{i=0}^{n} A_j = 2$. Let Q_N be the composite formula corresponding to Q applied to $[a, b]$ and suppose that $g \in C[a, b]$. Using upper and lower Riemann sums, show that $Q_N(g) \to \int_a^b g(z)\,dz$.
12. Discuss how the composite Simpson's rule given in (6.13a) can be modified slightly so as to integrate cubic splines exactly.

6.2.5. Multiple Integrals

A fairly common problem is that of evaluating the multiple integral

$$\int_Q\int f(x, y)dA$$

where $f(x, y)$ is real valued and defined on a region Q of the xy-plane. An elementary but useful approach to this important problem is based on techniques familiar from calculus: if the region is simple enough and if the integrand satisfies mild continuity conditions, then we can express the multiple integral as an iterated integral. Specifically, suppose that Q is a region in the xy-plane and has the form pictured in Fig. 6.1. In Fig. 6.1, Q is bounded on the left and right

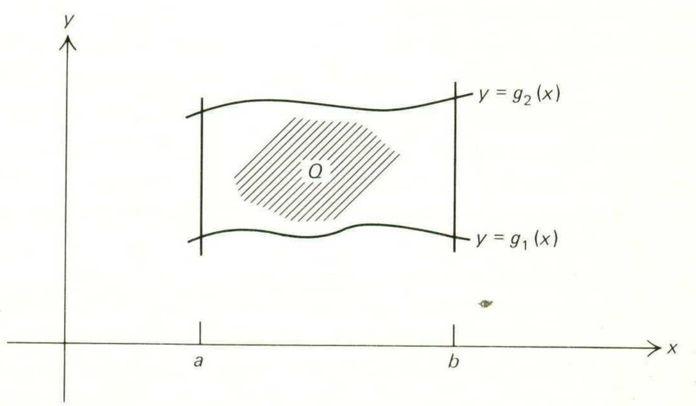

Figure 6.1 A region in the xy-plane