# 6 Numerical Integration and Differentiation

## 6.1 INTRODUCTION

In Chapter 5 we developed numerous ways for efficiently approximating a function, $f(x) \in C[a, b]$. If $g(x)$ is any approximation whatsoever to $f(x)$, and we wish to approximate either the integral or the derivative of $f(x)$, then our first inclination is to use either the integral or the derivative of $g(x)$, respectively, as our approximation. In the case of approximating derivatives, we have already pointed out that the derivative of the interpolatory cubic spline is fairly reliable whereas the derivative of the $n$th degree interpolating polynomial usually is not because of its oscillatory behavior. One other fairly reliable means of derivative approximation is to use the derivative of the discrete least-squares approximation of Section 5.3.1. [This method is especially reliable when the values of $f(x)$ are given in tabular form since this approximation tends to "smooth" the data when the degree of the approximation is fairly small.] In general, however, it remains true that numerical differentiation is a particularly unstable process and quite difficult to analyze carefully. We shall present in detail only one more numerical-differentiation method (based on Richardson extrapolation—Section 6.4). The rest of this chapter will be primarily devoted to numerical integration procedures.

## 6.2 INTERPOLATORY NUMERICAL INTEGRATION

For any function $f(x)$ that is integrable on the interval $[a, b]$, we define

$$I(f) \equiv \int_a^b f(x)w(x)\,dx \tag{6.1}$$

where $w(x)$ is a fixed nonnegative weight function as defined in (5.1a) or (5.1b). [Often we shall be using $w(x) \equiv 1$, but we shall see some important cases later where we shall desire more flexibility in choosing $w(x)$.] Any formula that approximates $I(f)$ is called a numerical integration or quadrature formula. As mentioned above, if $g(x)$ approximates $f(x)$ on $[a, b]$, then we expect $I(g) \approx I(f)$. For example if $g(x)$ is a cubic interpolating spline, then it is usually true that $I(g)$ approximates $I(f)$ quite well. However, because of the complex formula for the cubic spline we shall not pursue this point further here. We shall instead concentrate on the use of interpolating polynomials, and we shall find that they yield quite favorable results and lead to efficient, yet simple formulas. Formulas of this type are called *interpolatory quadratures*.

Interpolatory quadratures all have one standard form. From (5.4), the interpolating polynomial in $\mathcal{P}_n$ at the points $\{x_j\}_{j=0}^{n}$ can be written as

$$p_n(x) = \sum_{j=0}^{n} f(x_j)\ell_j(x);$$

and we define $Q_n(f) \equiv I(p_n)$ as the quadrature formula to approximate $I(f)$. Thus

$$\begin{aligned} Q_n(f) \equiv I(p_n) &= \int_a^b p_n(x)w(x)\,dx = \int_a^b \left(\sum_{j=0}^{n} f(x_j)\ell_j(x)\right) w(x)\,dx \\ &= \sum_{j=0}^{n} f(x_j) \int_a^b \ell_j(x)w(x)\,dx \equiv \sum_{j=0}^{n} A_j f(x_j) \end{aligned} \tag{6.2}$$

where

$$A_j \equiv \int_a^b \ell_j(x)w(x)\,dx, \qquad 0 \le j \le n.$$

The values $\{A_j\}_{j=0}^{n}$ are called the *weights* of the quadrature and the points $\{x_j\}_{j=0}^{n}$ are called the *nodes*. Thus an interpolatory quadrature formula,

$$Q_n(f) = \sum_{j=0}^{n} A_j f(x_j),$$

is nothing more than a *weighted* sum of the function values $f(x_0), f(x_1), \ldots, f(x_n)$. The weights, $A_j$, are computed once and for all and depend only on the nodes $x_0, x_1, \ldots, x_n$, the weight function $w(x)$, and the interval $[a, b]$. That is, the same weights are used no matter what function $f(x)$ appears in the integral $\int_a^b w(x)f(x)\,dx$ that we are trying to estimate. This simple form makes interpolatory quadrature formulas easy both to use and to analyze.

We note again that if $f(x)$ is a polynomial of degree $n$ or less [that is, $f(x) \in \mathcal{P}_n$], then $f(x) = p_n(x)$ by Theorem 5.3 [$f(x)$ is its own interpolating polynomial]. Hence for any $f(x) \in \mathcal{P}_n$, $Q_n(f) = I(f)$; and so the quadrature of (6.2) gives the exact value for the integral. If for some integer $m$, $Q_n(f) = I(f)$ for all $f(x) \in \mathcal{P}_m$, then we say that the quadrature has *precision m*. From our remarks above, we see that any $(n + 1)$-point interpolatory quadrature, $Q_n(f)$, always has precision at least $n$. Later we shall develop quadratures with precision strictly greater than $n$.

Since from (6.2) it has precision $n$, $Q_n(f)$ must give the exact values of the integrals of $1, x, x^2, \ldots, x^n$. This fact gives us an alternative way to determine the quadrature weights, $\{A_j\}_{j=0}^n$, once the nodes, $\{x_j\}_{j=0}^n$, are given and fixed. This procedure is similar to the method of undetermined coefficients in that we have a linear system of $(n + 1)$ equations in $(n + 1)$ unknowns (the weights). To be specific, for $f_k(x) = x^k$, $0 \le k \le n$, we get the $(n + 1)$ equations

$$I(f_k) = \int_a^b x^k w(x)\, dx = Q_n(f_k) = \sum_{j=0}^{n} A_j x_j^k, \qquad 0 \le k \le n. \tag{6.3}$$

In (6.3) the nodes, $\{x_j\}_{j=0}^n$, were fixed beforehand and the weights are determined by solving the linear system. If, however, we treat the nodes, as well as the weights, as unknowns, then we have $2(n + 1)$ unknowns. Considering Eq. (6.3) we might reason, as Gauss did in 1814, that it could be possible to let $k$ range from 0 to $2n + 1$ so that (6.3) represents a system (nonlinear this time) of $(2n + 2)$ equations in $(2n + 2)$ unknowns. If (6.3) has a solution, it will yield a quadrature of precision $(2n + 1)$. This procedure is indeed possible and we will study Gaussian quadrature in Section 6.5. For now we will be content to illustrate the construction of a quadrature with the following simple example.

**EXAMPLE 6.1.** Let $[a, b] = [-h, h]$ be the interval of integration where $h$ is a positive constant, and let $w(x) \equiv 1$. We shall derive two simple quadrature formulas: the first by direct integration of the interpolating polynomial, and the second by undetermined coefficients as in (6.3).

1. Let $x_0 = -h$ and $x_1 = h$; then the first-degree interpolating polynomial is

$$p_1(x) = f(-h)\,\frac{(h - x)}{2h} + f(h)\,\frac{(h + x)}{2h}.$$

Therefore

$$Q_1(f) = I(p_1) = \int_{-h}^{h} p_1(x)\, dx$$

$$= \frac{-f(-h)}{2h}\,\frac{(h - x)^2}{2}\bigg|_{-h}^{h} + \frac{f(h)}{2h}\,\frac{(h + x)^2}{2}\bigg|_{-h}^{h}.$$

So, $Q_1(f) = hf(-h) + hf(h)$, which is the familiar *trapezoidal rule* estimate for $\int_{-h}^{h} f(x)\, dx$.

2. Let $x_0 = -h$, $x_1 = 0$ and $x_2 = h$. By forcing the quadrature formula $Q_2(f) = A_0 f(x_0) + A_1 f(x_1) + A_2 f(x_2)$ to equal $\int_{-h}^{h} f(x)\,dx$ for $f(x) = 1, x, x^2$, we obtain this system:

$$I(1) = \int_{-h}^{h} 1\,dx = 2h = A_0 + A_1 + A_2$$

$$I(x) = \int_{-h}^{h} x\,dx = 0 = -A_0 h + A_2 h$$

$$I(x^2) = \int_{-h}^{h} x^2\,dx = \frac{2h^3}{3} = A_0 h^2 + A_2 h^2.$$

Solving these equations yields

$$A_0 = A_2 = \frac{h}{3} \quad \text{and} \quad A_1 = \frac{4h}{3}.$$

Thus

$$Q_2(f) = \frac{h}{3}[f(-h) + 4f(0) + f(h)],$$

which is the well-known *Simpson's rule* for estimating $\int_{-h}^{h} f(x)\,dx$. Note in this case that $I(x^3) = 0 = Q_2(x^3)$ but $I(x^4) \neq Q_2(x^4)$. Thus, Simpson's rule has precision 3 and integrates all cubic polynomials exactly. For small values of $h$, these formulas often provide quite good estimates. For example, for $h = 0.2$ and $f(x) = \cos(x)$, we have

$$I(f) = 0.397339,\ Q_2(f) = 0.397342,\ Q_1(f) = 0.392027;$$

and for $f(x) = e^x$ and $h = 0.2$, we obtain

$$I(f) = 0.402672, \qquad Q_2(f) = 0.402676, \qquad Q_1(f) = 0.408027.$$

It is natural at this point to ask if the interpolatory quadratures of formula (6.2) will converge to $\int_a^b w(x)f(x)\,dx$ as we increase the number of interpolating points, that is, as $n \to \infty$. The following theorem provides a condition for which this result is true.

**Theorem 6.1**

For any positive integer $n$ and any $f \in C[a, b]$, let $Q_n(f) = \sum_{j=0}^{n} A_j^{(n)} f(x_j^{(n)})$ be the interpolatory quadrature given by (6.2). If there exists a constant $K > 0$ such that $\sum_{j=0}^{n} |A_j^{(n)}| \leq K$ for all $n$, then $\lim_{n\to\infty} Q_n(f) = I(f)$ for all $f \in C[a, b]$.

*Proof.* By the Weierstrass theorem, for any $\varepsilon > 0$ there exists a polynomial $q_N(x) \in \mathcal{P}_N$ (where $N$ depends on $\varepsilon$) such that

$$\max_{a \leq x \leq b} |f(x) - q_N(x)| = \|f - q_N\|_\infty \leq \varepsilon.$$

We note, since the quadrature formula is interpolatory, that $Q_n(q_N) = I(q_N)$ when $n \geq N$. Choosing $n \geq N$ and letting $\int_a^b w(x)\,dx = c$, we obtain

$$\begin{aligned}|I(f) - Q_n(f)| &= |I(f) - I(q_N) + Q_n(q_N) - Q_n(f)| \\ &\leq |I(f) - I(q_N)| + |Q_n(q_N) - Q_n(f)|.\end{aligned}$$

Now,

$$\begin{aligned}|I(f) - I(q_N)| &= \left|\int_a^b w(x)[f(x) - q_N(x)]\,dx\right| \\ &\leq \|f - q_N\|_\infty \int_a^b w(x)\,dx \leq c\varepsilon\end{aligned}$$

and

$$\begin{aligned}|Q_n(q_N) - Q_n(f)| &= \left|\sum_{j=0}^{n} A_j^{(n)}[q_N(x_j^{(n)}) - f(x_j^{(n)})]\right| \\ &\leq \|f - q_N\|_\infty \sum_{j=0}^{n} |A_j^{(n)}| \leq K\varepsilon.\end{aligned}$$

Thus, for any $\varepsilon > 0$, there is an integer $N$ such that $|I(f) - Q_n(f)| \leq (K + c)\varepsilon$ whenever $n \geq N$. Therefore, $\lim_{n\to\infty} Q_n(f) = I(f)$ for every $f$ in $C[a, b]$. ■

It can also be shown that the converse of this theorem is true. That is, if $\lim_{n\to\infty} Q_n(f) = I(f)$ for each $f \in C[a, b]$ [where $Q_n(f)$ is an interpolatory quadrature], then there must be a number $K$ such that $\sum_{j=0}^{n} |A_j^{(n)}| \leq K$ for all $n$. However, it goes beyond the scope of this text to prove the converse. Theorem 6.1 (and its converse) do have some practical applications in terms of selecting quadrature formulas. We note first that any interpolatory formula has the property that $Q_n(1) = \int_a^b w(x)\,dx$ since the constant polynomial 1 is integrated exactly. Since $w(x)$ is a nonnegative weight function, we must have

$$0 < I(1) = \int_a^b w(x)\,dx = Q_n(1) = \sum_{j=0}^{n} A_j^{(n)}.$$

Therefore, if the weights $A_j^{(n)}$ are all positive for $0 \leq j \leq n$, $\int_a^b w(x)\,dx = \sum_{j=0}^{n} |A_j^{(n)}|$. If for each $n$ we can choose the nodes $x_0^{(n)}, x_1^{(n)}, \ldots, x_n^{(n)}$ so that the corresponding weights $A_0^{(n)}, A_1^{(n)}, \ldots, A_n^{(n)}$ are positive, then the hypotheses of Theorem 6.1 are satisfied and convergence is guaranteed. A further advantage of positive-weight quadrature formulas is that they have good rounding-error properties. For example, if $Q_N(f) = \sum_{j=0}^{N} A_j f(x_j)$, we can usually expect that the round-off error for the evaluation of the $f(x_j)$'s will be on the high side approximately as often as on the low side. Thus, if the $A_j$'s are all positive, the errors to the high side will tend to cancel the errors to the low side when forming the sum, $Q_n(f)$. Furthermore, the expected value of the total rounding error will be minimized if the $A_j$'s are nearly equal. (We shall see two examples of equal weight formulas when we investigate the composite trapezoidal rule and Gauss-Chebyshev quadrature.)

### 6.2.1. Transforming Quadrature Formulas to Other Intervals

Frequently we have a quadrature formula, $Q_n(g) = \sum_{j=0}^{n} A_j g(t_j)$, that is derived for a specific interval, say $[-1, 1]$, and is designed to approximate $\int_{-1}^{1} g(t)\, dt$. If the problem is to estimate $\int_a^b f(x)\, dx$, we can use the results of Section 5.2.4 to transform the formula from $[-1, 1]$ to $[a, b]$. To be specific, suppose $Q_n(g)$ is a given quadrature formula for $[-1, 1]$ and suppose $f(x)$ is defined on $[a, b]$. With the change of variable $x = \alpha t + \beta$ where $\alpha = (b - a)/2$ and $\beta = (a + b)/2$, we have

$$\int_a^b f(x)\, dx = \int_{-1}^{1} f(\alpha t + \beta)\alpha\, dt.$$

Letting $g(t) = \alpha f(\alpha t + \beta)$, we find $Q_n(g) = \sum_{j=0}^{n} \alpha A_j f(\alpha t_j + \beta)$ as an approximation to $\int_{-1}^{1} g(t)\, dt$. Thus we can define the corresponding transformed quadrature formula, $Q_n^*(f)$, for the interval $[a, b]$ by

$$\begin{aligned} Q_n^*(f) &= \sum_{j=0}^{n} A_j^* f(x_j) = \frac{b-a}{2}\sum_{j=0}^{n} A_j f(x_j) \\ x_j &= \frac{b-a}{2} t_j + \frac{a+b}{2}. \end{aligned} \tag{6.4}$$

We leave as a problem for the reader to show that if $Q_n$ has precision $m$ on $[-1, 1]$, then $Q_n^*$ has precision $m$ on $[a, b]$.

### 6.2.2. Newton-Cotes Formulas

Given $\int_a^b f(x)\, dx$ to approximate, probably the most natural choice of nodes $x_i$ to use in a quadrature formula are nodes that are equally spaced in $[a, b]$. Let $h = (b - a)/n$ and let $x_i = x_0 + ih$ where $x_0 = a$. An interpolatory quadrature formula $Q_n(f) = \sum_{j=0}^{n} A_j f(x_j)$ constructed using these equally spaced nodes is called a *closed* Newton-Cotes formula. The interpolatory quadrature formula constructed using the equally spaced nodes $y_i = a + ih$, $i = 1, 2, \ldots, n + 1$; $h = (b - a)/(n + 2)$ is called an *open* Newton-Cotes formula. (The closed formula uses the end-points $a$ and $b$; the open formula has $a < y_1$, and $y_{n+1} < b$.)

From Example 6.1 with $h = 1$, we see that

$$Q_1(f) = f(-1) + f(1)$$

$$Q_2(f) = \frac{1}{3}[f(-1) + 4f(0) + f(1)]$$

are the two- and three-point closed Newton-Cotes rules for $[-1, 1]$. Using the results of Section 6.2.1 on these formulas, we have for an arbitrary interval $[a, b]$, that

$$T(f) = \frac{(b-a)}{2}[f(a) + f(b)] \tag{6.5}$$

$$S(f) = \frac{(b-a)}{6}\left[f(a) + 4f\left(\frac{a+b}{2}\right) + f(b)\right] \tag{6.6}$$

are respectively the closed two-point and the three-point Newton-Cotes formulas. [Formula (6.5) is the trapezoidal rule for $[a, b]$ and (6.6) is Simpson's rule for $[a, b]$.] As two more examples of Newton-Cotes formulas, we have the three-point open formula for $[-1, 1]$ and the four-point closed formula for $[-1, 1]$ (see Problem 9):

$$\int_{-1}^{1} f(x)\,dx \approx \frac{2}{3}\left[2f\left(-\frac{1}{2}\right) - f(0) + 2f\left(\frac{1}{2}\right)\right]$$

$$\int_{-1}^{1} f(x)\,dx \approx \frac{1}{4}\left[f(-1) + 3f\left(-\frac{1}{3}\right) + 3f\left(\frac{1}{3}\right) + f(1)\right].$$

Note in the three-point open formula above that not all the weights are positive. In fact, it is known for $n \geq 10$ that the weights of any Newton-Cotes formula are of mixed sign. As we noted, this is a bad feature in terms of rounding error. Moreover, as $n$ increases, the weights themselves grow without bound; thus there are continuous functions for which the quadratures do not converge to the integral. For these reasons, higher order Newton-Cotes formulas are rarely used in practice. However, lower order Newton-Cotes formulas such as the trapezoidal rule and Simpson's rule are *extremely* useful, and the time invested in analyzing their properties in the next section will be well spent.

We now give one further type of quadrature that involves derivative evaluations of $f(x)$ as well as values of $f(x)$ itself. The cubic polynomial, $p_3(x)$, which satisfies $p_3(a) = f(a)$, $p_3'(a) = f'(a)$, $p_3(b) = f(b)$, and $p_3'(b) = f'(b)$ is given by formula (5.37); and we can approximate $I(f)$ by $\tilde{Q}_3(f) \equiv I(p_3)$. We could laboriously compute $I(p_3) \equiv \int_a^b p_3(x)\,dx$ by direct integration, but we can simplify this task by noting, since Simpson's rule has precision 3, that $S(p_3) = I(p_3)$. From

Eq. (5.37) we can easily verify that $p_3(a) = f(a)$, $p_3((a + b)/2) = 1/2(f(a) + f(b)) + ((b - a)/8)(f'(a) - f'(b))$, and $p_3(b) = f(b)$. Then, using Eq. (6.6), we have

$$\tilde{Q}_3(f) = S(p_3) = \frac{(b - a)}{2}[f(a) + f(b)] + \frac{(b - a)^2}{12}[f'(a) - f'(b)],$$

or

$$\tilde{Q}_3(f) = T(f) + \frac{(b - a)^2}{12}[f'(a) - f'(b)]. \tag{6.7}$$

Because of the presence of $T(f)$ in this formula, $\tilde{Q}_3(f)$ is called the *corrected trapezoidal rule* and is often denoted by $CT(f) \equiv \tilde{Q}_3(f)$. By the uniqueness of the Hermite interpolating polynomial in Theorem 5.7, if $f(x)$ is any polynomial of degree 3 or less, then $f(x) = p_3(x)$; and so $I(f) = CT(f)$. We can easily check that $I(x^4) \neq CT(x^4)$, and therefore $CT(f)$ has precision 3.

**EXAMPLE 6.2.** Given $\int_{-1}^{1} \cos(x)\,dx$ to estimate, we find for $f(x) = \cos(x)$ that

$$I(f) = 1.683$$

$$T(f) = 1.081$$

$$CT(f) = T(f) + 0.561 = 1.642.$$

This example indicates that when derivative data are readily available, the corrected trapezoidal rule may be expected to provide better answers. The theoretical analysis in the next section bears this out.

## PROBLEMS, SECTION 6.2.2

1. By integrating the Lagrange basis functions as in (6.2), derive an interpolatory quadrature formula of the form

$$\int_0^{2h} f(x)dx \simeq A_0 f(0) + A_1 f(h).$$

2. Use the method of undetermined coefficients to derive an interpolatory quadrature formula

$$\int_0^{3h} f(x)dx \simeq A_0 f(0) + A_1 f(h) + A_2 f(3h).$$

3. Use each of (6.5), (6.6), and (6.7) to estimate the integrals and compare your results with the exact result.

a) $\int_0^1 x^4 dx$ b) $\int_{.1}^{.2} \ell n(x)dx$ c) $\int_0^{.3} \frac{1}{1 + x}dx$

4. Determine the precision of the formulas for $\int_{-1}^{1} f(x)dx$; use the results of Problem 8.
 a) $\frac{2}{3}[2f(-\frac{1}{2}) - f(0) + 2f(\frac{1}{2})]$  b) $\frac{1}{4}[f(-1) + 3f(-\frac{1}{3}) + 3f(\frac{1}{3}) + f(1)]$

5. Apply each of the formulas in Problem 4 to the integrals in Problem 3; use (6.4) to translate the formulas to the proper interval.

6. Interpolatory numerical differentiation formulas can be constructed using techniques similar to (6.2) and (6.3). If $p_n(x)$ interpolates $f(x)$ at $x_0, x_1, \ldots, x_n$, and if $\alpha$ is some point, then $f'(\alpha) \simeq p_n'(\alpha)$. Furthermore, using the Lagrange form for $p_n(x)$, $p_n'(\alpha) = \sum_{j=0}^{n} A_j f(x_j)$ where $A_j = \ell_j'(\alpha)$. Derive a numerical differentiation formula of the form

$$f'(\alpha) \simeq A_0 f(\alpha - h) + A_1 f(\alpha) + A_2 f(\alpha + h),$$

and test the formula on $f(x) = \cos(x)$ with $\alpha = 2$ and $h = .05$.

7. Use undetermined coefficients, as in (6.3), to derive a differentiation formula of the form

$$f'(\alpha) \simeq A_0 f(\alpha - 2h) + A_1 f(\alpha - h) + A_2 f(\alpha).$$

[That is, choose $A_0, A_1, A_2$ so that the approximation above is exact for $f(x) = 1$, $f(x) = x$, and $f(x) = x^2$.] Test your formula on $f(x) = \cos(x)$, $f(x) = e^x$, and $f(x) = \sqrt{x}$ with $\alpha = 1$ and $h = .05$.

8. Suppose $Q_n(f) = \sum_{j=0}^{n} A_j f(x_j)$. Show that $Q_n(f + g) = Q_n(f) + Q_n(g)$. Next, suppose that $Q_n(f) = \int_a^b w(x)f(x)dx$ for the functions $1, x, \ldots, x^m$. Use the fact that $Q_n(f + g) = Q_n(f) + Q_n(g)$ to show that $Q_n$ has precision at least $m$.

9. Using (6.3), construct the open Newton-Cotes formula for $\int_{-1}^{1} f(x)\,dx$ with nodes $-1/2, 0, 1/2$ and the closed Newton-Cotes formula with nodes $-1, -1/3, 1/3, 1$.

10. Construct the interpolatory quadrature for $\int_{-1}^{1} f(x)\,dx$ with nodes $-1, -1/2, 1/2, 1$.

11. Prove that the quadrature formula $Q_n^*$ given in (6.4) has precision $m$ on $[a, b]$ whenever $Q_n$ has precision $m$ on $[-1, 1]$. [Hint: If $f(x)$ is a polynomial in $x$ of degree $m$ or less, what is $g(t)$?]

12. In Example 6.1 derive $Q_1(f)$ by undetermined coefficients and $Q_2(f)$ by integration of the interpolating polynomial.

13. Suppose that $\int_c^d g(t)dt$ is approximated by the quadrature $Q(g) = \sum_{i=0}^{n} A_i g(t_i)$. Find the corresponding quadrature $\tilde{Q}(f) = \sum_{i=0}^{n} B_i f(x_i)$ to approximate $\int_a^b f(x)dx$. [Hint: Let $x = mt + \beta$ where $x = a$ when $t = c$ and $x = b$ when $t = d$.]

14. a) Let $p(x) = b_3(x-1)^2(x+1) + b_2(x-1)(x+1)^2 + b_1(x-1)^2 + b_0(x+1)^2$. For a given $f(x)$ find $b_0$, $b_1$, $b_2$, and $b_3$ such that $p(-1) = f(-1)$, $p(1) = f(1)$, $p'(-1) = f'(-1)$, and $p'(1) = f'(1)$.
 b) Show that $p(x)$ in part (a) is unique in $\mathcal{P}_3$. [Hint: Let $q(x)$ in $\mathcal{P}_3$ satisfy $q(\pm 1) = f(\pm 1)$ and $q'(\pm 1) = f'(\pm 1)$, and consider $s(x) = p(x) - q(x)$.]

c) Let $Q(f) = \int_{-1}^{1} p(x)dx$ and express $Q(f)$ in the form $B_0 f(-1) + B_1 f(1) + B_2 f'(-1) + B_3 f'(1)$.

d) Transform $Q(f)$ in part (c) to approximate $\int_a^b f(x)dx$ and obtain the corrected trapezoidal rule (6.7).

e) Use part (b) and Exercise 11 to argue that the precision of $Q$ is at least 3.

**15.** a) With $\tilde{Q}_3(f)$ as in (6.7) show that $\tilde{Q}_3(\alpha f + \beta g) = \alpha\tilde{Q}_3(f) + \beta\tilde{Q}_3(g)$, $\alpha$ and $\beta$ constants, $f$ and $g$ functions.

b) Show that $\tilde{Q}_3(x^4) \neq \int_a^b x^4 dx$. If $q(x) = a_4x^4 + a_3x^3 + a_2x^2 + a_1x + a_0$ with $a_4 \neq 0$, show that $\tilde{Q}_3(q) \neq \int_a^b q(x)dx$.

**16.** For the interpolatory quadrature formula (6.2), show that at least one of the weights is positive. [Hint: Consider $I(1)$.]

### 6.2.3. Errors of Quadrature Formulas

In this section, we consider ways of estimating the quadrature error $I(f) - Q_n(f)$ and derive specific estimates for the important cases of the trapezoidal rule, Simpson's rule, and the corrected trapezoidal rule. By formula (5.27), the error of regular polynomial interpolation for $f(x) \in C^{n+1}[a, b]$ is given by

$$e_n(x) \equiv f(x) - p_n(x) = \frac{f^{(n+1)}(\xi)}{(n+1)!} W(x).$$

We can therefore express the error of interpolatory quadrature as

$$e_n = \int_a^b e_n(x)w(x)\,dx,$$

or

$$e_n \equiv \int_a^b f(x)w(x)\,dx - \int_a^b p_n(x)w(x)\,dx = \int_a^b \frac{f^{(n+1)}(\xi)}{(n+1)!} W(x)w(x)\,dx. \tag{6.8a}$$

Recalling that $f^{(n+1)}(\xi)$ is actually an unknown function of $x$, we see that the right-hand integral in (6.8a) cannot usually be evaluated explicitly. We can, however, obtain a computable bound on the error, $e_n$, from (6.8a) by using

$$|e_n| \leq \max_{a \leq x \leq b} |f^{(n+1)}(x)| \int_a^b \frac{|W(x)|}{(n+1)!} w(x)\,dx. \tag{6.8b}$$

We will use an error bound similar to this in a later section, but for now we consider two other ways of simplifying (6.8a). Recall that a simple form of the Second Mean-Value Theorem for integrals states that if $g(x)$ and $h(x)$ are continuous and if $g(x)$ does not change sign in the interval $(a, b)$, then there exists a mean value point, $\eta \in (a, b)$, such that $\int_a^b g(x)h(x)\,dx = h(\eta)\int_a^b g(x)\,dx$. We can use this theorem immediately in (6.5) and (6.7). For (6.5), (6.8a) gives the error for the trapezoidal rule:

$$I(f) - T(f) \equiv e^T = \frac{1}{2}\int_a^b f''(\xi)(x-a)(x-b)\,dx.$$

Now $[(x-a)(x-b)]$ is of constant sign on $(a, b)$; so the mean-value theorem above yields

$$e^{\mathrm{T}} = \frac{f''(\eta)}{2}\int_a^b (x-a)(x-b)\,dx = -\frac{f''(\eta)}{12}(b-a)^3. \tag{6.9}$$

Since (6.7) was the result of Hermite interpolation, we must use (5.39) instead of (5.27) to obtain the error. From (5.39), where $p_3(x)$ is given as in (6.7), we have

$$f(x) - p_3(x) = \frac{f^{(iv)}(\xi)}{4!}(x-a)^2(x-b)^2.$$

Now $[(x-a)^2(x-b)^2] > 0$ for $x \in (a, b)$; so the mean-value theorem yields

$$I(f) - CT(f) \equiv e^{CT} = \int_a^b \frac{f^{(iv)}(\xi)}{4!}(x-a)^2(x-b)^2\,dx$$

or

$$e^{\mathrm{CT}} = \frac{f^{(iv)}(\eta)}{4!}\int_a^b (x-a)^2(x-b)^2\,dx = \frac{f^{(iv)}(\eta)}{720}(b-a)^5. \tag{6.10}$$

The error for Simpson's rule is a bit more difficult to analyze since in (6.8a) the function $W(x)$ changes sign in $(a, b)$. First, let $x_0 = a$, $x_1 = (a+b)/2$, and $x_2 = b$. We can get at the error in Simpson's rule by defining an auxiliary cubic polynomial, $p_3(x)$, such that $p_3(x_0) = f(x_0)$, $p_3(x_1) = f(x_1)$, $p_3(x_2) = f(x_2)$, and $p_3'(x_1) = f'(x_1)$ (we leave as Problem 7 to show that such a polynomial exists). Next, note that $S(f) = S(p_3)$ since $p_3(x)$ interpolates $f(x)$ at $x_0$, $x_1$, and $x_2$. Further, since Simpson's rule has precision 3, $S(p_3) = I(p_3)$. Therefore we obtain an alternative expression for the error:

$$I(f) - S(f) = I(f) - S(p_3) = I(f) - I(p_3).$$

In order to use this expression, we need an error formula for $f(x) - p_3(x)$. This formula is easily obtained, as below, using a method similar to that in the proof of Theorem 5.5.

For a *fixed* $x$, different from $x_0$, $x_1$, and $x_2$, define $\phi(t)$ for $t \in [a, b]$ by

$$\phi(t) = [f(t) - p_3(t)] - [f(x) - p_3(x)]\frac{(t-x_0)(t-x_1)^2(t-x_2)}{(x-x_0)(x-x_1)^2(x-x_2)}.$$

Then $\phi(t)$ has at least 4 zeros in $[a, b]$; namely, $x_0$, $x_1$, $x_2$, and $x$. By Rolle's theorem, $\phi'(t)$ has at least 3 zeros in $(a, b)$ that are between the 4 zeros of $\phi(t)$. By construction, we see also that $\phi'(x_1) = 0$, and therefore $\phi'(t)$ has at least 4 *distinct* zeros in $(a, b)$. If $f \in C^4[a, b]$, we find (as in the proof of Theorem 5.5) that there is a point $\xi$ in $(a, b)$ (which depends on $x$) such that $\phi^{(iv)}(\xi) = 0$. Therefore

$$f(x) - p_3(x) = \frac{f^{(iv)}(\xi)}{4!}(x - x_0)(x - x_1)^2(x - x_2).$$

Since the function $[(x - x_0)(x - x_1)^2(x - x_2)]$ does not change sign on $(a, b)$, we can now use the Second Mean-Value Theorem to deduce

$$I(f) - I(p_3) = \int_a^b \frac{f^{(iv)}(\xi)}{4!}(x - x_0)(x - x_1)^2(x - x_2)\,dx,$$

or

$$I(f) - S(f) = \frac{f^{(iv)}(\eta)}{4!}\int_a^b (x - x_0)(x - x_1)^2(x - x_2)\,dx. \qquad (6.11a)$$

We can obviously evaluate the integral above directly to obtain the error. To illustrate another idea, however, we use a standard trick to evaluate

$$\int_a^b (x - x_0)(x - x_1)^2(x - x_2)\,dx$$

by choosing $\tilde{f}(x) = (x - x_1)^4$. From (6.11a), we have

$$I(\tilde{f}) - S(\tilde{f}) = \int_a^b (x - x_0)(x - x_1)^2(x - x_2)\,dx$$

since the fourth derivative of $\tilde{f}(x) = (x - x_1)^4$ is the constant $4!$. Letting $h = (b - a)/2 = x_1 - x_0 = x_2 - x_1$, we find

$$\int_{x_0}^{x_2} (x - x_1)^4\,dx = \frac{(x - x_1)^5}{5}\Bigg|_{x_0}^{x_2} = \frac{2h^5}{5}$$

and

$$S((x - x_1)^4) = \frac{2h}{6}[h^4 + h^4] = \frac{2h^5}{3}.$$

Thus for $\tilde{f}(x) = (x - x_1)^4$,

$$\int_a^b (x - x_0)(x - x_1)^2(x - x_2)\,dx = I(\tilde{f}) - S(\tilde{f}) = \frac{-4h^5}{15}.$$

Using this equation in (6.11a) with $e^S = I(f) - S(f)$, we have

$$e^S = \frac{-f^{(iv)}(\eta)}{90}\left(\frac{b-a}{2}\right)^5. \tag{6.11b}$$

**EXAMPLE 6.3.** The sine-integral, $Si(x)$, is defined by

$$Si(x) = \int_0^x \frac{\sin(t)}{t}\,dt.$$

To illustrate the error analysis of this section, we estimate $Si(1)$ by the trapezoidal rule, Simpson's rule, and the corrected trapezoidal rule. In order to use the error bounds derived above on the estimates for $Si(1)$, we need in (6.9) to bound $|f''(\eta)|$ for $\eta \in [0, 1]$; and in (6.10) and (6.11b) we need to bound $|f^{(iv)}(\eta)|$ for $\eta \in [0, 1]$.

To obtain these bounds, we use the expansion

$$\sin(t) = t - \frac{t^3}{3!} + \frac{t^5}{5!} - \frac{t^7}{7!} + \cdots$$

to obtain for $f(t) = (\sin(t)/t)$

$$f(t) = 1 - \frac{1}{3}\frac{t^2}{2!} + \frac{1}{5}\frac{t^4}{4!} - \frac{1}{7}\frac{t^6}{6!} + \cdots$$

$$f''(t) = -\frac{1}{3} + \frac{1}{5}\frac{t^2}{2!} - \frac{1}{7}\frac{t^4}{4!} + \cdots$$

$$f^{(iv)}(t) = \frac{1}{5} - \frac{1}{7}\frac{t^2}{2!} + \cdots.$$

Since all these series are alternating series, we see that $|f''(\eta)| \le 1/3$ and $|f^{(iv)}(\eta)| \le 1/5$ for $\eta \in [0, 1]$. Hence, the error bounds are $|e^{\mathrm{T}}| \le 1/36 = 0.027778$, $|e^{CT}| \le 1/3600 = 0.000278$, and $|e^S| \le 1/14400 = 0.000069$. From a table, we obtain $Si(1) = 0.946083$. Noting that $f(0) = 1$ and $f'(0) = 0$, we have

$$\begin{aligned} T(f) &= 0.920735; & e^{\mathrm{T}} &= 0.025348 \\ CT(f) &= 0.945832; & e^{\mathrm{CT}} &= 0.000251 \\ S(f) &= 0.946146; & e^{\mathrm{S}} &= -0.000063. \end{aligned}$$

### 6.2.4. Composite Rules for Numerical Integration

If we wish to derive a highly accurate quadrature formula for the interval $[a, b]$, we immediately see two obvious choices.

1. Take the number of nodes, $(n + 1)$, to be large so that the quadrature,

$$Q_n(f) = \sum_{j=0}^{n} A_j f(x_j),$$

is the integral of a high-degree interpolating polynomial.