to which the preceding work applies. By such manipulations, the applicability of the cases $w(x) = \log(x)$ and $w(x) = x^\alpha$ is much greater than might first be imagined.

For an asymptotic error analysis of product integration; see the work of de Hoog and Weiss (1973), in which some generalizations of the Euler–MacLaurin expansion are derived. Using their results, it can be shown that the error in the product Simpson rule is $O(h^4 \log(h))$. Thus the bound (5.6.24) based on the interpolation error $f(x) - f_n(x)$ does not predict the correct rate of convergence. This is similar to the result (5.1.17) for the Simpson rule error, in which the error was smaller than the use of quadratic interpolation would lead us to believe.

5.7 Numerical Differentiation

Numerical approximations to derivatives are used mainly in two ways. First, we are interested in calculating derivatives of given data that are often obtained empirically. Second, numerical differentiation formulas are used in deriving numerical methods for solving ordinary and partial differential equations. We begin this section by deriving some of the most commonly used formulas for numerical differentiation.

The problem of numerical differentiation is in some ways more difficult than that of numerical integration. When using empirically determined function values, the error in these values will usually lead to instability in the numerical differentiation of the function. In contrast, numerical integration is stable when faced with such errors (see Problem 13).

The classical formulas One of the main approaches to deriving a numerical approximation to $f'(x)$ is to use the derivative of a polynomial $p_n(x)$ that interpolates $f(x)$ at a given set of node points. Let $x_0, x_1, \dots, x_n$ be given, and let $p_n(x)$ interpolate $f(x)$ at these nodes. Usually $\{x_i\}$ are evenly spaced. Then use

$$f'(x) \doteq p_n'(x) \tag{5.7.1}$$

From (3.1.6), (3.2.4), and (3.2.11):

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

$$l_j(x) = \frac{\Psi_n(x)}{(x - x_j)\Psi_n'(x_j)}$$

$$= \frac{(x - x_0)\cdots(x - x_{j-1})(x - x_{j+1})\cdots(x - x_n)}{(x_j - x_0)\cdots(x_j - x_{j-1})(x_j - x_{j+1})\cdots(x_j - x_n)}$$

$$\Psi_n(x) = (x - x_0)\cdots(x - x_n)$$

$$f(x) - p_n(x) = \Psi_n(x) f[x_0, \dots, x_n, x] \tag{5.7.2}$$

Thus

$$f'(x) \doteq p_n'(x) = \sum_{j=0}^{n} f(x_j) l_j'(x) \equiv D_h f(x) \tag{5.7.3}$$

$$f'(x) - D_h f(x) = \Psi_n'(x) f[x_0, \dots, x_n, x] + \Psi_n(x) f[x_0, \dots, x_n, x, x] \tag{5.7.4}$$

with the last step using (3.2.17). Applying (3.2.12),

$$f'(x) - D_h f(x) = \Psi_n'(x) \frac{f^{(n+1)}(\xi_1)}{(n+1)!} + \Psi_n(x) \frac{f^{(n+2)}(\xi_2)}{(n+2)!} \tag{5.7.5}$$

with $\xi_1, \xi_2 \in \mathscr{H}\{x_0, \dots, x_n, x\}$. Higher order differentiation formulas and their error can be obtained by further differentiation of (5.7.3) and (5.7.4).

The most common application of the preceding is to evenly spaced nodes $\{x_i\}$. Thus let

$$x_i = x_0 + ih \qquad i \geq 0$$

with $h > 0$. In this case, it is straightforward to show that

$$\Psi_n(x) = O(h^{n+1}) \qquad \Psi_n'(x) = O(h^n) \tag{5.7.6}$$

Thus

$$f'(x) - p_n'(x) = \begin{cases} O(h^n) & \Psi_n'(x) \neq 0 \\ O(h^{n+1}) & \Psi_n'(x) = 0 \end{cases} \tag{5.7.7}$$

We now derive examples of each case.

Let $n = 1$, so that $p_n(x)$ is just the linear interpolate of $(x_0, f(x_0))$ and $(x_1, f(x_1))$. Then (5.7.3) yields

$$f'(x_0) \doteq D_h f(x_0) \equiv \frac{1}{h}[f(x_0 + h) - f(x_0)] \tag{5.7.8}$$

From (5.7.5),

$$f'(x_0) - D_h f(x_0) = \frac{h}{2} f''(\xi_1) \qquad x_0 \leq \xi_1 \leq x_1 \tag{5.7.9}$$

since $\Psi(x_0) = 0$.

To improve on this with linear interpolation, choose $x = m \equiv (x_0 + x_1)/2$. Then

$$f'(m) \doteq \frac{1}{h}[f(x_1) - f(x_0)]$$

We usually rewrite this by letting $\delta = h/2$, to obtain

$$f'(m) \doteq D_\delta f(m) = \frac{1}{2\delta}[f(m+\delta) - f(m-\delta)] \tag{5.7.10}$$

For the error, using (5.7.5) and $\Psi_1'(m) = 0$,

$$f'(m) - D_\delta f(m) = \frac{-\delta^2}{6} f^{(3)}(\xi_2) \qquad m - \delta \le \xi_2 \le m + \delta \tag{5.7.11}$$

In general, to obtain the higher order case in (5.7.7), we want to choose the nodes $\{x_i\}$ to have $\Psi_n'(x) = 0$. This will be true if n is odd and the nodes are placed symmetrically about x, as in (5.7.10).

To obtain higher order formulas in which the nodes all lie on one side of x, use higher values of n in (5.7.3). For example, with $x = x_0$ and $n = 2$,

$$f'(x_0) \doteq D_h f(x_0) \equiv \frac{1}{2h}[-3f(x_0) + 4f(x_1) - f(x_2)] \tag{5.7.12}$$

$$f'(x_0) - D_h f(x_0) = \frac{h^2}{3} f^{(3)}(\xi_1) \qquad x_0 \le \xi_1 \le x_2 \tag{5.7.13}$$

The method of undetermined coefficients Another method to derive formulas for numerical integration, differentiation, and interpolation is called the method of undetermined coefficients. It is often equivalent to the formulas obtained from a polynomial interpolation formula, but sometimes it results in a simpler derivation. We will illustrate the method by deriving a formula for $f''(x)$.

Assume

$$f''(x) \doteq D_h^{(2)} f(x) = Af(x+h) + Bf(x) + Cf(x-h) \tag{5.7.14}$$

with A, B, and C unspecified. Replace $f(x+h)$ and $f(x-h)$ by the Taylor expansions

$$f(x \pm h) = f(x) \pm hf'(x) + \frac{h^2}{2} f''(x) \pm \frac{h^3}{6} f^{(3)}(x) + \frac{h^4}{24} f^{(4)}(\xi_\pm)$$

with $x - h \le \xi_- \le x \le \xi_+ \le x + h$. Substitute into (5.7.14) and rearrange into a polynomial in powers of h:

$$\begin{aligned} &Af(x+h) + Bf(x) + Cf(x-h) \\ &\quad = (A + B + C)f(x) + h(A - C)f(x) + \frac{h^2}{2}(A + C)f''(x) \\ &\quad + \frac{h^3}{6}(A - C)f^{(3)}(x) + \frac{h^4}{24}[Af^{(4)}(\xi_+) + Bf^{(4)}(\xi_-)] \end{aligned} \tag{5.7.15}$$

In order for this to equal $f''(x)$, we set

$$A + B + C = 0 \qquad A - C = 0 \qquad A + C = \frac{2}{h^2}$$

The solution of this system is

$$A = C = \frac{1}{h^2} \qquad B = \frac{-2}{h^2} \tag{5.7.16}$$

This yields the formula

$$D_h^{(2)} f(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} \tag{5.7.17}$$

For the error, substitute (5.7.16) into (5.7.15) and use (5.7.17). This yields

$$f''(x) - D_h^{(2)} f(x) = \frac{h^2}{24}\left[f^{(4)}(\xi_+) + f^{(4)}(\xi_-)\right]$$

Using Problem 1 of Chapter 1, and assuming $f(x)$ is four times continuously differentiable,

$$f''(x) - D_h^{(2)} f(x) = -\frac{h^2}{12} f^{(4)}(\xi) \tag{5.7.18}$$

for some $x - h \le \xi \le x + h$. Formulas (5.7.17) and (5.7.18) could have been derived by calculating $p_2''(x)$ for the quadratic polynomial interpolating $f(x)$ at $x - h$, x, $x + h$, but the preceding is probably simpler.

The general idea of the method of undetermined coefficients is to choose the Taylor coefficients in an expansion in h so as to obtain the desired derivative (or integral) as closely as possible.

Effect of error in function values The preceding formulas are useful when deriving methods for solving ordinary and partial differential equations, but they can lead to serious errors when applied to function values that are obtained empirically. To illustrate a method for analyzing the effect of such errors, we consider the second derivative approximation (5.7.17).

Begin by rewriting (5.7.17) as

$$f''(x_1) \doteq D_h^{(2)} f(x_1) = \frac{f(x_2) - 2f(x_1) + f(x_0)}{h^2}$$

with $x_j = x_0 + jh$. Let the actual values used be $\tilde{f}_i$ with

$$f(x_i) = \tilde{f}_i + \epsilon_i \qquad i = 0, 1, 2 \tag{5.7.19}$$

The actual numerical derivative computed is

$$\tilde{D}_h^{(2)}f(x_1) = \frac{\tilde{f}_2 - 2\tilde{f}_1 + \tilde{f}_0}{h^2} \tag{5.7.20}$$

For its error, substitute (5.7.19) into (5.7.20), obtaining

$$\begin{aligned} f''(x_1) - \tilde{D}_h^{(2)}f(x_1) &= f''(x_1) - \frac{f(x_2) - 2f(x_1) + f(x_0)}{h^2} \\ &\quad + \frac{\epsilon_2 - 2\epsilon_1 + \epsilon_0}{h^2} \\ &= \frac{-h^2}{12} f^{(4)}(\xi) + \frac{\epsilon_2 - 2\epsilon_1 + \epsilon_0}{h^2} \end{aligned} \tag{5.7.21}$$

For the term involving $\{\epsilon_i\}$, assume these errors are random within some interval $-E \le \epsilon \le E$. Then

$$\left| f''(x_1) - \tilde{D}_h^{(2)}f(x_1) \right| \le \frac{h^2}{12} \left| f^{(4)}(\xi) \right| + \frac{4E}{h^2} \tag{5.7.22}$$

and the last bound would be attainable in many situations. An example of such errors would be rounding errors, with E a bound on their magnitude.

The error bound in (5.7.22) will initially get smaller as h decreases, but for h sufficiently close to zero, the error will begin to increase again. There is an optimal value of h, call it h^*, to minimize the right side of (5.7.22), and presumably there is a similar value for the actual error $f''(x_1) - \tilde{D}_h^{(2)}f(x_1)$.

Example Let $f(x) = -\cos(x)$, and compute $f''(0)$ using the numerical approximation (5.7.17). In Table 5.25, we give the errors in (1) $D_h^{(2)}f(0)$, computed exactly, and (2) $\tilde{D}_h^{(2)}f(0)$, computed using 8-digit rounded decimal arithmetic. In

Table 5.25 Example of $D_h^{(2)}f(0)$ and $\tilde{D}_h^{(2)}f(0)$

h	$f''(0) - D_h^{(2)}f(0)$	Ratio	$f''(0) - \tilde{D}_h^{(2)}f(0)$
.5	2.07E − 2		2.07E − 2
.25	5.20E − 3	3.98	5.20E − 3
.125	1.30E − 3	3.99	1.30E − 3
.0625	3.25E − 4	4.00	3.25E − 4
.03125	8.14E − 5	4.00	8.45E − 5
.015625	2.03E − 5	4.00	2.56E − 6
.0078125	5.09E − 6	4.00	−7.94E − 5
.00390625	1.27E − 6	4.00	−7.94E − 5
.001953125	3.18E − 7	4.00	−1.39E − 3

this last case,

$$\left|f''(0) - \tilde{D}_h^{(2)}f(0)\right| \leq \frac{h^2}{12} + \frac{2 \times 10^{-8}}{h^2} \tag{5.7.23}$$

This bound is minimized at $h^* = .0022$, which is consistent with the errors $f''(0) - \tilde{D}_h^{(2)}f(0)$ given in the table. For the exactly computed $D_h^{(2)}f(0)$, note that the errors decrease by four whenever h is halved, consistent with the error formula (5.7.18).

Discussion of the Literature

Even though the topic of numerical integration is one of the oldest in numerical analysis and there is a very large literature, new papers continue to appear at a fairly high rate. Many of these results give methods for special classes of problems, for example, oscillatory integrals, and others are a response to changes in computers, for example, the use of vector pipeline architectures. The best survey of numerical integration is the large and detailed work of Davis and Rabinowitz (1984). It contains a comprehensive survey of most quadrature methods, a very extensive bibliography, a set of computer programs, and a bibliography of published quadrature programs. It also contains the article "On the practical evaluation of integrals" by Abramowitz, which gives some excellent suggestions on analytic approaches to quadrature. Other important texts in numerical integration are Engels (1980), Krylov (1962), and Stroud (1971). For a history of the classical numerical integration methods, see Goldstine (1977).

For reasons of space, we have had to omit some important ideas. Chief among these are (1) Clenshaw–Curtis quadrature, and (2) multivariable quadrature. The former is based on integrating a Chebyshev expansion of the integrand; empirically the method has proved excellent for a wide variety of integrals. The original method is presented in Clenshaw and Curtis (1960); a current account of the method is given in Piessens et al. (1983, pp. 28–39). The area of multivariable quadrature is an active area of research, and the texts of Engels (1980) and Stroud (1971) are the best introductions to the area. Because of the widespread use of multivariable quadrature in the finite element method for solving partial differential equations, texts on the finite element method will often contain integration formulas for triangular and rectangular regions.

Automatic numerical integration was a very active area of research in the 1960s and 1970s, when it was felt that most numerical integrations could be done in this way. Recently, there has been a return to a greater use of nonautomatic quadrature especially adapted to the integral at hand. An excellent discussion of the relative advantages and disadvantages of automatic quadrature is given in Lyness (1983). The most powerful and flexible of the current automatic programs are probably those given in QUADPACK, which is discussed and illustrated in Piessens et al. (1983). Versions of QUADPACK are included in the IMSL and NAG libraries.