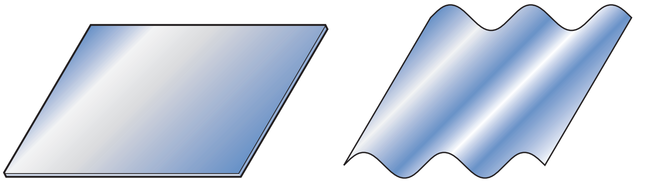
CHAPTER

4 Numerical Differentiation and Integration

Introduction

A sheet of corrugated roofing is constructed by pressing a flat sheet of aluminum into one whose cross section has the form of a sine wave.



A corrugated sheet 4 ft long is needed, the height of each wave is 1 in. from the center line, and each wave has a period of approximately 2π in. The problem of finding the length of the initial flat sheet is one of determining the length of the curve given by $f(x) = \sin x$ from $x = 0$ in. to $x = 48$ in. From calculus we know that this length is

$$L = \int_0^{48} \sqrt{1 + (f'(x))^2}\,dx = \int_0^{48} \sqrt{1 + (\cos x)^2}\,dx,$$

so the problem reduces to evaluating this integral. Although the sine function is one of the most common mathematical functions, the calculation of its length involves an elliptic integral of the second kind, which cannot be evaluated explicitly. Methods are developed in this chapter to approximate the solution to problems of this type. This particular problem is considered in Exercise 25 of Section 4.4 and Exercise 12 of Section 4.5.

We mentioned in the introduction to Chapter 3 that one reason for using algebraic polynomials to approximate an arbitrary set of data is that, given any continuous function defined on a closed interval, there exists a polynomial that is arbitrarily close to the function at every point in the interval. Also, the derivatives and integrals of polynomials are easily obtained and evaluated. It should not be surprising, then, that many procedures for approximating derivatives and integrals use the polynomials that approximate the function.

4.1 Numerical Differentiation

The derivative of the function f at x_0 is

$$f'(x_0) = \lim_{h \to 0} \frac{f(x_0 + h) - f(x_0)}{h}.$$

This formula gives an obvious way to generate an approximation to $f'(x_0)$; simply compute

$$\frac{f(x_0 + h) - f(x_0)}{h}$$

for small values of h. Although this may be obvious, it is not very successful, due to our old nemesis round-off error. But it is certainly a place to start.

To approximate $f'(x_0)$, suppose first that $x_0 \in (a, b)$, where $f \in C^2[a, b]$, and that $x_1 = x_0 + h$ for some $h \neq 0$ that is sufficiently small to ensure that $x_1 \in [a, b]$. We construct the first Lagrange polynomial $P_{0,1}(x)$ for f determined by x_0 and x_1, with its error term:

$$\begin{aligned} f(x) &= P_{0,1}(x) + \frac{(x - x_0)(x - x_1)}{2!} f''(\xi(x)) \\ &= \frac{f(x_0)(x - x_0 - h)}{-h} + \frac{f(x_0 + h)(x - x_0)}{h} + \frac{(x - x_0)(x - x_0 - h)}{2} f''(\xi(x)), \end{aligned}$$

for some $\xi(x)$ between x_0 and x_1. Differentiating gives

$$\begin{aligned} f'(x) &= \frac{f(x_0 + h) - f(x_0)}{h} + D_x \left[\frac{(x - x_0)(x - x_0 - h)}{2} f''(\xi(x)) \right] \\ &= \frac{f(x_0 + h) - f(x_0)}{h} + \frac{2(x - x_0) - h}{2} f''(\xi(x)) \\ &\quad + \frac{(x - x_0)(x - x_0 - h)}{2} D_x(f''(\xi(x))). \end{aligned}$$

Deleting the terms involving $\xi(x)$ gives

$$f'(x) \approx \frac{f(x_0 + h) - f(x_0)}{h}.$$

Difference equations were used and popularized by Isaac Newton in the last quarter of the 17th century, but many of these techniques had previously been developed by Thomas Harriot (1561–1621) and Henry Briggs (1561–1630). Harriot made significant advances in navigation techniques, and Briggs was the person most responsible for the acceptance of logarithms as an aid to computation.

One difficulty with this formula is that we have no information about $D_x f''(\xi(x))$, so the truncation error cannot be estimated. When x is x_0, however, the coefficient of $D_x f''(\xi(x))$ is 0, and the formula simplifies to

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2} f''(\xi). \tag{4.1}$$

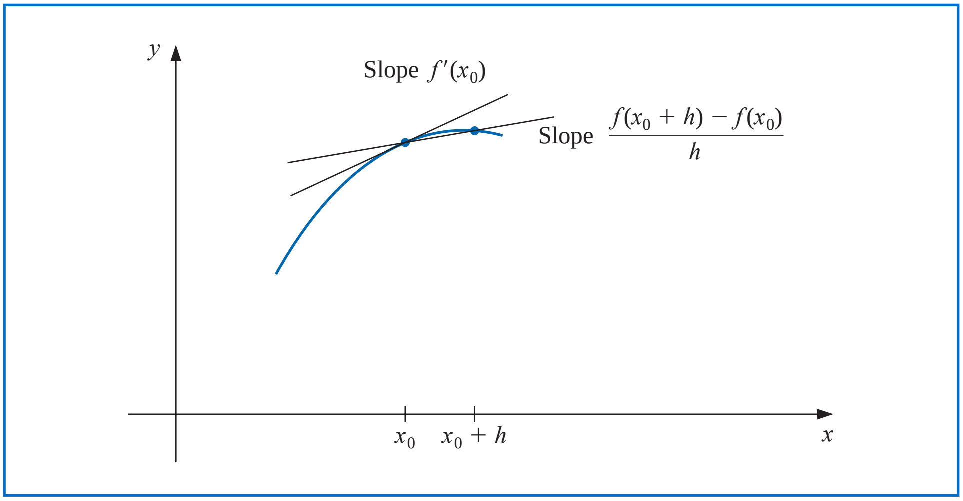
For small values of h, the difference quotient $[f(x_0 + h) - f(x_0)]/h$ can be used to approximate $f'(x_0)$ with an error bounded by $M|h|/2$, where M is a bound on $|f''(x)|$ for x between x_0 and $x_0 + h$. This formula is known as the **forward-difference formula** if $h > 0$ (see Figure 4.1) and the **backward-difference formula** if $h < 0$.

Example 1 Use the forward-difference formula to approximate the derivative of $f(x) = \ln x$ at $x_0 = 1.8$ using $h = 0.1$, $h = 0.05$, and $h = 0.01$, and determine bounds for the approximation errors.

Solution The forward-difference formula

$$\frac{f(1.8 + h) - f(1.8)}{h}$$

Figure 4.1



with $h = 0.1$ gives

$$\frac{\ln 1.9 - \ln 1.8}{0.1} = \frac{0.64185389 - 0.58778667}{0.1} = 0.5406722.$$

Because $f''(x) = -1/x^2$ and $1.8 < \xi < 1.9$, a bound for this approximation error is

$$\frac{|hf''(\xi)|}{2} = \frac{|h|}{2\xi^2} < \frac{0.1}{2(1.8)^2} = 0.0154321.$$

The approximation and error bounds when $h = 0.05$ and $h = 0.01$ are found in a similar manner and the results are shown in Table 4.1.

Table 4.1

h	$f(1.8+h)$	$\frac{f(1.8+h)-f(1.8)}{h}$	$\frac{\|h\|}{2(1.8)^2}$
0.1	0.64185389	0.5406722	0.0154321
0.05	0.61518564	0.5479795	0.0077160
0.01	0.59332685	0.5540180	0.0015432

Since $f'(x) = 1/x$, the exact value of $f'(1.8)$ is $0.55\overline{5}$, and in this case the error bounds are quite close to the true approximation error. ■

To obtain general derivative approximation formulas, suppose that $\{x_0, x_1, \ldots, x_n\}$ are $(n+1)$ distinct numbers in some interval I and that $f \in C^{n+1}(I)$. From Theorem 3.3 on page 112,

$$f(x) = \sum_{k=0}^{n} f(x_k)L_k(x) + \frac{(x-x_0)\cdots(x-x_n)}{(n+1)!} f^{(n+1)}(\xi(x)),$$

for some $\xi(x)$ in I, where $L_k(x)$ denotes the kth Lagrange coefficient polynomial for f at $x_0, x_1, \ldots, x_n$. Differentiating this expression gives

$$f'(x) = \sum_{k=0}^{n} f(x_k)L'_k(x) + D_x\left[\frac{(x-x_0)\cdots(x-x_n)}{(n+1!)}\right] f^{(n+1)}(\xi(x))$$
$$+ \frac{(x-x_0)\cdots(x-x_n)}{(n+1)!} D_x[f^{(n+1)}(\xi(x))].$$

We again have a problem estimating the truncation error unless x is one of the numbers x_j. In this case, the term multiplying $D_x[f^{(n+1)}(\xi(x))]$ is 0, and the formula becomes

$$f'(x_j) = \sum_{k=0}^{n} f(x_k)L'_k(x_j) + \frac{f^{(n+1)}(\xi(x_j))}{(n+1)!} \prod_{\substack{k=0\\k\neq j}}^{n}(x_j - x_k), \tag{4.2}$$

which is called an **$(n+1)$-point formula** to approximate $f'(x_j)$.

In general, using more evaluation points in Eq. (4.2) produces greater accuracy, although the number of functional evaluations and growth of round-off error discourages this somewhat. The most common formulas are those involving three and five evaluation points.

We first derive some useful three-point formulas and consider aspects of their errors. Because

$$L_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)}, \quad \text{we have} \quad L'_0(x) = \frac{2x - x_1 - x_2}{(x_0-x_1)(x_0-x_2)}.$$

Similarly,

$$L'_1(x) = \frac{2x - x_0 - x_2}{(x_1-x_0)(x_1-x_2)} \quad \text{and} \quad L'_2(x) = \frac{2x - x_0 - x_1}{(x_2-x_0)(x_2-x_1)}.$$

Hence, from Eq. (4.2),

$$f'(x_j) = f(x_0)\left[\frac{2x_j - x_1 - x_2}{(x_0-x_1)(x_0-x_2)}\right] + f(x_1)\left[\frac{2x_j - x_0 - x_2}{(x_1-x_0)(x_1-x_2)}\right]$$
$$+ f(x_2)\left[\frac{2x_j - x_0 - x_1}{(x_2-x_0)(x_2-x_1)}\right] + \frac{1}{6} f^{(3)}(\xi_j) \prod_{\substack{k=0\\k\neq j}}^{2}(x_j - x_k), \tag{4.3}$$

for each $j = 0, 1, 2$, where the notation ξ_j indicates that this point depends on x_j.

Three-Point Formulas

The formulas from Eq. (4.3) become especially useful if the nodes are equally spaced, that is, when

$$x_1 = x_0 + h \quad \text{and} \quad x_2 = x_0 + 2h, \quad \text{for some } h \neq 0.$$

We will assume equally-spaced nodes throughout the remainder of this section.

Using Eq. (4.3) with $x_j = x_0, x_1 = x_0 + h$, and $x_2 = x_0 + 2h$ gives

$$f'(x_0) = \frac{1}{h}\left[-\frac{3}{2}f(x_0) + 2f(x_1) - \frac{1}{2}f(x_2)\right] + \frac{h^2}{3} f^{(3)}(\xi_0).$$

Doing the same for $x_j = x_1$ gives

$$f'(x_1) = \frac{1}{h}\left[-\frac{1}{2}f(x_0) + \frac{1}{2}f(x_2)\right] - \frac{h^2}{6} f^{(3)}(\xi_1),$$

and for $x_j = x_2$,

$$f'(x_2) = \frac{1}{h}\left[\frac{1}{2}f(x_0) - 2f(x_1) + \frac{3}{2}f(x_2)\right] + \frac{h^2}{3}f^{(3)}(\xi_2).$$

Since $x_1 = x_0 + h$ and $x_2 = x_0 + 2h$, these formulas can also be expressed as

$$f'(x_0) = \frac{1}{h}\left[-\frac{3}{2}f(x_0) + 2f(x_0+h) - \frac{1}{2}f(x_0+2h)\right] + \frac{h^2}{3}f^{(3)}(\xi_0),$$

$$f'(x_0+h) = \frac{1}{h}\left[-\frac{1}{2}f(x_0) + \frac{1}{2}f(x_0+2h)\right] - \frac{h^2}{6}f^{(3)}(\xi_1),$$

and

$$f'(x_0+2h) = \frac{1}{h}\left[\frac{1}{2}f(x_0) - 2f(x_0+h) + \frac{3}{2}f(x_0+2h)\right] + \frac{h^2}{3}f^{(3)}(\xi_2).$$

As a matter of convenience, the variable substitution x_0 for $x_0 + h$ is used in the middle equation to change this formula to an approximation for $f'(x_0)$. A similar change, x_0 for $x_0 + 2h$, is used in the last equation. This gives three formulas for approximating $f'(x_0)$:

$$f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)] + \frac{h^2}{3}f^{(3)}(\xi_0),$$

$$f'(x_0) = \frac{1}{2h}[-f(x_0-h) + f(x_0+h)] - \frac{h^2}{6}f^{(3)}(\xi_1),$$

and

$$f'(x_0) = \frac{1}{2h}[f(x_0-2h) - 4f(x_0-h) + 3f(x_0)] + \frac{h^2}{3}f^{(3)}(\xi_2).$$

Finally, note that the last of these equations can be obtained from the first by simply replacing h with $-h$, so there are actually only two formulas:

Three-Point Endpoint Formula

- $f'(x_0) = \dfrac{1}{2h}[-3f(x_0) + 4f(x_0+h) - f(x_0+2h)] + \dfrac{h^2}{3}f^{(3)}(\xi_0),$ (4.4)

where ξ_0 lies between x_0 and $x_0 + 2h$.

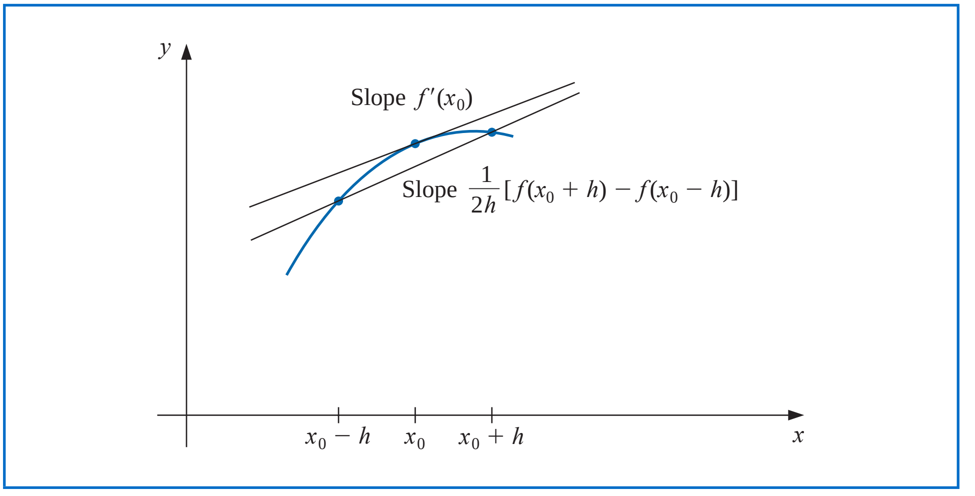
Three-Point Midpoint Formula

- $f'(x_0) = \dfrac{1}{2h}[f(x_0+h) - f(x_0-h)] - \dfrac{h^2}{6}f^{(3)}(\xi_1),$ (4.5)

where ξ_1 lies between $x_0 - h$ and $x_0 + h$.

Although the errors in both Eq. (4.4) and Eq. (4.5) are $O(h^2)$, the error in Eq. (4.5) is approximately half the error in Eq. (4.4). This is because Eq. (4.5) uses data on both sides of x_0 and Eq. (4.4) uses data on only one side. Note also that f needs to be evaluated at only two points in Eq. (4.5), whereas in Eq. (4.4) three evaluations are needed. Figure 4.2 on page 178 gives an illustration of the approximation produced from Eq. (4.5). The approximation in Eq. (4.4) is useful near the ends of an interval, because information about f outside the interval may not be available.

Figure 4.2



Five-Point Formulas

The methods presented in Eqs. (4.4) and (4.5) are called **three-point formulas** (even though the third point $f(x_0)$ does not appear in Eq. (4.5)). Similarly, there are **five-point formulas** that involve evaluating the function at two additional points. The error term for these formulas is $O(h^4)$. One common five-point formula is used to determine approximations for the derivative at the midpoint.

Five-Point Midpoint Formula

- $$f'(x_0) = \frac{1}{12h}[f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)] + \frac{h^4}{30}f^{(5)}(\xi), \tag{4.6}$$

  where ξ lies between $x_0 - 2h$ and $x_0 + 2h$.

The derivation of this formula is considered in Section 4.2. The other five-point formula is used for approximations at the endpoints.

Five-Point Endpoint Formula

- $$f'(x_0) = \frac{1}{12h}[-25f(x_0) + 48f(x_0+h) - 36f(x_0+2h) + 16f(x_0+3h) - 3f(x_0+4h)] + \frac{h^4}{5}f^{(5)}(\xi), \tag{4.7}$$

  where ξ lies between x_0 and $x_0 + 4h$.

Left-endpoint approximations are found using this formula with $h > 0$ and right-endpoint approximations with $h < 0$. The five-point endpoint formula is particularly useful for the clamped cubic spline interpolation of Section 3.5.

Example 2 Values for $f(x) = xe^x$ are given in Table 4.2. Use all the applicable three-point and five-point formulas to approximate $f'(2.0)$.

Table 4.2

x	$f(x)$
1.8	10.889365
1.9	12.703199
2.0	14.778112
2.1	17.148957
2.2	19.855030

Solution The data in the table permit us to find four different three-point approximations. We can use the endpoint formula (4.4) with $h = 0.1$ or with $h = -0.1$, and we can use the midpoint formula (4.5) with $h = 0.1$ or with $h = 0.2$.

Using the endpoint formula (4.4) with $h = 0.1$ gives

$$\frac{1}{0.2}[-3f(2.0) + 4f(2.1) - f(2.2] = 5[-3(14.778112) + 4(17.148957) - 19.855030)] = 22.032310,$$

and with $h = -0.1$ gives 22.054525.

Using the midpoint formula (4.5) with $h = 0.1$ gives

$$\frac{1}{0.2}[f(2.1) - f(1.9)] = 5(17.148957 - 12.7703199) = 22.228790,$$

and with $h = 0.2$ gives 22.414163.

The only five-point formula for which the table gives sufficient data is the midpoint formula (4.6) with $h = 0.1$. This gives

$$\begin{aligned}\frac{1}{1.2}[f(1.8) - 8f(1.9) + 8f(2.1) - f(2.2)] &= \frac{1}{1.2}[10.889365 - 8(12.703199) \\ &\quad + 8(17.148957) - 19.855030] \\ &= 22.166999\end{aligned}$$

If we had no other information we would accept the five-point midpoint approximation using $h = 0.1$ as the most accurate, and expect the true value to be between that approximation and the three-point mid-point approximation that is in the interval [22.166, 22.229].

The true value in this case is $f'(2.0) = (2+1)e^2 = 22.167168$, so the approximation errors are actually:

Three-point endpoint with $h = 0.1$: 1.35×10^{-1};

Three-point endpoint with $h = -0.1$: 1.13×10^{-1};

Three-point midpoint with $h = 0.1$: -6.16×10^{-2};

Three-point midpoint with $h = 0.2$: -2.47×10^{-1};

Five-point midpoint with $h = 0.1$: 1.69×10^{-4}. ■

Methods can also be derived to find approximations to higher derivatives of a function using only tabulated values of the function at various points. The derivation is algebraically tedious, however, so only a representative procedure will be presented.

Expand a function f in a third Taylor polynomial about a point x_0 and evaluate at $x_0 + h$ and $x_0 - h$. Then

$$f(x_0 + h) = f(x_0) + f'(x_0)h + \frac{1}{2}f''(x_0)h^2 + \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(\xi_1)h^4$$

and

$$f(x_0 - h) = f(x_0) - f'(x_0)h + \frac{1}{2}f''(x_0)h^2 - \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(\xi_{-1})h^4,$$

where $x_0 - h < \xi_{-1} < x_0 < \xi_1 < x_0 + h$.

If we add these equations, the terms involving $f'(x_0)$ and $-f'(x_0)$ cancel, so

$$f(x_0 + h) + f(x_0 - h) = 2f(x_0) + f''(x_0)h^2 + \frac{1}{24}[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})]h^4.$$

Solving this equation for $f''(x_0)$ gives

$$f''(x_0) = \frac{1}{h^2}[f(x_0 - h) - 2f(x_0) + f(x_0 + h)] - \frac{h^2}{24}[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})]. \qquad (4.8)$$

Suppose $f^{(4)}$ is continuous on $[x_0 - h, x_0 + h]$. Since $\frac{1}{2}[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})]$ is between $f^{(4)}(\xi_1)$ and $f^{(4)}(\xi_{-1})$, the Intermediate Value Theorem implies that a number ξ exists between ξ_1 and ξ_{-1}, and hence in $(x_0 - h, x_0 + h)$, with

$$f^{(4)}(\xi) = \frac{1}{2}\left[f^{(4)}(\xi_1) + f^{(4)}(\xi_{-1})\right].$$

This permits us to rewrite Eq. (4.8) in its final form.

Second Derivative Midpoint Formula

- $$f''(x_0) = \frac{1}{h^2}[f(x_0 - h) - 2f(x_0) + f(x_0 + h)] - \frac{h^2}{12}f^{(4)}(\xi), \qquad (4.9)$$

  for some ξ, where $x_0 - h < \xi < x_0 + h$.

If $f^{(4)}$ is continuous on $[x_0 - h, x_0 + h]$ it is also bounded, and the approximation is $O(h^2)$.

Example 3 In Example 2 we used the data shown in Table 4.3 to approximate the first derivative of $f(x) = xe^x$ at $x = 2.0$. Use the second derivative formula (4.9) to approximate $f''(2.0)$.

Table 4.3

x	$f(x)$
1.8	10.889365
1.9	12.703199
2.0	14.778112
2.1	17.148957
2.2	19.855030

Solution The data permits us to determine two approximations for $f''(2.0)$. Using (4.9) with $h = 0.1$ gives

$$\frac{1}{0.01}[f(1.9) - 2f(2.0) + f(2.1)] = 100[12.703199 - 2(14.778112) + 17.148957]$$
$$= 29.593200,$$

and using (4.9) with $h = 0.2$ gives

$$\frac{1}{0.04}[f(1.8) - 2f(2.0) + f(2.2)] = 25[10.889365 - 2(14.778112) + 19.855030]$$
$$= 29.704275.$$

Because $f''(x) = (x + 2)e^x$, the exact value is $f''(2.0) = 29.556224$. Hence the actual errors are -3.70×10^{-2} and -1.48×10^{-1}, respectively. ■

Round-Off Error Instability

It is particularly important to pay attention to round-off error when approximating derivatives. To illustrate the situation, let us examine the three-point midpoint formula Eq. (4.5),

$$f'(x_0) = \frac{1}{2h}[f(x_0 + h) - f(x_0 - h)] - \frac{h^2}{6}f^{(3)}(\xi_1),$$

more closely. Suppose that in evaluating $f(x_0 + h)$ and $f(x_0 - h)$ we encounter round-off errors $e(x_0 + h)$ and $e(x_0 - h)$. Then our computations actually use the values $\tilde{f}(x_0 + h)$ and $\tilde{f}(x_0 - h)$, which are related to the true values $f(x_0 + h)$ and $f(x_0 - h)$ by

$$f(x_0+h) = \tilde{f}(x_0+h) + e(x_0+h) \quad \text{and} \quad f(x_0-h) = \tilde{f}(x_0-h) + e(x_0-h).$$

The total error in the approximation,

$$f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h} = \frac{e(x_0+h) - e(x_0-h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi_1),$$

is due both to round-off error, the first part, and to truncation error. If we assume that the round-off errors $e(x_0 \pm h)$ are bounded by some number $\varepsilon > 0$ and that the third derivative of f is bounded by a number $M > 0$, then

$$\left| f'(x_0) - \frac{\tilde{f}(x_0+h) - \tilde{f}(x_0-h)}{2h} \right| \le \frac{\varepsilon}{h} + \frac{h^2}{6} M.$$

To reduce the truncation error, $h^2M/6$, we need to reduce h. But as h is reduced, the round-off error ε/h grows. In practice, then, it is seldom advantageous to let h be too small, because in that case the round-off error will dominate the calculations.

Illustration Consider using the values in Table 4.4 to approximate $f'(0.900)$, where $f(x) = \sin x$. The true value is $\cos 0.900 = 0.62161$. The formula

$$f'(0.900) \approx \frac{f(0.900+h) - f(0.900-h)}{2h},$$

with different values of h, gives the approximations in Table 4.5.

Table 4.4

x	$\sin x$	x	$\sin x$
0.800	0.71736	0.901	0.78395
0.850	0.75128	0.902	0.78457
0.880	0.77074	0.905	0.78643
0.890	0.77707	0.910	0.78950
0.895	0.78021	0.920	0.79560
0.898	0.78208	0.950	0.81342
0.899	0.78270	1.000	0.84147

Table 4.5

h	Approximation to $f'(0.900)$	Error
0.001	0.62500	0.00339
0.002	0.62250	0.00089
0.005	0.62200	0.00039
0.010	0.62150	−0.00011
0.020	0.62150	−0.00011
0.050	0.62140	−0.00021
0.100	0.62055	−0.00106

The optimal choice for h appears to lie between 0.005 and 0.05. We can use calculus to verify (see Exercise 29) that a minimum for

$$e(h) = \frac{\varepsilon}{h} + \frac{h^2}{6} M,$$

occurs at $h = \sqrt[3]{3\varepsilon/M}$, where

$$M = \max_{x \in [0.800, 1.00]} |f'''(x)| = \max_{x \in [0.800, 1.00]} |\cos x| = \cos 0.8 \approx 0.69671.$$

Because values of f are given to five decimal places, we will assume that the round-off error is bounded by $\varepsilon = 5 \times 10^{-6}$. Therefore, the optimal choice of h is approximately

$$h = \sqrt[3]{\frac{3(0.000005)}{0.69671}} \approx 0.028,$$

which is consistent with the results in Table 4.6. □

In practice, we cannot compute an optimal h to use in approximating the derivative, since we have no knowledge of the third derivative of the function. But we must remain aware that reducing the step size will not always improve the approximation. □

We have considered only the round-off error problems that are presented by the three-point formula Eq. (4.5), but similar difficulties occur with all the differentiation formulas. The reason can be traced to the need to divide by a power of h. As we found in Section 1.2 (see, in particular, Example 3), division by small numbers tends to exaggerate round-off error, and this operation should be avoided if possible. In the case of numerical differentiation, we cannot avoid the problem entirely, although the higher-order methods reduce the difficulty.

Keep in mind that difference method approximations might be unstable.

As approximation methods, numerical differentiation is *unstable*, since the small values of h needed to reduce truncation error also cause the round-off error to grow. This is the first class of unstable methods we have encountered, and these techniques would be avoided if it were possible. However, in addition to being used for computational purposes, the formulas are needed for approximating the solutions of ordinary and partial-differential equations.

EXERCISE SET 4.1

1. Use the forward-difference formulas and backward-difference formulas to determine each missing entry in the following tables.

a.

x	$f(x)$	$f'(x)$
0.5	0.4794	
0.6	0.5646	
0.7	0.6442	

b.

x	$f(x)$	$f'(x)$
0.0	0.00000	
0.2	0.74140	
0.4	1.3718	

2. Use the forward-difference formulas and backward-difference formulas to determine each missing entry in the following tables.

a.

x	$f(x)$	$f'(x)$
−0.3	1.9507	
−0.2	2.0421	
−0.1	2.0601	

b.

x	$f(x)$	$f'(x)$
1.0	1.0000	
1.2	1.2625	
1.4	1.6595	

3. The data in Exercise 1 were taken from the following functions. Compute the actual errors in Exercise 1, and find error bounds using the error formulas.

a. $f(x) = \sin x$ **b.** $f(x) = e^x - 2x^2 + 3x - 1$

4. The data in Exercise 2 were taken from the following functions. Compute the actual errors in Exercise 2, and find error bounds using the error formulas.

a. $f(x) = 2\cos 2x - x$ **b.** $f(x) = x^2 \ln x + 1$

5. Use the most accurate three-point formula to determine each missing entry in the following tables.

a.

x	$f(x)$	$f'(x)$
1.1	9.025013	
1.2	11.02318	
1.3	13.46374	
1.4	16.44465	

b.

x	$f(x)$	$f'(x)$
8.1	16.94410	
8.3	17.56492	
8.5	18.19056	
8.7	18.82091	

c.

x	$f(x)$	$f'(x)$
2.9	−4.827866	
3.0	−4.240058	
3.1	−3.496909	
3.2	−2.596792	

d.

x	$f(x)$	$f'(x)$
2.0	3.6887983	
2.1	3.6905701	
2.2	3.6688192	
2.3	3.6245909	

6. Use the most accurate three-point formula to determine each missing entry in the following tables.

a.

x	$f(x)$	$f'(x)$
-0.3	-0.27652	
-0.2	-0.25074	
-0.1	-0.16134	
0	0	

b.

x	$f(x)$	$f'(x)$
7.4	-68.3193	
7.6	-71.6982	
7.8	-75.1576	
8.0	-78.6974	

c.

x	$f(x)$	$f'(x)$
1.1	1.52918	
1.2	1.64024	
1.3	1.70470	
1.4	1.71277	

d.

x	$f(x)$	$f'(x)$
-2.7	0.054797	
-2.5	0.11342	
-2.3	0.65536	
-2.1	0.98472	

7. The data in Exercise 5 were taken from the following functions. Compute the actual errors in Exercise 5, and find error bounds using the error formulas.

a. $f(x) = e^{2x}$
b. $f(x) = x \ln x$
c. $f(x) = x \cos x - x^2 \sin x$
d. $f(x) = 2(\ln x)^2 + 3 \sin x$

8. The data in Exercise 6 were taken from the following functions. Compute the actual errors in Exercise 6, and find error bounds using the error formulas.

a. $f(x) = e^{2x} - \cos 2x$
b. $f(x) = \ln(x + 2) - (x + 1)^2$
c. $f(x) = x \sin x + x^2 \cos x$
d. $f(x) = (\cos 3x)^2 - e^{2x}$

9. Use the formulas given in this section to determine, as accurately as possible, approximations for each missing entry in the following tables.

a.

x	$f(x)$	$f'(x)$
2.1	-1.709847	
2.2	-1.373823	
2.3	-1.119214	
2.4	-0.9160143	
2.5	-0.7470223	
2.6	-0.6015966	

b.

x	$f(x)$	$f'(x)$
-3.0	9.367879	
-2.8	8.233241	
-2.6	7.180350	
-2.4	6.209329	
-2.2	5.320305	
-2.0	4.513417	

10. Use the formulas given in this section to determine, as accurately as possible, approximations for each missing entry in the following tables.

a.

x	$f(x)$	$f'(x)$
1.05	-1.709847	
1.10	-1.373823	
1.15	-1.119214	
1.20	-0.9160143	
1.25	-0.7470223	
1.30	-0.6015966	

b.

x	$f(x)$	$f'(x)$
-3.0	16.08554	
-2.8	12.64465	
-2.6	9.863738	
-2.4	7.623176	
-2.2	5.825013	
-2.0	4.389056	

11. The data in Exercise 9 were taken from the following functions. Compute the actual errors in Exercise 9, and find error bounds using the error formulas and Maple.

a. $f(x) = \tan x$
b. $f(x) = e^{x/3} + x^2$

12. The data in Exercise 10 were taken from the following functions. Compute the actual errors in Exercise 10, and find error bounds using the error formulas and Maple.

a. $f(x) = \tan 2x$
b. $f(x) = e^{-x} - 1 + x$

13. Use the following data and the knowledge that the first five derivatives of f are bounded on $[1, 5]$ by 2, 3, 6, 12 and 23, respectively, to approximate $f'(3)$ as accurately as possible. Find a bound for the error.

x	1	2	3	4	5
$f(x)$	2.4142	2.6734	2.8974	3.0976	3.2804

14. Repeat Exercise 13, assuming instead that the third derivative of f is bounded on $[1, 5]$ by 4.

15. Repeat Exercise 1 using four-digit rounding arithmetic, and compare the errors to those in Exercise 3.

16. Repeat Exercise 5 using four-digit chopping arithmetic, and compare the errors to those in Exercise 7.

17. Repeat Exercise 9 using four-digit rounding arithmetic, and compare the errors to those in Exercise 11.

18. Consider the following table of data:

x	0.2	0.4	0.6	0.8	1.0
$f(x)$	0.9798652	0.9177710	0.808038	0.6386093	0.3843735

a. Use all the appropriate formulas given in this section to approximate $f'(0.4)$ and $f''(0.4)$.

b. Use all the appropriate formulas given in this section to approximate $f'(0.6)$ and $f''(0.6)$.

19. Let $f(x) = \cos \pi x$. Use Eq. (4.9) and the values of $f(x)$ at $x = 0.25$, 0.5, and 0.75 to approximate $f''(0.5)$. Compare this result to the exact value and to the approximation found in Exercise 15 of Section 3.5. Explain why this method is particularly accurate for this problem, and find a bound for the error.

20. Let $f(x) = 3xe^x - \cos x$. Use the following data and Eq. (4.9) to approximate $f''(1.3)$ with $h = 0.1$ and with $h = 0.01$.

x	1.20	1.29	1.30	1.31	1.40
$f(x)$	11.59006	13.78176	14.04276	14.30741	16.86187

Compare your results to $f''(1.3)$.

21. Consider the following table of data:

x	0.2	0.4	0.6	0.8	1.0
$f(x)$	0.9798652	0.9177710	0.8080348	0.6386093	0.3843735

a. Use Eq. (4.7) to approximate $f'(0.2)$.

b. Use Eq. (4.7) to approximate $f'(1.0)$.

c. Use Eq. (4.6) to approximate $f'(0.6)$.

22. Derive an $O(h^4)$ five-point formula to approximate $f'(x_0)$ that uses $f(x_0 - h)$, $f(x_0)$, $f(x_0 + h)$, $f(x_0 + 2h)$, and $f(x_0 + 3h)$. [*Hint:* Consider the expression $Af(x_0 - h) + Bf(x_0 + h) + Cf(x_0 + 2h) + Df(x_0 + 3h)$. Expand in fourth Taylor polynomials, and choose A, B, C, and D appropriately.]

23. Use the formula derived in Exercise 22 and the data of Exercise 21 to approximate $f'(0.4)$ and $f'(0.8)$.

24. **a.** Analyze the round-off errors, as in Example 4, for the formula

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2} f''(\xi_0).$$

b. Find an optimal $h > 0$ for the function given in Example 2.

25. In Exercise 10 of Section 3.4 data were given describing a car traveling on a straight road. That problem asked to predict the position and speed of the car when $t = 10$ s. Use the following times and positions to predict the speed at each time listed.

Time	0	3	5	8	10	13
Distance	0	225	383	623	742	993

26. In a circuit with impressed voltage $\mathcal{E}(t)$ and inductance L, Kirchhoff's first law gives the relationship

$$\mathcal{E}(t) = L\frac{di}{dt} + Ri,$$

where R is the resistance in the circuit and i is the current. Suppose we measure the current for several values of t and obtain:

t	1.00	1.01	1.02	1.03	1.0
i	3.10	3.12	3.14	3.18	3.24

where t is measured in seconds, i is in amperes, the inductance L is a constant 0.98 henries, and the resistance is 0.142 ohms. Approximate the voltage $\mathcal{E}(t)$ when $t = 1.00$, 1.01, 1.02, 1.03, and 1.04.

27. All calculus students know that the derivative of a function f at x can be defined as

$$f'(x) = \lim_{h\to 0} \frac{f(x+h) - f(x)}{h}.$$

Choose your favorite function f, nonzero number x, and computer or calculator. Generate approximations $f'_n(x)$ to $f'(x)$ by

$$f'_n(x) = \frac{f(x + 10^{-n}) - f(x)}{10^{-n}},$$

for $n = 1, 2, \ldots, 20$, and describe what happens.

28. Derive a method for approximating $f'''(x_0)$ whose error term is of order h^2 by expanding the function f in a fourth Taylor polynomial about x_0 and evaluating at $x_0 \pm h$ and $x_0 \pm 2h$.

29. Consider the function

$$e(h) = \frac{\varepsilon}{h} + \frac{h^2}{6}M,$$

where M is a bound for the third derivative of a function. Show that $e(h)$ has a minimum at $\sqrt[3]{3\varepsilon/M}$.

4.2 Richardson's Extrapolation

Richardson's extrapolation is used to generate high-accuracy results while using low-order formulas. Although the name attached to the method refers to a paper written by L. F. Richardson and J. A. Gaunt [RG] in 1927, the idea behind the technique is much older. An interesting article regarding the history and application of extrapolation can be found in [Joy].

Lewis Fry Richardson (1881–1953) was the first person to systematically apply mathematics to weather prediction while working in England for the Meteorological Office. As a conscientious objector during World War I, he wrote extensively about the economic futility of warfare, using systems of differential equations to model rational interactions between countries. The extrapolation technique that bears his name was the rediscovery of a technique with roots that are at least as old as Christiaan Hugyens (1629–1695), and possibly Archimedes (287–212 B.C.E.).

Extrapolation can be applied whenever it is known that an approximation technique has an error term with a predictable form, one that depends on a parameter, usually the step size h. Suppose that for each number $h \neq 0$ we have a formula $N_1(h)$ that approximates an unknown constant M, and that the truncation error involved with the approximation has the form

$$M - N_1(h) = K_1 h + K_2 h^2 + K_3 h^3 + \cdots,$$

for some collection of (unknown) constants $K_1, K_2, K_3, \ldots$.

The truncation error is $O(h)$, so unless there was a large variation in magnitude among the constants $K_1, K_2, K_3, \ldots$,

$$M - N_1(0.1) \approx 0.1K_1, \quad M - N_1(0.01) \approx 0.01K_1,$$

and, in general, $M - N_1(h) \approx K_1 h$.

The object of extrapolation is to find an easy way to combine these rather inaccurate $O(h)$ approximations in an appropriate way to produce formulas with a higher-order truncation error.

Suppose, for example, we can combine the $N_1(h)$ formulas to produce an $O(h^2)$ approximation formula, $N_2(h)$, for M with

$$M - N_2(h) = \hat{K}_2 h^2 + \hat{K}_3 h^3 + \cdots,$$

for some, again unknown, collection of constants $\hat{K}_2, \hat{K}_3, \ldots$. Then we would have

$$M - N_2(0.1) \approx 0.01\hat{K}_2, \quad M - N_2(0.01) \approx 0.0001\hat{K}_2,$$

and so on. If the constants K_1 and $\hat{K}_2$ are roughly of the same magnitude, then the $N_2(h)$ approximations would be much better than the corresponding $N_1(h)$ approximations. The extrapolation continues by combining the $N_2(h)$ approximations in a manner that produces formulas with $O(h^3)$ truncation error, and so on.

To see specifically how we can generate the extrapolation formulas, consider the $O(h)$ formula for approximating M

$$M = N_1(h) + K_1 h + K_2 h^2 + K_3 h^3 + \cdots. \tag{4.10}$$

The formula is assumed to hold for all positive h, so we replace the parameter h by half its value. Then we have a second $O(h)$ approximation formula

$$M = N_1\left(\frac{h}{2}\right) + K_1\frac{h}{2} + K_2\frac{h^2}{4} + K_3\frac{h^3}{8} + \cdots. \tag{4.11}$$

Subtracting Eq. (4.10) from twice Eq. (4.11) eliminates the term involving K_1 and gives

$$M = N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right] + K_2\left(\frac{h^2}{2} - h^2\right) + K_3\left(\frac{h^3}{4} - h^3\right) + \cdots. \tag{4.12}$$

Define

$$N_2(h) = N_1\left(\frac{h}{2}\right) + \left[N_1\left(\frac{h}{2}\right) - N_1(h)\right].$$

Then Eq. (4.12) is an $O(h^2)$ approximation formula for M:

$$M = N_2(h) - \frac{K_2}{2}h^2 - \frac{3K_3}{4}h^3 - \cdots. \tag{4.13}$$

Example 1 In Example 1 of Section 4.1 we use the forward-difference method with $h = 0.1$ and $h = 0.05$ to find approximations to $f'(1.8)$ for $f(x) = \ln(x)$. Assume that this formula has truncation error $O(h)$ and use extrapolation on these values to see if this results in a better approximation.

Solution In Example 1 of Section 4.1 we found that

$$\text{with } h = 0.1\text{: } f'(1.8) \approx 0.5406722, \quad \text{and} \quad \text{with } h = 0.05\text{: } f'(1.8) \approx 0.5479795.$$

This implies that

$$N_1(0.1) = 0.5406722 \quad \text{and} \quad N_1(0.05) = 0.5479795.$$

Extrapolating these results gives the new approximation

$$N_2(0.1) = N_1(0.05) + (N_1(0.05) - N_1(0.1)) = 0.5479795 + (0.5479795 - 0.5406722)$$
$$= 0.555287.$$

The $h = 0.1$ and $h = 0.05$ results were found to be accurate to within 1.5×10^{-2} and 7.7×10^{-3}, respectively. Because $f'(1.8) = 1/1.8 = 0.\overline{5}$, the extrapolated value is accurate to within 2.7×10^{-4}. ∎

Extrapolation can be applied whenever the truncation error for a formula has the form

$$\sum_{j=1}^{m-1} K_j h^{\alpha_j} + O(h^{\alpha_m}),$$

for a collection of constants K_j and when $\alpha_1 < \alpha_2 < \alpha_3 < \cdots < \alpha_m$. Many formulas used for extrapolation have truncation errors that contain only even powers of h, that is, have the form

$$M = N_1(h) + K_1 h^2 + K_2 h^4 + K_3 h^6 + \cdots . \tag{4.14}$$

The extrapolation is much more effective than when all powers of h are present because the averaging process produces results with errors $O(h^2)$, $O(h^4)$, $O(h^6)$, $\ldots$, with essentially no increase in computation, over the results with errors, $O(h)$, $O(h^2)$, $O(h^3)$, $\ldots$.

Assume that approximation has the form of Eq. (4.14). Replacing h with $h/2$ gives the $O(h^2)$ approximation formula

$$M = N_1\left(\frac{h}{2}\right) + K_1\frac{h^2}{4} + K_2\frac{h^4}{16} + K_3\frac{h^6}{64} + \cdots .$$

Subtracting Eq. (4.14) from 4 times this equation eliminates the h^2 term,

$$3M = \left[4N_1\left(\frac{h}{2}\right) - N_1(h)\right] + K_2\left(\frac{h^4}{4} - h^4\right) + K_3\left(\frac{h^6}{16} - h^6\right) + \cdots .$$

Dividing this equation by 3 produces an $O(h^4)$ formula

$$M = \frac{1}{3}\left[4N_1\left(\frac{h}{2}\right) - N_1(h)\right] + \frac{K_2}{3}\left(\frac{h^4}{4} - h^4\right) + \frac{K_3}{3}\left(\frac{h^6}{16} - h^6\right) + \cdots .$$

Defining

$$N_2(h) = \frac{1}{3}\left[4N_1\left(\frac{h}{2}\right) - N_1(h)\right] = N_1\left(\frac{h}{2}\right) + \frac{1}{3}\left[N_1\left(\frac{h}{2}\right) - N_1(h)\right],$$

produces the approximation formula with truncation error $O(h^4)$:

$$M = N_2(h) - K_2\frac{h^4}{4} - K_3\frac{5h^6}{16} + \cdots . \tag{4.15}$$

Now replace h in Eq. (4.15) with $h/2$ to produce a second $O(h^4)$ formula

$$M = N_2\left(\frac{h}{2}\right) - K_2\frac{h^4}{64} - K_3\frac{5h^6}{1024} - \cdots .$$

Subtracting Eq. (4.15) from 16 times this equation eliminates the h^4 term and gives

$$15M = \left[16N_2\left(\frac{h}{2}\right) - N_2(h)\right] + K_3\frac{15h^6}{64} + \cdots .$$

Dividing this equation by 15 produces the new $O(h^6)$ formula

$$M = \frac{1}{15}\left[16N_2\left(\frac{h}{2}\right) - N_2(h)\right] + K_3\frac{h^6}{64} + \cdots .$$

We now have the $O(h^6)$ approximation formula

$$N_3(h) = \frac{1}{15}\left[16N_2\left(\frac{h}{2}\right) - N_2(h)\right] = N_2\left(\frac{h}{2}\right) + \frac{1}{15}\left[N_2\left(\frac{h}{2}\right) - N_2(h)\right].$$

Continuing this procedure gives, for each $j = 2, 3, \ldots,$ the $O(h^{2j})$ approximation

$$N_j(h) = N_{j-1}\left(\frac{h}{2}\right) + \frac{N_{j-1}(h/2) - N_{j-1}(h)}{4^{j-1} - 1}.$$

Table 4.6 shows the order in which the approximations are generated when

$$M = N_1(h) + K_1h^2 + K_2h^4 + K_3h^6 + \cdots. \tag{4.16}$$

It is conservatively assumed that the true result is accurate at least to within the agreement of the bottom two results in the diagonal, in this case, to within $|N_3(h) - N_4(h)|$.

Table 4.6

$O(h^2)$	$O(h^4)$	$O(h^6)$	$O(h^8)$
1: $N_1(h)$			
2: $N_1(\frac{h}{2})$	**3:** $N_2(h)$		
4: $N_1(\frac{h}{4})$	**5:** $N_2(\frac{h}{2})$	**6:** $N_3(h)$	
7: $N_1(\frac{h}{8})$	**8:** $N_2(\frac{h}{4})$	**9:** $N_3(\frac{h}{2})$	**10:** $N_4(h)$

Example 2 Taylor's theorem can be used to show that centered-difference formula in Eq. (4.5) to approximate $f'(x_0)$ can be expressed with an error formula:

$$f'(x_0) = \frac{1}{2h}[f(x_0 + h) - f(x_0 - h)] - \frac{h^2}{6}f'''(x_0) - \frac{h^4}{120}f^{(5)}(x_0) - \cdots.$$

Find approximations of order $O(h^2)$, $O(h^4)$, and $O(h^6)$ for $f'(2.0)$ when $f(x) = xe^x$ and $h = 0.2$.

Solution The constants $K_1 = -f'''(x_0)/6$, $K_2 = -f^{(5)}(x_0)/120, \cdots$, are not likely to be known, but this is not important. We only need to know that these constants exist in order to apply extrapolation.

We have the $O(h^2)$ approximation

$$f'(x_0) = N_1(h) - \frac{h^2}{6}f'''(x_0) - \frac{h^4}{120}f^{(5)}(x_0) - \cdots, \tag{4.17}$$

where

$$N_1(h) = \frac{1}{2h}[f(x_0 + h) - f(x_0 - h)].$$

This gives us the first $O(h^2)$ approximations

$$N_1(0.2) = \frac{1}{0.4}[f(2.2) - f(1.8)] = 2.5(19.855030 - 10.889365) = 22.414160,$$

and

$$N_1(0.1) = \frac{1}{0.2}[f(2.1) - f(1.9)] = 5(17.148957 - 12.703199) = 22.228786.$$

Combining these to produce the first $O(h^4)$ approximation gives

$$N_2(0.2) = N_1(0.1) + \frac{1}{3}(N_1(0.1) - N_1(0.2))$$
$$= 22.228786 + \frac{1}{3}(22.228786 - 22.414160) = 22.166995.$$

To determine an $O(h^6)$ formula we need another $O(h^4)$ result, which requires us to find the third $O(h^2)$ approximation

$$N_1(0.05) = \frac{1}{0.1}[f(2.05) - f(1.95)] = 10(15.924197 - 13.705941) = 22.182564.$$

We can now find the $O(h^4)$ approximation

$$N_2(0.1) = N_1(0.05) + \frac{1}{3}(N_1(0.05) - N_1(0.1))$$
$$= 22.182564 + \frac{1}{3}(22.182564 - 22.228786) = 22.167157.$$

and finally the $O(h^6)$ approximation

$$N_3(0.2) = N_2(0.1) + \frac{1}{15}(N_2(0.1) - N_1(0.2))$$
$$= 22.167157 + \frac{1}{15}(22.167157 - 22.166995) = 22.167168.$$

We would expect the final approximation to be accurate to at least the value 22.167 because the $N_2(0.2)$ and $N_3(0.2)$ give this same value. In fact, $N_3(0.2)$ is accurate to all the listed digits. ■

Each column beyond the first in the extrapolation table is obtained by a simple averaging process, so the technique can produce high-order approximations with minimal computational cost. However, as k increases, the round-off error in $N_1(h/2^k)$ will generally increase because the instability of numerical differentiation is related to the step size $h/2^k$. Also, the higher-order formulas depend increasingly on the entry to their immediate left in the table, which is the reason we recommend comparing the final diagonal entries to ensure accuracy.

In Section 4.1, we discussed both three- and five-point methods for approximating $f'(x_0)$ given various functional values of f. The three-point methods were derived by differentiating a Lagrange interpolating polynomial for f. The five-point methods can be obtained in a similar manner, but the derivation is tedious. Extrapolation can be used to more easily derive these formulas, as illustrated below.

Illustration Suppose we expand the function f in a fourth Taylor polynomial about x_0. Then

$$f(x) = f(x_0) + f'(x_0)(x - x_0) + \frac{1}{2}f''(x_0)(x - x_0)^2 + \frac{1}{6}f'''(x_0)(x - x_0)^3$$
$$+ \frac{1}{24}f^{(4)}(x_0)(x - x_0)^4 + \frac{1}{120}f^{(5)}(\xi)(x - x_0)^5,$$

for some number ξ between x and x_0. Evaluating f at $x_0 + h$ and $x_0 - h$ gives

$$f(x_0 + h) = f(x_0) + f'(x_0)h + \frac{1}{2}f''(x_0)h^2 + \frac{1}{6}f'''(x_0)h^3$$
$$+ \frac{1}{24}f^{(4)}(x_0)h^4 + \frac{1}{120}f^{(5)}(\xi_1)h^5 \tag{4.18}$$

and

$$f(x_0 - h) = f(x_0) - f'(x_0)h + \frac{1}{2}f''(x_0)h^2 - \frac{1}{6}f'''(x_0)h^3$$
$$+ \frac{1}{24}f^{(4)}(x_0)h^4 - \frac{1}{120}f^{(5)}(\xi_2)h^5, \tag{4.19}$$

where $x_0 - h < \xi_2 < x_0 < \xi_1 < x_0 + h$.

Subtracting Eq. (4.19) from Eq. (4.18) gives a new approximation for $f'(x)$.

$$f(x_0+h) - f(x_0-h) = 2hf'(x_0) + \frac{h^3}{3}f'''(x_0) + \frac{h^5}{120}[f^{(5)}(\xi_1) + f^{(5)}(\xi_2)], \quad (4.20)$$

which implies that

$$f'(x_0) = \frac{1}{2h}[f(x_0+h) - f(x_0-h)] - \frac{h^2}{6}f'''(x_0) - \frac{h^4}{240}[f^{(5)}(\xi_1) + f^{(5)}(\xi_2)].$$

If $f^{(5)}$ is continuous on $[x_0 - h, x_0 + h]$, the Intermediate Value Theorem 1.11 implies that a number $\tilde{\xi}$ in $(x_0 - h, x_0 + h)$ exists with

$$f^{(5)}(\tilde{\xi}) = \frac{1}{2}\left[f^{(5)}(\xi_1) + f^{(5)}(\xi_2)\right].$$

As a consequence,we have the $O(h^2)$ approximation

$$f'(x_0) = \frac{1}{2h}[f(x_0+h) - f(x_0-h)] - \frac{h^2}{6}f'''(x_0) - \frac{h^4}{120}f^{(5)}(\tilde{\xi}). \quad (4.21)$$

Although the approximation in Eq. (4.21) is the same as that given in the three-point formula in Eq. (4.5), the unknown evaluation point occurs now in $f^{(5)}$, rather than in f'''. Extrapolation takes advantage of this by first replacing h in Eq. (4.21) with $2h$ to give the new formula

$$f'(x_0) = \frac{1}{4h}[f(x_0+2h) - f(x_0-2h)] - \frac{4h^2}{6}f'''(x_0) - \frac{16h^4}{120}f^{(5)}(\hat{\xi}), \quad (4.22)$$

where $\hat{\xi}$ is between $x_0 - 2h$ and $x_0 + 2h$.

Multiplying Eq. (4.21) by 4 and subtracting Eq. (4.22) produces

$$3f'(x_0) = \frac{2}{h}[f(x_0+h) - f(x_0-h)] - \frac{1}{4h}[f(x_0+2h) - f(x_0-2h)]$$
$$- \frac{h^4}{30}f^{(5)}(\tilde{\xi}) + \frac{2h^4}{15}f^{(5)}(\hat{\xi}).$$

Even if $f^{(5)}$ is continuous on $[x_0 - 2h, x_0 + 2h]$, the Intermediate Value Theorem 1.11 cannot be applied as we did to derive Eq. (4.21) because here we have the *difference* of terms involving $f^{(5)}$. However, an alternative method can be used to show that $f^{(5)}(\tilde{\xi})$ and $f^{(5)}(\hat{\xi})$ can still be replaced by a common value $f^{(5)}(\xi)$. Assuming this and dividing by 3 produces the five-point midpoint formula Eq. (4.6) that we saw in Section 4.1

$$f'(x_0) = \frac{1}{12h}[f(x_0-2h) - 8f(x_0-h) + 8f(x_0+h) - f(x_0+2h)] + \frac{h^4}{30}f^{(5)}(\xi). \quad \square$$

Other formulas for first and higher derivatives can be derived in a similar manner. See, for example, Exercise 8.

The technique of extrapolation is used throughout the text. The most prominent applications occur in approximating integrals in Section 4.5 and for determining approximate solutions to differential equations in Section 5.8.

EXERCISE SET 4.2

1. Apply the extrapolation process described in Example 1 to determine $N_3(h)$, an approximation to $f'(x_0)$, for the following functions and stepsizes.
   a. $f(x) = \ln x$, $x_0 = 1.0$, $h = 0.4$
   b. $f(x) = x + e^x$, $x_0 = 0.0$, $h = 0.4$
   c. $f(x) = 2^x \sin x$, $x_0 = 1.05$, $h = 0.4$
   d. $f(x) = x^3 \cos x$, $x_0 = 2.3$, $h = 0.4$
2. Add another line to the extrapolation table in Exercise 1 to obtain the approximation $N_4(h)$.
3. Repeat Exercise 1 using four-digit rounding arithmetic.
4. Repeat Exercise 2 using four-digit rounding arithmetic.
5. The following data give approximations to the integral

$$M = \int_0^{\pi} \sin x \, dx.$$

$$N_1(h) = 1.570796, \quad N_1\left(\frac{h}{2}\right) = 1.896119, \quad N_1\left(\frac{h}{4}\right) = 1.974232, \quad N_1\left(\frac{h}{8}\right) = 1.993570.$$

   Assuming $M = N_1(h) + K_1h^2 + K_2h^4 + K_3h^6 + K_4h^8 + O(h^{10})$, construct an extrapolation table to determine $N_4(h)$.
6. The following data can be used to approximate the integral

$$M = \int_0^{3\pi/2} \cos x \, dx.$$

$$N_1(h) = 2.356194, \qquad N_1\left(\frac{h}{2}\right) = -0.4879837,$$

$$N_1\left(\frac{h}{4}\right) = -0.8815732, \quad N_1\left(\frac{h}{8}\right) = -0.9709157.$$

   Assume a formula exists of the type given in Exercise 5 and determine $N_4(h)$.
7. Show that the five-point formula in Eq. (4.6) applied to $f(x) = xe^x$ at $x_0 = 2.0$ gives $N_2(0.2)$ in Table 4.6 when $h = 0.1$ and $N_2(0.1)$ when $h = 0.05$.
8. The forward-difference formula can be expressed as

$$f'(x_0) = \frac{1}{h}[f(x_0 + h) - f(x_0)] - \frac{h}{2}f''(x_0) - \frac{h^2}{6}f'''(x_0) + O(h^3).$$

   Use extrapolation to derive an $O(h^3)$ formula for $f'(x_0)$.
9. Suppose that $N(h)$ is an approximation to M for every $h > 0$ and that

$$M = N(h) + K_1h + K_2h^2 + K_3h^3 + \cdots,$$

   for some constants $K_1, K_2, K_3, \ldots$. Use the values $N(h)$, $N\left(\frac{h}{3}\right)$, and $N\left(\frac{h}{9}\right)$ to produce an $O(h^3)$ approximation to M.
10. Suppose that $N(h)$ is an approximation to M for every $h > 0$ and that

$$M = N(h) + K_1h^2 + K_2h^4 + K_3h^6 + \cdots,$$

   for some constants $K_1, K_2, K_3, \ldots$. Use the values $N(h)$, $N\left(\frac{h}{3}\right)$, and $N\left(\frac{h}{9}\right)$ to produce an $O(h^6)$ approximation to M.
11. In calculus, we learn that $e = \lim_{h\to 0}(1 + h)^{1/h}$.
   a. Determine approximations to e corresponding to $h = 0.04$, 0.02, and 0.01.
   b. Use extrapolation on the approximations, assuming that constants $K_1, K_2, \ldots$ exist with $e = (1 + h)^{1/h} + K_1h + K_2h^2 + K_3h^3 + \cdots$, to produce an $O(h^3)$ approximation to e, where $h = 0.04$.
   c. Do you think that the assumption in part (b) is correct?

12. **a.** Show that

$$\lim_{h \to 0} \left(\frac{2+h}{2-h} \right)^{1/h} = e.$$

b. Compute approximations to e using the formula $N(h) = \left(\frac{2+h}{2-h}\right)^{1/h}$, for $h = 0.04, 0.02$, and 0.01.

c. Assume that $e = N(h) + K_1 h + K_2 h^2 + K_3 h^3 + \cdots$. Use extrapolation, with at least 16 digits of precision, to compute an $O(h^3)$ approximation to e with $h = 0.04$. Do you think the assumption is correct?

d. Show that $N(-h) = N(h)$.

e. Use part (d) to show that $K_1 = K_3 = K_5 = \cdots = 0$ in the formula

$$e = N(h) + K_1 h + K_2 h^2 + K_3 h^3 K_4 h^4 + K_5 h^5 + \cdots,$$

so that the formula reduces to

$$e = N(h) + K_2 h^2 + K_4 h^4 + K_6 h^6 + \cdots.$$

f. Use the results of part (e) and extrapolation to compute an $O(h^6)$ approximation to e with $h = 0.04$.

13. Suppose the following extrapolation table has been constructed to approximate the number M with $M = N_1(h) + K_1 h^2 + K_2 h^4 + K_3 h^6$:

$N_1(h)$		
$N_1\left(\frac{h}{2}\right)$	$N_2(h)$	
$N_1\left(\frac{h}{4}\right)$	$N_2\left(\frac{h}{2}\right)$	$N_3(h)$

a. Show that the linear interpolating polynomial $P_{0,1}(h)$ through $(h^2, N_1(h))$ and $(h^2/4, N_1(h/2))$ satisfies $P_{0,1}(0) = N_2(h)$. Similarly, show that $P_{1,2}(0) = N_2(h/2)$.

b. Show that the linear interpolating polynomial $P_{0,2}(h)$ through $(h^4, N_2(h))$ and $(h^4/16, N_2(h/2))$ satisfies $P_{0,2}(0) = N_3(h)$.

14. Suppose that $N_1(h)$ is a formula that produces $O(h)$ approximations to a number M and that

$$M = N_1(h) + K_1 h + K_2 h^2 + \cdots,$$

for a collection of positive constants $K_1, K_2, \ldots$. Then $N_1(h)$, $N_1(h/2)$, $N_1(h/4)$, $\ldots$ are all lower bounds for M. What can be said about the extrapolated approximations $N_2(h), N_3(h), \ldots$?

15. The semiperimeters of regular polygons with k sides that inscribe and circumscribe the unit circle were used by Archimedes before 200 B.C.E. to approximate π, the circumference of a semicircle. Geometry can be used to show that the sequence of inscribed and circumscribed semiperimeters $\{p_k\}$ and $\{P_k\}$, respectively, satisfy

$$p_k = k \sin\left(\frac{\pi}{k}\right) \quad \text{and} \quad P_k = k \tan\left(\frac{\pi}{k}\right),$$

with $p_k < \pi < P_k$, whenever $k \geq 4$.

a. Show that $p_4 = 2\sqrt{2}$ and $P_4 = 4$.

b. Show that for $k \geq 4$, the sequences satisfy the recurrence relations

$$P_{2k} = \frac{2p_k P_k}{p_k + P_k} \quad \text{and} \quad p_{2k} = \sqrt{p_k P_{2k}}.$$

c. Approximate π to within 10^{-4} by computing p_k and P_k until $P_k - p_k < 10^{-4}$.

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

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

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

$$\int_a^b f(x)\,dx = \int_{x_0}^{x_1} \left[\frac{(x - x_1)}{(x_0 - x_1)} f(x_0) + \frac{(x - x_0)}{(x_1 - x_0)} f(x_1) \right] dx + \frac{1}{2} \int_{x_0}^{x_1} f''(\xi(x))(x - x_0)(x - x_1)\,dx. \tag{4.23}$$

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),

$$\begin{aligned}\int_{x_0}^{x_1} f''(\xi(x))(x - x_0)(x - x_1)\,dx &= f''(\xi) \int_{x_0}^{x_1} (x - x_0)(x - x_1)\,dx \\ &= f''(\xi) \left[\frac{x^3}{3} - \frac{(x_1 + x_0)}{2} x^2 + x_0 x_1 x \right]_{x_0}^{x_1} \\ &= -\frac{h^3}{6} f''(\xi).\end{aligned}$$

When we use the term *trapezoid* we mean a four-sided figure that has at least two of its sides parallel. The European term for this figure is *trapezium*. To further confuse the issue, the European word trapezoidal refers to a four-sided figure with no sides equal, and the American word for this type of figure is trapezium.

Consequently, Eq. (4.23) implies that

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

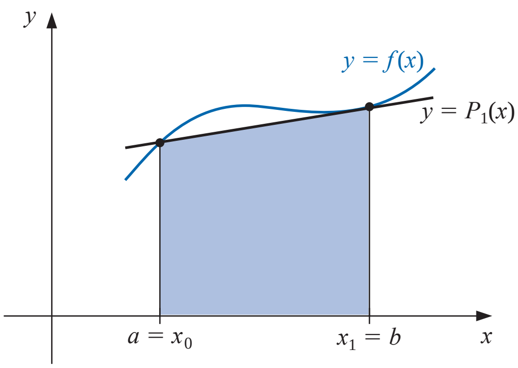
Using the notation $h = x_1 - x_0$ gives the following rule:

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

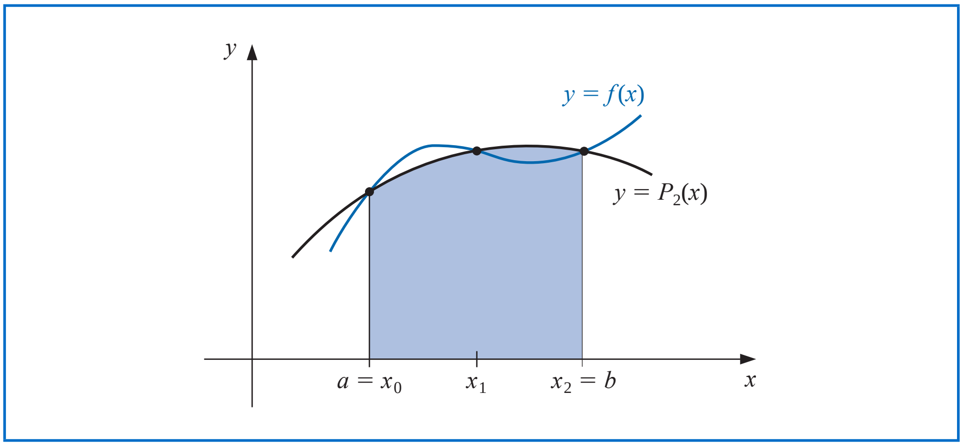


The error term for the Trapezoidal rule involves f'', so the rule gives the exact result when applied to any function whose second derivative is identically zero, that is, any polynomial of degree one or less.

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

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

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

$$\int_{x_0}^{x_2} f(x)\,dx = \left[f(x_1)(x-x_1) + \frac{f'(x_1)}{2}(x-x_1)^2 + \frac{f''(x_1)}{6}(x-x_1)^3 + \frac{f'''(x_1)}{24}(x-x_1)^4 \right]_{x_0}^{x_2} + \frac{1}{24}\int_{x_0}^{x_2} f^{(4)}(\xi(x))(x-x_1)^4\,dx. \quad (4.24)$$

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

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

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

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

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

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

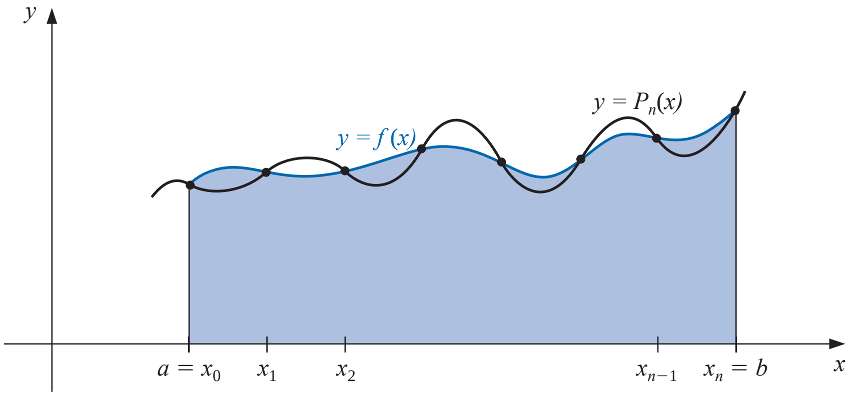
- The degree of precision of a quadrature formula is n if and only if the error is zero for all polynomials of degree $k = 0, 1, \ldots, n$, but is not zero for some polynomial of degree $n + 1$.

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 $f \in C^{n+1}[a, b]$. ■

Roger Cotes (1682–1716) rose from a modest background to become, in 1704, the first Plumian Professor at Cambridge University. He made advances in numerous mathematical areas including numerical methods for interpolation and integration. Newton is reputed to have said of Cotes ...*if he had lived we might have known something.*

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

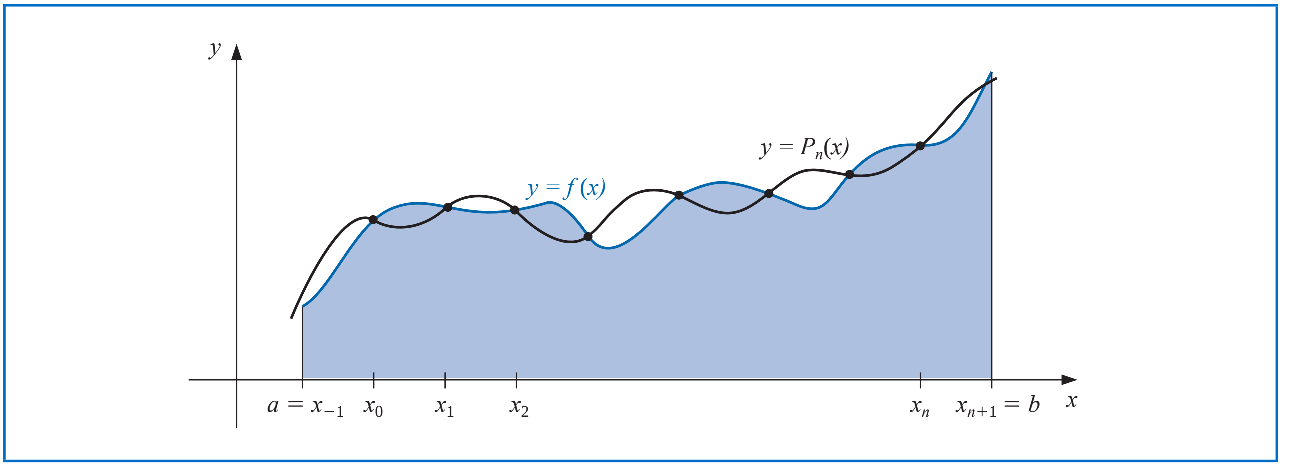
The *open Newton-Cotes formulas* do not include the endpoints of $[a, b]$ as nodes. They use the nodes $x_i = x_0 + ih$, for each $i = 0, 1, \ldots, n$, where $h = (b-a)/(n+2)$ and $x_0 = a + h$. This implies that $x_n = b - h$, so we label the endpoints by setting $x_{-1} = a$ and $x_{n+1} = b$, as 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

$$\int_{a}^{b} f(x)\,dx = \frac{9}{4}hf(x_1) + \frac{3}{4}hf(x_2).$$

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 $\int_3^4 e^x\, dx$.