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:

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

= $\frac{f(x_0)(x - x_0 - h)}{-h} + \frac{f(x_0 + h)(x - x_0)}{h} + \frac{(x - x_0)(x - x_0 - h)}{2} f''(\xi(x)),$

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

$$
f'(x) = \frac{f(x_0 + h) - f(x_0)}{h} + D_x \left[\frac{(x - x_0)(x - x_0 - h)}{2} f''(\xi(x)) \right]
$$

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

+
$$
\frac{(x - x_0)(x - x_0 - h)}{2} D_x(f''(\xi(x))).
$$

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

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

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

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

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.

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with $h = 0.1$ gives

Table 4.1

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

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.

Since $f'(x) = 1/x$, the exact value of $f'(1.8)$ is 0.555, and in this case the error bounds are quite close to the true approximation error. Ē.

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 *k*th 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

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

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

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

 $x_1 = x_0 + h$ and $x_2 = x_0 + 2h$, 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

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

Doing the same for $x_i = x_1$ gives

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

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

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

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

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

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

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

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

Three-Point Midpoint Formula

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

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

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

•
$$
f'(x_0) = \frac{1}{12h}[-25f(x_0) + 48f(x_0 + h) - 36f(x_0 + 2h) + 16f(x_0 + 3h) - 3f(x_0 + 4h)] + \frac{h^4}{5}f^{(5)}(\xi),
$$
 (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 $f'(2.0)$.

п

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

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

$$
= 22.166999
$$

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

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

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

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 $f''(2.0)$.

> **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 $f(x_0 + h)$ and $\hat{f}(x_0 - h)$, which are related to the true values $f(x_0 + h)$ and $f(x_0 - h)$ by

Table 4.3 $x \qquad f(x)$ 1.8 10.889365 1.9 12.703199 2.0 14.778112 2.1 17.148957 2.2 19.855030

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

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

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

To reduce the truncation error, $h^2M/6$, we need to reduce h. But as h is reduced, the roundoff 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.

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.

 \Box

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. \Box

We have considered only the round-off error problems that are presented by the threepoint 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.

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.

Keep in mind that difference method approximations might be unstable.

EXERCISE SET 4.1

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

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

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.

$$
f(x) = \sin x
$$

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. $f(x) = x^2 \ln x + 1$

b.
$$
f(x) = x^2 \ln x +
$$

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

a.	\boldsymbol{x}	f(x)	f'(x)	b.	\boldsymbol{x}	f(x)	f'(x)
	1.1	9.025013			8.1	16.94410	
	1.2	11.02318			8.3	17.56492	
	1.3	13.46374			8.5	18.19056	
	1.4	16.44465			8.7	18.82091	
c.	\boldsymbol{x}	f(x)	f'(x)	d.	\boldsymbol{x}	f(x)	f'(x)
	2.9	-4.827866			2.0	3.6887983	
	3.0	-4.240058			2.1	3.6905701	
	3.1	-3.496909			2.2	3.6688192	
	3.2	-2.596792			2.3	3.6245909	

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