Numerical Differentiation

4.1.3 Numerical Differentiation

Equation (4.14) is given a formal label in numerical methods—it is called a *finite divided difference.* It can be represented generally as

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i} + O(x_{i+1} - x_i) \tag{4.17}$$

or

$$f'(x_i) = \frac{\Delta f_i}{h} + O(h) \tag{4.18}$$

where Δf_i is referred to as the *first forward difference* and h is called the step size, that is, the length of the interval over which the approximation is made. It is termed a "forward" difference because it utilizes data at i and $i + 1$ to estimate the derivative (Fig. 4.6*a*). The entire term $\Delta f/h$ is referred to as a *first finite divided difference.*

This forward divided difference is but one of many that can be developed from the Taylor series to approximate derivatives numerically. For example, backward and centered difference approximations of the first derivative can be developed in a fashion similar to the derivation of Eq. (4.14). The former utilizes values at x_{i-1} and x_i (Fig. 4.6*b*), whereas the latter uses values that are equally spaced around the point at which the derivative is estimated (Fig. 4.6*c*). More accurate approximations of the first derivative can be developed by including higher-order terms of the Taylor series. Finally, all the above versions can also be developed for second, third, and higher derivatives. The following sections provide brief summaries illustrating how some of these cases are derived.

Backward Difference Approximation of the First Derivative. The Taylor series can be expanded backward to calculate a previous value on the basis of a present value, as in

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \cdots \tag{4.19}$$

Truncating this equation after the first derivative and rearranging yields

$$f'(x_i) \cong \frac{f(x_i) - f(x_{i-1})}{h} = \frac{\nabla f_i}{h} \tag{4.20}$$

where the error is $O(h)$, and ∇f_i is referred to as the *first backward difference.* See Fig. 4.6*b* for a graphical representation.

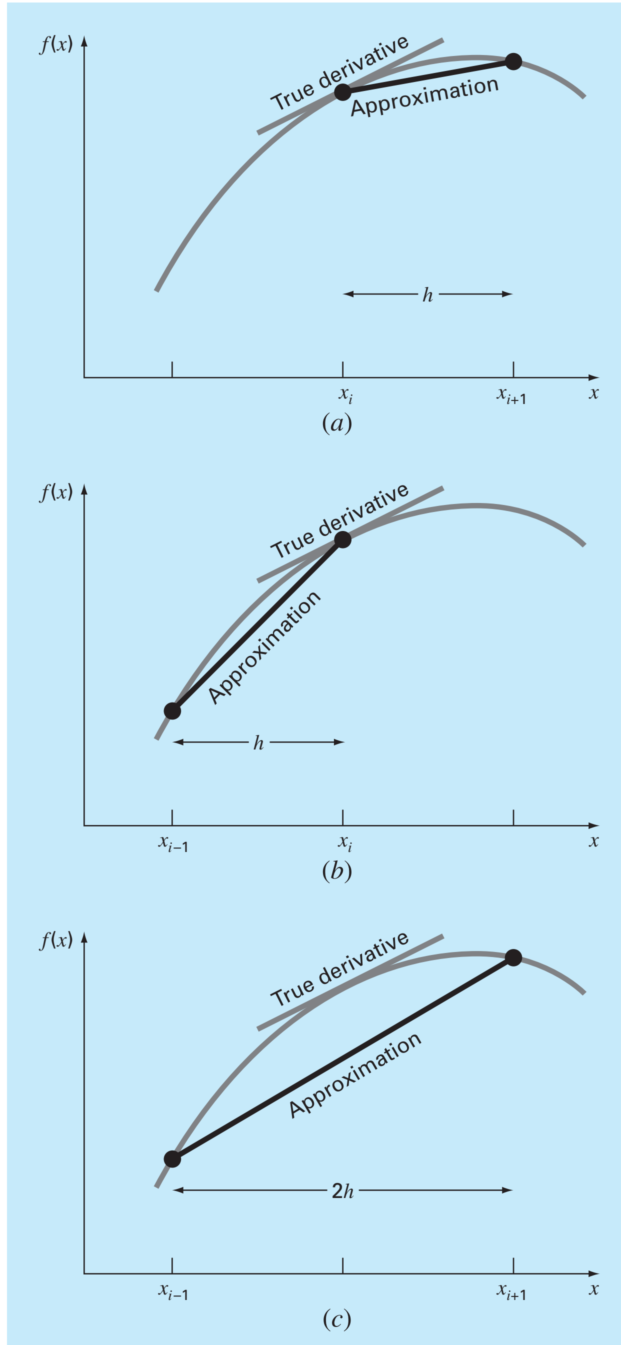

FIGURE 4.6
Graphical depiction of (*a*) forward, (*b*) backward, and (*c*) centered finite-divided-difference approximations of the first derivative.

Centered Difference Approximation of the First Derivative. A third way to approximate the first derivative is to subtract Eq. (4.19) from the forward Taylor series expansion:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \cdots \tag{4.21}$$

to yield

$$f(x_{i+1}) = f(x_{i-1}) + 2f'(x_i)h + \frac{2f^{(3)}(x_i)}{3!}h^3 + \cdots$$

which can be solved for

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} - \frac{f^{(3)}(x_i)}{6}h^2 - \cdots$$

or

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} - O(h^2) \tag{4.22}$$

Equation (4.22) is a *centered difference* representation of the first derivative. Notice that the truncation error is of the order of h^2 in contrast to the forward and backward approximations that were of the order of h. Consequently, the Taylor series analysis yields the practical information that the centered difference is a more accurate representation of the derivative (Fig. 4.6*c*). For example, if we halve the step size using a forward or backward difference, we would approximately halve the truncation error, whereas for the central difference, the error would be quartered.

EXAMPLE 4.4 Finite-Divided-Difference Approximations of Derivatives

Problem Statement. Use forward and backward difference approximations of $O(h)$ and a centered difference approximation of $O(h^2)$ to estimate the first derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.25$$

at $x = 0.5$ using a step size $h = 0.5$. Repeat the computation using $h = 0.25$. Note that the derivative can be calculated directly as

$$f'(x) = -0.4x^3 - 0.45x^2 - 1.0x - 0.25$$

and can be used to compute the true value as $f'(0.5) = -0.9125$.

Solution. For $h = 0.5$, the function can be employed to determine

$$\begin{aligned} x_{i-1} &= 0 & f(x_{i-1}) &= 1.2 \\ x_i &= 0.5 & f(x_i) &= 0.925 \\ x_{i+1} &= 1.0 & f(x_{i+1}) &= 0.2 \end{aligned}$$

These values can be used to compute the forward divided difference [Eq. (4.17)],

$$f'(0.5) \cong \frac{0.2 - 0.925}{0.5} = -1.45 \qquad |\varepsilon_t| = 58.9\%$$

the backward divided difference [Eq. (4.20)],

$$f'(0.5) \cong \frac{0.925 - 1.2}{0.5} = -0.55 \qquad |\varepsilon_t| = 39.7\%$$

and the centered divided difference [Eq. (4.22)],

$$f'(0.5) \cong \frac{0.2 - 1.2}{1.0} = -1.0 \qquad |\varepsilon_t| = 9.6\%$$

For $h = 0.25$,

$$\begin{array}{llll} x_{i-1} & = 0.25 & f(x_{i-1}) & = 1.10351563 \\ x_i & = 0.5 & f(x_i) & = 0.925 \\ x_{i+1} & = 0.75 & f(x_{i+1}) & = 0.63632813 \end{array}$$

which can be used to compute the forward divided difference,

$$f'(0.5) \cong \frac{0.63632813 - 0.925}{0.25} = -1.155 \qquad |\varepsilon_t| = 26.5\%$$

the backward divided difference,

$$f'(0.5) \cong \frac{0.925 - 1.10351563}{0.25} = -0.714 \qquad |\varepsilon_t| = 21.7\%$$

and the centered divided difference,

$$f'(0.5) \cong \frac{0.63632813 - 1.10351563}{0.5} = -0.934 \qquad |\varepsilon_t| = 2.4\%$$

For both step sizes, the centered difference approximation is more accurate than forward or backward differences. Also, as predicted by the Taylor series analysis, halving the step size approximately halves the error of the backward and forward differences and quarters the error of the centered difference.

CHAPTER 23

Numerical Differentiation

We have already introduced the notion of numerical differentiation in Chap. 4. Recall that we employed Taylor series expansions to derive finite-divided-difference approximations of derivatives. In Chap. 4, we developed forward, backward, and centered difference approximations of first and higher derivatives. Recall that, at best, these estimates had errors that were $O(h^2)$—that is, their errors were proportional to the square of the step size. This level of accuracy is due to the number of terms of the Taylor series that were retained during the derivation of these formulas. We will now illustrate how to develop more accurate formulas by retaining more terms.

23.1 HIGH-ACCURACY DIFFERENTIATION FORMULAS

As noted above, high-accuracy divided-difference formulas can be generated by including additional terms from the Taylor series expansion. For example, the forward Taylor series expansion can be written as [Eq. (4.21)]

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2}h^2 + \cdots \tag{23.1}$$

which can be solved for

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f''(x_i)}{2}h + O(h^2) \tag{23.2}$$

In Chap. 4, we truncated this result by excluding the second- and higher-derivative terms and were thus left with a final result of

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h) \tag{23.3}$$

In contrast to this approach, we now retain the second-derivative term by substituting the following approximation of the second derivative [recall Eq. (4.24)]

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} + O(h) \tag{23.4}$$

into Eq. (23.2) to yield

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{2h^2}h + O(h^2)$$

or, by collecting terms,

$$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O(h^2) \tag{23.5}$$

Notice that inclusion of the second-derivative term has improved the accuracy to $O(h^2)$. Similar improved versions can be developed for the backward and centered formulas as well as for the approximations of the higher derivatives. The formulas are summarized in Figs. 23.1 through 23.3 along with all the results from Chap. 4. The following example illustrates the utility of these formulas for estimating derivatives.

FIGURE 23.1
Forward finite-divided-difference formulas: two versions are presented for each derivative. The latter version incorporates more terms of the Taylor series expansion and is, consequently, more accurate.

First Derivative — Error

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} \qquad O(h)$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} \qquad O(h^2)$$

Second Derivative

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2} \qquad O(h)$$

$$f''(x_i) = \frac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2} \qquad O(h^2)$$

Third Derivative

$$f'''(x_i) = \frac{f(x_{i+3}) - 3f(x_{i+2}) + 3f(x_{i+1}) - f(x_i)}{h^3} \qquad O(h)$$

$$f'''(x_i) = \frac{-3f(x_{i+4}) + 14f(x_{i+3}) - 24f(x_{i+2}) + 18f(x_{i+1}) - 5f(x_i)}{2h^3} \qquad O(h^2)$$

Fourth Derivative

$$f''''(x_i) = \frac{f(x_{i+4}) - 4f(x_{i+3}) + 6f(x_{i+2}) - 4f(x_{i+1}) + f(x_i)}{h^4} \qquad O(h)$$

$$f''''(x_i) = \frac{-2f(x_{i+5}) + 11f(x_{i+4}) - 24f(x_{i+3}) + 26f(x_{i+2}) - 14f(x_{i+1}) + 3f(x_i)}{h^4} \qquad O(h^2)$$

First Derivative	Error
$f'(x_i) = \dfrac{f(x_i) - f(x_{i-1})}{h}$	$O(h)$
$f'(x_i) = \dfrac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h}$	$O(h^2)$
Second Derivative	
$f''(x_i) = \dfrac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2}$	$O(h)$
$f''(x_i) = \dfrac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3})}{h^2}$	$O(h^2)$
Third Derivative	
$f'''(x_i) = \dfrac{f(x_i) - 3f(x_{i-1}) + 3f(x_{i-2}) - f(x_{i-3})}{h^3}$	$O(h)$
$f'''(x_i) = \dfrac{5f(x_i) - 18f(x_{i-1}) + 24f(x_{i-2}) - 14f(x_{i-3}) + 3f(x_{i-4})}{2h^3}$	$O(h^2)$
Fourth Derivative	
$f''''(x_i) = \dfrac{f(x_i) - 4f(x_{i-1}) + 6f(x_{i-2}) - 4f(x_{i-3}) + f(x_{i-4})}{h^4}$	$O(h)$
$f''''(x_i) = \dfrac{3f(x_i) - 14f(x_{i-1}) + 26f(x_{i-2}) - 24f(x_{i-3}) + 11f(x_{i-4}) - 2f(x_{i-5})}{h^4}$	$O(h^2)$

FIGURE 23.2
Backward finite-divided-difference formulas: two versions are presented for each derivative. The latter version incorporates more terms of the Taylor series expansion and is, consequently, more accurate.

FIGURE 23.3
Centered finite-divided-difference formulas: two versions are presented for each derivative. The latter version incorporates more terms of the Taylor series expansion and is, consequently, more accurate.

First Derivative	Error
$f'(x_i) = \dfrac{f(x_{i+1}) - f(x_{i-1})}{2h}$	$O(h^2)$
$f'(x_i) = \dfrac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h}$	$O(h^4)$
Second Derivative	
$f''(x_i) = \dfrac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2}$	$O(h^2)$
$f''(x_i) = \dfrac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2}$	$O(h^4)$
Third Derivative	
$f'''(x_i) = \dfrac{f(x_{i+2}) - 2f(x_{i+1}) + 2f(x_{i-1}) - f(x_{i-2})}{2h^3}$	$O(h^2)$
$f'''(x_i) = \dfrac{-f(x_{i+3}) + 8f(x_{i+2}) - 13f(x_{i+1}) + 13f(x_{i-1}) - 8f(x_{i-2}) + f(x_{i-3})}{8h^3}$	$O(h^4)$
Fourth Derivative	
$f''''(x_i) = \dfrac{f(x_{i+2}) - 4f(x_{i+1}) + 6f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{h^4}$	$O(h^2)$
$f''''(x_i) = \dfrac{-f(x_{i+3}) + 12f(x_{i+2}) - 39f(x_{i+1}) + 56f(x_i) - 39f(x_{i-1}) + 12f(x_{i-2}) - f(x_{i-3})}{6h^4}$	$O(h^4)$

23.3 DERIVATIVES OF UNEQUALLY SPACED DATA

The approaches discussed to this point are primarily designed to determine the derivative of a given function. For the finite-divided-difference approximations of Sec. 23.1, these data had to be evenly spaced. For the Richardson extrapolation technique of Sec. 23.2, these data had to be evenly spaced and generated for successively halved intervals. Such control of data spacing is usually available only in cases where we can use a function to generate a table of values.

In contrast, empirically derived information—that is, data from experiments or field studies—is often collected at unequal intervals. Such information cannot be analyzed with the techniques discussed to this point.

One way to handle nonequispaced data is to fit a second-order Lagrange interpolating polynomial [recall Eq. (18.23)] to each set of three adjacent points. Remember that this polynomial does not require that the points be equispaced. The second-order polynomial can be differentiated analytically to give

$$f'(x) = f(x_{i-1})\frac{2x - x_i - x_{i+1}}{(x_{i-1} - x_i)(x_{i-1} - x_{i+1})} + f(x_i)\frac{2x - x_{i-1} - x_{i+1}}{(x_i - x_{i-1})(x_i - x_{i+1})} + f(x_{i+1})\frac{2x - x_{i-1} - x_i}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} \quad (23.9)$$

where x is the value at which you want to estimate the derivative. Although this equation is certainly more complicated than the first-derivative approximations from Figs. 23.1 through 23.3, it has some important advantages. First, it can be used to estimate the derivative anywhere within the range prescribed by the three points. Second, the points themselves do not have to be equally spaced. Third, the derivative estimate is of the same accuracy as the centered difference [Eq. (4.22)]. In fact, for equispaced points, Eq. (23.9) evaluated at $x = x_i$ reduces to Eq. (4.22).

EXAMPLE 23.3 Differentiating Unequally Spaced Data

Problem Statement. As in Fig. 23.4, a temperature gradient can be measured down into the soil. The heat flux at the soil-air interface can be computed with Fourier's law,

$$q(z = 0) = -k\rho C \left.\frac{dT}{dz}\right|_{z=0}$$

where q = heat flux (W/m^2), k = coefficient of thermal diffusivity in soil ($\cong 3.5 \times 10^{-7}$ m^2/s), ρ = soil density ($\cong$ 1800 kg/m^3), and C = soil specific heat ($\cong$ 840 J/(kg · °C)). Note that a positive value for flux means that heat is transferred from the air to the soil. Use numerical differentiation to evaluate the gradient at the soil-air interface and employ this estimate to determine the heat flux into the ground.

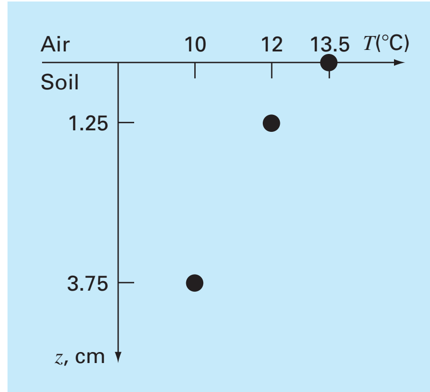

FIGURE 23.4
Temperature versus depth into the soil.

Solution. Equation (23.9) can be used to calculate the derivative as

$$f'(x) = 13.5\frac{2(0) - 1.25 - 3.75}{(0 - 1.25)(0 - 3.75)} + 12\frac{2(0) - 0 - 3.75}{(1.25 - 0)(1.25 - 3.75)} + 10\frac{2(0) - 0 - 1.25}{(3.75 - 0)(3.75 - 1.25)}$$

$$= -14.4 + 14.4 - 1.333333 = -1.333333°\text{C/cm}$$

which can be used to compute (note that 1 W = 1 J/s),

$$q(z = 0) = -3.5 \times 10^{-7}\frac{\text{m}^2}{\text{s}}\left(1800\frac{\text{kg}}{\text{m}^3}\right)\left(840\frac{\text{J}}{\text{kg} \cdot °\text{C}}\right)\left(-133.3333\frac{°\text{C}}{\text{m}}\right)$$

$$= 70.56 \text{ W/m}^2$$

PROBLEMS

23.1 Compute forward and backward difference approximations of $O(h)$ and $O(h^2)$, and central difference approximations of $O(h^2)$ and $O(h^4)$ for the first derivative of $y = \cos x$ at $x = \pi/4$ using a value of $h = \pi/12$. Estimate the true percent relative error ε_t for each approximation.

23.2 Repeat Prob. 23.1, but for $y = \log x$ evaluated at $x = 25$ with $h = 2$.

23.3 Use centered difference approximations to estimate the first and second derivatives of $y = e^x$ at $x = 2$ for $h = 0.1$. Employ both $O(h^2)$ and $O(h^4)$ formulas for your estimates.

23.4 Use Richardson extrapolation to estimate the first derivative of $y = \cos x$ at $x = \pi/4$ using step sizes of $h_1 = \pi/3$ and $h_2 = \pi/6$. Employ centered differences of $O(h^2)$ for the initial estimates.

23.5 Repeat Prob. 23.4, but for the first derivative of $\ln x$ at $x = 5$ using $h_1 = 2$ and $h_2 = 1$.

23.6 Employ Eq. (23.9) to determine the first derivative of $y = 2x^4 - 6x^3 - 12x - 8$ at $x = 0$ based on values at $x_0 = -0.5$, $x_1 = 1$, and $x_2 = 2$. Compare this result with the true value and with an estimate obtained using a centered difference approximation based on $h = 1$.

23.7 Prove that for equispaced data points, Eq. (23.9) reduces to Eq. (4.22) at $x = x_i$.

23.8 Compute the first-order central difference approximations of $O(h^4)$ for each of the following functions at the specified location and for the specified step size:

(a) $y = x^3 + 4x - 15$ at $x = 0$, $h = 0.25$
(b) $y = x^2 \cos x$ at $x = 0.4$, $h = 0.1$
(c) $y = \tan(x/3)$ at $x = 3$, $h = 0.5$
(d) $y = \sin(0.5\sqrt{x})/x$ at $x = 1$, $h = 0.2$
(e) $y = e^x + x$ at $x = 2$, $h = 0.2$

Compare your results with the analytical solutions.

23.9 The following data were collected for the distance traveled versus time for a rocket:

t, s	0	25	50	75	100	125
y, km	0	32	58	78	92	100

Use numerical differentiation to estimate the rocket's velocity and acceleration at each time.

in other words, find dy/dt , d^2y/dt^2 at each time.

23.11 Find the 1st derivative estimates for the following data at x=2

x	1	1.5	1.6	2.5	3.5
$f(x)$	0.6767	0.3734	0.3261	0.08422	0.01596

where $f(x) = 5e^{-2x}x$. Compare your results with the true derivatives.

23.12 The following data are provided for the velocity of an object as a function of time,

t, s	0	4	8	12	16	20	24	28	32	36
v, m/s	0	34.7	61.8	82.8	99.2	112.0	121.9	129.7	135.7	140.4

find dv/dt at x=1, 14, and 35

23.19 The objective of this problem is to compare second-order accurate forward, backward, and centered finite-difference approximations of the first derivative of a function to the actual value of the derivative. This will be done for

$$f(x) = e^{-2x} - x$$

(a) Use calculus to determine the correct value of the derivative at $x = 2$.

(b) To evaluate the centered finite-difference approximations, start with $x = 0.5$. Thus, for the first evaluation, the x values for the centered difference approximation will be $x = 2 \pm 0.5$ or $x = 1.5$ and 2.5. Then, x = 1.8 and 2.2 . Compare

(c) Repeat part **(b)** for the second-order forward and backward differences.

(d) Plot the results of **(b)** and **(c)** versus x. Include the exact result on the plot for comparison.