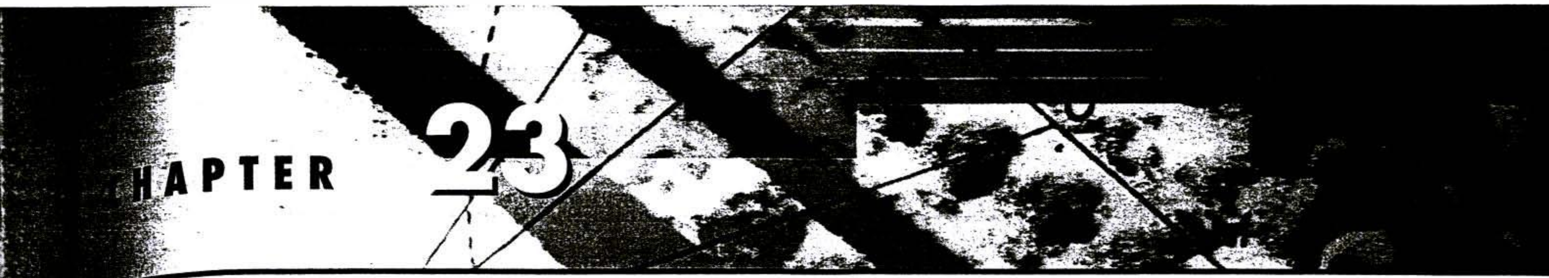

Numerical Differentiation

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,

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

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.

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

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.

First Derivative — Error

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

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

Second Derivative

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

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

Third Derivative

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

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

Fourth Derivative

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

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

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

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

$$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h} \qquad O(h^4)$$

Second Derivative

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

$$f''(x_i) = \frac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2} \qquad O(h^4)$$

Third Derivative

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

$$f'''(x_i) = \frac{-f(x_{i+3}) + 8f(x_{i+2}) - 13f(x_{i+1}) + 13f(x_{i-1}) - 8f(x_{i-2}) + f(x_{i-3})}{8h^3} \qquad O(h^4)$$

Fourth Derivative

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

$$f''''(x_i) = \frac{-f(x_{i+3}) + 12f(x_{i+2}) + 39f(x_{i+1}) + 56f(x_i) - 39f(x_{i-1}) + 12f(x_{i-2}) + f(x_{i-3})}{6h^4} \qquad O(h^4)$$

EXAMPLE 23.1 High-Accuracy Differentiation Formulas

Problem Statement. Recall that in Example 4.4 we estimated the derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at $x = 0.5$ using finite divided differences and a step size of $h = 0.25$,

	Forward $O(h)$	Backward $O(h)$	Centered $O(h^2)$
Estimate	−1.155	−0.714	−0.934
ε_t (%)	−26.5	21.7	−2.4

where the errors were computed on the basis of the true value of −0.9125. Repeat this computation, but employ the high-accuracy formulas from Figs. 23.1 through 23.3.

Solution. The data needed for this example is

$$\begin{aligned} x_{i-2} &= 0 & f(x_{i-2}) &= 1.2 \\ x_{i-1} &= 0.25 & f(x_{i-1}) &= 1.1035156 \\ x_i &= 0.5 & f(x_i) &= 0.925 \\ x_{i+1} &= 0.75 & f(x_{i+1}) &= 0.6363281 \\ x_{i+2} &= 1 & f(x_{i+2}) &= 0.2 \end{aligned}$$

The forward difference of accuracy $O(h^2)$ is computed as (Fig. 23.1)

$$f'(0.5) = \frac{-0.2 + 4(0.6363281) - 3(0.925)}{2(0.25)} = -0.859375 \qquad \varepsilon_t = 5.82\%$$

The backward difference of accuracy $O(h^2)$ is computed as (Fig. 23.2)

$$f'(0.5) = \frac{3(0.925) - 4(1.1035156) + 1.2}{2(0.25)} = -0.878125 \qquad \varepsilon_t = 3.77\%$$

The centered difference of accuracy $O(h^4)$ is computed as (Fig. 23.3)

$$f'(0.5) = \frac{-0.2 + 8(0.6363281) - 8(1.1035156) + 1.2}{12(0.25)} = -0.9125 \qquad \varepsilon_t = 0\%$$

As expected, the errors for the forward and backward differences are considerably more accurate than the results from Example 4.4. However, surprisingly, the centered difference yields a perfect result. This is because the formulas based on the Taylor series are equivalent to passing polynomials through the data points.

23.2 RICHARDSON EXTRAPOLATION

To this point, we have seen that there are two ways to improve derivative estimates when employing finite divided differences: (1) decrease the step size or (2) use a higher-order formula that employs more points. A third approach, based on Richardson extrapolation, uses two derivative estimates to compute a third, more accurate approximation.

SOFTWARE

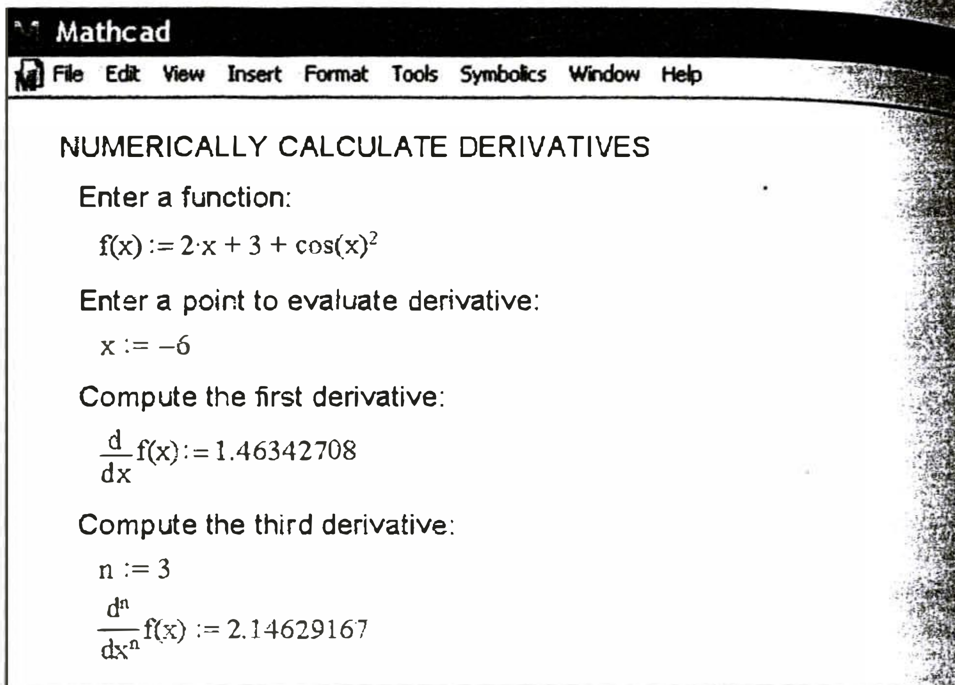

FIGURE 23.9
Mathcad screen to implement numerical differentiation.

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 $y = \sin x$ 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. reduces to Eq. (4. 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 $x = 0$,	$h = 0.$
(b) $y = x^2 \cos x$	at $x = 0.$	$h = 0.1$
(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 was 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.

23.10 Develop a user-friendly program to apply a Romberg algorithm to estimate the derivative of a given function.

a user-friendly program to obtain first-derivative
ɜqually spaced data. Test it with the following data:

1.5	1.6	2.5	3.5
0.3734	0.3261	0.08422	0.01596

^{-2x}x. Compare your results with the true derivatives.
wing data is provided for the velocity of an object as
ɿe,

8	12	16	20	24	28	32	36
51.8	82.8	99.2	112.0	121.9	129.7	135.7	140.4

ɔest numerical method available, how far does the
:l from $t = 0$ to 28 s?
est numerical method available, what is the object's
ɿ at $t = 28$ s.
ɩest numerical method available, what is the object's
ɿ at $t = 0$ s.
ɿat for the falling parachutist problem, the velocity

$$(1 - e^{-(c/m)t}) \qquad \text{(P23.13}a\text{)}$$

e traveled can be obtained by

$$\int_0^t \left(1 - e^{-(c/m)t}\right) dt \qquad \text{(P23.13}b\text{)}$$

, $m = 70$, and $c = 12$,
ĹAB or Mathcad to integrate Eq. (P23.13a) from

ly integrate Eq. (P23.13b) with the initial condition
at $t = 0$. Evaluate the result at $t = 10$ to confirm **(a)**.
ĹAB or Mathcad to differentiate Eq. (P23.13a) at

y differentiate Eq. (P23.13a) at $t = 10$ to confirm **(c)**.
mal distribution is defined as

$$= e^{-x^2/2}$$
$$\pi$$

ĹAB or Mathcad to integrate this function from
1 and from −2 to 2.
ĹAB or Mathcad to determine the inflection points of
ɔn.
llowing data was generated from the normal

	−1.5	−1	−0.5	0	0.5	1	1.5	2
9	0.12952	0.24197	0.35207	0.39894	0.35207	0.24197	0.12952	0.05399

(a) Use MATLAB to integrate this data from $x = -1$ to 1 and −2 to 2 with the `trap` function.

(b) Use MATLAB to estimate the inflection points of this data.

23.16 Evaluate $\partial f/\partial x$, $\partial f/\partial y$, and $\partial f/(\partial x \partial y)$ for the following function at $x = y = 1$ **(a)** analytically and **(b)** numerically $\Delta x = \Delta y = 0.0001$,

$$f(x, y) = 3xy + 3x - x^3 - 3y^3$$

23.17 Evaluate the following integral with MATLAB,

$$\int_0^{2\pi} \frac{\sin t}{t}\, dt$$

using both the `quad` and `quadl` functions. To learn more about `quadl`, type `help quadl` at the MATLAB prompt.

23.18 Use the `diff` command in MATLAB and compute the finite-difference approximation to the first and second derivative at each x-value in the table below, excluding the two end points. Use finite-difference approximations that are second-order correct, $O(\Delta x^2)$.

x	0	1	2	3	4	5	6	7	8	9	10
y	1.4	2.1	3.3	4.8	6.8	6.6	8.6	7.5	8.9	10.9	10

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, decrease in increments of 0.01 down to a minimum value of $\Delta x = 0.01$.

(c) Repeat part **(b)** for the second-order forward and backward differences. (Note that these can be done at the same time that the centered difference is computed in the loop.)

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

23.20 Use a Taylor series expansion to derive a centered finite-difference approximation to the third derivative that is second-order accurate. To do this, you will have to use four different expansions for the points x_{i-2}, x_{i-1}, x_{i+1}, and x_{i+2}. In each case, the expansion will be around the point x_i. The interval Δx will be used in each case of $i-1$ and $i+1$, and $2\Delta x$ will be used in each case of $i-2$ and $i+2$. The four equations must then be combined in a way to eliminate the first and second derivatives. Carry enough terms along in each expansion to evaluate the first term that will be truncated to determine the order of the approximation.

23.21 Use the following data to find the velocity and acceleration at $t = 10$ seconds:

Time, t, s	0	2	4	6	8	10	12	14	16
Position, x, m	0	0.7	1.8	3.4	5.1	6.3	7.3	8.0	8.4

Use second-order correct (**a**) centered finite-difference, (**b**) forward finite-difference, and (**c**) backward finite-difference methods.

23.22 A plane is being tracked by radar, and data is taken every second in polar coordinates θ and r.

t, s	200	202	204	206	208	210
θ, rad	0.75	0.72	0.70	0.68	0.67	0.66
r, m	5120	5370	5560	5800	6030	6240

At 206 seconds, use the centered finite difference (second-order correct) to find the vector expressions for velocity $\vec{v}$, and acceleration $\vec{a}$. The velocity and acceleration given in polar coordinates are:

$$\vec{v} = \dot{r}\vec{e}_r + r\dot{\theta}\vec{e}_\theta \qquad \text{and} \qquad \vec{a} = (\ddot{r} - r\dot{\theta}^2)\vec{e}_r + (r\ddot{\theta} + 2\dot{r}\dot{\theta})\vec{e}_\theta$$

23.23 Develop an Excel VBA macro program to read in adjacent columns of x and y values from a worksheet. Evaluate the derivatives at each point using Eq. 23.9, and display the results in a third column adjacent to the x and y values back on the spreadsheet. Test your program by applying it to evaluate the velocities for the time–position values from Prob. 23.21.

23.24 Use regression to estimate the acceleration at each time for the following data with second-, third-, and fourth-order polynomials. Plot the results.

t	1	2	3.25	4.5	6	7	8	8.5	9.3	10
v	10	12	11	14	17	16	12	14	14	10

23.25 You have to measure the flow rate of water through a small pipe. In order to do it, you place a bucket at the pipe's outlet and measure the volume in the bucket as a function of time as tabulated below. Estimate the flow rate at $t = 7$ s.

Time, s	0	1	5	8
Volume, cm^3	0	1	8	16.4

23.26 The velocity v (m/s) of air flowing past a flat surface is measured at several distances y (m) away from the surface. Determine the shear stress τ (N/m^2) at the surface ($y = 0$), using Newton's viscosity law

$$\tau = \mu \frac{dv}{dy}$$

Assume a value of dynamic viscosity $\mu = 1.8 \times 10^{-5}$ N · s/m^2.

y, m	0	0.002	0.006	0.012	0.018	0.024
v, m/s	0	0.287	0.899	1.915	3.048	4.299

23.27 Chemical reactions often follow the model:

$$\frac{dc}{dt} = -kc^n$$

where c = concentration, t = time, k = reaction rate, and n = reaction order. Given values of c and dc/dt, k and n can be evaluated by a linear regression of the logarithm of this equation:

$$\log\left(-\frac{dc}{dt}\right) = \log k + n \log c$$

Use this approach along with the following data to estimate k and n.

t	10	20	30	40	50	60
c	3.52	2.48	1.75	1.23	0.87	0.61

23.28 The velocity profile of a fluid in a circular pipe can be represented as

$$v = 10\left(1 - \frac{r}{r_0}\right)^{1/n}$$

where v = velocity, r = radial distance measured out from the pipe's centerline, r_0 = the pipe's radius and n = a parameter. Determine the flow in the pipe if $r_0 = 0.75$ and $n = 7$ using (**a**) Romberg integration to a tolerance of 0.1%, (**b**) two-point Gauss-Legendre formula, and (**c**) the MATLAB `quad` function. Note that flow is equal to velocity times area.

23.29 The amount of mass transported via a pipe over a period of time can be computed as

$$M = \int_{t_1}^{t_2} Q(t)c(t)\,dt$$

where M = mass (mg), t_1 = the initial time (min), t_2 = the final time (min), $Q(t)$ = flow rate (m^3/min), and $c(t)$ = concentration (mg/m^3). The following functional representations define the temporal variations in flow and concentration,

$$Q(t) = 9 + 4\cos^2(0.4t)$$
$$c(t) = 5e^{-0.5t} + 2e^{0.15t}$$

Determine the mass transported between $t_1 = 2$ and $t_2 = 8$ min with (**a**) Romberg integration to a tolerance of 0.1%, and (**b**) the MATLAB `quad` function.