Chapter 8

Numerical Differentiation

Core Topics

Finite difference approximation of the derivative (8.2).

Finite difference formulas using Taylor series expansion (8.3).

Summary of finite difference formulas for numerical differentiation (8.4).

Differentiation formulas using Lagrange polynomials (8.5).

Differentiation using curve fitting (8.6).

Use of MATLAB built-in functions for numerical differentiation (8.7).

Complementary Topics

Richardson's extrapolation (8.8).

Error in numerical differentiation (8.9).

Numerical partial differentiation (8.10).

8.1 BACKGROUND

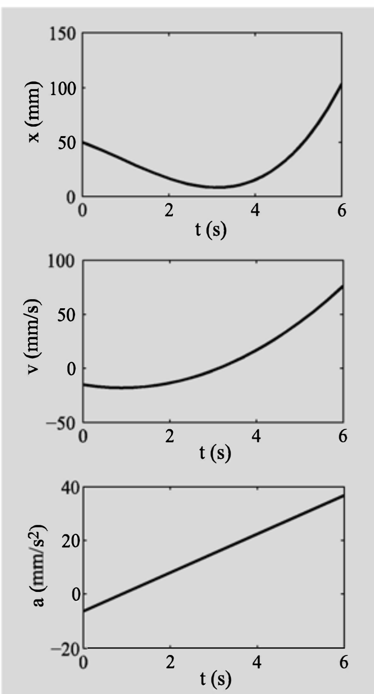


Figure 8-1: Position, velocity, and acceleration as a function of time.

Differentiation gives a measure of the rate at which a quantity changes. Rates of change of quantities appear in many disciplines, especially science and engineering. One of the more fundamental of these rates is the relationship between position, velocity, and acceleration. If the position, x of an object that is moving along a straight line is known as a function of time, t, (the top curve in Fig. 8-1):

$$x = f(t) \tag{8.1}$$

the object's velocity, $v(t)$, is the derivative of the position with respect to time (the middle curve in Fig. 8-1):

$$v = \frac{df(t)}{dt} \tag{8.2}$$

The velocity v is the slope of the position–time curve. Similarly, the object's acceleration, $a(t)$, is the derivative of the velocity with respect to time (the bottom curve in Fig. 8-1):

$$a = \frac{dv(t)}{dt} \tag{8.3}$$

The acceleration a is the slope of the velocity–time curve.

Many models in physics and engineering are expressed in terms of rates. In an electrical circuit, the current in a capacitor is related to the time derivative of the voltage. In analyzing conduction of heat, the amount of heat flow is determined from the derivative of the temperature. Differentiation is also used for finding the maximum and minimum values of functions.

The need for numerical differentiation

The function to be differentiated can be given as an analytical expression or as a set of discrete points (tabulated data). When the function is given as a simple mathematical expression, the derivative can be determined analytically. When analytical differentiation of the expression is difficult or not possible, numerical differentiation has to be used. When the function is specified as a set of discrete points, differentiation is done by using a numerical method.

Numerical differentiation also plays an important role in some of the numerical methods used for solving differential equations, as shown in Chapters 10 and 11.

Approaches to numerical differentiation

Numerical differentiation is carried out on data that are specified as a set of discrete points. In many cases the data are measured or are recorded in experiments, or they may be the result of large-scale numerical calculations. If there is a need to calculate the numerical derivative of a function that is given in an analytical form, then the differentiation is done by using discrete points of the function. This means that in all cases numerical integration is done by using the values of points.

For a given set of points, two approaches can be used to calculate a numerical approximation of the derivative at one of the points. One approach is to use a ***finite difference approximation*** for the derivative. A finite difference approximation of a derivative at a point x_i is an approximate calculation based on the value of points in the neighborhood of x_i. This approach is illustrated in Fig. 8-2*a* where the derivative at point x_i is approximated by the slope of the line that connects the point before x_i with the point after x_i. The accuracy of a finite difference approximation depends on the accuracy of the data points, the spacing between the points, and the specific formula used for the approximation. The simplest formula approximates the derivative as the slope of the line that connects two adjacent points. Finite difference approximation is covered in Sections 8.2 and 8.3.

The second approach is to approximate the points with an analytical expression that can be easily differentiated, and then to calculate the derivative by differentiating the analytical expression. The approximate analytical expression can be derived by using curve fitting. This approach is illustrated in Fig. 8-2*b*, where the points are curve fitted by $f(x)$, and the derivative at point x_i is obtained by analytically differentiating the approximating function and evaluating the result at the point x_i. This approach for numerical differentiation is described in Section 8.6.

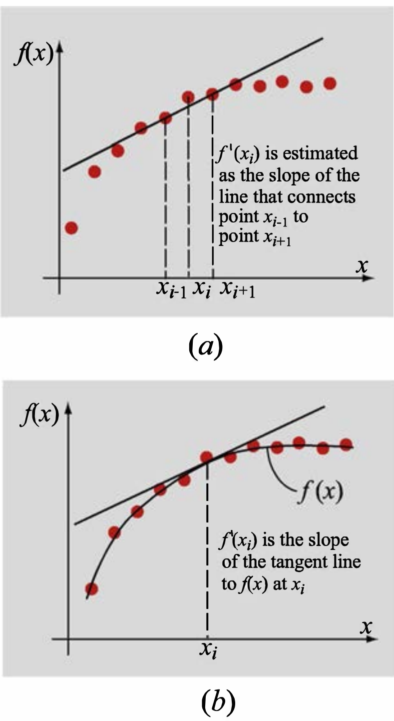


Figure 8-2: Numerical differentiation using (*a*) finite difference approximation and (*b*) function approximation.

Noise and scatter in the data points

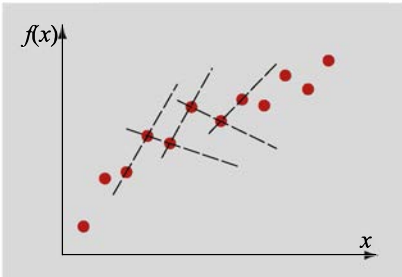


Figure 8-3: Numerical differentiation of data with scatter.

When the data to be differentiated is obtained from experimental measurements, usually there is scatter in the data because of the experimental errors or uncertainties in the measurement (e.g., electrical noise). A set of data points that contains scatter is shown schematically in Fig. 8-3. If this data set is differentiated using a two-point finite difference approximation, which is the simplest form of finite difference approximation (slope of the line that connects two adjacent points), then large variations (positive and negative values) will be seen in the value of the derivative from point to point. It is obvious from the data in the figure that the value of y generally increases with increasing x, which means that the derivative of y w.r.t x is positive. Better results can be obtained by using higher-order formulas of finite difference approximation that take into account the values from more than two points. For example, (see the formulas in Section 8.4) there are four, five, and seven-point finite difference formulas. As mentioned before, the differentiation can also be done by curve fitting the data with an analytical function that is then differentiated. In this case, the data is smoothed out before it is differentiated, eliminating the problem of wrongly amplified slopes between successive points.

8.2 FINITE DIFFERENCE APPROXIMATION OF THE DERIVATIVE

The derivative $f'(x)$ of a function $f(x)$ at the point $x = a$ is defined by:

$$\left.\frac{df(x)}{dx}\right|_{x=a} = f'(a) = \lim_{x \to a} \frac{f(x) - f(a)}{x - a} \tag{8.4}$$

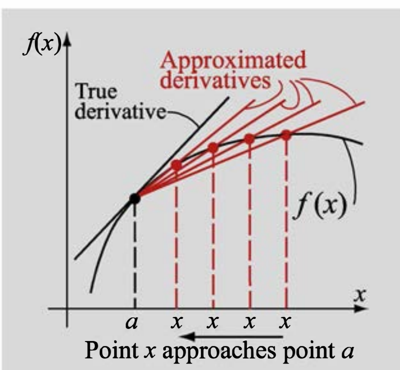


Figure 8-4: Definition of derivative.

Graphically, the definition is illustrated in Fig. 8-4. The derivative is the value of the slope of the tangent line to the function at $x = a$. The derivative is obtained by taking a point x near $x = a$ and calculating the slope of the line that connects the two points. The accuracy of calculating the derivative in this way increases as point x is closer to point a. In the limit as point x approaches point a, the derivative is the slope of the line that is tangent to $f(x)$ at $x = a$. In Calculus, application of the limit condition in Eq. (8.4), which means that point x approaches point a, is used for deriving rules of differentiation that give an analytic expression for the derivative.

In finite difference approximations of the derivative, values of the function at different points in the neighborhood of the point $x=a$ are used for estimating the slope. It should be remembered that the function that is being differentiated is prescribed by a set of discrete points. Various finite difference approximation formulas exist. Three such formulas, where the derivative is calculated from the values of two points, are presented in this section.

Forward, backward, and central difference formulas for the first derivative

The forward, backward, and central finite difference formulas are the simplest finite difference approximations of the derivative. In these approximations, illustrated in Fig. 8-5, the derivative at point (x_i) is calculated from the values of two points. The derivative is estimated as the value of the slope of the line that connects the two points.

- ***Forward difference*** is the slope of the line that connects points $(x_i, f(x_i))$ and $(x_{i+1}, f(x_{i+1}))$:

$$\left.\frac{df}{dx}\right|_{x=x_i} = \frac{f(x_{i+1})-f(x_i)}{x_{i+1}-x_i} \tag{8.5}$$

- ***Backward difference*** is the slope of the line that connects points $(x_{i-1}, f(x_{i-1}))$ and $(x_i, f(x_i))$:

$$\left.\frac{df}{dx}\right|_{x=x_i} = \frac{f(x_i)-f(x_{i-1})}{x_i-x_{i-1}} \tag{8.6}$$

- ***Central difference*** is the slope of the line that connects points $(x_{i-1}, f(x_{i-1}))$ and $(x_{i+1}, f(x_{i+1}))$:

$$\left.\frac{df}{dx}\right|_{x=x_i} = \frac{f(x_{i+1})-f(x_{i-1})}{x_{i+1}-x_{i-1}} \tag{8.7}$$

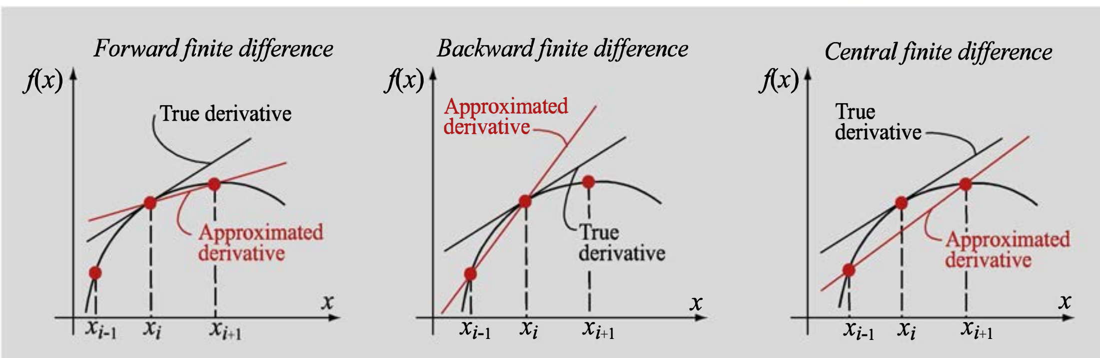


Figure 8-5: Finite difference approximation of derivative.

The first two examples show applications of the forward, backward, and central finite difference formulas. Example 8-1 compares numerical differentiation with analytical differentiation, and in Example 8-2 the formulas are used for differentiation of discrete data.

Example 8-1: Comparing numerical and analytical differentiation.

Consider the function $f(x) = x^3$. Calculate its first derivative at point $x = 3$ numerically with the forward, backward, and central finite difference formulas and using:
(a) Points $x = 2$, $x = 3$, and $x = 4$.
(b) Points $x = 2.75$, $x = 3$, and $x = 3.25$.
Compare the results with the exact (analytical) derivative.

SOLUTION

Analytical differentiation: The derivative of the function is $f'(x) = 3x^2$, and the value of the derivative at $x = 3$ is $f'(3) = 3 \cdot 3^2 = 27$.

Numerical differentiation

(a) The points used for numerical differentiation are:

x:	2	3	4
$f(x)$:	8	27	64

Using Eqs. (8.5) through (8.7), the derivatives using the forward, backward, and central finite difference formulas are:

Forward finite difference:

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(4)-f(3)}{4-3} = \frac{64-27}{1} = 37 \qquad error = \left|\frac{37-27}{27}\cdot 100\right| = 37.04\,\%$$

Backward finite difference:

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(3)-f(2)}{3-2} = \frac{27-8}{1} = 19 \qquad error = \left|\frac{19-27}{27}\cdot 100\right| = 29.63\,\%$$

Central finite difference:

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(4)-f(2)}{4-2} = \frac{64-8}{2} = 28 \qquad error = \left|\frac{28-27}{27}\cdot 100\right| = 3.704\,\%$$

(b) The points used for numerical differentiation are:

x:	2.75	3	3.25
$f(x)$:	2.75^3	3^3	3.25^3

Using Eqs. (8.5) through (8.7), the derivatives using the forward, backward, and central finite difference formulas are:

Forward finite difference:

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(3.25)-f(3)}{3.25-3} = \frac{3.25^3-27}{0.25} = 29.3125 \qquad error = \left|\frac{29.3125-27}{27}\right|\cdot 100 = 8.565\ \%$$

Backward finite difference:

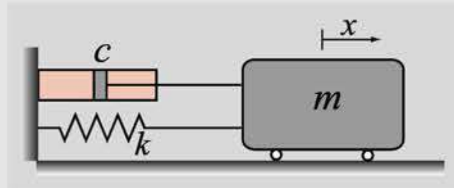
$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(3)-f(2.75)}{3-2.75} = \frac{27-2.75^3}{0.25} = 24.8125 \qquad error = \left|\frac{24.8125-27}{27}\right|\cdot 100 = 8.102\ \%$$

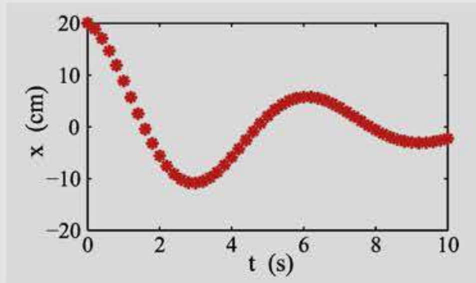
Central finite difference:

$$\left.\frac{df}{dx}\right|_{x=3} = \frac{f(3.25)-f(2.75)}{3.25-2.75} = \frac{3.25^3-2.75^3}{0.5} = 27.0625 \qquad error = \left|\frac{27.0625-27}{27}\right|\cdot 100 = 0.2315\ \%$$

The results show that the central finite difference formula gives a more accurate approximation. This will be discussed further in the next section. In addition, smaller separation between the points gives a significantly more accurate approximation.

Example 8-2: Damped vibrations.





In a vibration experiment, a block of mass m is attached to a spring of stiffness k, and a dashpot with damping coefficient c, as shown in the figure. To start the experiment the block is moved from the equilibrium position and then released from rest. The position of the block as a function of time is recorded at a frequency of 5 Hz (5 times a second). The recorded data for the first 10 s is shown in the figure. The data points for $4 \le t \le 8$ s are given in the table below.

(*a*) The velocity of the block is the derivative of the position w.r.t. time. Use the central finite difference formula to calculate the velocity at time $t = 5$ and $t = 6$ s.

(*b*) Write a user-defined MATLAB function that calculates the derivative of a function that is given by a set of discrete points. Name the function `dx=derivative(x,y)` where `x` and `y` are vectors with the coordinates of the points, and `dx` is a vector with the value of the derivative $\frac{dy}{dx}$ at each point. The function should calculate the derivative at the ***first*** and ***last*** points using the ***forward*** and ***backward finite difference formulas***, respectively, and using the central finite difference formula for all of the other points.

Use the given data points to calculate the velocity of the block for $4 \le t \le 8$ s. Calculate the acceleration of the block by differentiating the velocity. Make a plot of the displacement, velocity, and acceleration, versus time for $4 \le t \le 8$ s.

t (s)	4.0	4.2	4.4	4.6	4.8	5.0	5.2	5.4	5.6	5.8	6.0	6.2	6.4	6.6
x (cm)	–5.87	–4.23	–2.55	–0.89	0.67	2.09	3.31	4.31	5.06	5.55	5.78	5.77	5.52	5.08

t (s)	6.8	7.0	7.2	7.4	7.6	7.8	8.0
x (cm)	4.46	3.72	2.88	2.00	1.10	0.23	–0.59

SOLUTION

(*a*) The velocity is calculated by using Eq. (8.7):

for $t = 5$ s: $$\left.\frac{dx}{dt}\right|_{x=5} = \frac{f(5.2)-f(4.8)}{5.2-4.8} = \frac{3.31-0.67}{0.4} = 6.6 \quad \text{cm/s}$$

for $t = 6$ s: $$\left.\frac{dx}{dt}\right|_{x=5} = \frac{f(6.2)-f(5.8)}{6.2-5.8} = \frac{5.77-5.55}{0.4} = 0.55 \quad \text{cm/s}$$

(*b*) The user-defined function `dx=derivative(x,y)` that is listed next calculates the derivative of a function that is given by a set of discrete points.

Program 8-1: Function file. Derivative of a function given by points.

```
function dx = derivative(x,y)
% derivative calculates the derivative of a function that is given by a set
% of points. The derivatives at the first and last points are calculated by
% using the forward and backward finite difference formula, respectively.
% The derivative at all the other points is calculated by the central
```

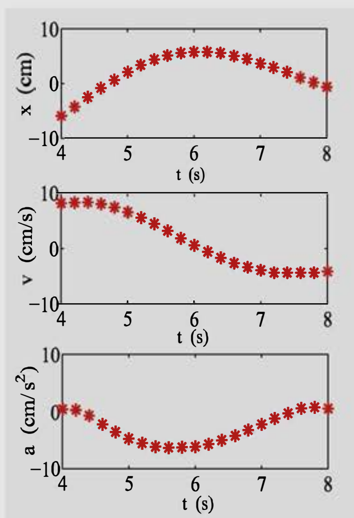
```
% finite difference formula.
% Input variables:
% x  A vector with the coordinates x of the data points.
% y  A vector with the coordinates y of the data points.
% Output variable:
% dx  A vector with the value of the derivative at each point.

n = length(x);
dx(1) = (y(2) - y(1))/(x(2) - x(1));
for i = 2:n - 1
   dx(i) = (y(i + 1) - y(i - 1))/(x(i + 1) - x(i - 1));
end
dx(n) = (y(n) - y(n - 1))/(x(n) - x(n - 1));
```

The user-defined function `derivative` is used in the following script file. The program determines the velocity (the derivative of the given data points) and the acceleration (the derivative of the velocity) and then displays three plots.

```
t = 4:0.2:8;
x = [-5.87 -4.23 -2.55 -0.89 0.67 2.09 3.31 4.31 5.06 5.55 5.78 5.77 5.52 5.08 4.46
3.72 2.88 2.00 1.10 0.23 -0.59];
vel = derivative(t,x)
acc = derivative(t,vel);
subplot (3,1,1)
plot(t,x)
subplot (3,1,2)
plot(t,vel)
subplot (3,1,3)
plot(t,acc)
```

When the script file is executed, the following plots are displayed (the plots were formatted in the Figure Window):



8.3 FINITE DIFFERENCE FORMULAS USING TAYLOR SERIES EXPANSION

The forward, backward, and central difference formulas, as well as many other finite difference formulas for approximating derivatives, can be derived by using Taylor series expansion. The formulas give an estimate of the derivative at a point from the values of points in its neighborhood. The number of points used in the calculation varies with the formula, and the points can be ahead, behind, or on both sides of the point at which the derivative is calculated. One advantage of using Taylor series expansion for deriving the formulas is that it also provides an estimate for the truncation error in the approximation.

In this section, several finite difference formulas are derived. Although the formulas can be derived for points that are not evenly spaced, the derivation here is for points are equally spaced. Section 8.3.1 gives formulas for approximating the first derivative, and Section 8.3.2 deals with finite difference formulas for the second derivative. The methods used for deriving the formulas can also be used for obtaining finite difference formulas for approximating higher-order derivatives. A summary of finite difference formulas for evaluating derivatives up to the fourth derivative is presented in Section 8.4.

8.3.1 Finite Difference Formulas of First Derivative

Several formulas for approximating the first derivative at point x_i based on the values of the points near x_i are derived by using the Taylor series expansion. All the formulas derived in this section are for the case where the points are equally spaced.

Two-point forward difference formula for first derivative

The value of a function at point x_{i+1} can be approximated by a Taylor series in terms of the value of the function and its derivatives at point x_i:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{3!}h^3 + \frac{f^{(4)}(x_i)}{4!}h^4 + \dots \quad (8.8)$$

where $h = x_{i+1} - x_i$ is the spacing between the points. By using two-term Taylor series expansion with a remainder (see Chapter 2), Eq. (8.8) can be rewritten as:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(\xi)}{2!}h^2 \quad (8.9)$$

where ξ is a value of x between x_i and x_{i+1}.
Solving Eq. (8.9) for $f'(x_i)$ yields:

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f''(\xi)}{2!}h \quad (8.10)$$

An approximate value of the derivative $f'(x_i)$ can now be calculated if the second term on the right-hand side of Eq. (8.10) is ignored. Ignoring this second term introduces a truncation (discretization) error. Since this term is proportional to h, the truncation error is said to be on the order of h (written as $O(h)$):

$$truncation\ \ error = -\frac{f''(\xi)}{2!}h = O(h) \tag{8.11}$$

It should be pointed out here that the magnitude of the truncation error is not really known since the value of $f''(\xi)$ is not known. Nevertheless, Eq. (8.11) is valuable since it implies that smaller h gives a smaller error. Moreover, as will be shown later in this chapter, it provides a means for comparing the size of the error in different finite difference formulas.

Using the notation of Eq. (8.11), the approximated value of the first derivative is:

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} + O(h) \tag{8.12}$$

The approximation in Eq. (8.12) is the same as the forward difference formula in Eq. (8.5).

Two-point backward difference formula for first derivative

The backward difference formula can also be derived by application of Taylor series expansion. The value of the function at point x_{i-1} is approximated by a Taylor series in terms of the value of the function and its derivatives at point x_i:

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f'''(x_i)}{3!}h^3 + \frac{f^{(4)}(x_i)}{4!}h^4 + \ldots \tag{8.13}$$

where $h = x_i - x_{i-1}$. By using a two-term Taylor series expansion with a remainder (see Chapter 2), Eq. (8.13) can be rewritten as:

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(\xi)}{2!}h^2 \tag{8.14}$$

where ξ is a value of x between x_{i-1} and x_i. Solving Eq. (8.14) for $f'(x_i)$ yields:

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} + \frac{f''(\xi)}{2!}h \tag{8.15}$$

An approximate value of the derivative, $f'(x_i)$, can be calculated if the second term on the right-hand side of Eq. (8.15) is ignored. This yields:

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h} + O(h) \tag{8.16}$$

The approximation in Eq. (8.16) is the same as the backward difference formula in Eq. (8.6).

Two-point central difference formula for first derivative

The central difference formula can be derived by using three terms in the Taylor series expansion and a remainder. The value of the function at point x_{i+1} in terms of the value of the function and its derivatives at point x_i is given by:

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(\xi_1)}{3!}h^3 \tag{8.17}$$

where ξ_1 is a value of x between x_i and x_{i+1}. The value of the function at point x_{i-1} in terms of the value of the function and its derivatives at point x_i is given by:

$$f(x_{i-1}) = f(x_i) - f'(x_i)h + \frac{f''(x_i)}{2!}h^2 - \frac{f'''(\xi_2)}{3!}h^3 \tag{8.18}$$

where ξ_2 is a value of x between x_{i-1} and x_i. In the last two equations, the spacing of the intervals is taken to be equal so that $h = x_{i+1} - x_i = x_i - x_{i-1}$. Subtracting Eq. (8.18) from Eq. (8.17) gives:

$$f(x_{i+1}) - f(x_{i-1}) = 2f'(x_i)h + \frac{f'''(\xi_1)}{3!}h^3 + \frac{f'''(\xi_2)}{3!}h^3 \tag{8.19}$$

An estimate for the first derivative is obtained by solving Eq. (8.19) for $f'(x_i)$ while neglecting the remainder terms, which introduces a truncation error, which is of the order of h^2:

$$\boxed{f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h} + O(h^2)} \tag{8.20}$$

The approximation in Eq. (8.20) is the same as the central difference formula Eq. (8.7) for equally spaced intervals. A comparison of Eqs. (8.12), (8.16), and (8.20) shows that in the forward and backward difference approximation the truncation error is of the order of h, while in the central difference approximation the truncation error is of the order of h^2. This indicates that the central difference approximation gives a more accurate approximation of the derivative. This can be observed schematically in Fig. 8-5, where the slope of the line that represents the approximated derivative in the central difference approximation appears to be closer to the slope of the tangent line than the lines from the forward and backward approximations.

Three-point forward and backward difference formulas for the first derivative

The forward and backward difference formulas, Eqs. (8.12) and (8.16), give an estimate for the first derivative with a truncation error of $O(h)$. The forward difference formula evaluates the derivative at point x_i based on the values at that point and the point immediately to the right of it x_{i+1}. The backward difference formula evaluates the derivative at point x_i based on the values at that point and the one immediately to the left of it, x_{i-1}. Clearly, the forward difference formula can be useful for evaluating the first derivative at the first point x_1 and at all interior points, while the backward difference formula is useful for evaluating the first derivative at the last point and all interior points. The central difference formula, Eq. (8.20), gives an estimate for the first derivative with an error of $O(h^2)$. The central difference formula evaluates the first derivative at a given point x_i by using the points x_{i-1} and x_{i+1}. Consequently, for a function that is given by a discrete set of n points, the central difference formula is useful only for ***interior points*** and not for the endpoints (x_1 or x_n). An estimate for the first derivative at the endpoints, with error of $O(h^2)$, can be calculated with three-point forward and backward difference formulas, which are derived next.

The ***three-point forward difference*** formula calculates the derivative at point x_i from the value at that point and the next two points, x_{i+1} and x_{i+2}. It is assumed that the points are equally spaced such that $h = x_{i+2}-x_{i+1} = x_{i+1}-x_i$. (The procedure can be applied to unequally spaced points.) The derivation of the formula starts by using three terms of the Taylor series expansion with a remainder, for writing the value of the function at point x_{i+1} and at point x_{i+2} in terms of the value of the function and its derivatives at point x_i:

$$f(x_{i+1}) = f(x_i)+f'(x_i)h+\frac{f''(x_i)}{2!}h^2+\frac{f'''(\xi_1)}{3!}h^3 \tag{8.21}$$

$$f(x_{i+2}) = f(x_i)+f'(x_i)2h+\frac{f''(x_i)}{2!}(2h)^2+\frac{f'''(\xi_2)}{3!}(2h)^3 \tag{8.22}$$

where ξ_1 is a value of x between x_i and x_{i+1}, and ξ_2 is a value of x between x_i and x_{i+2}. Equations (8.21) and (8.22) are next combined such that the terms with the second derivative vanish. This is done by multiplying Eq. (8.21) by 4 and subtracting Eq. (8.22):

$$4f(x_{i+1})-f(x_{i+2}) = 3f(x_i)+2f'(x_i)h+\frac{4f'''(\xi_1)}{3!}h^3-\frac{f'''(\xi_2)}{3!}(2h)^3 \tag{8.23}$$

An estimate for the first derivative is obtained by solving Eq. (8.23) for $f'(x_i)$ while neglecting the remainder terms, which introduces a truncation error of the order of h^2:

$$f'(x_i) = \frac{-3f(x_i)+4f(x_{i+1})-f(x_{i+2})}{2h}+O(h^2) \tag{8.24}$$

Equation (8.24) is the three-point forward difference formula that estimates the first derivative at point x_i from the value of the function at that point and at the next two points, x_{i+1} and x_{i+2}, with an error of $O(h^2)$. The formula can be used for calculating the derivative at the first point of a function that is given by a discrete set of n points.

The ***three-point backward difference*** formula yields the derivative at point x_i from the value of the function at that point and at the previous two points, x_{i-1} and x_{i-2}. The formula is derived in the same way that Eq. (8.24) was derived. The three-term Taylor series expansion with a remainder is written for the value of the function at point x_{i-1}, and at point x_{i-2} in terms of the value of the function and its derivatives at point x_i. The equations are then manipulated to obtain an equation without the second derivative terms, which is then solved for $f'(x_i)$. The formula that is obtained is:

$$f'(x_i) = \frac{f(x_{i-2}) - 4f(x_{i-1}) + 3f(x_i)}{2h} + O(h^2) \tag{8.25}$$

where $h = x_i - x_{i-1} = x_{i-1} - x_{i-2}$ is the distance between the points.

Example 8-3 shows application of the three-point forward difference formula for the first derivative.

Example 8-3: Comparing numerical and analytical differentiation.

Consider the function $f(x) = x^3$. Calculate the first derivative at point $x = 3$ numerically with the three-point forward difference formula, using:

(*a*) Points $x = 3$, $x = 4$, and $x = 5$.

(*b*) Points $x = 3$, $x = 3.25$, and $x = 3.5$.

Compare the results with the exact value of the derivative, obtained analytically.

SOLUTION

Analytical differentiation: The derivative of the function is $f'(x) = 3x^2$, and the value of the derivative at $x = 3$ is $f'(3) = 3 \cdot 3^2 = 27$.

Numerical differentiation

(*a*) The points used for numerical differentiation are:

x:	3	4	5
$f(x)$:	27	64	125

Using Eq. (8.24), the derivative using the three-point forward difference formula is:

$$f'(3) = \frac{-3f(3) + 4f(4) - f(5)}{2 \cdot 1} = \frac{-3 \cdot 27 + 4 \cdot 64 - 125}{2} = 25 \qquad error = \left|\frac{25-27}{27}\right| \cdot 100 = 7.41 \ \%$$

(*b*) The points used for numerical differentiation are:

x:	3	3.25	3.5
$f(x)$:	27	3.25^3	3.5^3

Using Eq. (8.24), the derivative using the three points forward finite difference formula is:

$$f'(3) = \frac{-3f(3) + 4f(3.25) - f(3.5)}{2 \cdot 0.25} = \frac{-3 \cdot 27 + 4 \cdot 3.25^3 - 3.5^3}{0.5} = 26.875$$

$$error = \left|\frac{26.875 - 27}{27}\right| \cdot 100 = 0.46 \ \%$$

The results show that the three-point forward difference formula gives a much more accurate value for the first derivative than the two-point forward finite difference formula in Example 8-1. For $h = 1$ the error reduces from 37.04% to 7.4%, and for $h = 0.25$ the error reduces from 8.57% to 0.46%.

8.3.2 Finite Difference Formulas for the Second Derivative

The same approach used in Section 8.3.1 to develop finite difference formulas for the first derivative can be used to develop expressions for higher-order derivatives. In this section, expressions based on central differences, one-sided forward differences, and one-sided backward differences are presented for approximating the second derivative at a point x_i.

Three-point central difference formula for the second derivative

Central difference formulas for the second derivative can be developed using any number of points on either side of the point x_i, where the second derivative is to be evaluated. The formulas are derived by writing the Taylor series expansion with a remainder at points on either side of x_i in terms of the value of the function and its derivatives at point x_i. Then, the equations are combined in such a way that the terms containing the first derivatives are eliminated. For example, for points x_{i+1}, and x_{i-1} the four-term Taylor series expansion with a remainder is:

$$f(x_{i+1}) = f(x_i)+f'(x_i)h+\frac{f''(x_i)}{2!}h^2+\frac{f'''(x_i)}{3!}h^3+\frac{f^{(4)}(\xi_1)}{4!}h^4 \tag{8.26}$$

$$f(x_{i-1}) = f(x_i)-f'(x_i)h+\frac{f''(x_i)}{2!}h^2-\frac{f'''(x_i)}{3!}h^3+\frac{f^{(4)}(\xi_2)}{4!}h^4 \tag{8.27}$$

where ξ_1 is a value of x between x_i and x_{i+1}, and ξ_2 is a value of x between x_i and x_{i-1}. Adding Eq. (8.26) and Eq. (8.27) gives:

$$f(x_{i+1})+f(x_{i-1}) = 2f(x_i)+2\frac{f''(x_1)}{2!}h^2+\frac{f^{(4)}(\xi_1)}{4!}h^4+\frac{f^{(4)}(\xi_2)}{4!}h^4 \tag{8.28}$$

An estimate for the second derivative can be obtained by solving Eq. (8.28) for $f''(x_i)$ while neglecting the remainder terms. This introduces a truncation error of the order of h^2.

$$f''(x_i) = \frac{f(x_{i-1})-2f(x_i)+f(x_{i+1})}{h^2}+O(h^2) \tag{8.29}$$

Equation (8.29) is the three-point central difference formula that provides an estimate of the second derivative at point x_i from the value of the function at that point, at the previous point, x_{i-1}, and at the next point x_{i+1}, with a truncation error of $O(h^2)$.

The same procedure can be used to develop a higher-order (fourth-order) accurate formula involving the five points x_{i-2}, x_{i-1}, x_i, x_{i+1}, and x_{i+2}:

$$f''(x_i) = \frac{-f(x_{i-2})+16f(x_{i-1})-30f(x_i)+16f(x_{i+1})-f(x_{i+2})}{12h^2}+O(h^4) \quad (8.30)$$

Three-point forward and backward difference formulas for the second derivative

The ***three-point forward difference*** formula that estimates the second derivative at point x_i from the value of that point and the next two points, x_{i+1} and x_{i+2}, is developed by multiplying Eq. (8.21) by 2 and subtracting it from Eq. (8.22). The resulting equation is then solved for $f''(x_i)$:

$$f''(x_i) = \frac{f(x_i)-2f(x_{i+1})+f(x_{i+2})}{h^2}+O(h) \quad (8.31)$$

The ***three-point backward difference*** formula that estimates the second derivative at point x_i from the value of that point and the previous two points, x_{i-1} and x_{i-2}, is derived similarly. It is done by writing the three-term Taylor series expansion with a remainder, for the value of the function at point x_{i-1} and at point x_{i-2}, in terms of the value of the function and its derivatives at point x_i. The equations are then manipulated to obtain an equation without the terms that include the first derivative, which is then solved for $f''(x_i)$. The resulting formula is:

$$f''(x_i) = \frac{f(x_{i-2})-2f(x_{i-1})+f(x_i)}{h^2}+O(h) \quad (8.32)$$

Formulas for higher-order derivatives can be derived by using the same methods that are used here for the second derivative. A list of such formulas is given in the next section. Example 8-3 shows application of the three-point forward difference formula for the second derivative.

Example 8-4: Comparing numerical and analytical differentiation.

Consider the function $f(x) = \frac{2^x}{x}$. Calculate the second derivative at $x = 2$ numerically with the three-point central difference formula using:

(a) Points $x = 1.8$, $x = 2$, and $x = 2.2$.

(b) Points $x = 1.9$, $x = 2$, and $x = 2.1$.

Compare the results with the exact (analytical) derivative.

SOLUTION

Analytical differentiation: The second derivative of the function $f(x) = \frac{2^x}{x}$ is:

$$f''(x) = \frac{2^x[\ln(2)]^2}{x} - \frac{2 \cdot 2^x \ln(2)}{x^2} + \frac{2 \cdot 2^x}{x^3}$$

and the value of the derivative at $x = 2$ is $f''(2) = 0.574617$.

Numerical differentiation

(a) The numerical differentiation is done by substituting the values of the points $x = 1.8$, $x = 2$, and $x = 2.2$ in Eq. (8.29). The operations are done with MATLAB, in the Command Window:

```
>> xa = [1.8 2 2.2];
>> ya = 2.^xa./xa;
>> df = (ya(1) - 2*ya(2) + ya(3))/0.2^2
df =
   0.57748177389232
```

(b) The numerical differentiation is done by substituting the values of the points $x = 1.9$, $x = 2$, and $x = 2.1$ in Eq. (8.29). The operations are done with MATLAB, in the Command Window:

```
>> xb = [1.9 2 2.1];
>> yb = 2.^xb./xb;
>> dfb = (yb(1) - 2*yb(2) + yb(3))/0.1^2
dfb =
   0.57532441566441
```

Error in part (a): $error = \frac{0.577482 - 0.574617}{0.574617} \cdot 100 = 0.4986\ \%$

Error in part (b): $error = \frac{0.575324 - 0.574617}{0.574617} \cdot 100 = 0.1230\ \%$

The results show that the three-point central difference formula gives a quite accurate approximation for the value of the second derivative.

8.4 SUMMARY OF FINITE DIFFERENCE FORMULAS FOR NUMERICAL DIFFERENTIATION

Table 8-1 lists difference formulas, of various accuracy, that can be used for numerical evaluation of first, second, third, and fourth derivatives. The formulas can be used when the function that is being differentiated is specified as a set of discrete points with the independent variable equally spaced.

Table 8-1: Finite difference formulas.

First Derivative		
Method	**Formula**	**Truncation Error**
Two-point forward difference	$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h}$	$O(h)$
Three-point forward difference	$f'(x_i) = \frac{-3f(x_i) + 4f(x_{i+1}) - f(x_{i+2})}{2h}$	$O(h^2)$

Table 8-1: Finite difference formulas.

Two-point backward difference	$f'(x_i) = \dfrac{f(x_i)-f(x_{i-1})}{h}$	$O(h)$
Three-point backward difference	$f'(x_i) = \dfrac{f(x_{i-2})-4f(x_{i-1})+3f(x_i)}{2h}$	$O(h^2)$
Two-point central difference	$f'(x_i) = \dfrac{f(x_{i+1})-f(x_{i-1})}{2h}$	$O(h^2)$
Four-point central difference	$f'(x_i) = \dfrac{f(x_{i-2})-8f(x_{i-1})+8f(x_{i+1})-f(x_{i+2})}{12h}$	$O(h^4)$
	Second Derivative	
Method	**Formula**	**Truncation Error**
Three-point forward difference	$f''(x_i) = \dfrac{f(x_i)-2f(x_{i+1})+f(x_{i+2})}{h^2}$	$O(h)$
Four-point forward difference	$f''(x_i) = \dfrac{2f(x_i)-5f(x_{i+1})+4f(x_{i+2})-f(x_{i+3})}{h^2}$	$O(h^2)$
Three-point backward difference	$f''(x_i) = \dfrac{f(x_{i-2})-2f(x_{i-1})+f(x_i)}{h^2}$	$O(h)$
Four-point backward difference	$f''(x_i) = \dfrac{-f(x_{i-3})+4f(x_{i-2})-5f(x_{i-1})+2f(x_i)}{h^2}$	$O(h^2)$
Three-point central difference	$f''(x_i) = \dfrac{f(x_{i-1})-2f(x_i)+f(x_{i+1})}{h^2}$	$O(h^2)$
Five-point central difference	$f''(x_i) = \dfrac{-f(x_{i-2})+16f(x_{i-1})-30f(x_i)+16f(x_{i+1})-f(x_{i+2})}{12h^2}$	$O(h^4)$
	Third Derivative	
Method	**Formula**	**Truncation Error**
Four-point forward difference	$f'''(x_i) = \dfrac{-f(x_i)+3f(x_{i+1})-3f(x_{i+2})+f(x_{i+3})}{h^3}$	$O(h)$
Five-point forward difference	$f'''(x_i) = \dfrac{-5f(x_i)+18f(x_{i+1})-24f(x_{i+2})+14f(x_{i+3})-3f(x_{i+4})}{2h^3}$	$O(h^2)$
Four-point backward difference	$f'''(x_i) = \dfrac{-f(x_{i-3})+3f(x_{i-2})-3f(x_{i-1})+f(x_i)}{h^3}$	$O(h)$
Five-point backward difference	$f'''(x_i) = \dfrac{3f(x_{i-4})-14f(x_{i-3})+24f(x_{i-2})-18f(x_{i-1})+5f(x_i)}{2h^3}$	$O(h^2)$
Four-point central difference	$f'''(x_i) = \dfrac{-f(x_{i-2})+2f(x_{i-1})-2f(x_{i+1})+f(x_{i+2})}{2h^3}$	$O(h^2)$
Six-point central difference	$f'''(x_i) = \dfrac{f(x_{i-3})-8f(x_{i-2})+13f(x_{i-1})-13f(x_{i+1})+8f(x_{i+2})-f(x_{i+3})}{8h^3}$	$O(h^4)$

Table 8-1: Finite difference formulas.

Fourth Derivative		
Method	**Formula**	**Truncation Error**
Five-point forward difference	$f^{iv}(x_i) = \dfrac{f(x_i)-4f(x_{i+1})+6f(x_{i+2})-4f(x_{i+3})+f(x_{i+4})}{h^4}$	$O(h)$
Six-point forward difference	$f^{iv}(x_i)=\dfrac{3f(x_i)-14f(x_{i+1})+26f(x_{i+2})-24f(x_{i+3})+11f(x_{i+4})-2f(x_{i+5})}{h^4}$	$O(h^2)$
Five-point backward difference	$f^{iv}(x_i) = \dfrac{f(x_{i-4})-4f(x_{i-3})+6f(x_{i-2})-4f(x_{i-1})+f(x_i)}{h^4}$	$O(h)$
Six-point backward difference	$f^{iv}(x_i)=\dfrac{-2f(x_{i-5})+11f(x_{i-4})-24f(x_{i-3})+26f(x_{i-2})-14f(x_{i-1})+3f(x_i)}{h^4}$	$O(h^2)$
Five-point central difference	$f^{iv}(x_i) = \dfrac{f(x_{i-2})-4f(x_{i-1})+6f(x_i)-4f(x_{i+1})+f(x_{i+2})}{h^4}$	$O(h^2)$
Seven-point central difference	$f^{iv}(x_i)=\dfrac{-f(x_{i-3})+12f(x_{i-2})-39f(x_{i-1})+56f(x_i)-39f(x_{i+1})+12f(x_{i+2})-f(x_{i+3})}{6h^4}$	$O(h^4)$

8.5 DIFFERENTIATION FORMULAS USING LAGRANGE POLYNOMIALS

The differentiation formulas can also be derived by using Lagrange polynomials. For the first derivative, the two-point central, three-point forward, and three-point backward difference formulas are obtained by considering three points (x_i, y_i), (x_{i+1}, y_{i+1}), and (x_{i+2}, y_{i+2}). The polynomial, in Lagrange form, that passes through the points is given by:

$$f(x) = \frac{(x-x_{i+1})(x-x_{i+2})}{(x_i-x_{i+1})(x_i-x_{i+2})}y_i + \frac{(x-x_i)(x-x_{i+2})}{(x_{i+1}-x_i)(x_{i+1}-x_{i+2})}y_{i+1} + \frac{(x-x_i)(x-x_{i+1})}{(x_{i+2}-x_i)(x_{i+2}-x_{i+1})}y_{i+2} \tag{8.33}$$

Differentiating Eq. (8.33) gives:

$$f'(x) = \frac{2x-x_{i+1}-x_{i+2}}{(x_i-x_{i+1})(x_i-x_{i+2})}y_i + \frac{2x-x_i-x_{i+2}}{(x_{i+1}-x_i)(x_{i+1}-x_{i+2})}y_{i+1} + \frac{2x-x_i-x_{i+1}}{(x_{i+2}-x_i)(x_{i+2}-x_{i+1})}y_{i+2} \tag{8.34}$$

The first derivative at either one of the three points is calculated by substituting the corresponding value of x (x_i, x_{i+1} or x_{i+2}) in Eq. (8.34). This gives the following three formulas for the first derivative at the three points.

$$f'(x) = \frac{2x_i - x_{i+1} - x_{i+2}}{(x_i - x_{i+1})(x_i - x_{i+2})} y_i + \frac{x_i - x_{i+2}}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})} y_{i+1} + \frac{x_i - x_{i+1}}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} y_{i+2} \tag{8.35}$$

$$f'(x_{i+1}) = \frac{x_{i+1} - x_{i+2}}{(x_i - x_{i+1})(x_i - x_{i+2})} y_i + \frac{2x_{i+1} - x_i - x_{i+2}}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})} y_{i+1} + \frac{x_{i+1} - x_i}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} y_{i+2} \tag{8.36}$$

$$f'(x_{i+2}) = \frac{x_{i+2} - x_{i+1}}{(x_i - x_{i+1})(x_i - x_{i+2})} y_i + \frac{x_{i+2} - x_i}{(x_{i+1} - x_i)(x_{i+1} - x_{i+2})} y_{i+1} + \frac{2x_{i+2} - x_i - x_{i+1}}{(x_{i+2} - x_i)(x_{i+2} - x_{i+1})} y_{i+2} \tag{8.37}$$

When the points are equally spaced, Eq. (8.35) reduces to the three-point forward difference formula (Eq. (8.24)), Eq. (8.36) reduces to the two-point central difference formula (Eq. (8.20)), and Eq. (8.37) reduces to the three-point backward difference formula (Eq. (8.25)).

Equation (8.34) has two other important features. It can be used when the points ***are not*** spaced equally, and it can be used for calculating the value of the first derivative at any point between x_i and x_{i+2}.

Other difference formulas with more points and for higher-order derivatives can also be derived by using Lagrange polynomials. Use of Lagrange polynomials to derive finite difference formulas is sometimes easier than using the Taylor series. However, the Taylor series provides an estimate of the truncation error.

8.6 DIFFERENTIATION USING CURVE FITTING

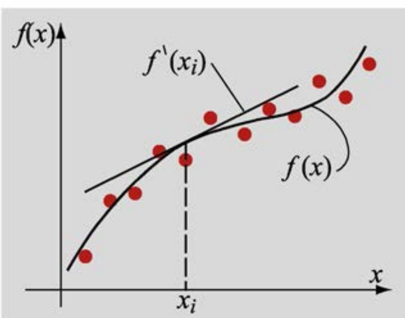


Figure 8-6: Numerical differentiation using curve fitting.

A different approach to differentiation of data specified by a set of discrete points is to first approximate with an analytical function that can be easily differentiated. The approximate function is then differentiated for calculating the derivative at any of the points (Fig. 8-6). Curve fitting is described in Chapter 6. For data that shows a nonlinear relationship, curve fitting is often done by using least squares with an exponential function, a power function, low-order polynomial, or a combination of a nonlinear functions, which are simple to differentiate. This procedure may be preferred when the data contains scatter, or noise, since the curved-fitted function smooths out the noise.

8.7 USE OF MATLAB BUILT-IN FUNCTIONS FOR NUMERICAL DIFFERENTIATION

In general, it is recommended that the techniques described in this chapter be used to develop script files that perform the desired differentiation. MATLAB does not have built-in functions that perform numerical differentiation of an arbitrary function or discrete data. There is, however, a built-in function called `diff`, which can be used to perform numerical differentiation, and another built-in function called `polyder`, which determines the derivative of polynomial.

The `diff` command

The built-in function `diff` calculates the differences between adjacent elements of a vector. The simplest form of the command is:

`d = diff(x)`

`d` is a vector with the differences between elements of x: $d = [(x_2 - x_1), (x_3 - x_2), \ldots, (x_n - x_{n-1})]$

`x` is a vector: $[x_1, x_2, x_3, x_4, \ldots, x_{n-1}, x_n]$

The vector `d` is one element shorter than the vector `x`.

For a function represented by a discrete set of n points (x_1, y_1), (x_2, y_2), (x_3, y_3), …, (x_n, y_n), the first derivative with the two-point forward difference formula, Eq. (8.5), can be calculated using the `diff` command by entering `diff(y)./diff(x)`. The result is a vector whose elements are:

$$\left[\frac{(y_2 - y_1)}{(x_2 - x_1)}, \frac{(y_3 - y_2)}{(x_3 - x_2)}, \frac{(y_4 - y_3)}{(x_4 - x_3)}, \ldots, \frac{(y_n - y_{n-1})}{(x_n - x_{n-1})}\right]$$

When the spacing between the points is the same such that $h = (x_2 - x_1) = (x_3 - x_2) = \ldots = (x_n - x_{n-1})$, then the first derivative with the two-point forward difference formula, Eq. (8.12), can be calculated using the `diff` command by entering `diff(y)/h`.

The `diff` command has an additional optional input argument that can be used for calculating higher-order derivatives. Its form is:

`d = diff(x,n)`

where `n` is a number (integer) that specifies the number of times that `diff` is applied recursively. For example, `diff(x,2)` is the same as `diff(diff(x))`. In other words, for an n-element vector $x_1, \ldots, x_n$ `diff(x)` calculates a vector with $n-1$ elements:

$$x_{i+1} - x_i \quad \text{for} \quad i = 1, \ldots, n-1 \tag{8.38}$$

and `diff(x,2)` gives the vector with $n-2$ elements:

$$((x_{i+2} - x_{i+1}) - (x_{i+1} - x_i)) = x_i - 2x_{i+1} + x_{i+2} \quad \text{for} \quad i = 1, \ldots, n-1 \tag{8.39}$$

The right-hand side of Eq. (8.39) is the same as the numerator of the three-point forward difference formula for the second derivative at $x = x_i$, Eq. (8.31). Consequently, for a function represented by a discrete set of n points (x_i, y_i), where the distance, h, between the points is the same, an estimate of the second derivative according to the three-point forward difference formula can be calculated with MATLAB by entering `diff(y,2)/h^2`.

Similarly, `diff(y,3)` yields the numerator of the third derivative in the four-point forward difference formula (see Table 8-1). In general, `diff(y,n)` gives the numerator in the forward difference formula of the nth derivative.

The `polyder` *command*

The built-in function `polyder` can calculate the derivative of a polynomial (it can also calculate the derivative of a product and quotient of two polynomials). The simplest form of the command is:

`dp = polyder(p)`

`dp` is a vector with the coefficients of the polynomial that is the derivative of the polynomial `p`.

`p` is a vector with the coefficients of the polynomial that is differentiated.

In MATLAB, polynomials are represented by a row vector in which the elements are the coefficients of the polynomial in order from the coefficient of the highest order term to the zeroth order term. If `p` is a vector of length n, then `dp` will be a vector of length $n-1$. For example, to find the derivative of the polynomial $f(x) = 4x^3+5x+7$, define a vector `p = [4 0 5 7]`, and type `df = polyder(p)`. The output will be `df = [12 0 5]`, representing $12x^2+5$, which is the derivative of $f(x)$.

```
>> p = [4 0 5 7];
>> dp = polyder(p)
dp =
    12     0     5
```

The `polyder` command can be useful for calculating the derivative when a function represented by a set of discrete data points is approximated by a curve-fitted polynomial.

8.8 RICHARDSON'S EXTRAPOLATION

Richardson's extrapolation is a method for calculating a more accurate approximation of a derivative from two less accurate approximations of that derivative.

In general terms, consider the value, D, of a derivative (unknown) that is calculated by the difference formula:

$$D = D(h)+k_2h^2+k_4h^4 \tag{8.40}$$

where $D(h)$ is a function that approximates the value of the derivative and k_2h^2 and k_4h^4 are error terms in which the coefficients, k_2 and k_4 are independent of the spacing h. Using the same formula for calculating the value of D but using a spacing of $h/2$ gives:

$$D = D\left(\frac{h}{2}\right) + k_2\left(\frac{h}{2}\right)^2 + k_4\left(\frac{h}{2}\right)^4 \tag{8.41}$$

Equation (8.41) can be rewritten (after multiplying by 4) as:

$$4D = 4D\left(\frac{h}{2}\right) + k_2h^2 + k_4\frac{h^4}{4} \tag{8.42}$$

Subtracting Eq. (8.40) from Eq. (8.42) eliminates the terms with h^2, and gives:

$$3D = 4D\left(\frac{h}{2}\right) - D(h) - k_4\frac{3h^4}{4} \tag{8.43}$$

Solving Eq. (8.43) for D yields a new approximation for the derivative:

$$D = \frac{1}{3}\left(4D\left(\frac{h}{2}\right) - D(h)\right) - k_4\frac{h^4}{4} \tag{8.44}$$

The error term in Eq. (8.44) is now $O(h^4)$. The value, D, of the derivative can now be approximated by:

$$\boxed{D = \frac{1}{3}\left(4D\left(\frac{h}{2}\right) - D(h)\right) + O(h^4)} \tag{8.45}$$

This means that an approximated value of D with error $O(h^4)$ is obtained from two lower-order approximations ($D(h)$ and $D\left(\frac{h}{2}\right)$) that were calculated with an error $O(h^2)$. Equation (8.45) can be used for obtaining a more accurate approximation for any formula that calculates the derivative with an error $O(h^2)$. The formula is used for calculating one approximation with a spacing of h and a second approximation with a spacing of $h/2$. The two approximations are then substituted in Eq. (8.45), which gives a new estimate with an error of $O(h^4)$. The procedure is illustrated in Example 8-5.

Equation (8.45) can also be derived directly from a particular finite difference formula. As an example, consider the two-point central difference formula for the first derivative for points with equal spacing of h, such that $x_{i+1} = x_i + h$ and $x_{i-1} = x_i - h$. Writing the five-term Taylor series expansion with a remainder for the value of the function at point x_{i+1} in terms of the value of the function and its derivatives at point x_i gives:

$$f(x_i+h) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2!}h^2 + \frac{f'''(x_i)}{3!}h^3 + \frac{f^{\text{iv}}(x_i)}{4!}h^4 + \frac{f^{\text{v}}(\xi_1)}{5!}h^5 \tag{8.46}$$

where ξ_1 is a value of x between x_i and x_i+h. In the same manner, the value of the function at point x_{i-1} is expressed in terms of the value of the function and its derivatives at point x_i:

$$f(x_i-h)=f(x_i)-f'(x_i)h+\frac{f''(x_i)}{2!}h^2-\frac{f'''(x_i)}{3!}h^3+\frac{f^{\text{iv}}(x_i)}{4!}h^4-\frac{f^{\text{v}}(\xi_2)}{5!}h^5 \quad (8.47)$$

where ξ_2 is a value of x between x_i-h and x_i. Subtracting Eq. (8.47) from Eq. (8.46) gives:

$$f(x_i+h)-f(x_i-h) = 2f'(x_i)h+2\frac{f'''(x_i)}{3!}h^3+\frac{f^{\text{v}}(\xi_1)}{5!}h^5+\frac{f^{\text{v}}(\xi_2)}{5!}h^5 \quad (8.48)$$

Assuming that the fifth derivative is continuous in the interval $[x_{i-1}, x_{i+1}]$, the two remainder terms in Eq. (8.48) can be combined and written as $O(h^5)$. Then, solving Eq. (8.48) for $f'(x_i)$ gives:

$$f'(x_i) = \frac{f(x_i+h)-f(x_i-h)}{2h}-\frac{f'''(x_i)}{3!}h^2+O(h^4) \quad (8.49)$$

which is the approximation for the first derivative with a spacing of h.

The derivation of Eqs. (8.46)–(8.49) can be repeated if the spacing between the points is changed to $h/2$. For this case the equation for the value of the derivative is:

$$f'(x_i) = \frac{f(x_i+h/2)-f(x_i-h/2)}{2(h/2)}-\frac{f'''(x_i)}{3!}\left(\frac{h}{2}\right)^2+O(h^4) \quad (8.50)$$

or

$$f'(x_i) = \frac{f(x_i+h/2)-f(x_i-h/2)}{h}-\frac{f'''(x_i)}{4\cdot 3!}h^2+O(h^4) \quad (8.51)$$

Multiplying Eq. (8.51) by 4 gives:

$$4f'(x_i) = 4\frac{f(x_i+h/2)-f(x_i-h/2)}{h}-\frac{f'''(x_i)}{3!}h^2+O(h^4) \quad (8.52)$$

Subtracting Eq. (8.49) from Eq. (8.52) and dividing the result by 3 yields an approximation for the first derivative with error $O(h^4)$:

$$f'(x_i)=\frac{1}{3}\left[4\frac{f(x_i+h/2)-f(x_i-h/2)}{h}-\frac{f(x_i+h)-f(x_i-h)}{2h}\right]+O(h^4) \quad (8.53)$$

First derivative calculated with two-point central difference formula, Eq. (8.20), with error $O(h^2)$ for points with spacing of $h/2$.

First derivative calculated with two-point central difference formula, Eq. (8.20), with error $O(h^2)$ for points with spacing of h.

Equation (8.53) is a special case of Eq. (8.45) where the derivatives are calculated with the two-point central difference formula. Equation

(8.45) can be used with any difference formula with an error $O(h^2)$.

Richardson's extrapolation method can also be used with approximations that have errors of higher order. Two approximations with an error $O(h^4)$—one calculated from points with spacing of h and the other from points with spacing of $h/2$ —can be used for calculating a more accurate approximation with an error $O(h^6)$. The formula for this case is:

$$D = \frac{1}{15}\left(16D\left(\frac{h}{2}\right) - D(h)\right) + O(h^6) \tag{8.54}$$

Application of Richardson's extrapolation is shown in Example 8-5.

Example 8-5: Using Richardson's extrapolation in differentiation.

Use Richardson's extrapolation with the results in Example 8-4 to calculate a more accurate approximation for the derivative of the function $f(x) = \frac{2^x}{x}$ at the point $x = 2$.

Compare the results with the exact (analytical) derivative.

SOLUTION

In Example 8-4 two approximations of the derivative of the function at $x = 2$ were calculated using the central difference formula in which the error is $O(h^2)$. In one approximation $h = 0.2$, and in the other $h = 0.1$. The results from Example 8-4 are:

for $h = 0.2$, $f''(2) = 0.577482$. The error in this approximation is 0.5016 %.

for $h = 0.1$, $f''(2) = 0.575324$. The error in this approximation is 0.126 %.

Richardson's extrapolation can be used by substituting these results in Eq. (8.45) (or Eq. (8.53)):

$$D = \frac{1}{3}\left(4D\left(\frac{h}{2}\right) - D(h)\right) + O(h^4) = \frac{1}{3}(4 \cdot 0.575324 - 0.577481) = 0.574605$$

The error now is $error = \frac{0.574605 - 0.5746}{0.5746} \cdot 100 = 0.00087\ \%$

This result shows that a much more accurate approximation is obtained by using Richardson's extrapolation.

8.9 ERROR IN NUMERICAL DIFFERENTIATION

Throughout this chapter, expressions have been given for the truncation error, also known as the discretization error. These expressions are generated by the particular numerical scheme used for deriving a specific finite difference formula to estimate the derivative. In each case, the truncation error depends on h (the spacing between the points) raised to some power. Clearly, the implication is that as h is made smaller and smaller, the error could be made arbitrarily small. When the function to be differentiated is specified as a set of discrete data points, the spacing is fixed, and the truncation error cannot be reduced by reducing the size of h. In this case, a smaller truncation error can be obtained by using a finite difference formula that has a higher-order truncation error.

When the function that is being differentiated is given by a mathematical expression, the spacing h for the points that are used in the finite difference formulas can be defined by the user. It might appear then that h can be made arbitrarily small and there is no limit to how small the error can be made. This, however, is not true because the total error is composed of two parts. One is the truncation error arising from the numerical method (the specific finite difference formula) that is used. The second part is a round-off error arising from the finite precision of the particular computer used. Therefore, even if the truncation error can be made vanishingly small by choosing smaller and smaller values of h, the round-off error still remains, or can even grow as h is made smaller and smaller. Example 8-6 illustrates this point.

Example 8-6: Comparing numerical and analytical differentiation.

Consider the function $f(x) = e^x$. Write an expression for the first derivative of the function at $x = 0$ using the two-point central difference formula in Eq. (8.20). Investigate the effect that the spacing, h, between the points has on the truncation and round-off errors.

SOLUTION

The two-point central difference formula in Eq. (8.20) is:

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

where ξ is a value of x between x_{i-1} and x_{i+1}

The points used for calculating the derivative of $f(x) = e^x$ at $x = 0$ are $x_{i-1} = -h$ and $x_{i+1} = h$. Substituting these points in the formula gives:

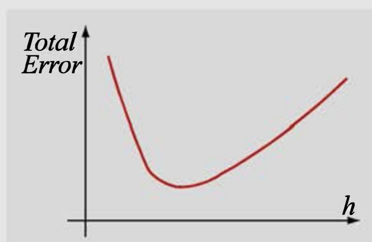
$$f'(0) = \frac{e^h - e^{-h}}{2h} - 2\frac{f'''(\xi)}{3!}h^2 \tag{8.55}$$

When the computer calculates the values of e^h and e^{-h}, a round-off error is introduced, since the computer has finite precision. Consequently, the terms e^h and e^{-h} in Eq. (8.55) are replaced by $e^h + R_1$ and $e^{-h} + R_2$ where now e^h and e^{-h} are the exact values, and R_1 and R_2 are the round-off errors:

$$f'(0) = \frac{e^h + R_1 - e^{-h} - R_2}{2h} - 2\frac{f'''(\xi)}{3!}h^2 = \frac{e^h - e^{-h}}{2h} + \frac{R_1 - R_2}{2h} - 2\frac{f'''(\xi)}{3!}h^2 \tag{8.56}$$

In Eq. (8.56) the last term on the right-hand side is the truncation error. In this term, the value of $f'''(\xi)$ is not known, but it is bounded. This means that as h decreases the truncation error decreases.

The round-off error is $(R_1 - R_2)/(2h)$. As h decreases the round-off error increases. The total error is the sum of the truncation error and round-off error. Its behavior is shown schematically in the figure on the right. As h decreases, the total error initially decreases, but after a certain value (which depends on the precision of the computer used) the total error increases as h decreases further.



8.10 NUMERICAL PARTIAL DIFFERENTIATION

All the numerical differentiation methods presented so far considered functions with one independent variable. Most problems in engineering or science involve functions of several independent variables since real-life applications are either two or three-dimensional, and in addition may be a function of time. For example, the temperature distribution in an object is a function of the three coordinates used to describe the object: $T(x, y, z)$, or $T(r, \theta, z)$, or $T(r, \theta, \phi)$. The temperature may also be a function of time: $T(x, y, z, t)$. If there is a need for evaluating the amount of heat flow in a given direction, say z, the partial derivative in the z direction is required: $\frac{\partial T(x, y, z, t)}{\partial z}$. Another example is the determination of strains from displacements. If two-dimensional displacements are measured on the surface of a structure, the strains are determined from the partial derivatives of the displacements.

For a function of several independent variables, the partial derivative of the function with respect to one of the variables represents the rate of change of the value of the function with respect to this variable, while all the other variables are kept constant (see Section 2.6). For a function $f(x, y)$ with two independent variables, the partial derivatives with respect to x and y at the point (a, b) are defined as:

$$\left.\frac{\partial f(x, y)}{\partial x}\right|_{\substack{x=a \\ y=b}} = \lim_{x \to a} \frac{f(x, b) - f(a, b)}{x - a} \tag{8.57}$$

$$\left.\frac{\partial f(x, y)}{\partial y}\right|_{\substack{x=a \\ y=b}} = \lim_{y \to b} \frac{f(a, y) - f(a, b)}{y - b} \tag{8.58}$$

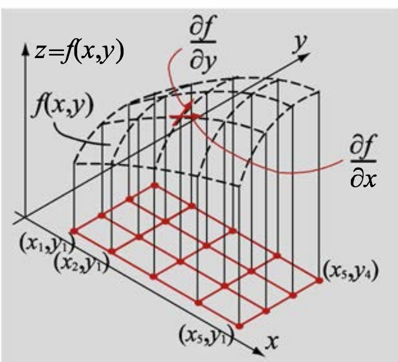


Figure 8-7: A function with two independent variables.

This means that the finite difference formulas that are used for approximating the derivatives of functions with one independent variable can be adopted for calculating partial derivatives. The formulas are applied for one of the variables, while the other variables are kept constant. For example, consider a function of two independent variables $f(x, y)$ specified as a set of discrete $m \cdot n$ points (x_1, y_1), (x_1, y_2), ... , (x_n, y_m). The spacing between the points in each direction is constant such that $h_x = x_{i+1} - x_i$ and $h_y = y_{i+1} - y_i$. Figure 8-7 shows a case where $n = 5$ and $m = 4$. An approximation for the partial derivative at point (x_i, y_i) with the two-point forward difference formula is:

$$\left.\frac{\partial f}{\partial x}\right|_{\substack{x=x_i \\ y=y_i}} = \frac{f(x_{i+1}, y_i) - f(x_i, y_i)}{h_x} \tag{8.59}$$

$$\left.\frac{\partial f}{\partial y}\right|_{\substack{x=x_i \\ y=y_i}} = \frac{f(x_i, y_{i+1}) - f(x_i, y_i)}{h_y} \tag{8.60}$$

In the same way, the two-point backward and central difference formulas are:

$$\left.\frac{\partial f}{\partial x}\right|_{\substack{x = x_i \\ y = y_i}} = \frac{f(x_i, y_i) - f(x_{i-1}, y_i)}{h_x} \qquad \left.\frac{\partial f}{\partial y}\right|_{\substack{x = x_i \\ y = y_i}} = \frac{f(x_i, y_i) - f(x_i, y_{i-1})}{h_y} \tag{8.61}$$

$$\left.\frac{\partial f}{\partial x}\right|_{\substack{x = x_i \\ y = y_i}} = \frac{f(x_{i+1}, y_i) - f(x_{i-1}, y_i)}{2h_x} \qquad \left.\frac{\partial f}{\partial y}\right|_{\substack{x = x_i \\ y = y_i}} = \frac{f(x_i, y_{i+1}) - f(x_i, y_{i-1})}{2h_y} \tag{8.62}$$

The second partial derivatives with the three-point central difference formula are:

$$\left.\frac{\partial^2 f}{\partial x^2}\right|_{\substack{x = x_i \\ y = y_i}} = \frac{f(x_{i-1}, y_i) - 2f(x_i, y_i) + f(x_{i+1}, y_i)}{h_x^2} \tag{8.63}$$

$$\left.\frac{\partial^2 f}{\partial y^2}\right|_{\substack{x = x_i \\ y = y_i}} = \frac{f(x_i, y_{i-1}) - 2f(x_i, y_i) + f(x_i, y_{i+1})}{h_y^2} \tag{8.64}$$

Similarly, all the finite difference formulas listed in Section 8.4 can be adapted for calculating partial derivatives of different orders with respect to one of the variables.

A second-order partial derivative can also be mixed $\frac{\partial^2 f}{\partial x \partial y}$. This derivative is carried out successively $\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x}\right) = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right)$. A finite difference formula for the mixed derivative can be obtained by using the first-order finite difference formulas for partial derivatives. For example, the second-order mixed four-point central finite difference formula is obtained from Eqs. (8.62):

$$\left.\frac{\partial^2 f}{\partial x \partial y}\right|_{\substack{x = x_i \\ y = y_i}} = \frac{[f(x_{i+1}, y_{i+1}) - f(x_{i-1}, y_{i+1})] - [f(x_{i+1}, y_{i-1}) - f(x_{i-1}, y_{i-1})]}{2h_x \cdot 2h_y} \tag{8.65}$$

Application of finite difference formulas for numerical partial differentiation is shown in Example 8-7.

Example 8-7: Numerical partial differentiation.

The following two-dimensional data for the x component of velocity u as a function of the two coordinates x and y is measured from an experiment:

	$x = 1.0$	$x = 1.5$	$x = 2.0$	$x = 2.5$	$x = 3.0$
$y = 1.0$	163	205	250	298	349
$y = 2.0$	228	291	361	437	517
$y = 3.0$	265	350	448	557	676

(*a*) Using central difference approximations, calculate $\partial u/\partial x$, $\partial u/(\partial y)$, $\partial^2 u/\partial y^2$, and $\partial^2 u/\partial x \partial y$ at the point $(2, 2)$.

(*b*) Using a three-point forward difference approximation, calculate $\partial u/\partial x$ at the point (2,2).
(*c*) Using a three-point forward difference approximation, calculate $\partial u/\partial y$ at the point $(2, 1)$.

SOLUTION

(*a*) In this part $x_i = 2$, $y_i = 2$, $x_{i-1} = 1.5$, $x_{i+1} = 2.5$, $y_{i-1} = 1$, $y_{i+1} = 3$, $h_x = 0.5$, $h_y = 1$.

Using Eqs. (8.59) and (8.60), the partial derivatives $\partial f/\partial x$ and $\partial u/\partial y$ are:

$$\left.\frac{\partial u}{\partial x}\right|_{\substack{x = x_i \\ y = y_i}} = \frac{u(x_{i+1}, y_i) - u(x_{i-1}, y_i)}{2h_x} = \frac{u(2.5, 2) - u(1.5, 2)}{2 \cdot 0.5} = \frac{437 - 291}{1} = 146$$

$$\left.\frac{\partial u}{\partial y}\right|_{\substack{x = x_i \\ y = y_i}} = \frac{u(x_i, y_{i+1}) - u(x_i, y_{i-1})}{2h_y} = \frac{u(2, 3) - u(2, 1)}{2 \cdot 1} = \frac{448 - 250}{2} = 99$$

The second partial derivative $\partial^2 u/\partial y^2$ is calculated with Eq. (8.64):

$$\left.\frac{\partial^2 u}{\partial y^2}\right|_{\substack{x = x_i \\ y = y_i}} = \frac{u(x_i, y_{i-1}) - 2u(x_i, y_i) + u(x_i, y_{i+1})}{h_y^2} = \frac{250 - (2 \cdot 361) + 448}{1^2} = -24$$

The second mixed derivative $\partial^2 u/\partial x \partial y$ is given by Eq. (8.65):

$$\left.\frac{\partial^2 u}{\partial x \partial y}\right|_{\substack{x = x_i \\ y = y_i}} = \frac{[u(x_{i+1}, y_{i+1}) - u(x_{i-1}, y_{i+1})] - [u(x_{i+1}, y_{i-1}) - u(x_{i-1}, y_{i-1})]}{2h_x \cdot 2h_y}$$

$$= \frac{[u(2.5, 3) - u(1.5, 3)] - [u(2.5, 1) - u(1.5, 1)]}{2 \cdot 0.5 \cdot 2 \cdot 1} = \frac{[557 - 350] - [298 - 205]}{2 \cdot 0.5 \cdot 2 \cdot 1} = 57$$

(*b*) In this part $x_i = 2$, $x_{i+1} = 2.5$, $x_{i+2} = 3.0$, $y_i = 2$, and $h_x = 0.5$. The formula for the partial derivative $\partial u/\partial x$ with the three-points forward finite difference formula can be written from the formula for the first derivative in Section 8.4.

$$\left.\frac{\partial u}{\partial x}\right|_{\substack{x = x_i \\ y = y_i}} = \frac{-3u(x_i, y_i) + 4u(x_{i+1}, y_i) - u(x_{i+2}, y_i)}{2h_x} =$$

$$= \frac{-3u(2, 2) + 4u(2.5, 2) - u(3.0, 2)}{2 \cdot 0.5} = \frac{-3 \cdot 361 + 4 \cdot 437 - 517}{2 \cdot 0.5} = 148$$

(*c*) In this part $y_i = 1$, $y_{i+1} = 2$, $y_{i+2} = 3$, $x_i = 2$, and $h_y = 1.0$. The formula for the partial derivative $\partial u/\partial y$ with the three-points forward difference formula can be written from the formula for the first derivative in Section 8.4.

$$\left.\frac{\partial u}{\partial y}\right|_{\substack{x = x_i \\ y = y_i}} = \frac{-3u(x_i, y_i) + 4u(x_i, y_{i+1}) - u(x_i, y_{i+2})}{2h_y} =$$

$$= \frac{-3u(2, 1) + 4u(2, 2) - u(2, 3)}{2 \cdot 1} = \frac{-3 \cdot 250 + 4 \cdot 361 - 448}{2 \cdot 1} = 123$$

8.11 PROBLEMS

Problems to be solved by hand

Solve the following problems by hand. When needed, use a calculator, or write a MATLAB script file to carry out the calculations. If using MATLAB, do not use built-in functions for differentiation.

8.1 Given the following data:

x	1.1	1.2	1.3	1.4	1.5
$f(x)$	0.6133	0.7822	0.9716	1.1814	1.4117

find the first derivative $f'(x)$ at the point $x = 1.3$.
(*a*) Use the three-point forward difference formula.
(*b*) Use the three-point backward difference formula.
(*c*) Use the two-point central difference formula.

8.2 Given the following data:

x	0.6	0.7	0.8	0.9	1.0
$f(x)$	5.2296	3.6155	2.7531	2.2717	2

find the second derivative $f''(x)$ at the point $x = 0.8$.
(*a*) Use the three-point forward difference formula.
(*b*) Use the three-point backward difference formula.
(*c*) Use the three-point central difference formula.

8.3 The following data show estimates of the population of Liberia in selected years between 1960 and 2010:

Year	1960	1970	1980	1990	2000	2010
Population (millions)	1.1	1.4	1.9	2.1	2.8	4

Calculate the rate of growth of the population in millions per year for 2010.
(*a*) Use two-point backward difference formula.
(*b*) Use three-point backward difference formula.
(*c*) Using the slope in 2010 from part (*b*), apply the two-point central difference formula to extrapolate and predict the population in the year 2020.

8.4 The following data is given for the stopping distance of a car on a wet road versus the speed at which it begins braking.

v (mi/h)	12.5	25	37.5	50	62.5	75
d (ft)	20	59	118	197	299	420

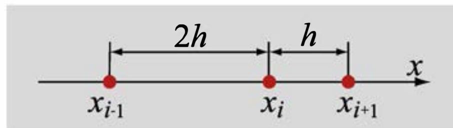
(*a*) Calculate the rate of change of the stopping distance at a speed of 62.5 mph using (*i*) the two-point backward difference formula, and (*ii*) the three-point backward difference formula.

(*b*) Calculate an estimate for the stopping distance at 75 mph by using the results from part (*a*) for the slope and the two-point central difference formula applied at the speed of 62.5 mph. How does the estimate compares with tha data?

8.5 Given three ***unequally*** spaced points (x_i, y_i), (x_{i+1}, y_{i+1}), and (x_{i+2}, y_{i+2}), use Taylor series expansion to develop a finite difference formula to evaluate the first derivative dy/dx at the point $x = x_i$. Verify that when the spacing between these points is equal, the three-point forward difference formula is obtained. The answer should involve y_i, y_{i+1}, and y_{i+2}.

8.6 Using a four-term Taylor series expansion, derive a four-point backward difference formula for evaluating the first derivative of a function given by a set of unequally spaced points. The formula should give the derivative at point $x = x_i$, in terms of x_i, x_{i-1}, x_{i-2}, x_{i-3}, $f(x_i)$, $f(x_{i-1})$, $f(x_{i-2})$, and $f(x_{i-3})$.

8.7 Derive a finite difference approximation formula for $f''(x_i)$ using three points x_{i-1}, x_i, and x_{i+1}, where the spacing is such that $x_i - x_{i-1} = 2h$ and $x_{i+1} - x_i = h$.



8.8 A particular finite difference formula for the first derivative of a function is:

$$f'(x_i) = \frac{-f(x_{i+3}) + 9f(x_{i+1}) - 8f(x_i)}{6h}$$

where the points x_i, x_{i+1}, x_{i+2}, and x_{i+3} are all equally spaced with step size h. What is the order of the truncation or discretization error?

8.9 The following data show the number of female and male physicians in the U.S. for various years (American Medical Association):

Year	1980	1990	2000	2002	2003	2006	2008
# males	413,395	511,227	618,182	638,182	646,493	665,647	677,807
# females	54,284	104,194	195,537	215,005	225,042	256,257	276,417

(*a*) Calculate the rate of change in the number of male and female physicians in 2006 by using the three-point backward difference formula for the derivative, with unequally spaced points, Eq. (8.37).
(*b*) Use the result from part (*a*) and the three-point central difference formula for the derivative with unequally spaced points, Eq. (8.36), to calculate (predict) the number of male and female physicians in 2008.

8.10 Use the data from Problem 8.9 and the four-point backward difference formula that was derived in Problem 8.6 for evaluating the first derivative of a function specified at unequally spaced points to calculate the following quantities.
(*a*) Evaluate the rate of change in the number of male and female physicians in 2008.
(*b*) Use the data from 2008, 2006, together with the slopes in 2008 from part (*a*) to estimate the year in which the number of female and male physicians will be equal. Use the three-point central difference formula for the derivative (Eq. (8.36)) of a function specified at unequally spaced points.

8.11 Use Lagrange interpolation polynomials to find the finite difference formula for the second derivative at the point $x = x_i$ using the unequally spaced points x_i, x_{i+1}, and x_{i+2}. What is the second derivative at $x = x_{i+1}$ and at $x = x_{i+2}$?

8.12 Given the function $f(x) = \dfrac{(x^2+\sqrt{x})\cos(x)}{\sin(x)}$, find the value of the first derivative at $x = 2$.
(*a*) Use analytical differentiation by hand.
(*b*) Use the four-point central difference formula with $x_{i-2} = 1.96$, $x_{i-1} = 1.98$, $x_{i+1} = 2.02$, and $x_{i+2} = 2.04$. Write a MATLAB program in a script file to carry out the calculations.

8.13 For the function given in Problem 8.12, find the value of the second derivative at $x = 2$.
(*a*) Use analytical differentiation by hand.
(*b*) Use the five-point central difference formula with $x_{i-2} = 1.96$, $x_{i-1} = 1.98$, $x_i = 2$, $x_{i+1} = 2.02$, and $x_{i+2} = 2.04$. Write a MATLAB program in a script file to carry out the calculations.

8.14 The following data for the velocity component in the *x*-direction, *u*, are obtained as a function of the two coordinates *x* and *y*:

	$x = 0$	$x = 1$	$x = 2$	$x = 3$	$x = 4$
$y = 0$	0	8	2	13	15
$y = 1$	3	10	7	15	18
$y = 2$	14	14	8	22	22
$y = 3$	7	12	9	16	17
$y = 4$	5	10	7	9	14

Use the four-point central difference formula for $\dfrac{\partial^2 u}{\partial y \partial x}$ to evaluate this derivative at the point $(2, 3)$.

8.15 Use Lagrange polynomials to develop a difference formula for the second derivative of a function that is specified by a discrete set of data points with unequal spacing. The formula determines the second derivative at point (x_i, y_i) using points (x_{i-1}, y_{i-1}), (x_i, y_i), and (x_{i+1}, y_{i+1}).

8.16 Using Lagrange polynomials, develop a difference formula for the third derivative of a function that is specified by a discrete set of data points. The formula determines the third derivative at point (x_i, y_i) using points (x_{i-1}, y_{i-1}), (x_i, y_i), (x_{i+1}, y_{i+1}), and (x_{i+2}, y_{i+2}). The points are spaced such that $x_i - x_{i-1} = x_{i+2} - x_{i+1} = h$ and $x_{i+1} - x_i = 2h$.

Problems to be programmed in MATLAB
Solve the following problems using MATLAB environment.

8.17 Write a MATLAB user-defined function that determines the first derivative of a function that is given by a set of discrete points with equal spacing. For the function name use `yd = FirstDeriv(x,y)`. The input arguments `x` and `y` are vectors with the coordinates of the points, and the output argument `yd` is a vector with the values of the derivative at each point. At the first and last points, the function should calculate the derivative with the three-point forward and backward difference formulas, respectively. At all the other points `FirstDeriv` should use the two-point central difference formula. Use `FirstDeriv` to calculate the derivative of the function that is given in Problem 8.1.

8.18 Write a MATLAB user-defined function that calculates the second derivative of a function that is given by a set of discrete data points with equal spacing. For the function name and arguments use `ydd=SecDeriv(x,y)`, where the input arguments `x` and `y` are vectors with the coordinates of the points, and `ydd` is a vector with the values of the second derivative at each point. For calculating the second derivative, the function `SecDeriv` should use the finite difference formulas that have a truncation error of $O(h^2)$. Use `SecDeriv` for calculating the second derivative of the function that is given by the following set of points:

x	–1	–0.5	0	0.5	1	1.5	2	2.5	3	3.5	4	4.5
$f(x)$	–3.632	–0.3935	1	0.6487	–1.282	–4.518	–8.611	–12.82	–15.91	–15.88	–9.402	9.017

8.19 Write a MATLAB user-defined function that determines the first and second derivatives of a function that is given by a set of discrete points with equal spacing. For the function name use `[yd,ydd] = FrstScndDeriv(x,y)`. The input arguments `x` and `y` are vectors with the coordinates of the points, and the output arguments `yd` and `ydd` are vectors with the values of the first and second derivatives, respectively, at each point. For calculating both derivatives, the function should use the finite difference formulas that have a truncation error of $O(h^2)$.

(*a*) Use the function `FrstScndDeriv` to calculate the derivatives of the function that is given by the data in Problem 8.18.

(*b*) Modify the function (rename it `FrstScndDerivPt`) such that it also creates three plots (one page in a column). The top plot should be of the function, the second plot of the first derivative, and the third of the second derivative. Apply the function `FrstScndDerivPt` to the data in Problem 8.18.

8.20 Write a MATLAB user-defined function that determines the first derivative of a function that is given in an analytical form. For the function name and arguments use `dfx = DiffAnaly(Fun,xi)`. `Fun` is a name for the function that is being differentiated. It is a dummy name for the function that is imported into `DiffAnaly`. The actual function that is differentiated should be written as an anonymous function, or as a user-defined function, that calculates the values of $f(x)$ for given values of x. It is entered as a function handle when `DiffAnaly` is used. `xi` is the value of x where the derivative is calculated. The user-defined function should calculate the derivative by using the two-point central difference formula. In the formula, the values of (x_{i+1}) and (x_{i-1}) should be taken to be 5% higher and 5% lower than the value of (x_i), respectively.

(*a*) Use `DiffAnaly` to calculate the first derivative of $f(x) = e^x \ln x$ at $x = 2$.

(*b*) Use `DiffAnaly` to calculate the first derivative of the function from Problem 8.12 at $x = 2$.

8.21 Modify the MATLAB user-defined function in Problem 8.20 to include Richardson's extrapolation. The function should calculate a first estimate for the derivative as described in Problem 8.20, and a second estimate by taking the values of (x_{i+1}) and (x_{i-1}) to be 2.5% higher and 2.5% lower than the value of (x_i), respectively. The two estimates should then be used with Richardson's extrapolation for calculating the derivative. For the function name and arguments use `dfx=DiffRichardson(Fun,xi)`.

(*a*) Use the function to calculate the derivative of $f(x) = e^x \ln x$ at $x = 2$.
(*b*) Use the function to calculate the first derivative of the function that is given in Problem 8.12 at $x = 2$.

8.22 Write a MATLAB user-defined function that calculates the second derivative of a function that is given in an analytical form. For the function name and arguments use `ddfx = DDiffAnaly(Fun,xi)`. `Fun` is a name for the function that is being differentiated. It is a dummy name for the function that is imported into `DiffAnaly`. The actual function that is differentiated should be written as an anonymous function, or as a user-defined function, that calculates the values of $f(x)$ for given values of x. It is entered as a function handle when `DiffAnaly` is used. `xi` is the value of x where the second derivative is calculated. The function should calculate the second derivative with the three-point central difference formula. In the formula, the values of (x_{i+1}) and (x_{i-1}) should be taken to be 5% higher and 5% lower than the value of (x_i), respectively.

(*a*) Use the function to calculate the second derivative of $f(x) = 2^x/x$ at $x = 2$.
(*b*) Use the function to calculate the second derivative of the function that is given in Problem 8.12 at $x = 2$.

8.23 Write a MATLAB user-defined function that evaluates the first derivative of a function that is given by a set of discrete points with unequal spacing. For the function name use `yd = FirstDerivUneq(x,y)`. The input arguments `x` and `y` are vectors with the coordinates of the points, and the output argument `yd` is a vector with the values of the first derivative at each point. The differentiation is done by using second-order Lagrange polynomials (Section 8.5). At the first and last points, the function should calculate the derivative with Eqs. (8.35) and (8.37), respectively. At all the other points the function should use Eq. (8.36). Use `FirstDerivUneq` to calculate the derivative of the function that is given by the following set of points:

x	–1	–0.6	–0.3	0	0.5	0.8	1.6	2.5	2.8	3.2	3.5	4
$f(x)$	–3.632	–0.8912	0.3808	1.0	0.6487	–0.3345	–5.287	–12.82	–14.92	–16.43	–15.88	–9.402

8.24 Write a MATLAB user-defined function that evaluates the second derivative of a function that is given by a set of discrete data points with unequal spacing. For the function name use `yd = SndDerivUneq(x,y)`. The input arguments `x` and `y` are vectors with the coordinates of the points, and the output argument `yd` is a vector with the values of the second derivative at each point. Use the following scheme for the differentiation. Write a third-order Lagrange polynomial $f(x)$ for four points (x_{i-1}), (x_i), (x_{i+1}), and (x_{i+2}), and derive formulas for the second derivative of the polynomial at each of the four points. `SndDerivUneq` uses the formula for $f''(x_{i-1})$ for calculating the second derivative at the first data point, and the formula for $f''(x_{i+2})$ and $f''(x_{i+1})$ for calculating the second derivative at the last data point and one point before the last, respectively. The formula for $f''(x_i)$ is used in all the points in between. Use the function to calculate the second derivative of the function that is given by the following set of points:

x	–1	–0.6	–0.3	0	0.5	0.8	1.6	2.5	2.8	3.2	3.5	4
$f(x)$	–3.632	–0.8912	0.3808	1.0	0.6487	–0.3345	–5.287	–12.82	–14.92	–16.43	–15.88	–9.402

8.25 Write a MATLAB user-defined function that evaluates the partial first derivatives $\frac{\partial f}{\partial x}$ and $\frac{\partial f}{\partial y}$ of a function $f(x, y)$ that is specified by discrete tabulated points with equal spacing. Use two-point central difference formulas at the interior points and one-sided three-point forward and backward difference formulas at the endpoints. For the function name use `[dfdx,dfdy]= ParDer(x,y,f)`. The input arguments `x` and `y` are vectors with the values of the independent variables. `f` is a vector with the value of f at each point. The output arguments `dfdx` and `dfdy` are vectors with the values of the partial derivatives at each point. Use `ParDer` to calculate the partial derivatives with respect to x and y of the function given in Problem 8.14.

8.26 Write a MATLAB user-defined function that evaluates the partial second derivatives $\frac{\partial^2 f}{\partial x^2}$ and $\frac{\partial^2 f}{\partial y^2}$ of a function $f(x, y)$ that is specified by discrete tabulated points with equal spacing. Use three-point central difference formulas for the interior points and one-sided four-point forward and backward difference formulas for the end points. For the function name use `[dfdx2,dfdy2]= ParDerSnd(x,y,f)`. The input arguments `x` and `y` are vectors with the values of the independent variables. `f` is a vector with the value of f at each point. The output arguments `dfdx2` and `dfdy2` are vectors with the values of the partial second derivatives at each point. Use `ParDerSnd` to calculate the partial second derivatives with respect to x and y of the function given in Problem 8.14.

Problems in math, science, and engineering

Solve the following problems using MATLAB environment. As stated, use the MATLAB programs that are presented in the chapter, programs developed in previously solved problems, or MATLAB's built-in functions.

8.27 The following data is obtained for the velocity of a vehicle during a crash test.:

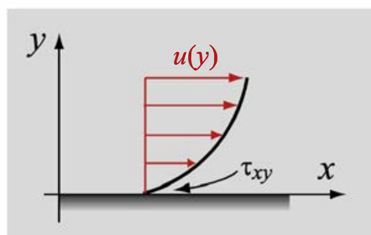
t (ms)	0	10	20	30	40	50	60	70	80
v (mph)	30	29.5	28	23	10	5	2	0.5	0

If the vehicle weight is 2,400 lb, determine the instantaneous force F acting on the vehicle during the crash. The force can be calculated by $F = m\frac{dv}{dt}$, and the mass of the car m is $2400/32.2$ slug. Note that 1 ms = 10^{-3} s and 1 mile = 5,280 ft.

(*a*) Solve by using the user-defined function `FirstDeriv` that was written in Problem 8.17.

(*b*) Solve by the using MATLAB built-in function `diff`.

8.28 The distribution of the x-component of the velocity u of a fluid near a flat surface is measured as a function of the distance y from the surface:



y (m)	0	0.002	0.004	0.006	0.008
u (m/s)	0	0.005	0.008	0.017	0.022

The shear stress τ_{yx} in the fluid is described by Newton's equation:

$$\tau_{yx} = \mu\frac{\partial u}{\partial y}$$

where μ is the coefficient of dynamic viscosity. The viscosity can be thought of as a measure of the internal friction within the fluid. Fluids that obey Newton's constitutive equation are called Newtonian fluids. Calculate the shear stress at $y = 0$ using (*i*) the two-point forward, and (*ii*) the three-point forward approximations for the derivative. Take $\mu = 0.00516$ N-s/m^2.

8.29 The refractive index n (how much the speed of light is reduced) of fused silica at different wavelengths λ is displayed in the table.

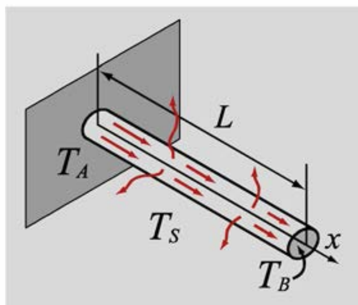
λ (μm)	0.2	0.25	0.3	0.36	0.45	0.6	1.0	1.6	2.2	3.37
n	1.551	1.507	1.488	1.475	1.466	1.458	1.450	1.443	1.435	1.410

Use the data to calculate the dispersion (spreading of light beam) defined by $\frac{dn}{d\lambda}$ at each wavelength.

(*a*) Use the user-defined function `FirstDerivUneq` written in Problem 8.23.
(*b*) Use MATLAB's built-in function `diff`.

8.30 A fin is an extended surface used to transfer heat from a base material (at $x = 0$) to an ambient. Heat flows from the base material through the base of the fin, through its outer surface, and through the tip. Measurement of the temperature distribution along a pin fin gives the following data:

x (cm)	0	1	2	3	4	5	6	7	8	9	10
T (K)	473	446.3	422.6	401.2	382	364.3	348.0	332.7	318.1	304.0	290.1



The fin has a length $L = 10$ cm, constant cross-sectional area of 1.6×10^{-5} m^2, and thermal conductivity $k = 240$ W/m/K. The heat flux (W/m^2) is given by $q_x = -k\frac{dT}{dx}$

(*a*) Determine the heat flux at $x = 0$. Use the three-point forward difference formula for calculating the derivative.
(*b*) Determine the heat flux at $x = L$. Use the three-point backward difference formula for calculating the derivative.
(*c*) Determine the amount of heat (in W) lost between $x = 0$ and $x = L$. (The heat flow per unit time in Watts is the heat flux multiplied by the cross-sectional area of the fin.)

8.31 The altitude of the space shuttle during the first two minutes of its ascent is displayed in the following table (www.nasa.gov):

t (s)	0	10	20	30	40	50	60	70	80	90	100	110	120
h (m)	–8	241	1,244	2,872	5,377	8,130	11,617	15,380	19,872	25,608	31,412	38,309	44,726

Assuming the shuttle is moving straight up, determine its velocity and acceleration at each point. Display the results in three plots (h versus time, velocity versus time, and acceleration versus time).

(*a*) Solve by using the user-defined function `FrstScndDerivPt` that was written in Problem 8.19.
(*b*) Solve by using the MATLAB built-in function `diff`.

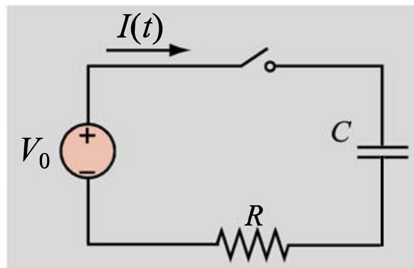
8.32 The position of an airplane at 5 s intervals as it accelerates on the runway is given in the following table:

t (s)	0	5	10	15	20	25	30	35	40
d (ft)	0	20	53	295	827	1437	2234	3300	4658

Write a MATLAB program in a script file that first determines the airplane's velocity ($v = \frac{dh}{dt}$) and the acceleration ($a = \frac{dv}{dt}$) at each point. Display the results in three plots (*d* versus time, velocity (in mph) versus time, and acceleration (in ft/s^2) versus time).
(*a*) Solve by using the user-defined function `FirstDeriv` that was written in Problem 8.17.
(*b*) Solve by using the MATLAB built-in function `diff`.

8.33 Use the user-defined function `FrstScndDeriv` written in Problem 8.19 to calculate the velocity and the acceleration of the airplane in Problem 8.32. Display the results in three plots (*h* versus time, velocity versus time, and acceleration versus time).

8.34 The charge on the capacitor in the RC circuit shown at various times after the switch is closed at time $t = 0$ is given in the following table. The current, *I*, as a function of time is given by $I(t) = \frac{dQ}{dt}$. Determine the current as a function of time by numerically differentiating the data.
(*a*) Use the user-defined function `FirstDerivUneq` that was written in Problem 8.23.
(*b*) Use the MATLAB built-in function `diff`.
In both parts plot *I* versus *t*.



$Q \times 10^6$ (C)	0	340	584	759	884	973	1038	1084	1117	1140	1157
t (ms)	0	50	100	150	200	250	300	350	400	450	500
$Q \times 10^6$ (C)	1169	1178	1184	1189	1192	1194	1196	1197	1198	1199	
t (ms)	550	600	650	700	750	800	850	900	950	1000	

8.35 The following data for mean velocity $\bar{u}$ near the wall in a fully developed turbulent pipe air flow was measured [J. Laufer, "The Structure of Turbulence in Fully Developed Pipe Flow," U.S. National Advisory Committee for Aeronautics (NACA), Technical Report 1174, 1954]:

y/R	0.0030	0.0034	0.0041	0.0051	0.0055	0.0061	0.0071	0.0075	0.0082
$\bar{u}/U$	0.140	0.152	0.179	0.221	0.228	0.264	0.300	0.318	0.343

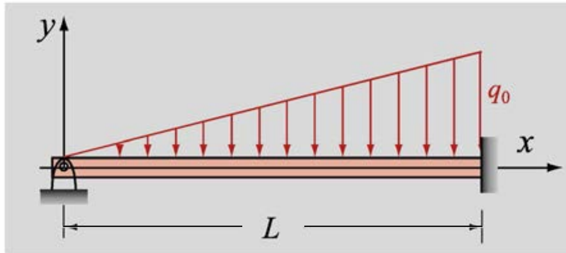
y is the distance from the wall, $R = 4.86$ in. is the radius of the pipe, and $U = 9.8$ ft/s. Use the data to calculate the shear stress τ defined by $\tau = \mu\frac{d\bar{u}}{dy} = \mu\frac{U}{R}\frac{d(\bar{u}/U)}{d(y/R)}$. $\mu = 3.8\times10^{-7}$ lb-s/ft^2 is the dynamic viscosity. Note that τ will have units of lb/ft^2.

(*a*) Use the user-defined function `FirstDerivUneq` written in Problem 8.23.

(*b*) Use MATLAB's built-in function `diff`.

8.36 A 30-ft-long uniform beam is simply supported at the left end and clamped at the right end. The beam is subjected to the triangular load shown. The deflection of the beam is given by the differential equation:

$$\frac{d^2y}{dx^2} = \frac{M(x)}{EI}$$

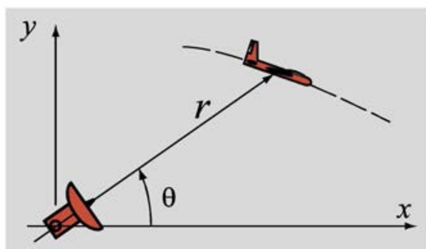


where y is the deflection, x is the coordinate measured along the length of the beam, $M(x)$ is the bending moment, $E = 29\times10^6$ psi is the elastic modulus, and $I = 720$ in^4 is its moment of inertia. The following data is obtained from measuring the deflection of the beam versus position:

x (in)	0	24	48	72	96	120	144	168
y (in)	0	–0.111	–0.216	–0.309	–0.386	–0.441	–0.473	–0.479
x (in)	192	216	240	264	288	312	336	360
y (in)	–0.458	–0.412	–0345	–0.263	–0.174	–0.090	–0.026	0

Using the data, determine the bending moment $M(x)$ at each location x. Solve the problem by using the user-defined function `SecDeriv` written in Problem 8.18. Make a plot of the bending moment diagram

8.37 A radar station is tracking the motion of an aircraft. The recorded distance to the aircraft, r, and the angle θ during a period of 60 s is given in the following table. The magnitude of the instantaneous velocity and acceleration of the aircraft can be calculated by:



$$v = \sqrt{\left(\frac{dr}{dt}\right)^2 + \left(r\frac{d\theta}{dt}\right)^2} \qquad a = \sqrt{\left[\frac{d^2r}{dt^2} - r\left(\frac{d\theta}{dt}\right)^2\right]^2 + \left[r\frac{d^2\theta}{dt^2} + 2\frac{dr}{dt}\frac{d\theta}{dt}\right]^2}$$

Determine the magnitudes of the velocity and acceleration at the times given in the table. Plot the velocity and acceleration versus time (two separate plots on the same page). Solve the problem by writing a program in a script file. The program evaluates the various derivatives that are required for calculating the velocity and acceleration, and then makes the plots. For calculating the derivatives use

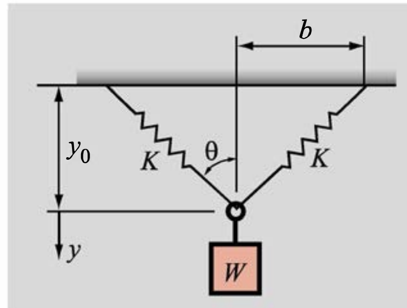
(*a*) the user-defined function `FrstScndDeriv` that was written in Problem 8.19;

(*b*) MATLAB's built-in function `diff`.

t (s)	0	4	8	12	16	20	24	28
r (km)	18.803	18.861	18.946	19.042	19.148	19.260	19.376	19.495

θ(rad)	0.7854	0.7792	0.7701	0.7594	0.7477	0.7350	0.7215	0.7073
t (s)	32	36	40	44	48	52	56	60
r (km)	19.617	19.741	19.865	19.990	20.115	20.239	20.362	20.484
θ(rad)	0.6925	0.6771	0.6612	0.6448	0.6280	0.6107	0.5931	0.5750

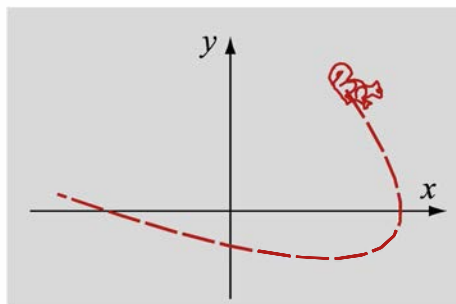
8.38 A scale is made of two springs ($K = 3$ lb/in.) as shown in the figure ($y = 3$ in., $b = 4$ in.). With no weight on the scale $y = 0$ and the length of the spring L_0 is given by $L_0 = \sqrt{b^2 + y_0^2}$. As weights are placed on the scale, it moves down a distance y and the length of the spring L is given by $L = \sqrt{b^2 + (y_0 + y)^2}$. The force in each spring is $F_s = K(L - L_0)$, and the relationship between W and F_s is $W = 2F\cos\theta$. The equivalent spring constant of the scale K_{eq} is given by $K_{eq} = \frac{dW}{dy}$. Derive an expression for K_{eq} as in terms of y and determine the derivative K_{eq} numerically for $0 \le y \le 2$ in. Make a plot of K_{eq} versus y.



(*a*) Determine the derivative by using the user-defined function `FirstDeriv` that was written in Problem 8.17.

(*b*) Determine the derivative by using MATLAB's built-in function `diff`.

8.39 The position of a squirrel (x and y coordinates) running around as a function of time, t, is given in the table that follows. The velocity of the squirrel, v, is given by $v = \sqrt{v_x^2 + v_y^2}$, where $v_x = \frac{dx}{dt}$ and $v_y = \frac{dy}{dt}$. The acceleration of the squirrel, a, is given by $a = \sqrt{a_x^2 + a_y^2}$, where $a_x = \frac{d^2x}{dt^2}$ and $a_y = \frac{d^2y}{\partial t^2}$. Write a MATLAB program in a script file that



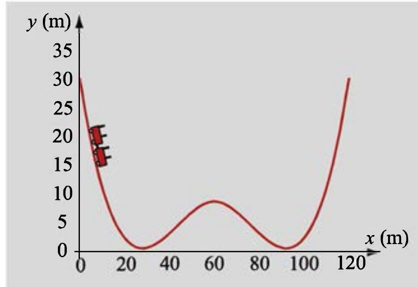
(*a*) determines v and a by using the user-defined function `FrstScndDeriv` that was written in Problem 8.19;

(*b*) displays a figure with plots of v_x, v_y and v as a function of time (three plots in one figure);

(*c*) displays a second figure with plots of a_x, a_y and a as a function of time (three plots in one figure).

t (s)	0	2	4	6	8	10	12	14
x (m)	61	72.8	81.9	87.9	90.9	90.8	87.3	80.5
y (m)	65	46.7	30.3	15.8	3.2	–7.4	–15.8	–22.1
t (s)	16	18	20	22	24	26	28	30
x (m)	70.4	56.9	39.9	19.4	–4.6	–32.2	–63.3	–98
y (m)	–26.2	–28.1	–27.9	–25.3	–20.5	–13.4	–4.1	7.6

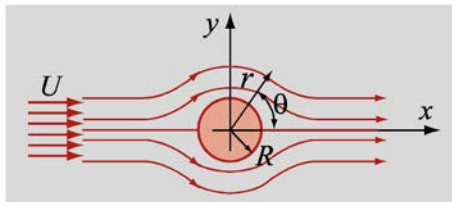
8.40 The position of the roller coaster cars (x and y coordinates) as a function of time, t, is given in the table that follows. Determine the velocity, v, given by $v = \sqrt{v_x^2 + v_y^2}$, where $v_x = \frac{dx}{dt}$ and $v_y = \frac{dy}{dt}$, and the acceleration, a, given by $a = \sqrt{a_x^2 + a_y^2}$, where $a_x = \frac{d^2x}{dt^2}$ and $a_y = \frac{d^2y}{\partial t^2}$ of the cars. Write a MATLAB program in a script file that:



(*a*) Determines v and a as a function of time. (The user-defined functions `FirstDerivUneq` and `SndDerivUneq` can be used if Problems 8.23 and 8.24 were solved.)
(*b*) Displays plots of y versus x, v versus x, and a versus x. (Three figures on one page.)

t (s)	0	1	2	2.5	3	3.5	4	4.5	5	5.5	6	7	8
x (m)	0	4.1	14.9	25.4	37.5	48.4	59	69.6	80.3	92.2	103.5	115.3	119.8
y (m)	31.6	22.3	7.1	2	3.54	7.6	10	8.2	4.3	1.8	5.7	21.2	31.1

8.41 The nondimensional stream function $\frac{\Psi}{UR}$ for potential flow over a cylinder of radius R in an incompressible flow of uniform velocity U is given in the following table as a function of the nondimensional coordinate r/R and the polar angle θ. The nondimensional radial component u_r/U and the azimuthal component u_θ/U of the velocity are given by:



$$\frac{u_r}{U} = \frac{1}{(r/R)} \frac{\partial\left(\frac{\Psi}{UR}\right)}{\partial\theta} \quad \text{and} \quad \frac{u_\theta}{U} = -\frac{\partial\left(\frac{\Psi}{UR}\right)}{\partial(r/R)}$$

Calculate u_r/U and u_θ/U at every point. Write a MATLAB program that uses two-point central difference formulas at the interior points and one-sided three-point forward and backward difference formulas at the endpoints. The user-defined function `ParDer` can be used instead if Problem 8.25 was solved.

	θ=0°	θ=36°	θ=72°	θ=108°	θ=144°	θ=180°	θ=216°	θ=252°	θ=288°	θ=324°	θ=360°
r/R=0.2	0	–2.8214	-4.5651	–4.5651	–2.8214	0	2.8214	4.5651	4.5651	2.8214	0
r/R=0.6	0	–0.6270	–1.0145	–1.014	–0.6270	0	0.6270	1.0145	1.0145	0.6270	0
r/R=1.0	0	0	0	0	0	0	0	0	0	0	0
r/R=1.4	0	0.4031	0.6522	0.6522	0.4031	0	–0.4031	–0.6522	–0.6522	–0.4031	0
r/R=1.8	0	0.7315	1.1835	1.1835	0.7315	0	–0.7315	–1.1835	–1.1835	–0.7315	0
r/R=2.2	0	1.0260	1.6600	1.6600	1.0260	0	–1.0260	–1.6600	–1.6600	–1.0260	0
r/R=2.6	0	1.3022	2.1070	2.1070	1.3022	0	–1.3022	–2.1070	–2.1070	–1.3022	0
r/R=3.0	0	1.5674	2.5362	2.5362	1.5674	0	–1.5674	–2.5362	–2.5362	–1.5674	0