PART SIX

NUMERICAL DIFFERENTIATION AND INTEGRATION

PT6.1 MOTIVATION

Calculus is the mathematics of change. Because engineers must continuously deal with systems and processes that change, calculus is an essential tool of our profession. Standing at the heart of calculus are the related mathematical concepts of differentiation and integration.

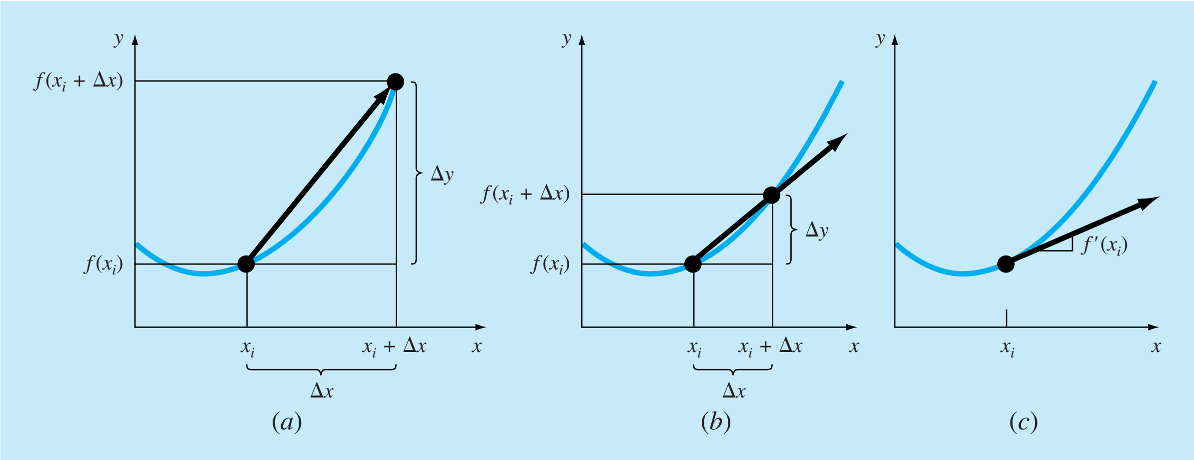
According to the dictionary definition, to *differentiate* means "to mark off by differences; distinguish; . . . to perceive the difference in or between." Mathematically, the *derivative,* which serves as the fundamental vehicle for differentiation, represents the rate of change of a dependent variable with respect to an independent variable. As depicted in Fig. PT6.1, the mathematical definition of the derivative begins with a difference approximation:

$$\frac{\Delta y}{\Delta x} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x} \tag{PT6.1}$$

where y and $f(x)$ are alternative representatives for the dependent variable and x is the independent variable. If Δx is allowed to approach zero, as occurs in moving from Fig. PT6.1a to c, the difference becomes a derivative

$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

FIGURE PT6.1
The graphical definition of a derivative: as Δx approaches zero in going from (a) to (c), the difference approximation becomes a derivative.



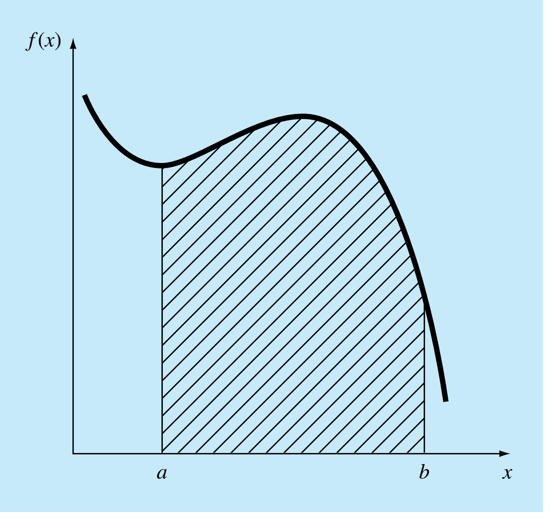


FIGURE PT6.2
Graphical representation of the integral of $f(x)$ between the limits $x = a$ to b. The integral is equivalent to the area under the curve.

where dy/dx [which can also be designated as y' or $f'(x_i)$] is the first derivative of y with respect to x evaluated at x_i. As seen in the visual depiction of Fig. PT6.1c, the derivative is the slope of the tangent to the curve at x_i.

The inverse process to differentiation in calculus is integration. According to the dictionary definition, to *integrate* means "to bring together, as parts, into a whole; to unite; to indicate the total amount . . . ." Mathematically, integration is represented by

$$I = \int_a^b f(x)\,dx \tag{PT6.2}$$

which stands for the integral of the function $f(x)$ with respect to the independent variable x, evaluated between the limits $x = a$ to $x = b$. The function $f(x)$ in Eq. (PT6.2) is referred to as the *integrand.*

As suggested by the dictionary definition, the "meaning" of Eq. (PT6.2) is the *total value,* or *summation,* of $f(x)\,dx$ over the range $x = a$ to b. In fact, the symbol $\int$ is actually a stylized capital S that is intended to signify the close connection between integration and summation.

Figure PT6.2 represents a graphical manifestation of the concept. For functions lying above the x axis, the integral expressed by Eq. (PT6.2) corresponds to the area under the curve of $f(x)$ between $x = a$ and b.[1]

As outlined above, the "marking off" or "discrimination" of differentiation and the "bringing together" of integration are closely linked processes that are, in fact, inversely

[1]It should be noted that the process represented by Eq. (PT6.2) and Fig. PT6.2 is called *definite integration.* There is another type called indefinite integration in which the limits a and b are unspecified. As will be discussed in Part Seven, *indefinite integration* deals with determining a function whose derivative is given.

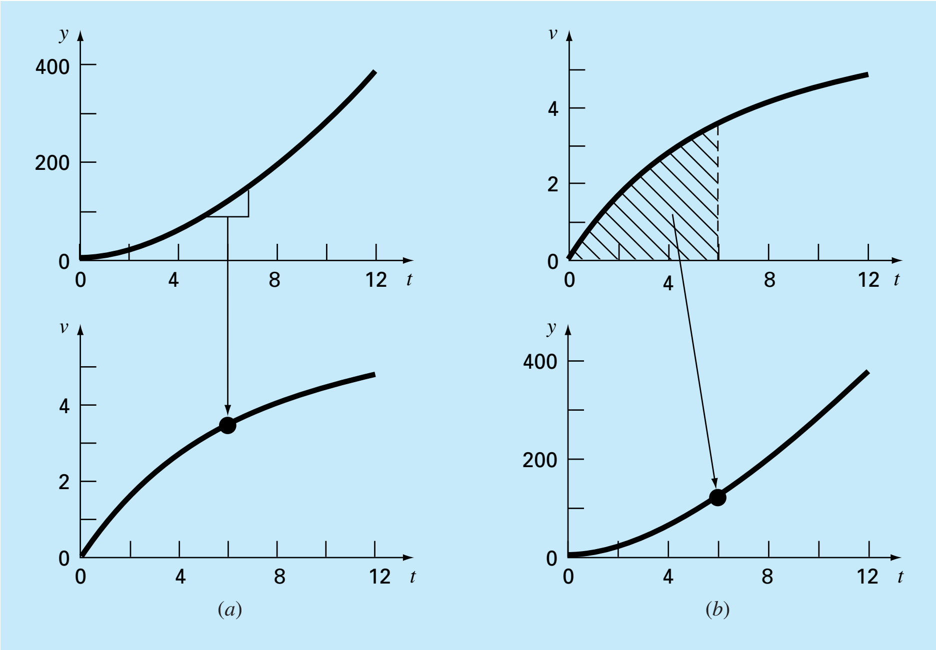


FIGURE PT6.3
The contrast between (*a*) differentiation and (*b*) integration.

related (Fig. PT6.3). For example, if we are given a function $y(t)$ that specifies an object's position as a function of time, differentiation provides a means to determine its velocity, as in (Fig. PT6.3*a*).

$$v(t) = \frac{d}{dt} y(t)$$

Conversely, if we are provided with velocity as a function of time, integration can be used to determine its position (Fig. PT6.3*b*),

$$y(t) = \int_0^t v(t)\, dt$$

Thus, we can make the general claim that the evaluation of the integral

$$I = \int_a^b f(x)\, dx$$

is equivalent to solving the differential equation

$$\frac{dy}{dx} = f(x)$$

for $y(b)$ given the initial condition $y(a) = 0$.

Because of this close relationship, we have opted to devote this part of the book to both processes. Among other things, this will provide the opportunity to highlight their similarities and differences from a numerical perspective. In addition, our discussion will have relevance to the next parts of the book where we will cover differential equations.

PT6.1.1 Noncomputer Methods for Differentiation and Integration

The function to be differentiated or integrated will typically be in one of the following three forms:

1. A simple continuous function such as a polynomial, an exponential, or a trigonometric function.
2. A complicated continuous function that is difficult or impossible to differentiate or integrate directly.
3. A tabulated function where values of x and $f(x)$ are given at a number of discrete points, as is often the case with experimental or field data.

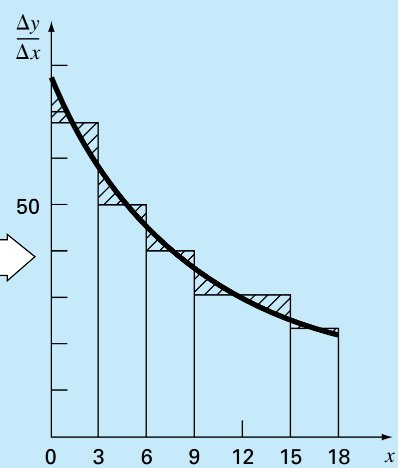
In the first case, the derivative or integral of a simple function may be evaluated analytically using calculus. For the second case, analytical solutions are often impractical, and sometimes impossible, to obtain. In these instances, as well as in the third case of discrete data, approximate methods must be employed.

A noncomputer method for determining derivatives from data is called *equal-area graphical differentiation.* In this method, the (x, y) data are tabulated and, for each interval, a simple divided difference $\Delta y/\Delta x$ is employed to estimate the slope. Then these values are plotted as a stepped curve versus x (Fig. PT6.4). Next, a smooth curve is drawn that attempts to approximate the area under the stepped curve. That is, it is drawn so that visually, the positive and negative areas are balanced. The rates at given values of x can then be read from the curve.

In the same spirit, visually oriented approaches were employed to integrate tabulated data and complicated functions in the precomputer era. A simple intuitive approach is to plot the function on a grid (Fig. PT6.5) and count the number of boxes that approximate the area. This number multiplied by the area of each box provides a rough estimate of the total

x	y	$\Delta y/\Delta x$
0	0	
		66.7
3	200	
		50
6	350	
		40
9	470	
		30
15	650	
		23.3
18	720	

(*a*)



(*b*)

x	dy/dx
0	76.50
3	57.50
6	45.00
9	36.25
15	25.00
18	21.50

(*c*)

FIGURE PT6.4
Equal-area differentiation. (*a*) Centered finite divided differences are used to estimate the derivative for each interval between the data points. (*b*) The derivative estimates are plotted as a bar graph. A smooth curve is superimposed on this plot to approximate the area under the bar graph. This is accomplished by drawing the curve so that equal positive and negative areas are balanced. (*c*) Values of dy/dx can then be read off the smooth curve.

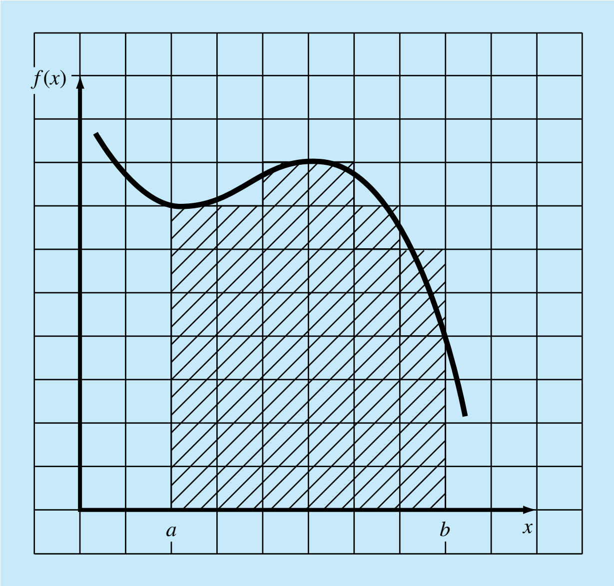


FIGURE PT6.5
The use of a grid to approximate an integral.

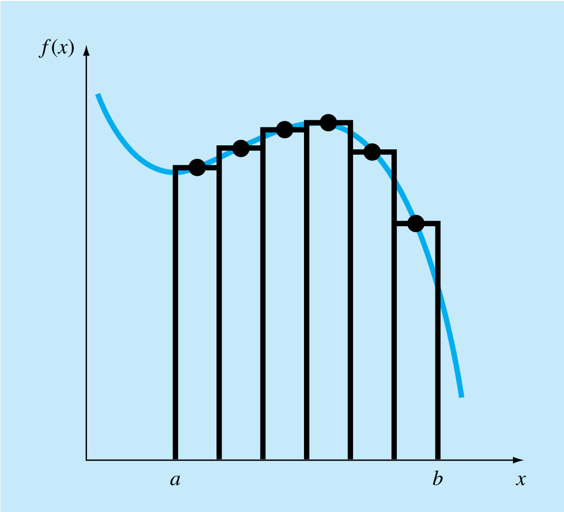


FIGURE PT6.6
The use of rectangles, or strips, to approximate the integral.

area under the curve. This estimate can be refined, at the expense of additional effort, by using a finer grid.

Another commonsense approach is to divide the area into vertical segments, or strips, with a height equal to the function value at the midpoint of each strip (Fig. PT6.6). The area of the rectangles can then be calculated and summed to estimate the total area. In this approach, it is assumed that the value at the midpoint provides a valid approximation of the average height of the function for each strip. As with the grid method, refined estimates are possible by using more (and thinner) strips to approximate the integral.

Although such simple approaches have utility for quick estimates, alternative numerical techniques are available for the same purpose. Not surprisingly, the simplest of these methods is similar in spirit to the noncomputer techniques.

For differentiation, the most fundamental numerical techniques use finite divided differences to estimate derivatives. For data with error, an alternative approach is to fit a smooth curve to the data with a technique such as least-squares regression and then differentiate this curve to obtain derivative estimates.

In a similar spirit, numerical integration or *quadrature* methods are available to obtain integrals. These methods, which are actually easier to implement than the grid approach, are similar in spirit to the strip method. That is, function heights are multiplied by strip widths and summed to estimate the integral. However, through clever choices of weighting factors, the resulting estimate can be made more accurate than that from the simple strip method.

As in the simple strip method, numerical integration and differentiation techniques utilize data at discrete points. Because tabulated information is already in such a form, it is naturally compatible with many of the numerical approaches. Although continuous functions are not originally in discrete form, it is usually a simple proposition to use the given equation to generate a table of values. As depicted in Fig. PT6.7, this table can then be evaluated with a numerical method.

PT6.1.2 Numerical Differentiation and Integration in Engineering

The differentiation and integration of a function has so many engineering applications that you were required to take differential and integral calculus in your first year at college. Many specific examples of such applications could be given in all fields of engineering.

Differentiation is commonplace in engineering because so much of our work involves characterizing the changes of variables in both time and space. In fact, many of the laws and other generalizations that figure so prominently in our work are based on the predictable ways in which change manifests itself in the physical world. A prime example is Newton's second law, which is not couched in terms of the position of an object but rather in its change of position with respect to time.

Aside from such temporal examples, numerous laws governing the spatial behavior of variables are expressed in terms of derivatives. Among the most common of these are those laws involving potentials or gradients. For example, *Fourier's law of heat conduction* quantifies the observation that heat flows from regions of high to low temperature. For the one-dimensional case, this can be expressed mathematically as

$$\text{Heat flux} = -k' \frac{dT}{dx}$$

Thus, the derivative provides a measure of the intensity of the temperature change, or *gradient,* that drives the transfer of heat. Similar laws provide workable models in many other areas of engineering, including the modeling of fluid dynamics, mass transfer, chemical reaction kinetics, and electromagnetic flux. The ability to accurately estimate derivatives is an important facet of our capability to work effectively in these areas.

(*a*)

$$\int_0^2 \frac{2 + \cos(1 + x^{3/2})}{\sqrt{1 + 0.5 \sin x}} \, e^{0.5x} \, dx$$

(*b*)

x	$f(x)$
0.25	2.599
0.75	2.414
1.25	1.945
1.75	1.993

(*c*)

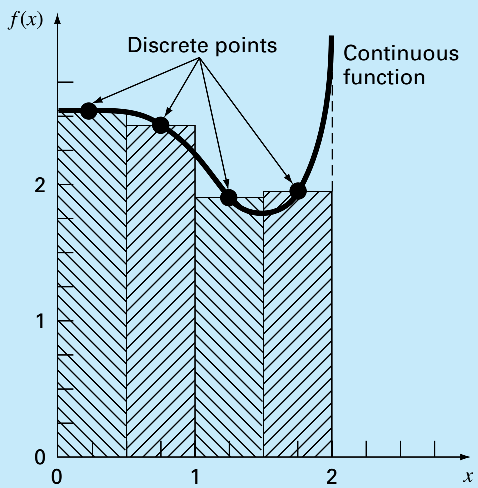


FIGURE PT6.7
Application of a numerical integration method: (*a*) A complicated, continuous function. (*b*) Table of discrete values of *f*(*x*) generated from the function. (*c*) Use of a numerical method (the strip method here) to estimate the integral on the basis of the discrete points. For a tabulated function, the data is already in tabular form (*b*); therefore, step (*a*) is unnecessary.

Just as accurate estimates of derivatives are important in engineering, the calculation of integrals is equally valuable. A number of examples relate directly to the idea of the integral as the area under a curve. Figure PT6.8 depicts a few cases where integration is used for this purpose.

Other common applications relate to the analogy between integration and summation. For example, a common application is to determine the mean of continuous functions. In Part Five, you were introduced to the concept of the mean of n discrete data points [recall Eq. (PT5.1)]:

$$\text{Mean} = \frac{\sum_{i=1}^{n} y_i}{n} \qquad \text{(PT6.3)}$$

where y_i are individual measurements. The determination of the mean of discrete points is depicted in Fig. PT6.9*a*.

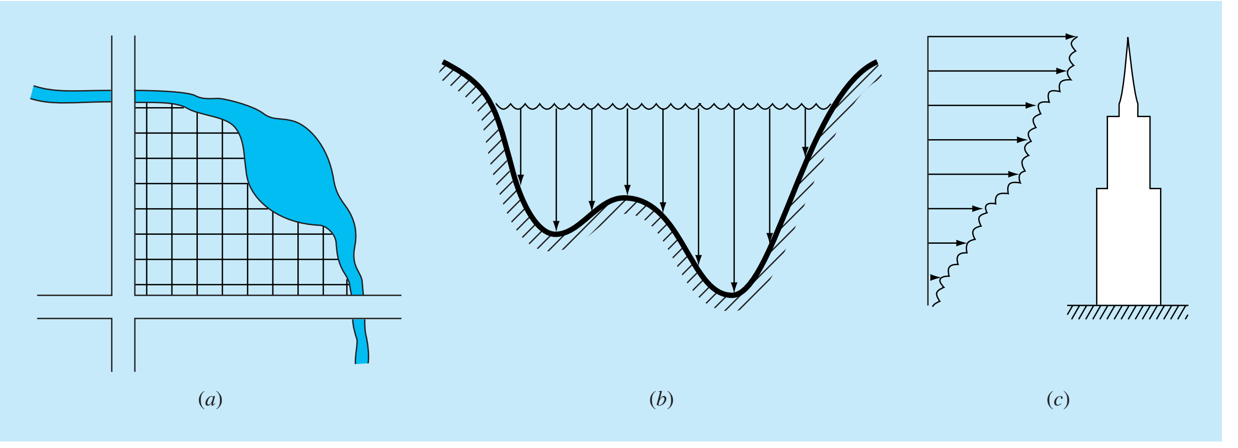
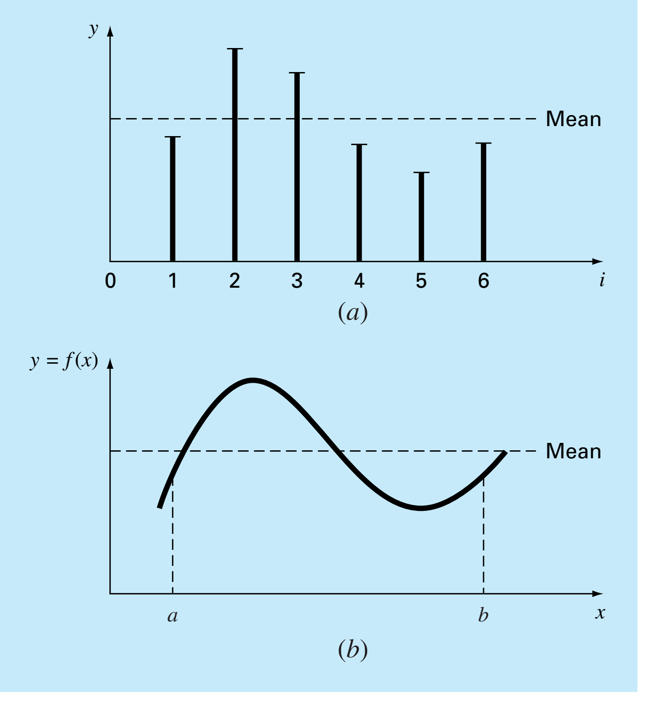


FIGURE PT6.8
Examples of how integration is used to evaluate areas in engineering applications. (*a*) A surveyor might need to know the area of a field bounded by a meandering stream and two roads. (*b*) A water-resource engineer might need to know the cross-sectional area of a river. (*c*) A structural engineer might need to determine the net force due to a nonuniform wind blowing against the side of a skyscraper.

FIGURE PT6.9
An illustration of the mean for (*a*) discrete and (*b*) continuous data.



In contrast, suppose that y is a continuous function of an independent variable x, as depicted in Fig. PT6.9b. For this case, there are an infinite number of values between a and b. Just as Eq. (PT6.3) can be applied to determine the mean of the discrete readings, you might also be interested in computing the mean or average of the continuous function $y = f(x)$ for the interval from a to b. Integration is used for this purpose, as specified by the formula

$$\text{Mean} = \frac{\int_a^b f(x)\,dx}{b-a} \tag{PT6.4}$$

This formula has hundreds of engineering applications. For example, it is used to calculate the center of gravity of irregular objects in mechanical and civil engineering and to determine the root-mean-square current in electrical engineering.

Integrals are also employed by engineers to evaluate the total amount or quantity of a given physical variable. The integral may be evaluated over a line, an area, or a volume. For example, the total mass of chemical contained in a reactor is given as the product of the concentration of chemical and the reactor volume, or

$$\text{Mass} = \text{concentration} \times \text{volume}$$

where concentration has units of mass per volume. However, suppose that concentration varies from location to location within the reactor. In this case, it is necessary to sum the products of local concentrations c_i and corresponding elemental volumes ΔV_i:

$$\text{Mass} = \sum_{i=1}^{n} c_i \,\Delta V_i$$

where n is the number of discrete volumes. For the continuous case, where $c(x, y, z)$ is a known function and x, y, and z are independent variables designating position in Cartesian coordinates, integration can be used for the same purpose:

$$\text{Mass} = \iiint c(x, y, z)\,dx\,dy\,dz$$

or

$$\text{Mass} = \iiint_V c(V)\,dV$$

which is referred to as a *volume integral.* Notice the strong analogy between summation and integration.

Similar examples could be given in other fields of engineering. For example, the total rate of energy transfer across a plane where the flux (in calories per square centimeter per second) is a function of position is given by

$$\text{Heat transfer} = \iint_A \text{flux}\,dA$$

which is referred to as an *areal integral,* where A = area.

Similarly, for the one-dimensional case, the total mass of a variable-density rod with constant cross-sectional area is given by

$$m = A \int_0^L \rho(x)\, dx$$

where m = total weight (kg), L = length of the rod (m), $\rho(x)$ = known density (kg/m^3) as a function of length x (m), and A = cross-sectional area of the rod (m^2).

Finally, integrals are used to evaluate differential or rate equations. Suppose the velocity of a particle is a known continuous function of time $v(t)$,

$$\frac{dy}{dt} = v(t)$$

The total distance y traveled by this particle over a time t is given by (Fig. PT6.3b)

$$y = \int_0^t v(t)\, dt \qquad \text{(PT6.5)}$$

These are just a few of the applications of differentiation and integration that you might face regularly in the pursuit of your profession. When the functions to be analyzed are simple, you will normally choose to evaluate them analytically. For example, in the falling parachutist problem, we determined the solution for velocity as a function of time [Eq. (1.10)]. This relationship could be substituted into Eq. (PT6.5), which could then be integrated easily to determine how far the parachutist fell over a time period t. For this case, the integral is simple to evaluate. However, it is difficult or impossible when the function is complicated, as is typically the case in more realistic examples. In addition, the underlying function is often unknown and defined only by measurement at discrete points. For both these cases, you must have the ability to obtain approximate values for derivatives and integrals using numerical techniques. Several such techniques will be discussed in this part of the book.

PT6.2 MATHEMATICAL BACKGROUND

In high school or during your first year of college, you were introduced to *differential* and *integral calculus.* There you learned techniques to obtain analytical or exact derivatives and integrals.

When we differentiate a function analytically, we generate a second function that can be used to compute the derivative for different values of the independent variable. General rules are available for this purpose. For example, in the case of the monomial

$$y = x^n$$

the following simple rule applies ($n \neq 0$):

$$\frac{dy}{dx} = nx^{n-1}$$

which is the expression of the more general rule for

$$y = u^n$$

where u = a function of x. For this equation, the derivative is computed via

$$\frac{dy}{dx} = nu^{n-1}\frac{du}{dx}$$

Two other useful formulas apply to the products and quotients of functions. For example, if the product of two functions of $x(u$ and $v)$ is represented as $y = uv$, then the derivative can be computed as

$$\frac{dy}{dx} = u\frac{dv}{dx} + v\frac{du}{dx}$$

For the division, $y = u/v$, the derivative can be computed as

$$\frac{dy}{dx} = \frac{v\dfrac{du}{dx} - u\dfrac{dv}{dx}}{v^2}$$

Other useful formulas are summarized in Table PT6.1.

Similar formulas are available for definite integration, which deals with determining an integral between specified limits, as in

$$I = \int_a^b f(x)\,dx \qquad \text{(PT6.6)}$$

According to the *fundamental theorem* of integral calculus, Eq. (PT6.6) is evaluated as

$$\int_a^b f(x)\,dx = F(x)\Big|_a^b$$

where $F(x)$ = the integral of $f(x)$—that is, any function such that $F'(x) = f(x)$. The nomenclature on the right-hand side stands for

$$F(x)\Big|_a^b = F(b) - F(a) \qquad \text{(PT6.7)}$$

TABLE PT6.1 Some commonly used derivatives.

$\frac{d}{dx}\sin x = \cos x$	$\frac{d}{dx}\cot x = -\csc^2 x$
$\frac{d}{dx}\cos x = -\sin x$	$\frac{d}{dx}\sec x = \sec x \tan x$
$\frac{d}{dx}\tan x = \sec^2 x$	$\frac{d}{dx}\csc x = -\csc x \cot x$
$\frac{d}{dx}\ln x = \frac{1}{x}$	$\frac{d}{dx}\log_a x = \frac{1}{x \ln a}$
$\frac{d}{dx}e^x = e^x$	$\frac{d}{dx}a^x = a^x \ln a$

An example of a definite integral is

$$I = \int_0^{0.8} (0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5)\, dx \qquad \text{(PT6.8)}$$

For this case, the function is a simple polynomial that can be integrated analytically by evaluating each term according to the rule

$$\int_a^b x^n\, dx = \left. \frac{x^{n+1}}{n+1} \right|_a^b \qquad \text{(PT6.9)}$$

where n cannot equal -1. Applying this rule to each term in Eq. (PT6.8) yields

$$I = 0.2x + 12.5x^2 - \frac{200}{3}x^3 + 168.75x^4 - 180x^5 + \left. \frac{400}{6}x^6 \right|_0^{0.8} \qquad \text{(PT6.10)}$$

which can be evaluated according to Eq. (PT6.7) as $I = 1.6405333$. This value is equal to the area under the original polynomial [Eq. (PT6.8)] between $x = 0$ and 0.8.

The foregoing integration depends on knowledge of the rule expressed by Eq. (PT6.9). Other functions follow different rules. These "rules" are all merely instances of *antidifferentiation,* that is, finding $F(x)$ so that $F'(x) = f(x)$. Consequently, analytical integration depends on prior knowledge of the answer. Such knowledge is acquired by training and

TABLE PT6.2 Some simple integrals that are used in Part Six. The a and b in this table are constants and should not be confused with the limits of integration discussed in the text.

$$\int u\, dv = uv - \int v\, du$$

$$\int u^n\, du = \frac{u^{n+1}}{n+1} + C \qquad n \neq -1$$

$$\int a^{bx}\, dx = \frac{a^{bx}}{b \ln a} + C \qquad a > 0,\ a \neq 1$$

$$\int \frac{dx}{x} = \ln |x| + C \qquad x \neq 0$$

$$\int \sin (ax + b)\, dx = -\frac{1}{a} \cos (ax + b) + C$$

$$\int \cos (ax + b)\, dx = \frac{1}{a} \sin (ax + b) + C$$

$$\int \ln |x|\, dx = x \ln |x| - x + C$$

$$\int e^{ax}\, dx = \frac{e^{ax}}{a} + C$$

$$\int xe^{ax}\, dx = \frac{e^{ax}}{a^2} (ax - 1) + C$$

$$\int \frac{dx}{a + bx^2} = \frac{1}{\sqrt{ab}} \tan^{-1} \frac{\sqrt{ab}}{a} x + C$$

experience. Many of the rules are summarized in handbooks and in tables of integrals. We list some commonly encountered integrals in Table PT6.2. However, many functions of practical importance are too complicated to be contained in such tables. One reason why the techniques in the present part of the book are so valuable is that they provide a means to evaluate relationships such as Eq. (PT6.8) without knowledge of the rules.

PT6.3 ORIENTATION

Before proceeding to the numerical methods for integration, some further orientation might be helpful. The following is intended as an overview of the material discussed in Part Six. In addition, we have formulated some objectives to help focus your efforts when studying the material.

PT6.3.1 Scope and Preview

Figure PT6.10 provides an overview of Part Six. *Chapter 21* is devoted to the most common approaches for numerical integration—the *Newton-Cotes formulas.* These relationships are based on replacing a complicated function or tabulated data with a simple polynomial that is easy to integrate. Three of the most widely used Newton-Cotes formulas are discussed in detail: the *trapezoidal rule, Simpson's 1/3 rule,* and *Simpson's 3/8 rule.* All these formulas are designed for cases where the data to be integrated is evenly spaced. In addition, we also include a discussion of numerical integration of unequally spaced data. This is a very important topic because many real-world applications deal with data that is in this form.

All the above material relates to closed integration, where the function values at the ends of the limits of integration are known. At the end of Chap. 21, we present *open integration formulas,* where the integration limits extend beyond the range of the known data. Although they are not commonly used for definite integration, open integration formulas are presented here because they are utilized extensively in the solution of ordinary differential equations in Part Seven.

The formulations covered in Chap. 21 can be employed to analyze both tabulated data and equations. *Chapter 22* deals with two techniques that are expressly designed to integrate equations and functions: *Romberg integration* and *Gauss quadrature.* Computer algorithms are provided for both of these methods. In addition, methods for evaluating *improper integrals* are discussed.

In *Chap. 23,* we present additional information on *numerical differentiation* to supplement the introductory material from Chap. 4. Topics include high-accuracy finite-difference formulas, Richardson's extrapolation, and the differentiation of unequally spaced data. The effect of errors on both numerical differentiation and integration is discussed. Finally, the chapter is concluded with a description of the application of several software packages and libraries for integration and differentiation.

Chapter 24 demonstrates how the methods can be applied for problem solving. As with other parts of the book, applications are drawn from all fields of engineering.

A review section, or *epilogue,* is included at the end of Part Six. This review includes a discussion of trade-offs that are relevant to implementation in engineering practice. In addition, important formulas are summarized. Finally, we present a short review of advanced

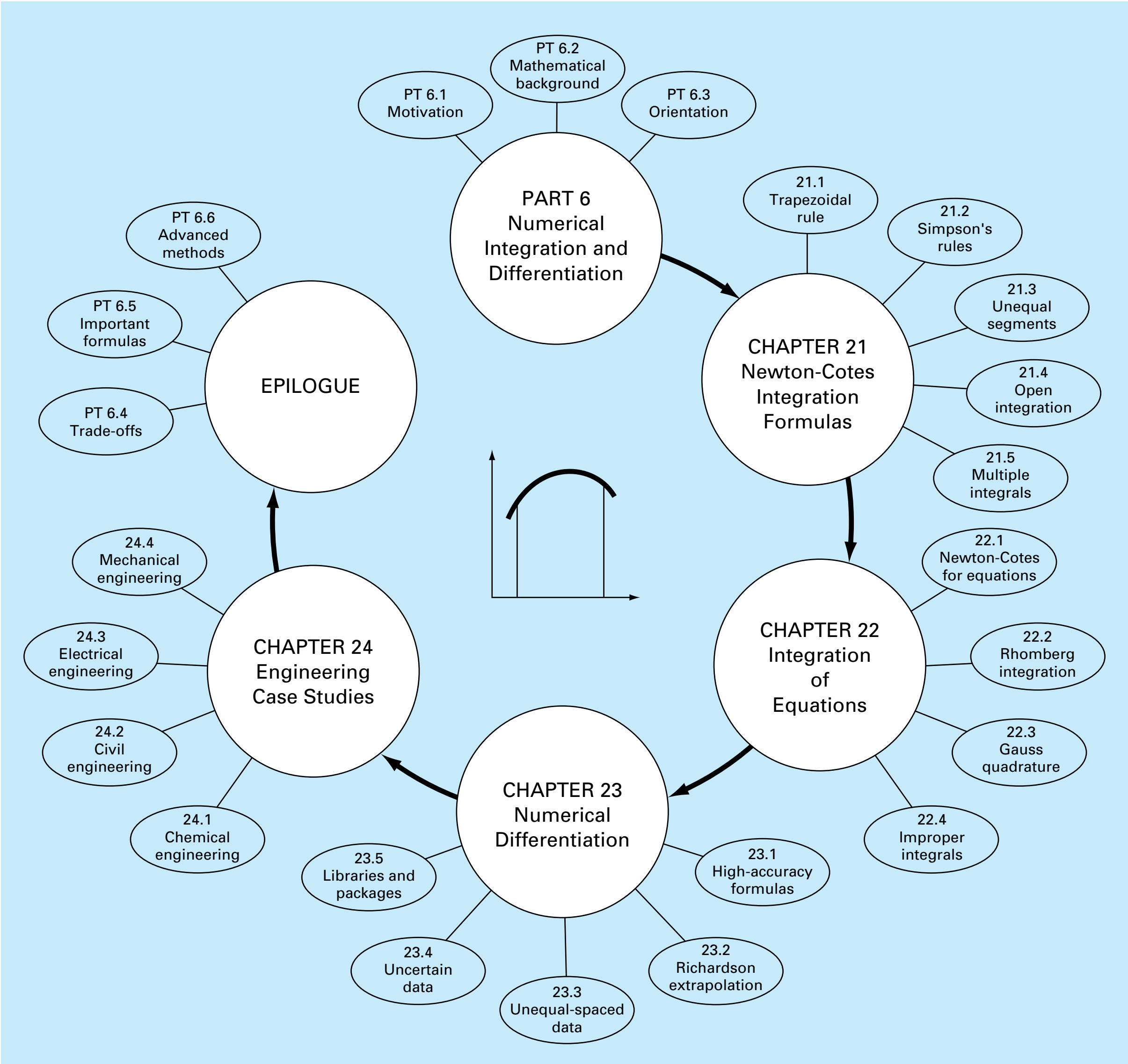


FIGURE PT6.10
Schematic of the organization of material in Part Six: Numerical Integration and Differentiation.

methods and alternative references that will facilitate your further studies of numerical differentiation and integration.

PT6.3.2 Goals and Objectives

Study Objectives. After completing Part Six, you should be able to solve many numerical integration and differentiation problems and appreciate their application for engineering

TABLE PT6.3 Specific study objectives for Part Six.

1. Understand the derivation of the Newton-Cotes formulas; know how to derive the trapezoidal rule and how to set up the derivation of both of Simpson's rules; recognize that the trapezoidal and Simpson's 1/3 and 3/8 rules represent the areas under first-, second-, and third-order polynomials, respectively.
2. Know the formulas and error equations for (*a*) the trapezoidal rule, (*b*) the multiple-application trapezoidal rule, (*c*) Simpson's 1/3 rule, (*d*) Simpson's 3/8 rule, and (*e*) the multiple-application Simpson's rule. Be able to choose the "best" among these formulas for any particular problem context.
3. Recognize that Simpson's 1/3 rule is fourth-order accurate even though it is based on only three points; realize that all the even-segment–odd-point Newton-Cotes formulas have similar enhanced accuracy.
4. Know how to evaluate the integral and derivative of unequally spaced data.
5. Recognize the difference between open and closed integration formulas.
6. Understand the theoretical basis of Richardson extrapolation and how it is applied in the Romberg integration algorithm and for numerical differentiation.
7. Understand the fundamental difference between Newton-Cotes and Gauss quadrature formulas.
8. Recognize why both Romberg integration and Gauss quadrature have utility when integrating equations (as opposed to tabular or discrete data).
9. Know how open integration formulas are employed to evaluate improper integrals.
10. Understand the application of high-accuracy numerical-differentiation formulas.
11. Know how to differentiate unequally spaced data.
12. Recognize the differing effects of data error on the processes of numerical integration and differentiation.

problem solving. You should strive to master several techniques and assess their reliability. You should understand the trade-offs involved in selecting the "best" method (or methods) for any particular problem. In addition to these general objectives, the specific concepts listed in Table PT6.3 should be assimilated and mastered.

Computer Objectives. You have been provided with software and simple computer algorithms to implement the techniques discussed in Part Six. All have utility as learning tools.

Algorithms are provided for most of the other methods in Part Six. This information will allow you to expand your software library to include techniques beyond the trapezoidal rule. For example, you may find it useful from a professional viewpoint to have software to implement numerical integration and differentiation of unequally spaced data. You may also want to develop your own software for Simpson's rules, Romberg integration, and Gauss quadrature, which are usually more efficient and accurate than the trapezoidal rule.

Finally, one of your most important goals should be to master several of the general-purpose software packages that are widely available. In particular, you should become adept at using these tools to implement numerical methods for engineering problem solving.