Numerical Differentiation and Integration

- Standing in the heart of calculus are the mathematical concepts of *differentiation* and *integration*:

$$\frac{\Delta y}{\Delta x} = \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

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

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

Figure PT6.1

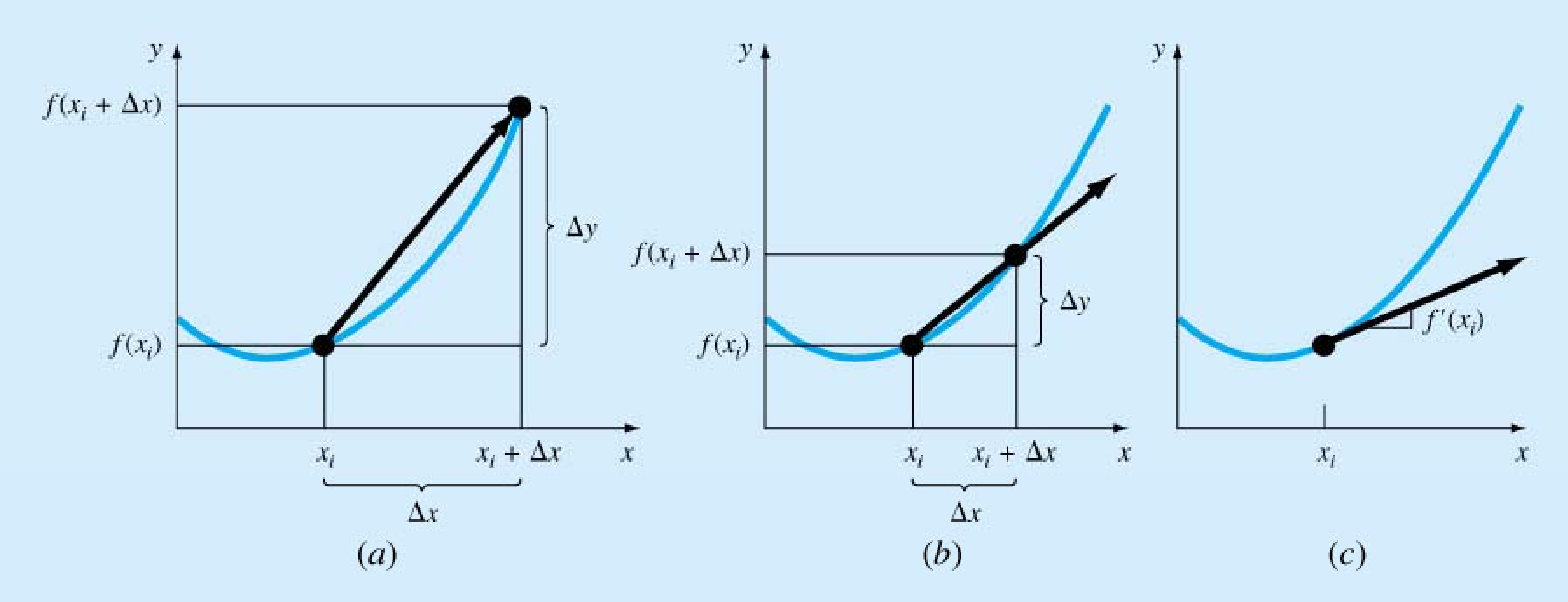
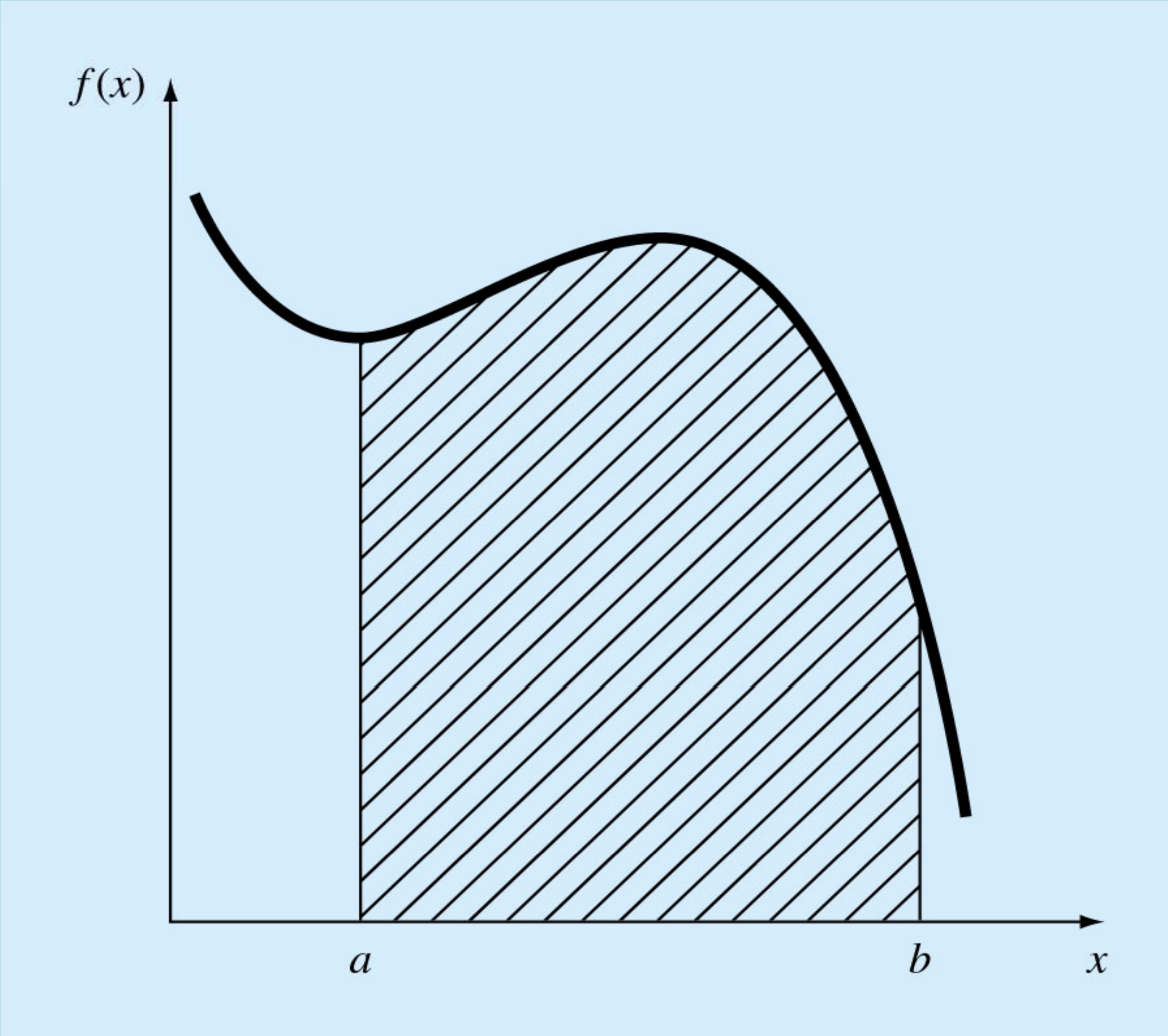

y
$f(x_i + \Delta x)$
Δy
$f(x_i)$
x_i
$x_i + \Delta x$
x
Δx
(a)
y
$f(x_i + \Delta x)$
Δy
$f(x_i)$
x_i
$x_i + \Delta x$
x
Δx
(b)
y
$f'(x_i)$
x_i
x
(c)

Figure PT6.2



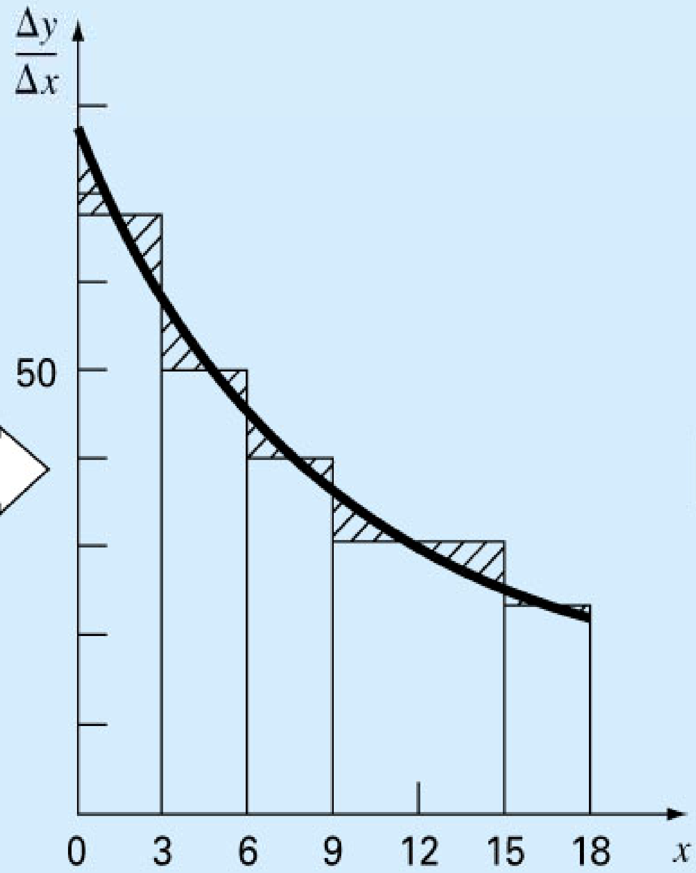
Noncomputer Methods for Differentiation and Integration

- The function to be differentiated or integrated will typically be in one of the following three forms:
  - A simple continuous function such as polynomial, an exponential, or a trigonometric function.
  - A complicated continuous function that is difficult or impossible to differentiate or integrate directly.
  - 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.

Figure PT6.4

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*)

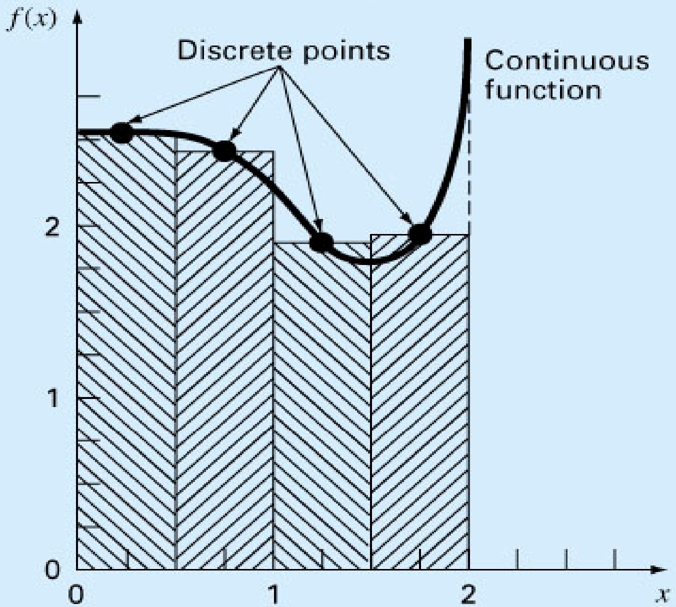
Figure PT6.7

(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)



Newton-Cotes Integration Formulas
Chapter 21

- The *Newton-Cotes formulas* are the most common numerical integration schemes.

- They are based on the strategy of replacing a complicated function or tabulated data with an approximating function that is easy to integrate:

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

$$f_n(x) = a_0 + a_1 x + \cdots + a_{n-1}x^{n-1} + a_n x^n$$

Figure 21.1

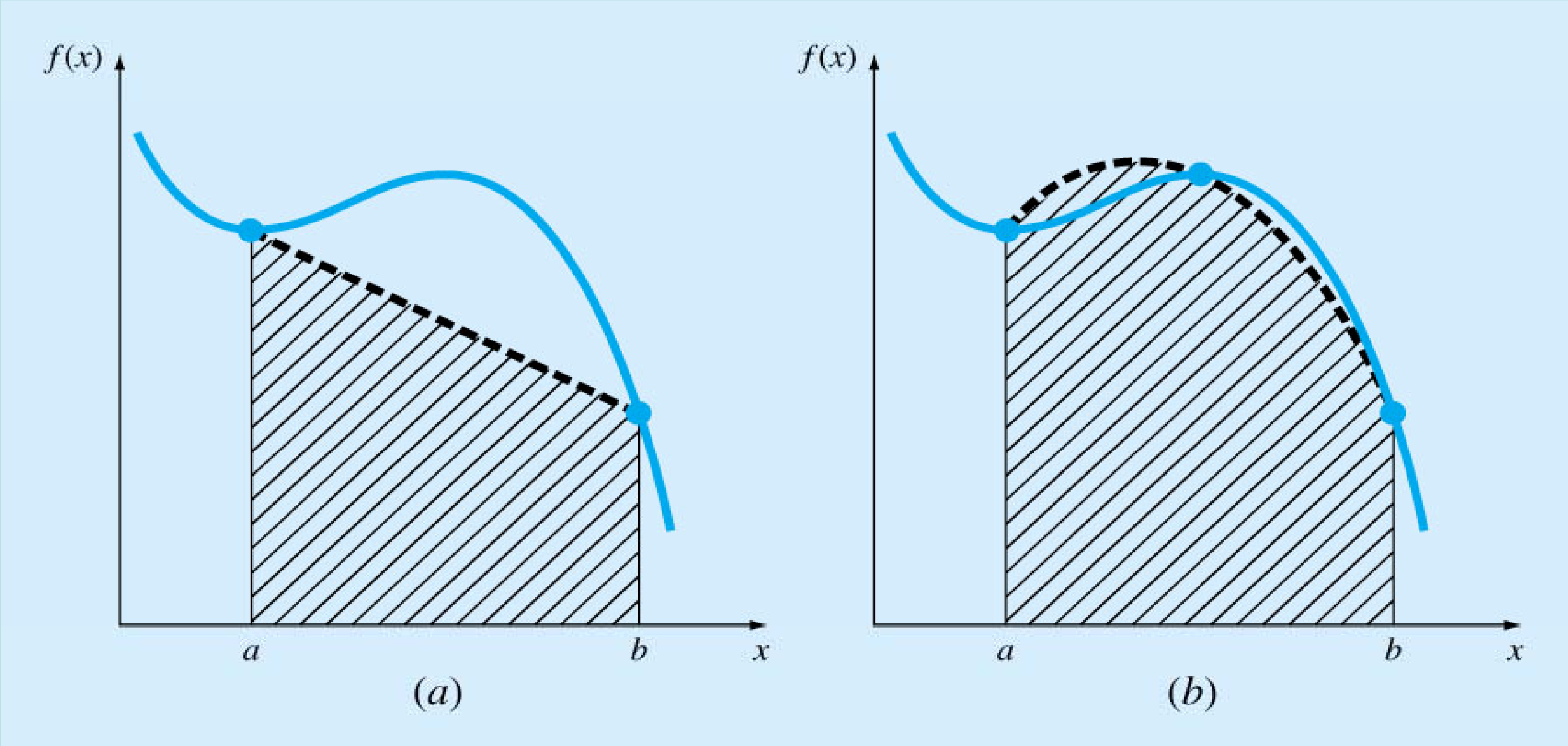
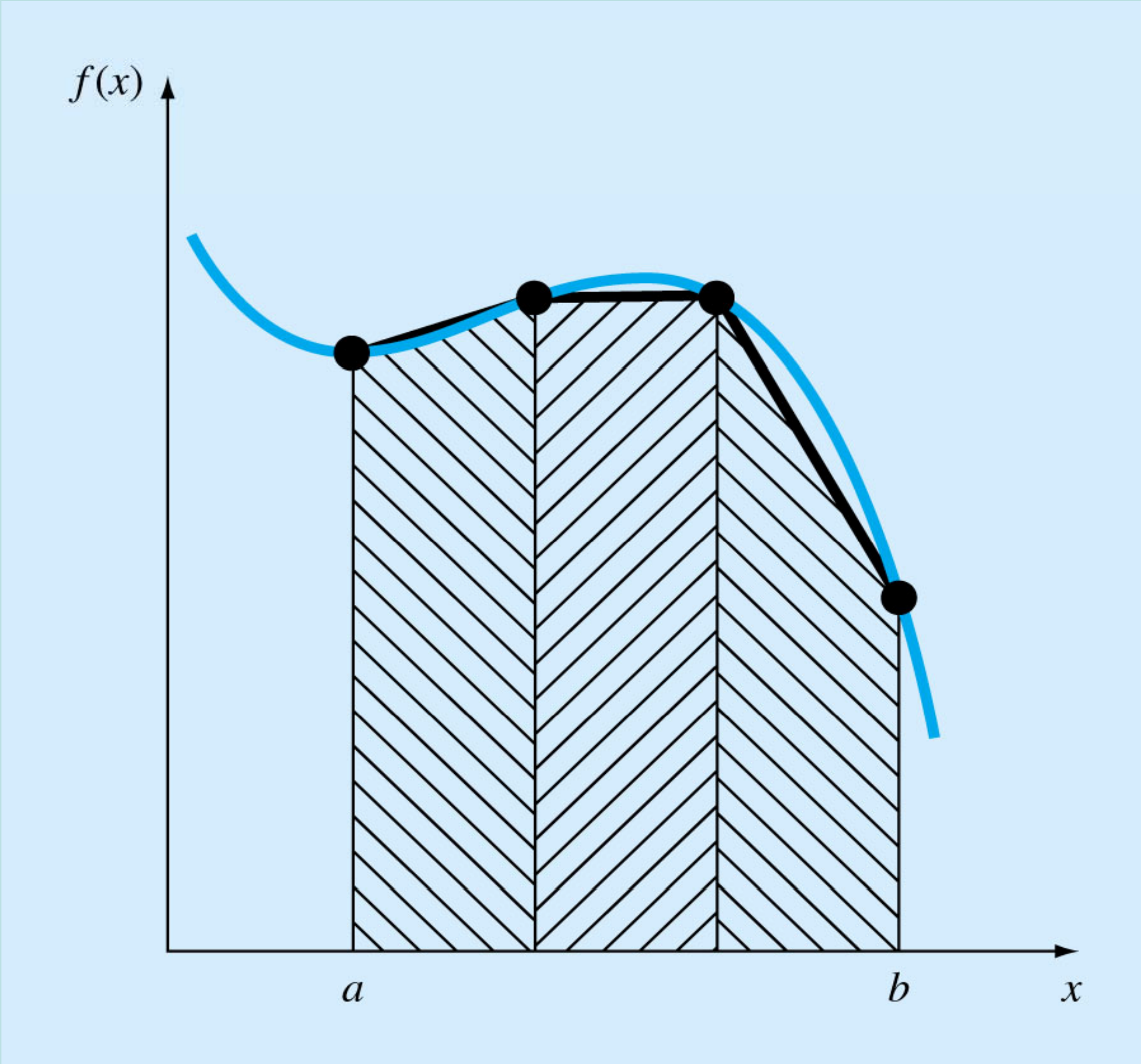


Figure 21.2



The Trapezoidal Rule

- The *Trapezoidal rule* is the first of the Newton-Cotes closed integration formulas, corresponding to the case where the polynomial is first order:

$$I = \int_a^b f(x)dx \cong \int_a^b f_1(x)dx$$

- The area under this first order polynomial is an estimate of the integral of *f(x)* between the limits of *a* and *b*:

$$\left. I = (b-a)\frac{f(a)+f(b)}{2} \right\} \textit{Trapezoidal rule}$$

Before integration, Eq. (21.2) can be expressed as

$$f_1(x) = \frac{f(b) - f(a)}{b - a}x + f(a) - \frac{af(b) - af(a)}{b - a}$$

Grouping the last two terms gives

$$f_1(x) = \frac{f(b) - f(a)}{b - a}x + \frac{bf(a) - af(a) - af(b) + af(a)}{b - a}$$

or

$$f_1(x) = \frac{f(b) - f(a)}{b - a}x + \frac{bf(a) - af(b)}{b - a}$$

which can be integrated between $x = a$ and $x = b$ to yield

$$I = \frac{f(b) - f(a)}{b - a}\frac{x^2}{2} + \frac{bf(a) - af(b)}{b - a}x\Big|_a^b$$

This result can be evaluated to give

$$I = \frac{f(b) - f(a)}{b - a}\frac{(b^2 - a^2)}{2} + \frac{bf(a) - af(b)}{b - a}(b - a)$$

Now, since $b^2 - a^2 = (b - a)(b + a)$,

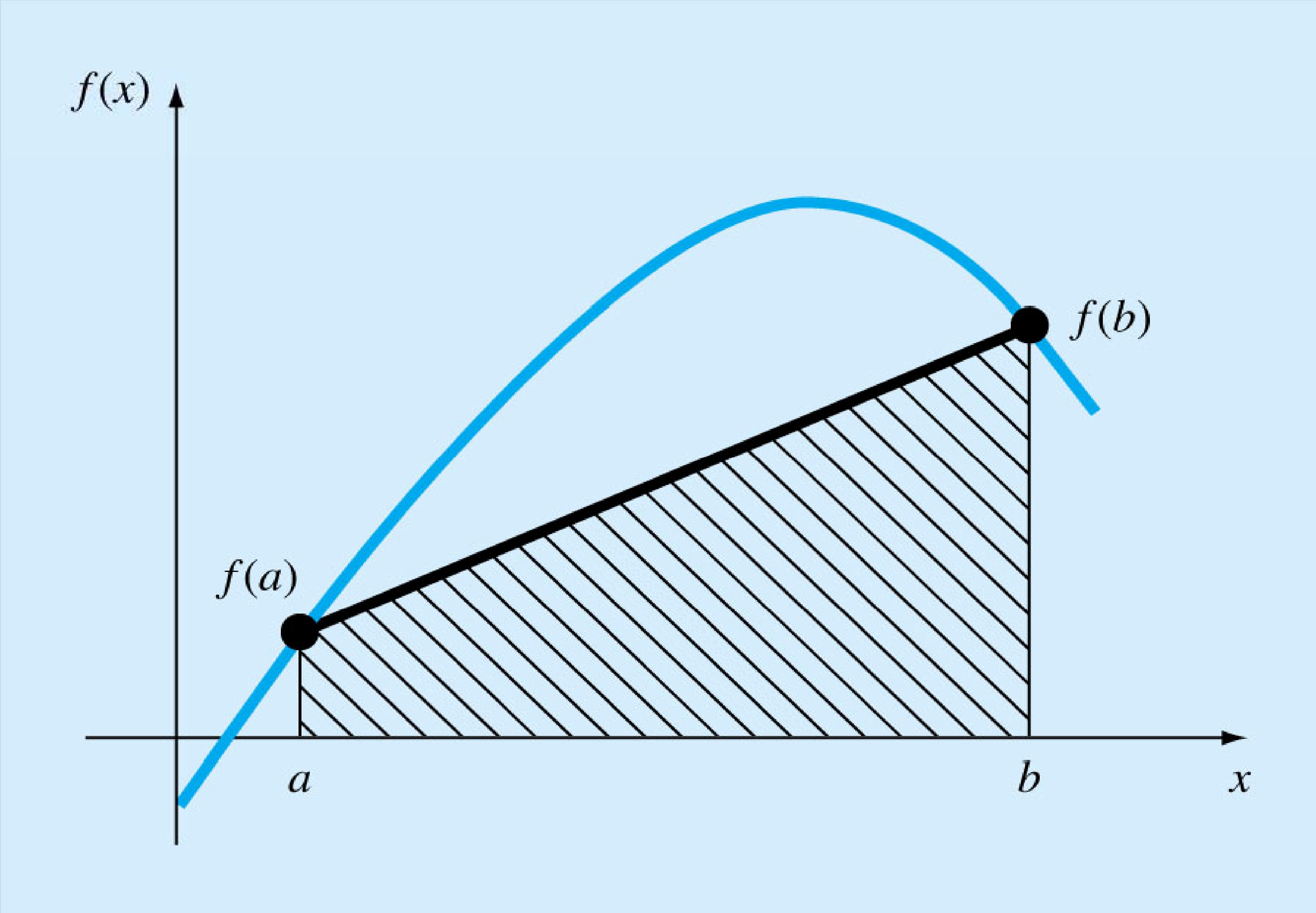
$$I = [f(b) - f(a)]\frac{b + a}{2} + bf(a) - af(b)$$

Multiplying and collecting terms yields

$$I = (b - a)\frac{f(a) + f(b)}{2}$$

which is the formula for the trapezoidal rule.

Figure 21.4



Error of the Trapezoidal Rule/

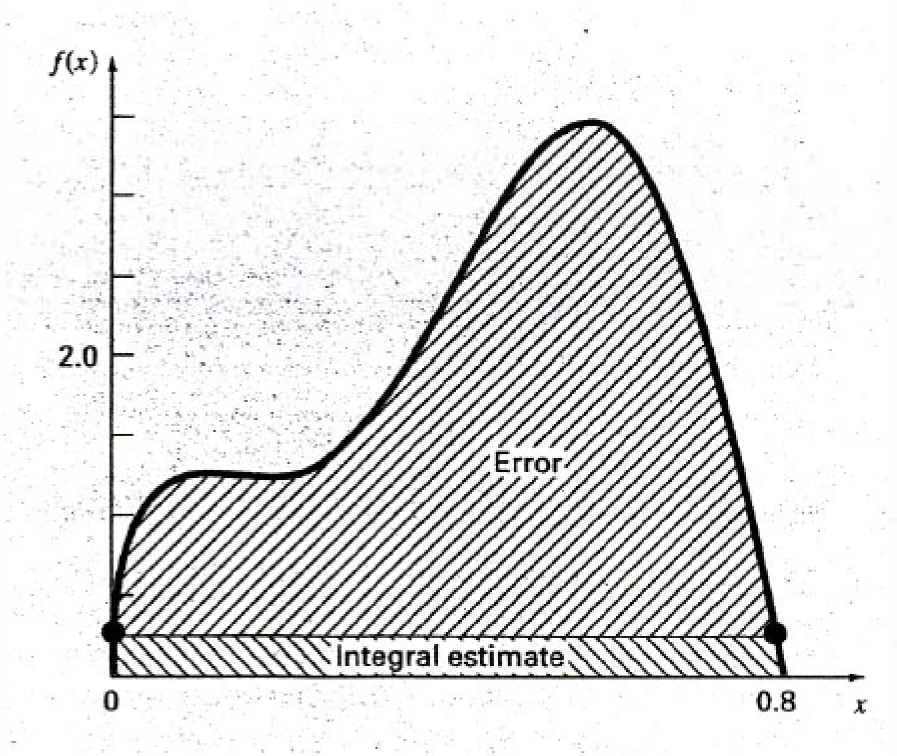
- When we employ the integral under a straight line segment to approximate the integral under a curve, error may be substantial:

$$E_t = -\frac{1}{12} f''(\xi)(b-a)^3$$

where ξ lies somewhere in the interval from a to b.

FIGURE 21.6

Graphical depiction of the use of a single application of the trapezoidal rule to approximate th integral of $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$ from $x = 0$ to 0.8.



Single Application of the Trapezoidal Rule

Problem Statement. Use Eq. (21.3) to numerically integrate

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from $a = 0$ to $b = 0.8$. Recall from Sec. PT6.2 that the exact value of the integral can be determined analytically to be 1.640533.

Solution. The function values

$$f(0) = 0.2$$
$$f(0.8) = 0.232$$

can be substituted into Eq. (21.3) to yield

$$I \cong 0.8 \frac{0.2 + 0.232}{2} = 0.1728$$

which represents an error of

$$E_t = 1.640533 - 0.1728 = 1.467733$$

The Multiple Application Trapezoidal Rule/

- One way to improve the accuracy of the trapezoidal rule is to divide the integration interval from a to b into a number of segments and apply the method to each segment.
- The areas of individual segments can then be added to yield the integral for the entire interval.

$$h = \frac{b-a}{n} \qquad a = x_0 \quad b = x_n$$

$$I = \int_{x_0}^{x_1} f(x)dx + \int_{x_1}^{x_2} f(x)dx + \cdots + \int_{x_{n-1}}^{x_n} f(x)dx$$

Substituting the trapezoidal rule for each integral yields:

$$I = h\frac{f(x_0)+f(x_1)}{2} + h\frac{f(x_1)+f(x_2)}{2} + \cdots + h\frac{f(x_{n-1})+f(x_n)}{2}$$

or, grouping terms,

$$I = \frac{h}{2}\left[f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)\right]$$

$$I = \underbrace{(b-a)}_{\text{Width}}\ \underbrace{\frac{f(x_0) + 2\sum_{i=1}^{n-1} f(x_i) + f(x_n)}{2n}}_{\text{Average height}} \tag{21.10}$$

Because the summation of the coefficients of $f(x)$ in the numerator divided by $2n$ is equal to 1, the average height represents a weighted average of the function values. According to Eq. (21.10), the interior points are given twice the weight of the two end points $f(x_0)$ and $f(x_n)$.

An error for the multiple-application trapezoidal rule can be obtained by summing the individual errors for each segment to give

$$E_t = -\frac{(b-a)^3}{12n^3}\sum_{i=1}^{n} f''(\xi_i) \tag{21.11}$$

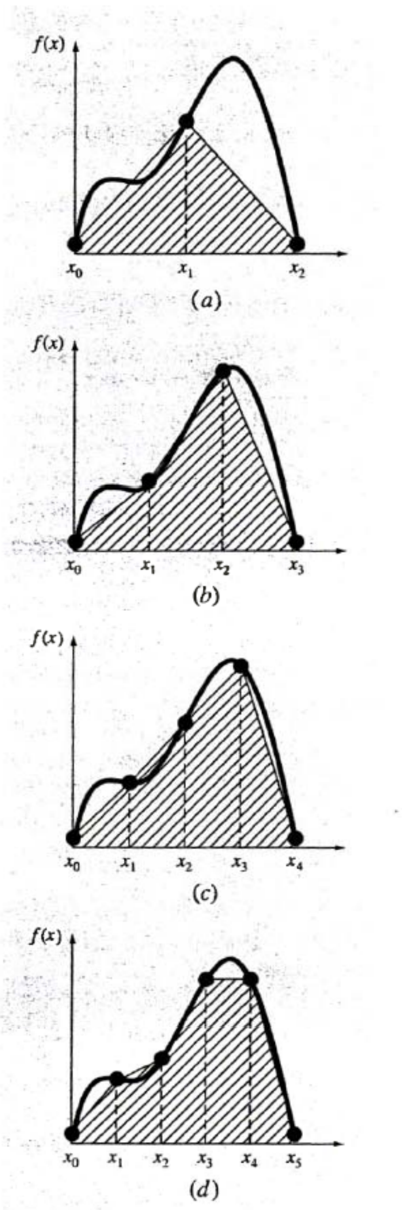
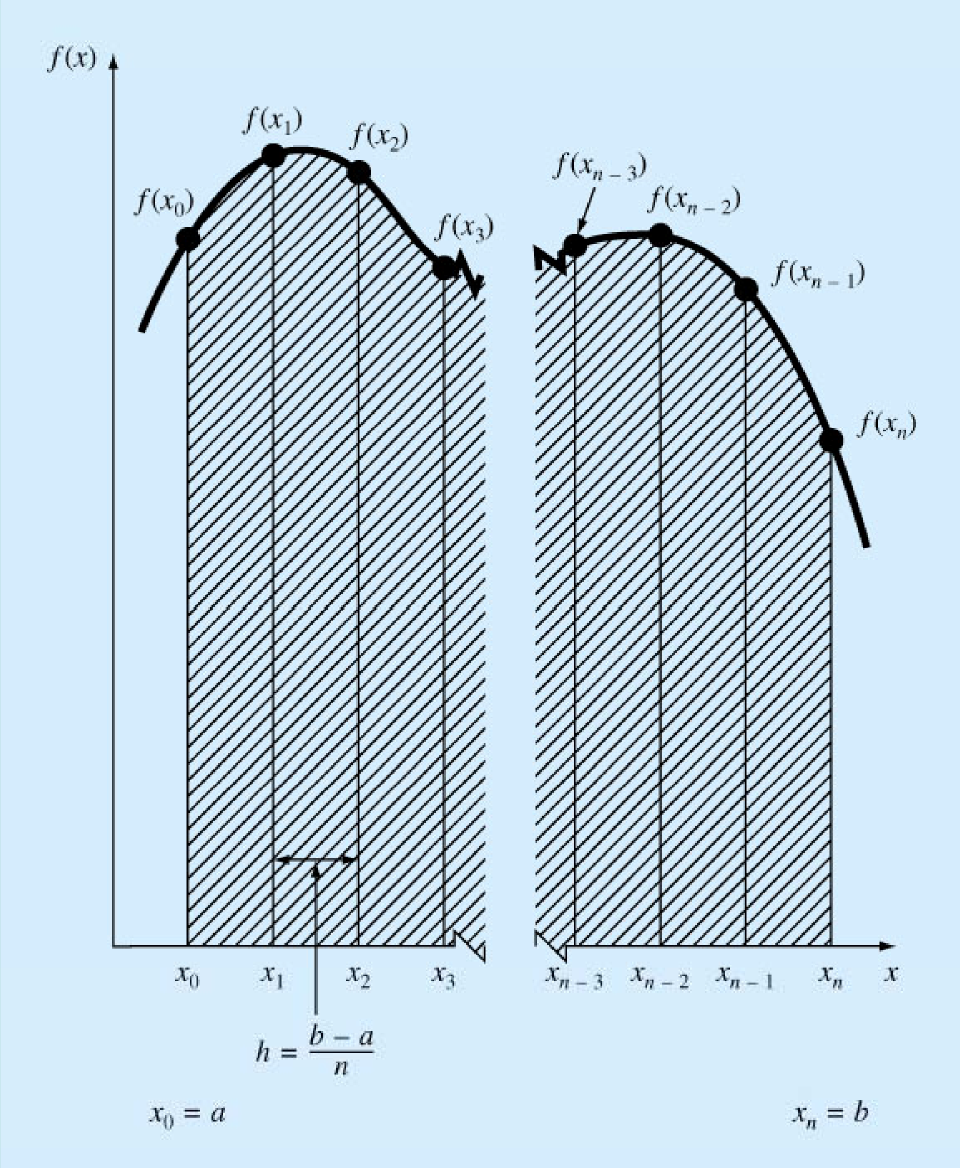


FIGURE 21.7
Illustration of the multiple-application trapezoidal rule. (a) Two segments, (b) three segments, (c) four segments, and (d) five segments.

Figure 21.8



f(x)
f(x1)
f(x2)
f(x0)
f(x3)
f(xn − 3)
f(xn − 2)
f(xn − 1)
f(xn)
x0
x1
x2
x3
xn − 3
xn − 2
xn − 1
xn
x
h = (b − a)/n
x0 = a
xn = b

(a) Single-segment

```
FUNCTION Trap (h, f0, f1)
  Trap = h * (f0 + f1)/2
END Trap
```

(b) Multiple-segment

```
FUNCTION Trapm (h, n, f)
  sum = f0
  OOFOR i = 1, n - 1
    sum = sum + 2 * fi
  END DO
  sum = sum + fn
  Trapm = h * sum / 2
END Trapm
```

FIGURE 21.9
Algorithms for the (*a*) single-segment and (*b*) multiple-segment trapezoidal rule.

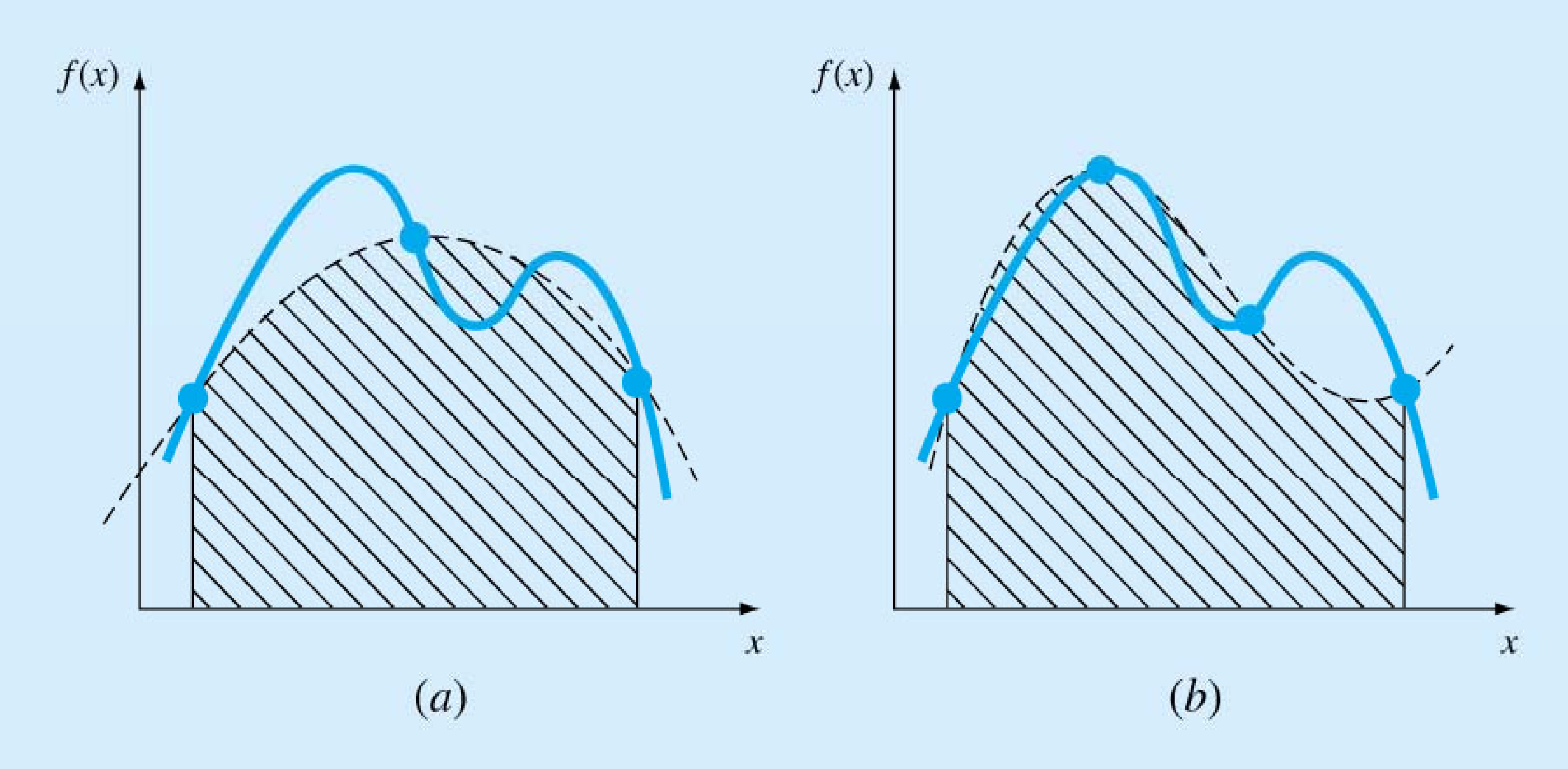
Simpson's Rules

- More accurate estimate of an integral is obtained if a high-order polynomial is used to connect the points. The formulas that result from taking the integrals under such polynomials are called *Simpson's rules*.

Simpson's 1/3 Rule/

- Results when a second-order interpolating polynomial is used.

Figure 21.10



$$I = \int_a^b f(x)dx \cong \int_a^b f_2(x)dx$$

$$a = x_0 \qquad b = x_2$$

$$I = \int_{x_0}^{x_2} \left[\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} f(x_0) + \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} f(x_1) + \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} f(x_2) \right] dx$$

$$\boxed{I \cong \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2) \right] \qquad h = \frac{b-a}{2}}$$

Simpson's 1/3 Rule

After integration and algebraic manipulation, the following formula results:

$$I \cong \frac{h}{3}[f(x_0) + 4f(x_1) + f(x_2)]$$

where, for this case, $h = (b - a)/2$.

Simpson's 1/3 rule can also be expressed using the format of Eq.

$$I \cong \underbrace{(b-a)}_{\text{Width}} \underbrace{\frac{f(x_0) + 4f(x_1) + f(x_2)}{6}}_{\text{Average height}}$$

It can be shown that a single-segment application of Simpson's 1/3 rule has a truncation error of (Box 21.3)

$$E_t = -\frac{1}{90}h^5 f^{(4)}(\xi)$$

or, because $h = (b - a)/2$,

$$E_t = -\frac{(b-a)^5}{2880} f^{(4)}(\xi) \tag{21.16}$$

EXAMPLE 21.4 Single Application of Simpson's 1/3 Rule

Problem Statement. Use Eq. (21.15) to integrate

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from $a = 0$ to $b = 0.8$. Recall that the exact integral is 1.640533.

Solution.

$$f(0) = 0.2 \qquad f(0.4) = 2.456 \qquad f(0.8) = 0.232$$

Therefore, Eq. (21.15) can be used to compute

$$I \cong 0.8 \frac{0.2 + 4(2.456) + 0.232}{6} = 1.367467$$

which represents an exact error of

$$E_t = 1.640533 - 1.367467 = 0.2730667 \qquad \varepsilon_t = 16.6\%$$

which is approximately 5 times more accurate than for a single application of the trapezoidal rule (Example 21.1).

21.2.2 The Multiple-Application Simpson's 1/3 Rule

Just as with the trapezoidal rule, Simpson's rule can be improved by dividing the integration interval into a number of segments of equal width (Fig. 21.11):

$$h = \frac{b-a}{n}$$

The total integral can be represented as

$$I = \int_{x_0}^{x_2} f(x)\,dx + \int_{x_2}^{x_4} f(x)\,dx + \cdots + \int_{x_{n-2}}^{x_n} f(x)\,dx$$

Substituting Simpson's 1/3 rule for the individual integral yields

$$I \cong 2h\frac{f(x_0) + 4f(x_1) + f(x_2)}{6} + 2h\frac{f(x_2) + 4f(x_3) + f(x_4)}{6} + \cdots + 2h\frac{f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)}{6}$$

or, combining terms and using Eq. (21.17),

$$I \cong \underbrace{(b-a)}_{\text{Width}} \underbrace{\frac{f(x_0) + 4\displaystyle\sum_{i=1,3,5}^{n-1} f(x_i) + 2\sum_{j=2,4,6}^{n-2} f(x_j) + f(x_n)}{3n}}_{\text{Average height}}$$

An error estimate for the multiple-application Simpson's rule is obtained in the same fashion as for the trapezoidal rule by summing the individual errors for the segments and averaging the derivative to yield

$$E_a = -\frac{(b-a)^5}{180n^4}\bar{f}^{(4)} \tag{21.19}$$

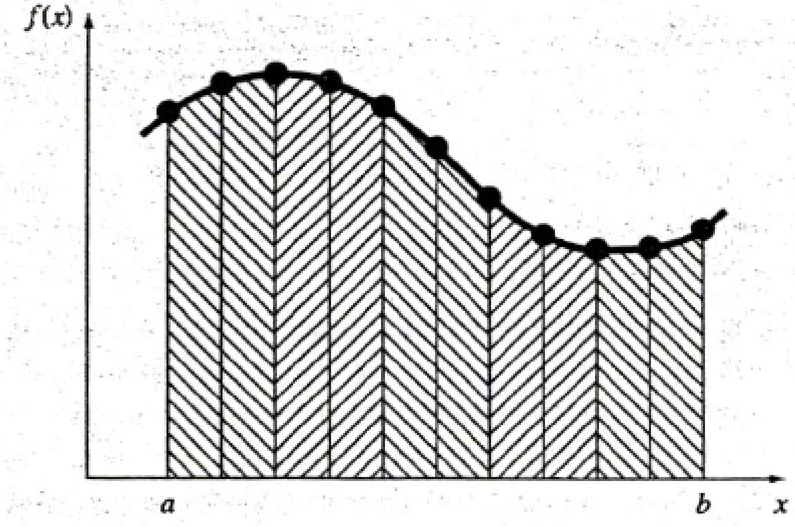


FIGURE 21.11
Graphical representation of the multiple application of Simpson's 1/3 rule. Note that the method can be employed only if the number of segments is even.

EXAMPLE 21.5 Multiple-Application Version of Simpson's 1/3 Rule

Problem Statement. Use Eq. (21.18) with $n = 4$ to estimate the integral of

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from $a = 0$ to $b = 0.8$. Recall that the exact integral is 1.640533.

Solution. $n = 4$ ($h = 0.2$):

$$f(0) = 0.2 \qquad f(0.2) = 1.288$$
$$f(0.4) = 2.456 \qquad f(0.6) = 3.464$$
$$f(0.8) = 0.232$$

From Eq. (21.18),

$$I = 0.8\,\frac{0.2 + 4(1.288 + 3.464) + 2(2.456) + 0.232}{12} = 1.623467$$

$$E_t = 1.640533 - 1.623467 = 0.017067 \qquad \varepsilon_t = 1.04\%$$

The estimated error [Eq. (21.19)] is

$$E_a = -\frac{(0.8)^5}{180(4)^4}(-2400) = 0.017067$$

21.2.3 Simpson's 3/8 Rule

In a similar manner to the derivation of the trapezoidal and Simpson's 1/3 rule, a th
order Lagrange polynomial can be fit to four points and integrated:

$$I = \int_a^b f(x)\,dx \cong \int_a^b f_3(x)\,dx$$

to yield

$$I \cong \frac{3h}{8}[f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)]$$

where $h = (b - a)/3$. This equation is called *Simpson's* 3/8 *rule* because h is multiplied b
3/8. It is the third Newton-Cotes closed integration formula. The 3/8 rule can also be e
pressed in the form of Eq. (21.5):

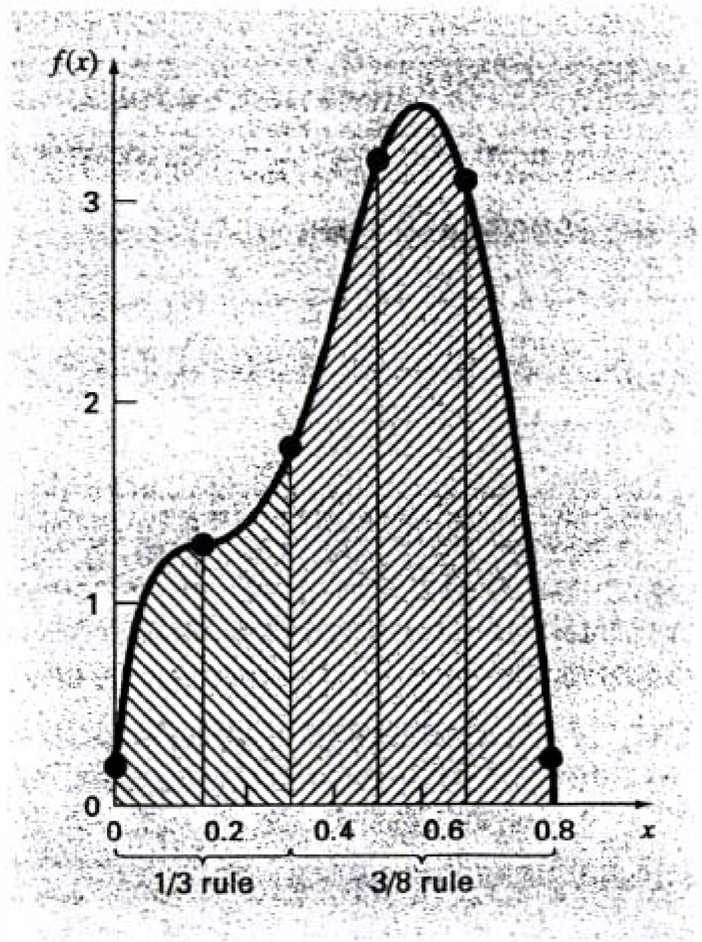
$$I \cong \underbrace{(b-a)}_{\text{Width}}\ \underbrace{\frac{f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)}{8}}_{\text{Average height}} \qquad (21.20)$$

Thus, the two interior points are given weights of three-eighths, whereas the end points ar
weighted with one-eighth. Simpson's 3/8 rule has an error of

$$E_t = -\frac{3}{80}h^5 f^{(4)}(\xi)$$

or, because $h = (b - a)/3$,

$$E_t = -\frac{(b-a)^5}{6480} f^{(4)}(\xi) \qquad (21.21)$$



GURE 21.12
stration of how Simpson's
and 3/8 rules can be
plied in tandem to handle
ltiple applications with odd
mbers of intervals.

EXAMPLE 21.6 Simpson's 3/8 Rule

Problem Statement.

(a) Use Simpson's 3/8 rule to integrate

$$f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

from $a = 0$ to $b = 0.8$.

(b) Use it in conjunction with Simpson's 1/3 rule to integrate the same function for five segments.

Solution.

(a) A single application of Simpson's 3/8 rule requires four equally spaced points:

$$f(0) = 0.2 \qquad f(0.2667) = 1.432724$$

$$f(0.5333) = 3.487177 \qquad f(0.8) = 0.232$$

Using Eq. (21.20),

$$I \cong 0.8\,\frac{0.2 + 3(1.432724 + 3.487177) + 0.232}{8} = 1.519170$$

$$E_t = 1.640533 - 1.519170 = 0.1213630 \qquad \varepsilon_t = 7.4\%$$

$$E_a = -\frac{(0.8)^5}{6480}(-2400) = 0.1213630$$

(b) The data needed for a five-segment application ($h = 0.16$) is

$$f(0) = 0.2 \qquad f(0.16) = 1.296919$$
$$f(0.32) = 1.743393 \qquad f(0.48) = 3.186015$$
$$f(0.64) = 3.181929 \qquad f(0.80) = 0.232$$

The integral for the first two segments is obtained using Simpson's 1/3 rule:

$$I \cong 0.32\,\frac{0.2 + 4(1.296919) + 1.743393}{6} = 0.3803237$$

For the last three segments, the 3/8 rule can be used to obtain

$$I \cong 0.48\,\frac{1.743393 + 3(3.186015 + 3.181929) + 0.232}{8} = 1.264754$$

The total integral is computed by summing the two results:

$$I = 0.3803237 + 1.264753 = 1.645077$$
$$E_t = 1.640533 - 1.645077 = -0.00454383 \qquad \varepsilon_t = -0.28\%$$

```
TION Simp13 (h, f0, f1, f2)
imp13 = 2*h* (f0+4*f1+f2) / 6
Simp13

TION Simp38 (h, f0, f1, f2, f3)
imp38 = 3*h* (f0+3*(f1+f2)+f3) / 8
Simp38

NCTION Simp13m (h, n, f)
um = f(0)
OFOR i = 1, n - 2, 2
  sum = sum + 4 * f_i + 2 * f_i+1
ND DO
um = sum + 4 * f_n-1 + f_n
imp13m = h * sum / 3
Simp13m
```

```
(d)
FUNCTION SimpInt(a,b,n,f)
  h = (b - a) / n
  IF n = 1 THEN
    sum = Trap(h, f_n-1, f_n)
  ELSE
    m = n
    odd = n / 2 - INT(n / 2)
    IF odd > 0 AND n > 1 THEN
      sum = sum+Simp38(h, f_n-3, f_n-2, f_n-1, f_n)
      m = n - 3
    END IF
    IF m > 1 THEN
      sum = sum + Simp13m(h,m,f)
    END IF
  END IF
  SimpInt = sum
END SimpInt
```

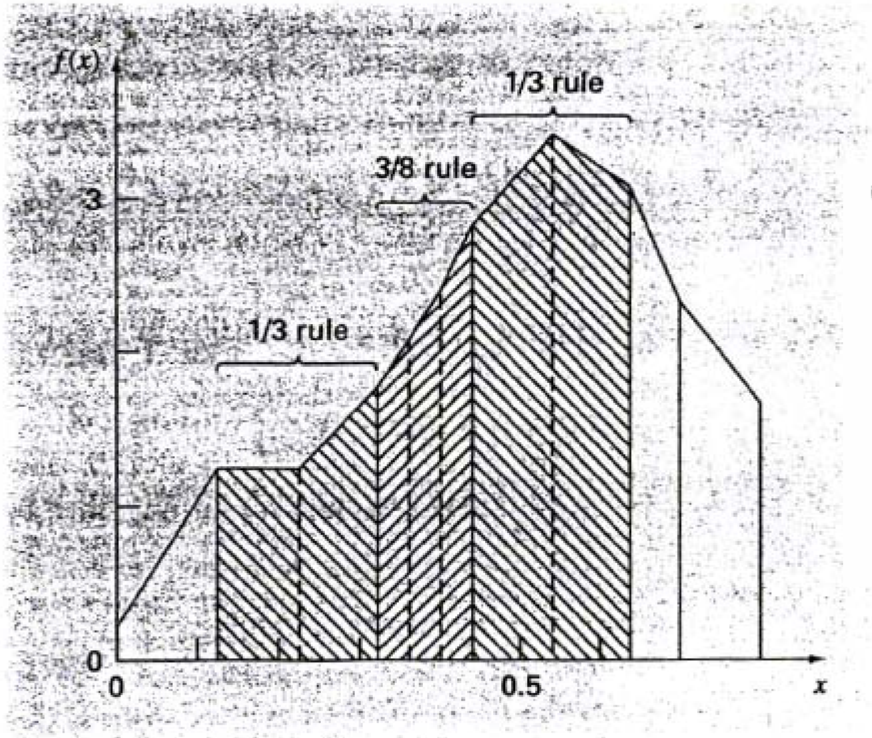
GURE 21.13

udocode for Simpson's rules. (a) Single-application Simpson's 1/3 rule, (b) single-application Simpson's 3/8 rule, (c) multiple-application Simpson's 1/3 rule, and (d) multiple-application Simpson's rule for both odd and even number of segments. Note that for all cases, must be ≥1.

21.3 INTEGRATION WITH UNEQUAL SEGMENTS

To this point, all formulas for numerical integration have been based on equally sp[...] data points. In practice, there are many situations where this assumption does not hold [...] we must deal with unequal-sized segments. For example, experimentally derived da[...] often of this type. For these cases, one method is to apply the trapezoidal rule to each [...] ment and sum the results:

$$I = h_1 \frac{f(x_0) + f(x_1)}{2} + h_2 \frac{f(x_1) + f(x_2)}{2} + \cdots + h_n \frac{f(x_{n-1}) + f(x_n)}{2}$$



(a)

```
FUNCTION Trapun (x, y, n)
  LOCAL i, sum
  sum = 0
  DOFOR i = 1, n
    sum = sum + (xi - xi-1)*(yi-1 + yi)/2
  END DO
  Trapun = sum
END Trapun
```

FIGURE 21.14
Use of the trapezoidal rule to determine the integral of unevenly spaced data. Notice how the shaded segments could be evaluated with Simpson's rule to attain higher accuracy.

21.5 MULTIPLE INTEGRALS

Multiple integrals are widely used in engineering. For example, a general equation to compute the average of a two-dimensional function can be written as (recall Eq. PT6.4)

$$\bar{f} = \frac{\int_c^d \left(\int_a^b f(x, y)\, dx \right) dy}{(d - c)(b - a)} \tag{21.23}$$

The numerator is called a double integral.

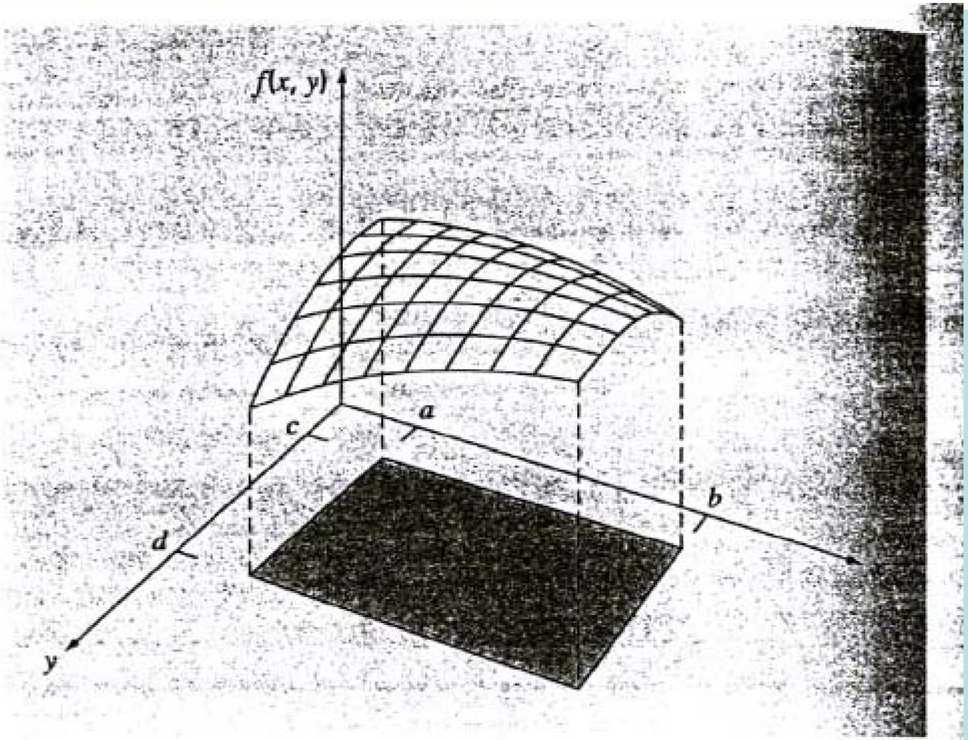


FIGURE 21.16
Double integral as the area under the function surface.

EXAMPLE 21.9 Using Double Integral to Determine Average Temperature

Problem Statement. Suppose that the temperature of a rectangular heated plate is described by the following function:

$$T(x, y) = 2xy + 2x - x^2 - 2y^2 + 72$$

If the plate is 8-m long (x dimension) and 6-m wide (y dimension), compute the average temperature.

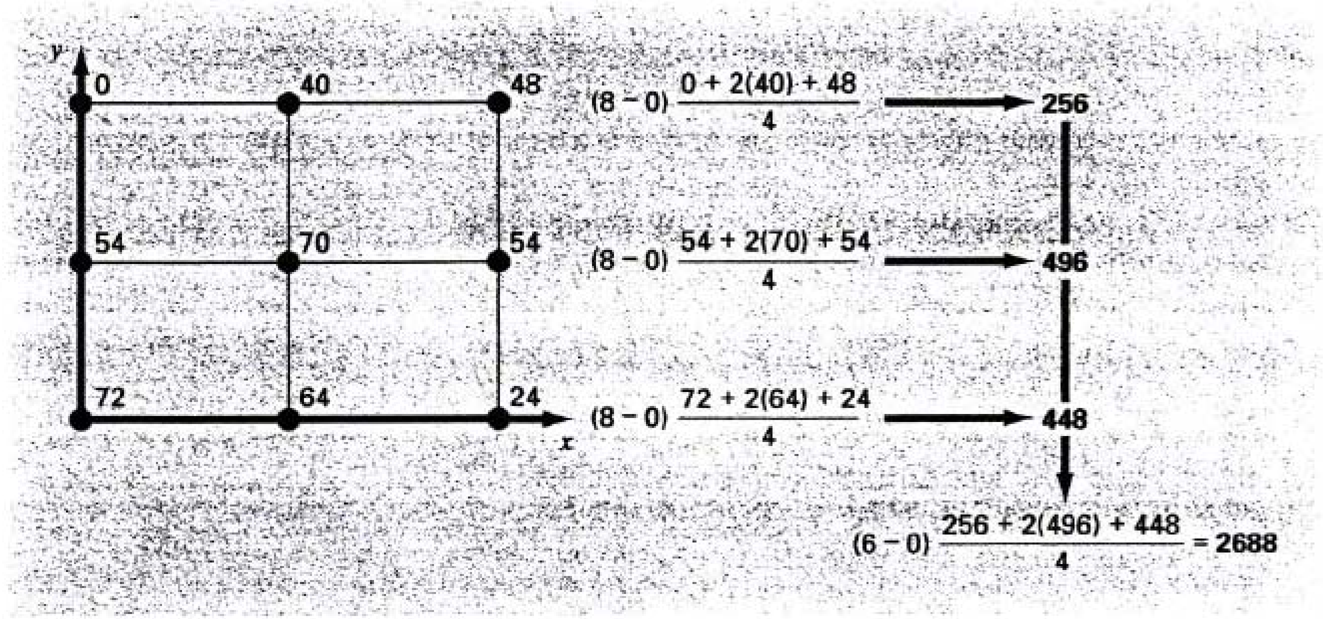


FIGURE 21.17
Numerical evaluation of a double integral using the two-segment trapezoidal rule.

FIGURE 22.1
Algorithms for multiple applications of the (*a*) trapezoidal and (*b*) Simpson's 1/3 rules, where the function is available.

(a)

```
FUNCTION TrapEq (n, a, b)
  h = (b - a) / n
  x = a
  sum = f(x)
  DOFOR i = 1, n - 1
    x = x + h
    sum = sum + 2 * f(x)
  END DO
  sum = sum + f(b)
  TrapEq = (b - a) * sum / (2 * n)
END TrapEq
```

(b)

```
FUNCTION SimpEq (n, a, b)
  h = (b - a) / n
  x = a
  sum = f(x)
  DOFOR i = 1, n - 2, 2
    x = x + h
    sum = sum + 4 * f(x)
    x = x + h
    sum = sum + 2 * f(x)
  END DO
  x = x + h
  sum = sum + 4 * f(x)
  sum = sum + f(b)
  SimpEq = (b - a) * sum /(3 * n)
END SimpEq
```

22.2 ROMBERG INTEGRATION

The estimate and error associated with a multiple-application trapezoidal rule can be represented generally as

$$I = I(h) + E(h)$$

where I = the exact value of the integral, $I(h)$ = the approximation from an n-segment application of the trapezoidal rule with step size $h = (b - a)/n$, and $E(h)$ = the truncation error. If we make two separate estimates using step sizes of h_1 and h_2 and have exact values for the error,

$$I(h_1) + E(h_1) = I(h_2) + E(h_2) \tag{22.1}$$

Now recall that the error of the multiple-application trapezoidal rule can be represented approximately by Eq. (21.13) [with $n = (b - a)/h$]:

$$E \cong -\frac{b-a}{12}h^2\bar{f}'' \tag{22.2}$$

If it is assumed that $\bar{f}''$ is constant regardless of step size, Eq. (22.2) can be used to determine that the ratio of the two errors will be

$$\frac{E(h_1)}{E(h_2)} \cong \frac{h_1^2}{h_2^2} \tag{22.3}$$

This calculation has the important effect of removing the term $\bar{f}''$ from the computation. In so doing, we have made it possible to utilize the information embodied by Eq. (22.2) without prior knowledge of the function's second derivative. To do this, we rearrange Eq. (22.3) to give

$$E(h_1) \cong E(h_2)\left(\frac{h_1}{h_2}\right)^2$$

which can be substituted into Eq. (22.1):

$$I(h_1) + E(h_2)\left(\frac{h_1}{h_2}\right)^2 \cong I(h_2) + E(h_2)$$

which can be solved for

$$E(h_2) \cong \frac{I(h_1) - I(h_2)}{1 - (h_1/h_2)^2}$$

Thus, we have developed an estimate of the truncation error in terms of the integral estimates and their step sizes. This estimate can then be substituted into

$$I = I(h_2) + E(h_2)$$

to yield an improved estimate of the integral:

$$I \cong I(h_2) + \frac{1}{(h_1/h_2)^2 - 1}[I(h_2) - I(h_1)] \tag{22.4}$$

It can be shown (Ralston and Rabinowitz, 1978) that the error of this estimate is $O(h^6)$. Thus, we have combined two trapezoidal rule estimates of $O(h^2)$ to yield a new estimate of $O(h^4)$. For the special case where the interval is halved ($h_2 = h_1/2$), this equation becomes

$$I \cong I(h_2) + \frac{1}{2^2 - 1}[I(h_2) - I(h_1)]$$

or, collecting terms,

$$I \cong \frac{4}{3}I(h_2) - \frac{1}{3}I(h_1) \tag{22.5}$$

EXAMPLE 22.1 Error Corrections of the Trapezoidal Rule

Problem Statement. In the previous chapter (Example 21.1 and Table 21.1), we used a variety of numerical integration methods to evaluate the integral of $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$ from $a = 0$ to $b = 0.8$. For example, single and multiple applications of the trapezoidal rule yielded the following results:

Segments	*h*	Integral	ε_t, %
1	0.8	0.1728	89.5
2	0.4	1.0688	34.9
4	0.2	1.4848	9.5

Use this information along with Eq. (22.5) to compute improved estimates of the integral.

Solution. The estimates for one and two segments can be combined to yield

$$I \cong \frac{4}{3}(1.0688) - \frac{1}{3}(0.1728) = 1.367467$$

The error of the improved integral is $E_t = 1.640533 - 1.367467 = 0.273067$ ($\varepsilon_t = 16.6\%$), which is superior to the estimates upon which it was based.

In the same manner, the estimates for two and four segments can be combined to give

$$I \cong \frac{4}{3}(1.4848) - \frac{1}{3}(1.0688) = 1.623467$$

which represents an error of $E_t = 1.640533 - 1.623467 = 0.017067$ ($\varepsilon_t = 1.0\%$).

Equation (22.4) provides a way to combine two applications of the trapezoidal rule with error $O(h^2)$ to compute a third estimate with error $O(h^4)$. This approach is a subset of a more general method for combining integrals to obtain improved estimates. For instance, in Example 22.1, we computed two improved integrals of $O(h^4)$ on the basis of three trapezoidal rule estimates. These two improved estimates can, in turn, be combined to yield an even better value with $O(h^6)$. For the special case where the original trapezoidal estimates are based on successive halving of the step size, the equation used for $O(h^6)$ accuracy is

$$I \cong \frac{16}{15} I_m - \frac{1}{15} I_l \tag{22.6}$$

where I_m and I_l are the more and less accurate estimates, respectively. Similarly, two $O(h^6)$ results can be combined to compute an integral that is $O(h^8)$ using

$$I \cong \frac{64}{63} I_m - \frac{1}{63} I_l \tag{22.7}$$

EXAMPLE 22.2 Higher-Order Error Correction of Integral Estimates

Problem Statement. In Example 22.1, we used Richardson's extrapolation to compute two integral estimates of $O(h^4)$. Utilize Eq. (22.6) to combine these estimates to compute an integral with $O(h^6)$.

Solution. The two integral estimates of $O(h^4)$ obtained in Example 22.1 were 1.367467 and 1.623467. These values can be substituted into Eq. (22.6) to yield

$$I = \frac{16}{15}(1.623467) - \frac{1}{15}(1.367467) = 1.640533$$

which is the correct answer to the seven significant figures that are carried in this example.

22.2.2 The Romberg Integration Algorithm

$$I_{j,k} \cong \frac{4^{k-1} I_{j+1,k-1} - I_{j,k-1}}{4^{k-1} - 1}$$

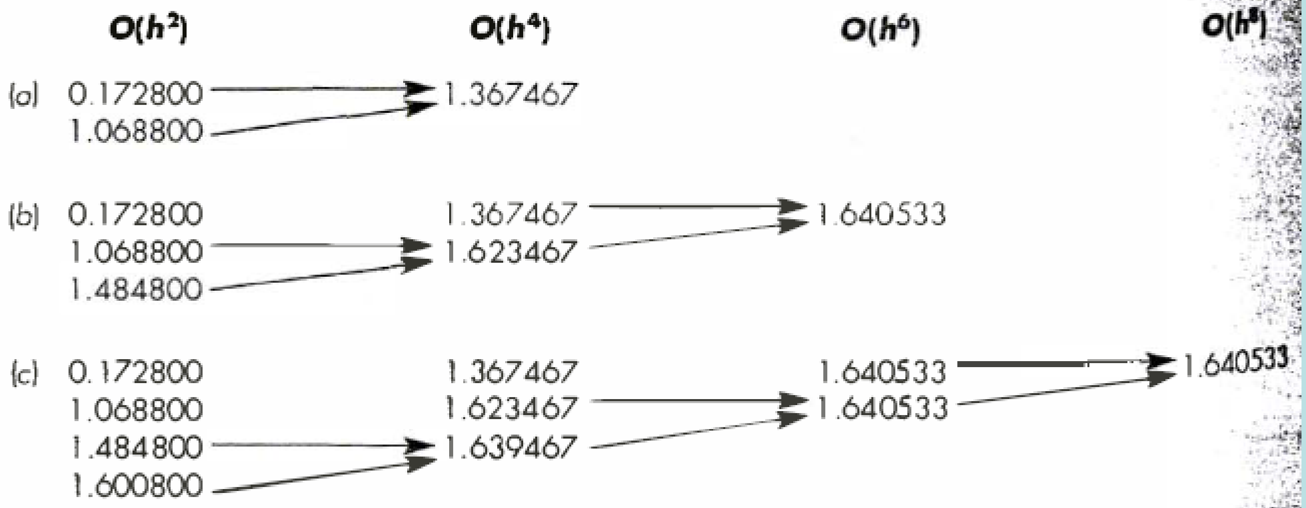
where $I_{j+1,k-1}$ and $I_{j,k-1}$ = the more and less accurate integrals, respectively,

The index k signifies the level of the integration,

The index j is used to distinguish between the more $(j+1)$ and the less (j) accurate estimates. For example, for $k = 2$ and $j = 1$,

$$I_{1,2} \cong \frac{4I_{2,1} - I_{1,1}}{3}$$

FIGURE 22.3
Graphical depiction of the sequence of integral estimates generated using Romberg integration. (*a*) First iteration. (*b*) Second iteration. (*c*) Third iteration.



For example, the first iteration (Fig. 22.3*a*) involves computing the one- and two-segment trapezoidal rule estimates ($I_{1,1}$ and $I_{2,1}$). Equation (22.8) is then used to compute the element $I_{1,2} = 1.367467$, which has an error of $O(h^4)$.

$$|\varepsilon_a| = \left| \frac{I_{1,k} - I_{2,k-1}}{I_{1,k}} \right| 100\%$$

```
FUNCTION Romberg (a, b, maxit, es)
  LOCAL I(10, 10)
  n = 1
  I1,1 = TrapEq(n, a, b)
  iter = 0
  DO
    iter = iter + 1
    n = 2^iter
    Iiter+1,1 = TrapEq(n, a, b)
    DOFOR k = 2, iter + 1
      j = 2 + iter - k
      Ij,k = (4^(k-1) * Ij+1,k-1 - Ij,k-1) / (4^(k-1) - 1)
    END DO
    ea = ABS((I1,iter+1 - I2,iter) / I1,iter+1) * 100
    IF (iter ≥ maxit OR ea ≤ es) EXIT
  END DO
  Romberg = I1,iter+1
END Romberg
```

FIGURE 22.4
Pseudocode for Romberg integration that uses the equal-size-segment version of the trapezoidal rule from Fig. 22.1.

HIGH-ACCURACY DIFFERENTIATION FORMULAS

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

which can be solved for

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

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

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

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

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

into Eq. (23.2) to yield

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

or, by collecting terms,

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

FIGURE 23.1

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

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

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

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

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

First Derivative | Error

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

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

Second Derivative

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

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

Third Derivative

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

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

Fourth Derivative

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

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

High-Accuracy Differentiation Formulas

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

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

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

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

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

Solution. The data needed for this example is

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

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

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

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

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

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

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

RICHARDSON EXTRAPOLATION

Recall from Sec. 22.1.1 that Richardson extrapolation provided a means to obtain an improved integral estimate I by the formula [Eq. (22.4)]

$$I \cong I(h_2) + \frac{1}{(h_1/h_2)^2 - 1}[I(h_2) - I(h_1)] \tag{23.6}$$

where $I(h_1)$ and $I(h_2)$ are integral estimates using two step sizes h_1 and h_2. Because of its convenience when expressed as a computer algorithm, this formula is usually written for the case where $h_2 = h_1/2$, as in

$$I \cong \frac{4}{3} I(h_2) - \frac{1}{3} I(h_1) \tag{23.7}$$

In a similar fashion, Eq. (23.7) can be written for derivatives as

$$D \cong \frac{4}{3} D(h_2) - \frac{1}{3} D(h_1) \tag{23.8}$$

For centered difference approximations with $O(h^2)$, the application of this formula will yield a new derivative estimate of $O(h^4)$.

Richardson Extrapolation

Problem Statement. Using the same function as in Example 23.1, estimate the first derivative at $x = 0.5$ employing step sizes of $h_1 = 0.5$ and $h_2 = 0.25$. Then use Eq. (23.8) to compute an improved estimate with Richardson extrapolation. Recall that the true value is -0.9125.

Solution. The first-derivative estimates can be computed with centered differences as

$$D(0.5) = \frac{0.2 - 1.2}{1} = -1.0 \qquad \varepsilon_t = -9.6\%$$

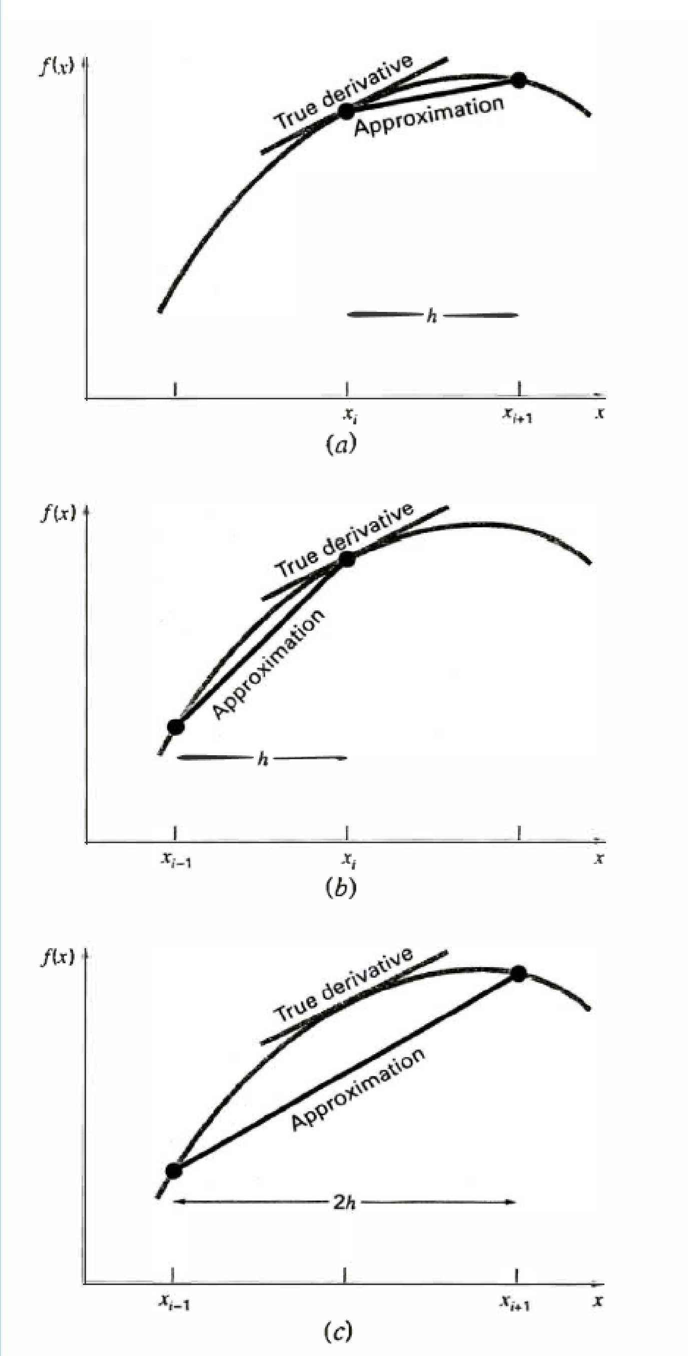
and

$$D(0.25) = \frac{0.6363281 - 1.1035156}{0.5} = -0.934375 \qquad \varepsilon_t = -2.4\%$$

The improved estimate can be determined by applying Eq. (23.8) to give

$$D = \frac{4}{3}(-0.934375) - \frac{1}{3}(-1) = -0.9125$$

which for the present case is a perfect result.



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

or

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

$$f'(x_i) \cong \frac{f(x_i) - f(x_{i-1})}{h} = \frac{\nabla f_1}{h}$$

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