# Part 6

## Numerical Differentiation and Integration

### MOTIVATION

- Calculus is the mathematics of change. Because engineers must continuously deal with systems and processes that change, calculus is an essential tool of engineering.
- Standing in the heart of calculus are the mathematical concepts of *differentiation* and *integration*:

to *differentiate* means "to mark off by differences; distinguish; . . . to perceive the difference in or between."

to *integrate* means "to bring together, as parts, into a whole; to unite; to indicate the total amount . . . ."

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

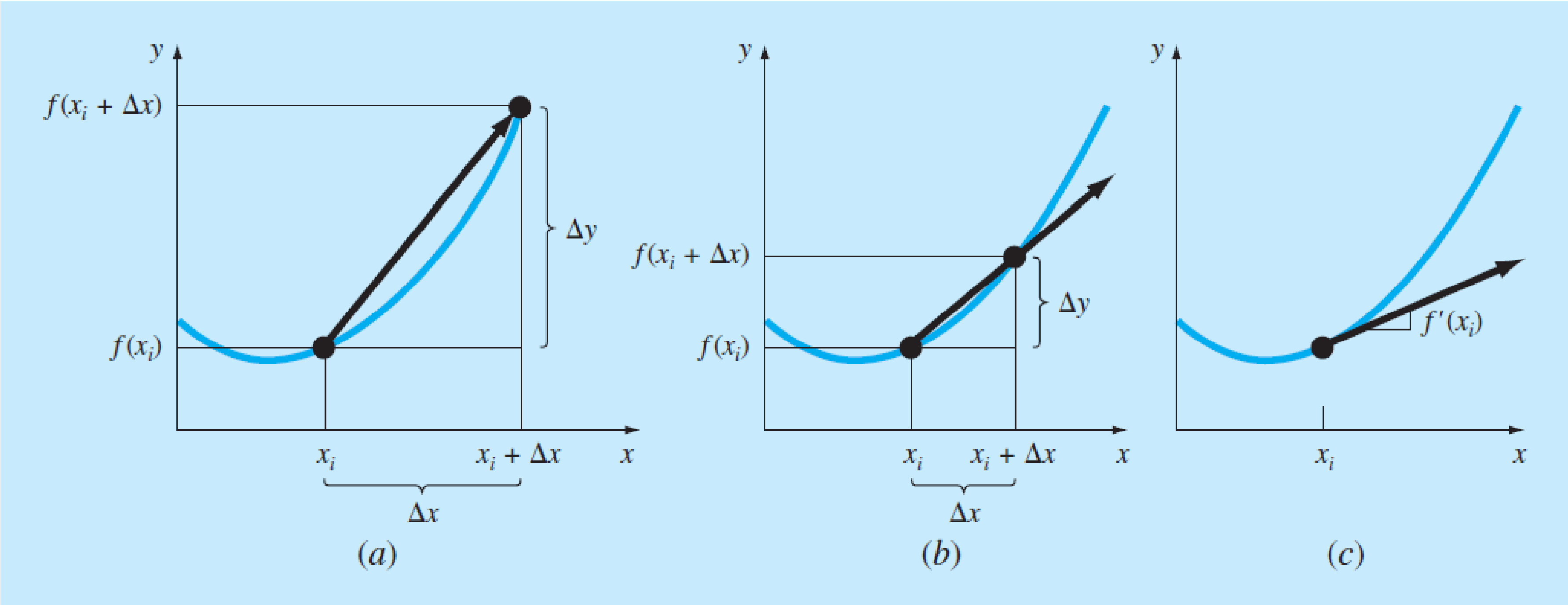
$$\frac{dy}{dx} = \lim_{\Delta x \to 0} \frac{f(x_i + \Delta x) - f(x_i)}{\Delta x}$$

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

- 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.

**FIGURE PT6.1**

The graphical definition of a derivative: as $\Delta x$ approaches zero in going from (a) to (c), the difference approximation becomes a derivative.




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

- Partial derivatives are used for functions that depend on more than one variable.
- Partial derivatives can be thought of as taking the derivative of the function at a point with all but one variable held constant.

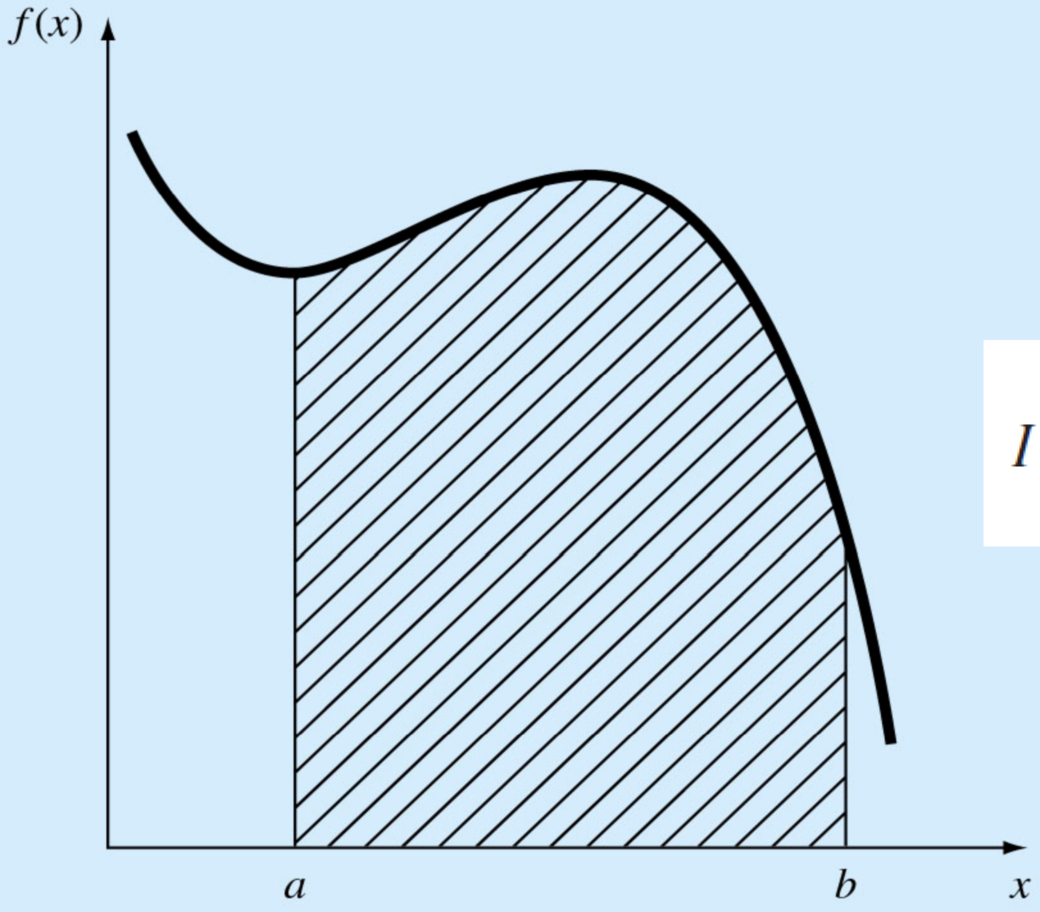
$$\frac{\partial f}{\partial x} = \lim_{\Delta x \to 0} \frac{f(x + \Delta x, y) - f(x, y)}{\Delta x}$$

$$\frac{\partial f}{\partial y} = \lim_{\Delta y \to 0} \frac{f(x, y + \Delta y) - f(x, y)}{\Delta y}$$

- 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 . . . ."

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

This is called the definite integral and it corresponds to the area under the curve of $f(x)$ between $x = a$ and $x = b$.




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

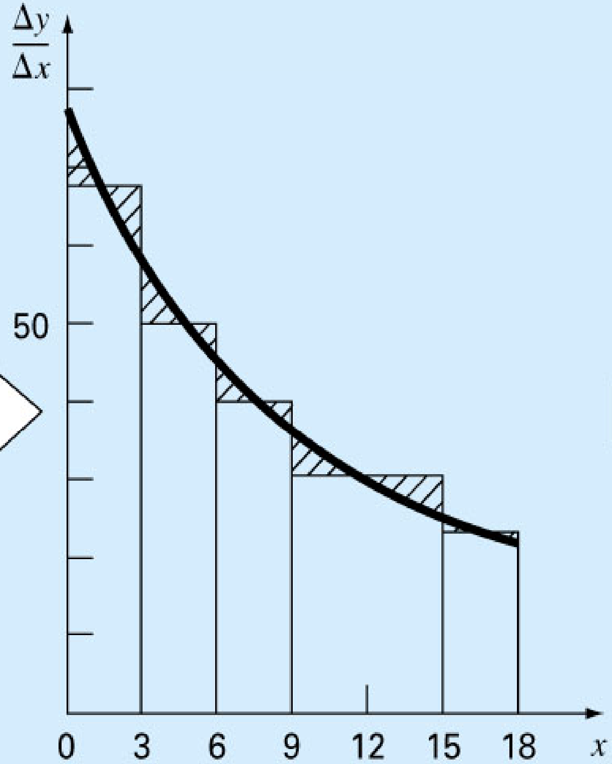
**FIGURE PT6.2**
Graphical representation of the integral of $f(x)$ between the limits $x = a$ to $b$. The integral is equivalent to the area under the curve.

# 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.

| $x$ | $y$ | $\Delta y/\Delta x$ |
|---|---|---|
| 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*)

**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.

## 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 are already in tabular form (b); therefore, step (a) is unnecessary.

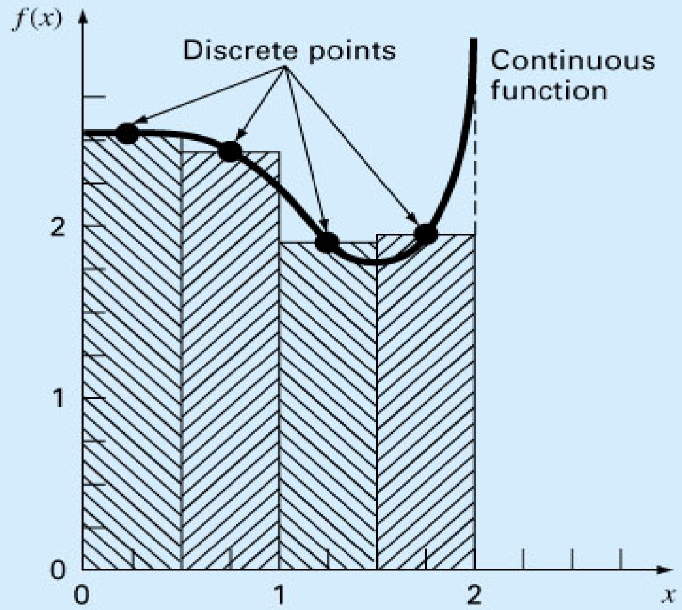
(a)

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

(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

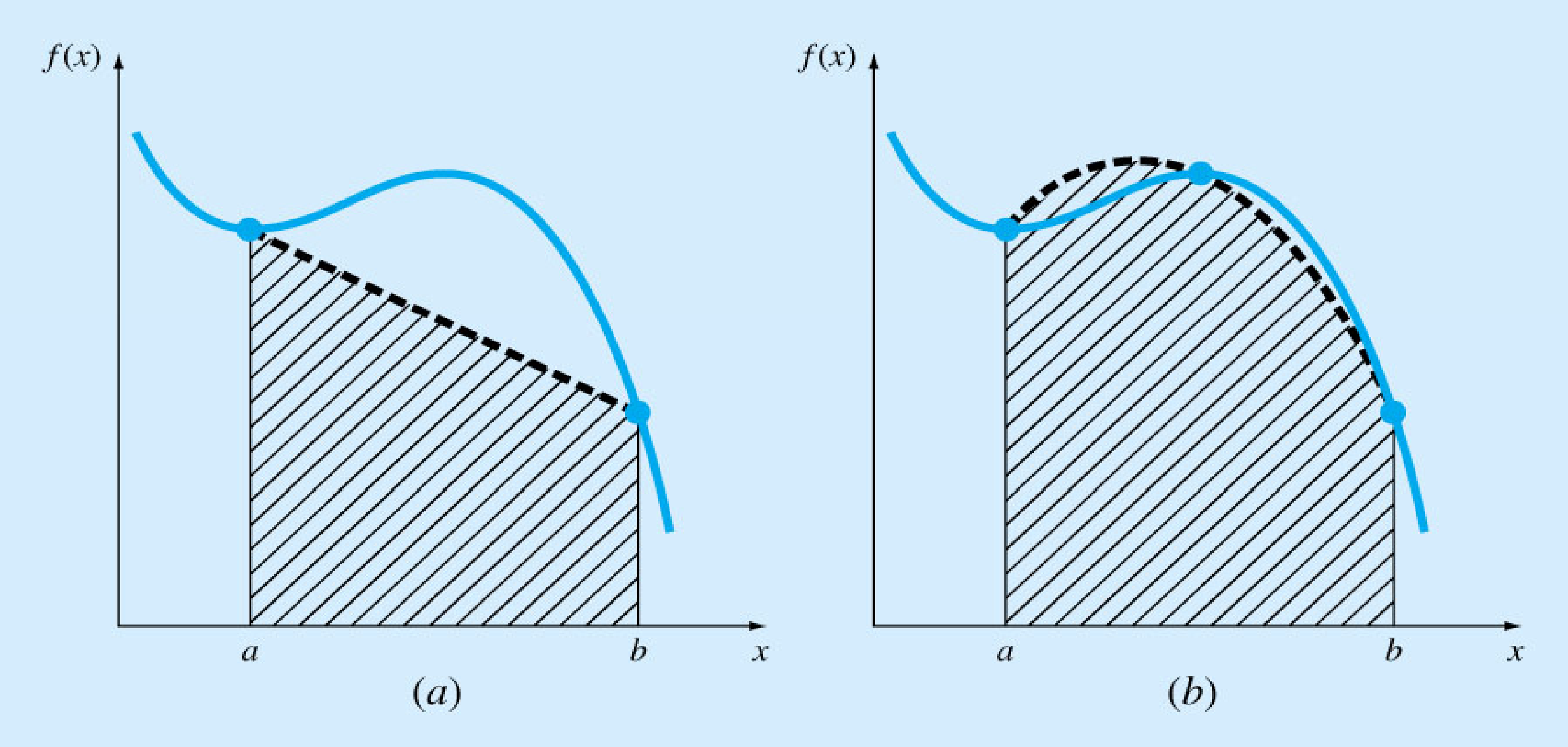
## Chapter 21

- 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:

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

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




The approximation of an integral by the area under
(a) a single straight line and
(b) a single parabola.

The integral can also be approximated using a series of polynomials applied piecewise to the function or data over segments of constant length.

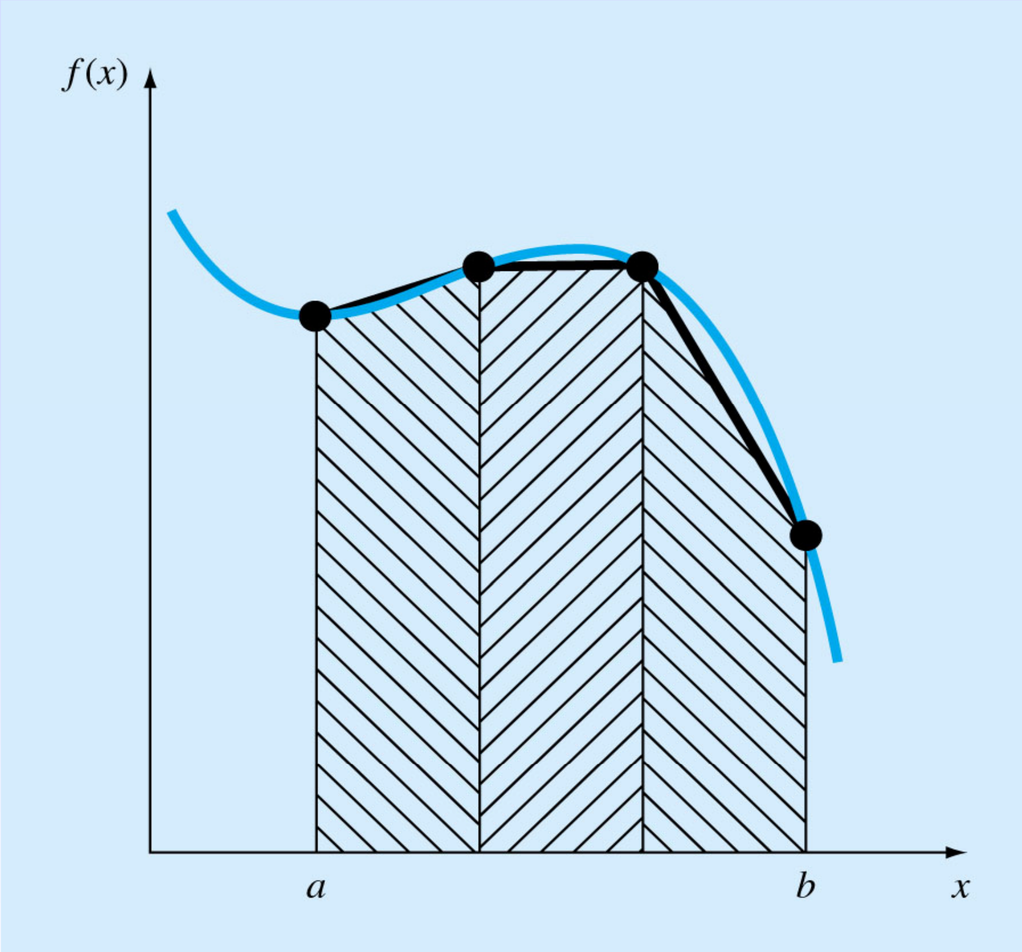



**FIGURE 21.2**
The approximation of an integral by the area under three straight-line segments.

# 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*:

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

# Proof of the 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 $b^2 - a^2 = (b - a)(b + a)$,

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

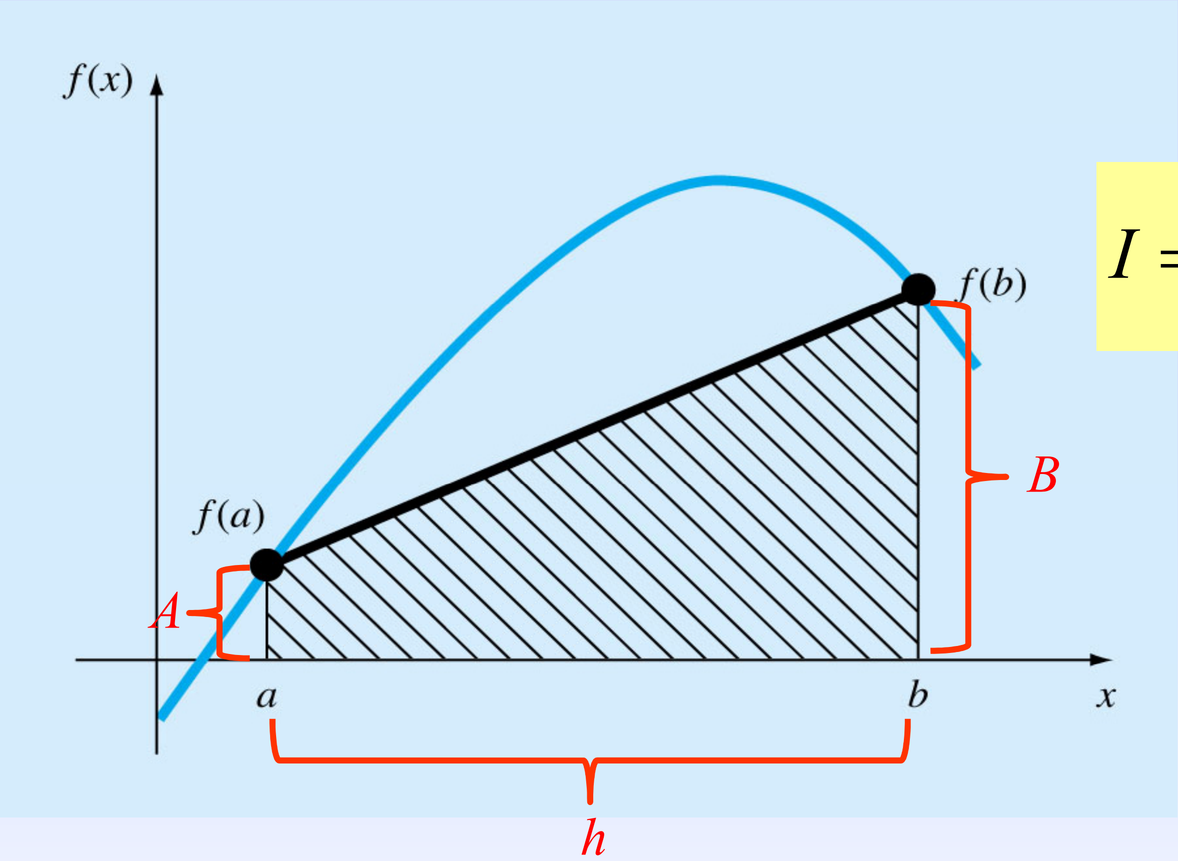
Multiplying and collecting terms yields

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

which is the formula for the trapezoidal rule.

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

**FIGURE 21.4**
Graphical depiction of the trapezoidal rule.

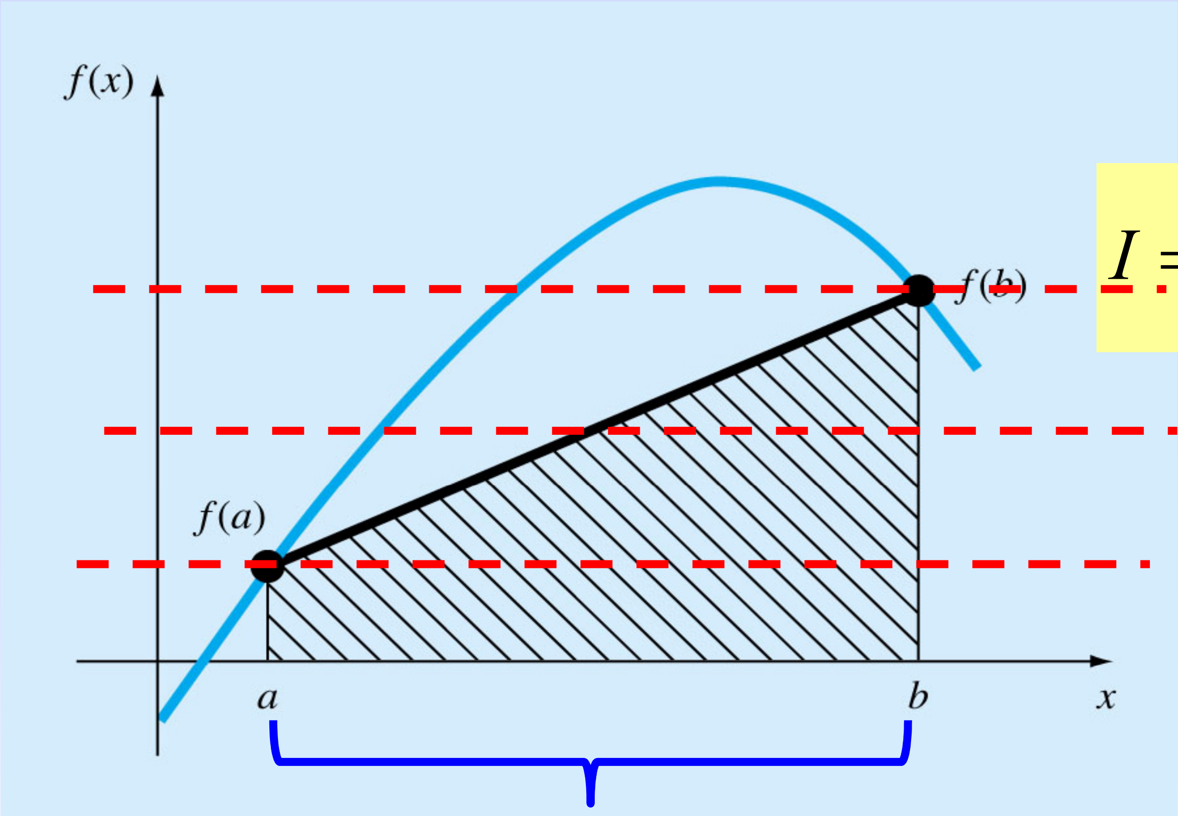



$$I = (b-a)\frac{f(a)+f(b)}{2}$$

Equals to the area under the trapezoid

Area of the Trapezoid = $(A + B)\ h\ /\ 2$

**FIGURE 21.4**
Graphical depiction of the trapezoidal rule.




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

**Average height**

**Width**

All Newton-Cotes formulas can be written in the form

“***I ≈ Average height*** × ***width***”.

Different formulas will have different expressions for average height.

- Newton-Cotes formulas can be derived by integrating Newton's Interpolating Polynomials.
- Newton-Gregory version can be used for equispaced data points.

Remember Newton-Gregory forward formula used for *n*th order approximation::

$$f_n(x) = f(x_0) + \Delta f(x_0)\alpha + \frac{\Delta^2 f(x_0)}{2!}\alpha(\alpha - 1) + \cdots + \frac{\Delta^n f(x_0)}{n!}\alpha(\alpha - 1)\cdots(\alpha - n + 1) + R_n$$

where $\alpha = \dfrac{x - x_0}{h}$ $\quad R_n = \dfrac{f^{(n+1)}(\xi)}{(n+1)!}h^{n+1}\alpha(\alpha - 1)(\alpha - 2)\cdots(\alpha - n)$

- This representation (the remainder term) also provide an estimate for the truncation error.

# Derivation of the trapezoidal rule ($n$=1 case) by using Newton-Gregory forward formula:

$$I = \int_a^b \left[ f(a) + \Delta f(a)\alpha + \frac{f''(\xi)}{2}\alpha(\alpha - 1)h^2 \right] dx$$

Substitution: $\alpha = (x - a)/h, \quad dx = h\,d\alpha$

$$I = h\int_0^1 \left[ f(a) + \Delta f(a)\alpha + \frac{f''(\xi)}{2}\alpha(\alpha - 1)h^2 \right] d\alpha$$

$f''(\xi)$ can be considered as constant for small $h$:

$$I = h\left[ \alpha f(a) + \frac{\alpha^2}{2}\Delta f(a) + \left(\frac{\alpha^3}{6} - \frac{\alpha^2}{4}\right) f''(\xi)h^2 \right]_0^1$$

$$I = h\left[ f(a) + \frac{\Delta f(a)}{2} \right] - \frac{1}{12} f''(\xi)h^3 \qquad \text{replacing } \Delta f(a) = f(b) - f(a).$$

$$I = \underbrace{h\frac{f(a) + f(b)}{2}}_{\text{Trapezoidal rule}} - \underbrace{\frac{1}{12} f''(\xi)h^3}_{\text{Truncation error}}$$

## Error of the Trapezoidal Rule/

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

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

where $\xi$ lies somewhere in the interval from $a$ to $b$.

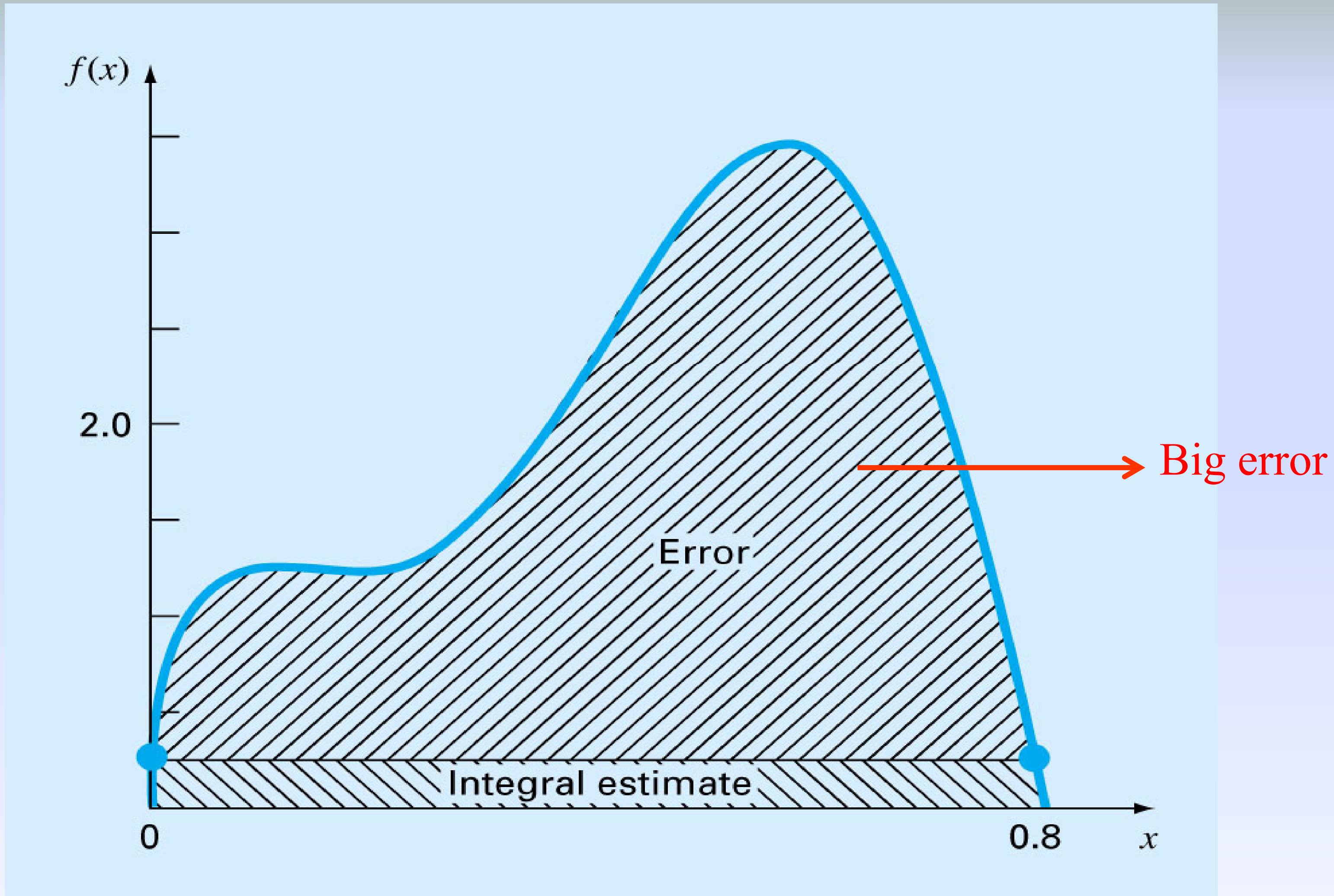



**FIGURE 21.6**
Graphical depiction of the use of a single application of the trapezoidal rule to approximate the integral of $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$ from $x = 0$ to $0.8$.

# 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:

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

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

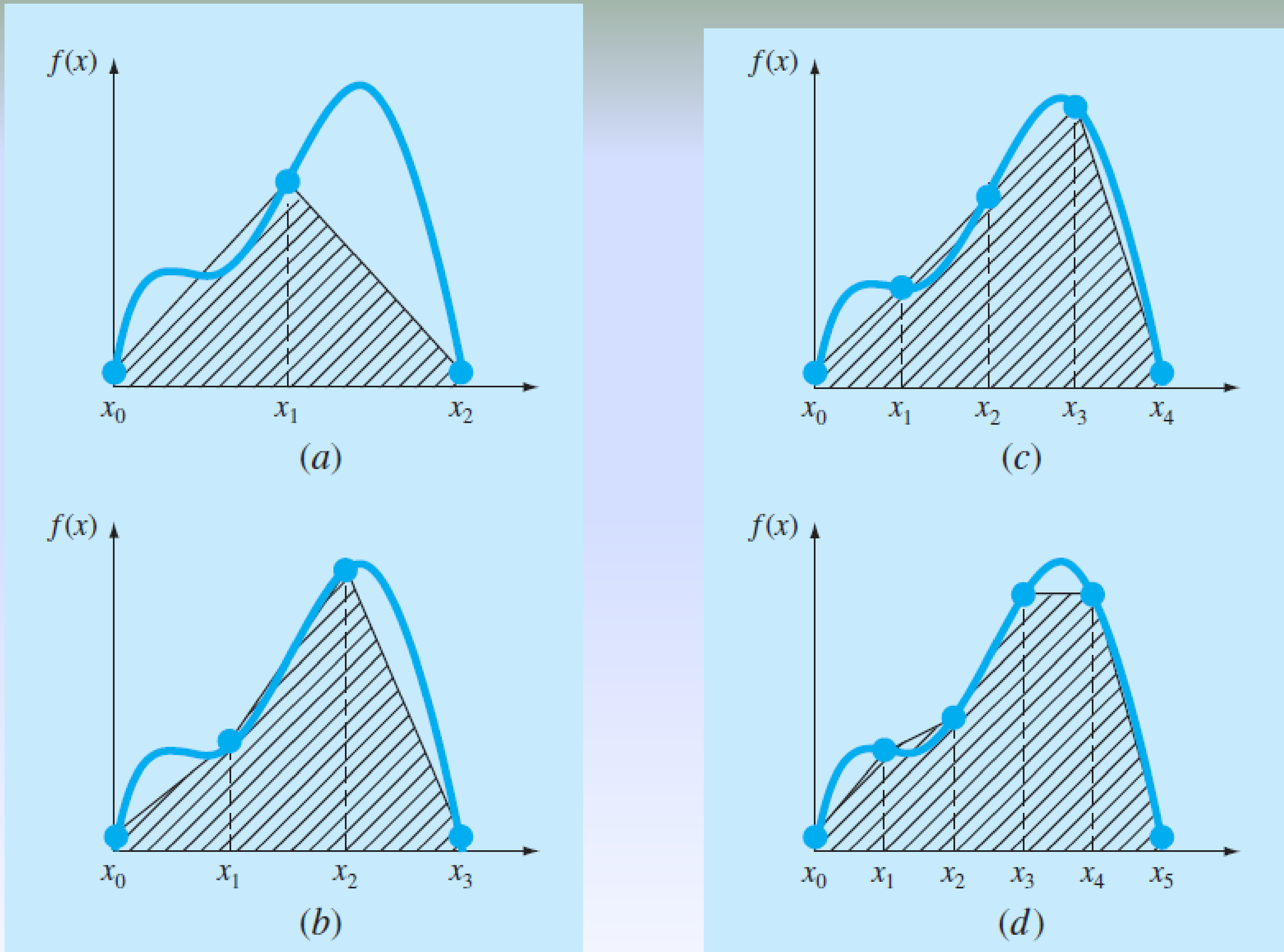



**FIGURE 21.7**

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

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

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

$f''(\xi_i)$ is the second derivative at a point $i$ located in segment $i$. This result can be simplified by estimating the mean or average value of the second derivative for the entire interval as $\bar{f}''$:

$$\sum f''(\xi i) \cong n\bar{f}''$$

$$E_a = -\frac{(b-a)^3}{12n^2}\bar{f}''$$

Thus, if the number of segments is doubled, the truncation error will be quartered.

# Homework:

- Try the following pseudocodes in MATLAB to examine with Examples 21.1, 21.2 and 21.3.

**(*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
  DOFOR i = 1, n − 1
    sum = sum + 2 * fi
  END DO
  sum = sum + fn
  Trapm = h * sum / 2
END Trapm
```

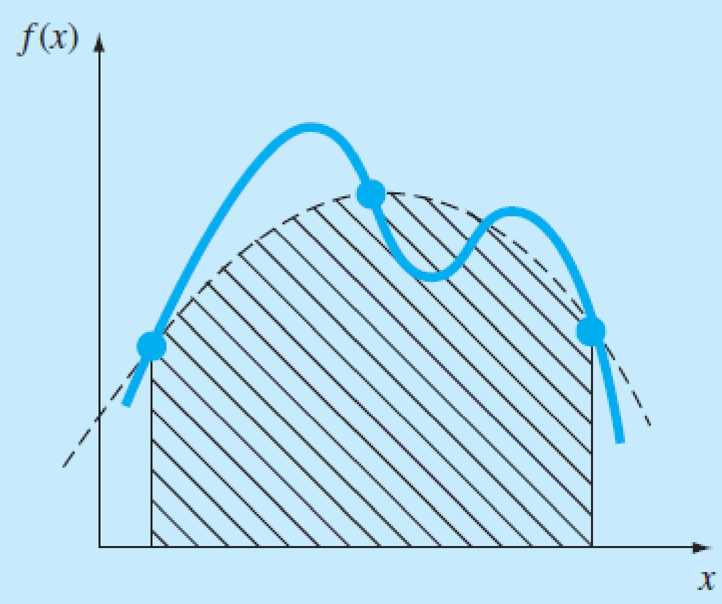
**FIGURE 21.9**
Algorithms for the (*a*) single-segment and (*b*) multiple-segment trapezoidal rule.

# 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.
- It is the second Newton-Cotes closed integration formula.




(a)

Graphical depiction of Simpson's 1/3 rule: It consists of taking the area under a parabola connecting three points.

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

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

This equation is known as Simpson's 1/3 rule. It is the second Newton-Cotes closed integration formula. The label "1/3" stems from the fact that $h$ is divided by 3 .

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

$$a = x_0 \quad b = x_2$$

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

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

Simpson's 1/3 Rule

Single segment application of Simpson's 1/3 rule has a truncation error of:

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

- Simpson's 1/3 Rule uses 3 points, therefore it is expected to integrate 2nd order polynomials exactly.
- However it can integrate cubics exactly. This is due to the vanishing third term in integrating the Newton-Gregory polynomial.
- Simpson's 1/3 rule is more accurate than trapezoidal rule in general.

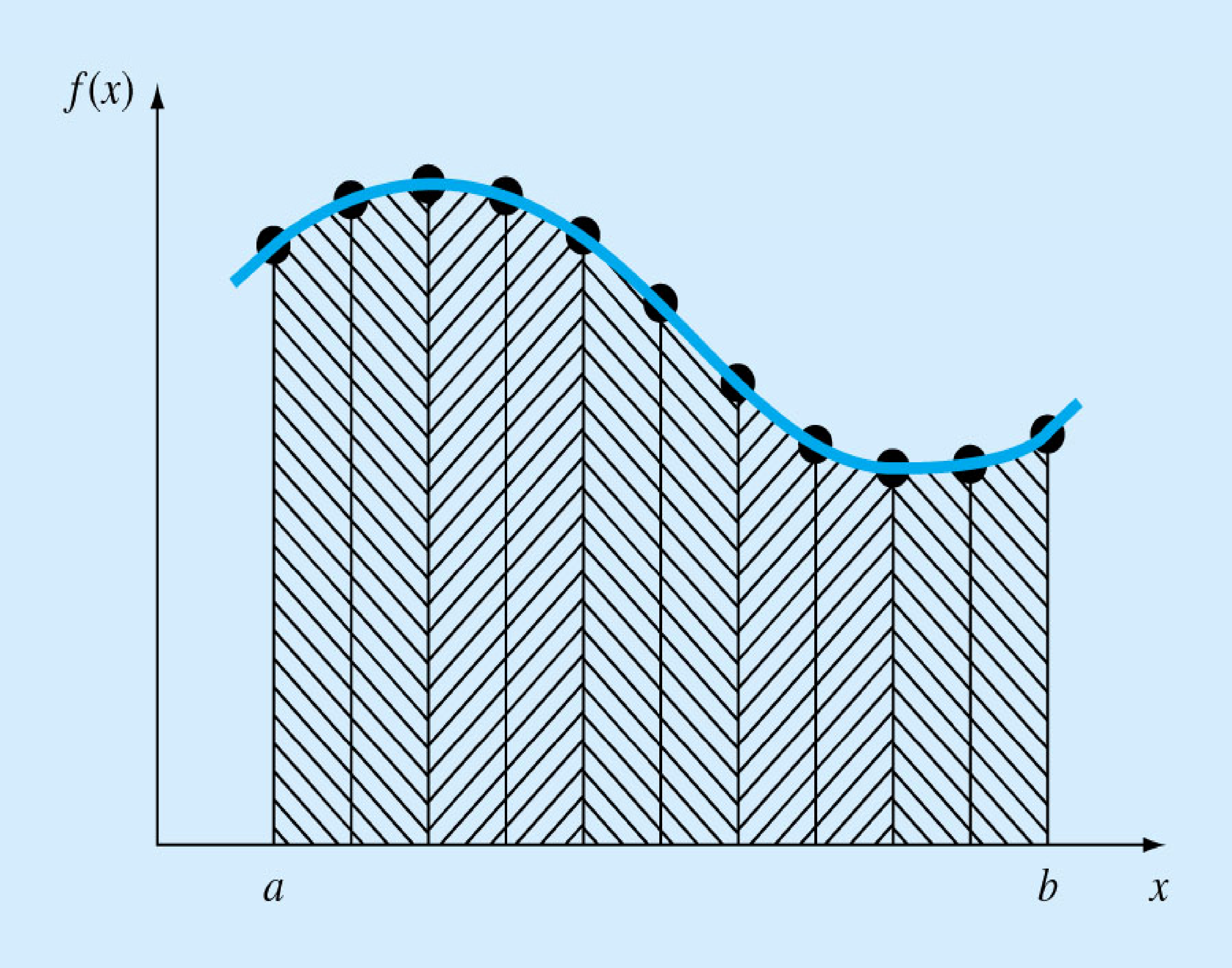
$$I = \underbrace{\frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right]}_{\text{Simpson's 1/3}} - \underbrace{\frac{1}{90}f^{(4)}(\xi)h^5}_{\text{Truncation error}}$$

**Proof**: Home Study (*see* box 21.3 pp. 616)

$h = (b - a)/2$

# The Multiple-Application Simpson's of 1/3 Rule

- Just as the trapezoidal rule, Simpson's rule can be improved by dividing the integration interval into a number of segments of equal width.
- Yields accurate results and considered superior to trapezoidal rule for most applications.
- *However*, it is limited to cases where values are equispaced.
- *Further*, it is limited to situations where there are an even number of segments and odd number of points.




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:

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

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

# Simpson's 3/8 Rule:

- A third order Lagrange polynomial can be fit to four points and integrated as:

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

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

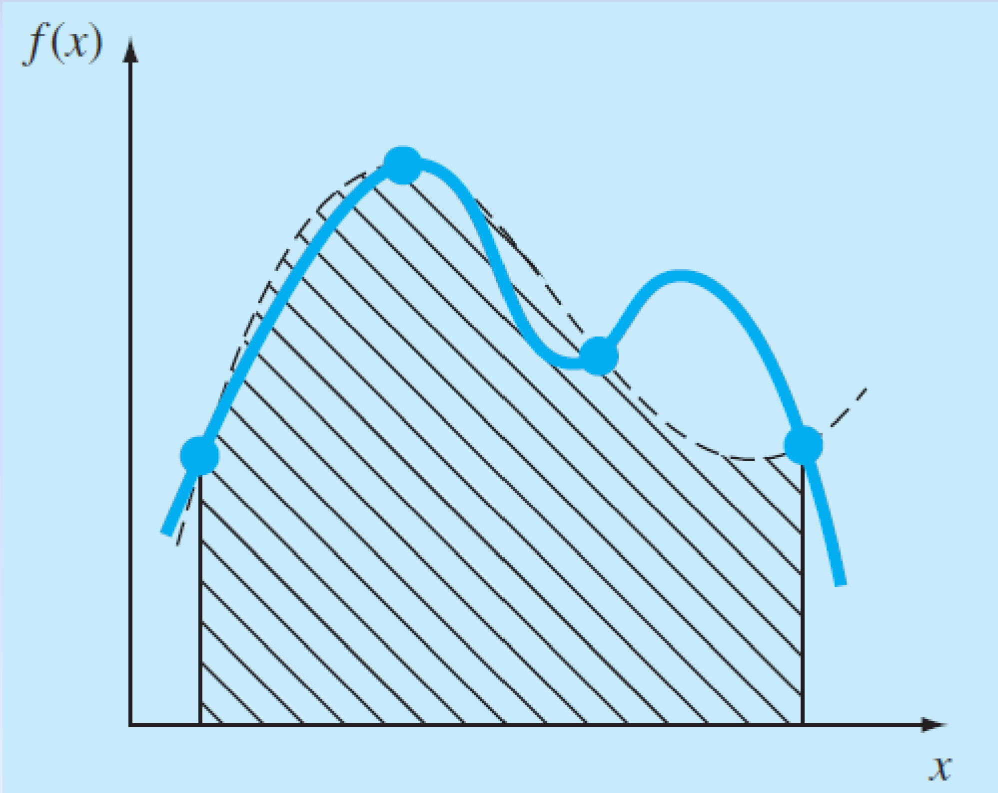
$$h = \frac{(b-a)}{3}$$

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

This equation is called Simpson's 3/8 rule because $h$ is multiplied by 3/8.

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

More accurate (error is smaller)




Graphical depiction of Simpson's 3/8 rule:
It consists of taking the area under a cubic equation connecting four points.

- Simpson's 1/3 rule is usually the method of preference because it attains third order accuracy with three points rather than the four points required for the 3/8 version.
- However, the 3/8 rule has utility when the number of segments is odd.
- Suppose that you desired an estimate for five segments. One option would be to use a multiple-application version of the trapezoidal rule. This may not be advisable, however, because of the large truncation error associated with this method.
- An alternative would be to apply Simpson's 1/3 rule to the first two segments and Simpson's 3/8 rule to the last three (Fig. 21.12).
- In this way, we could obtain an estimate with third-order accuracy across the entire interval.

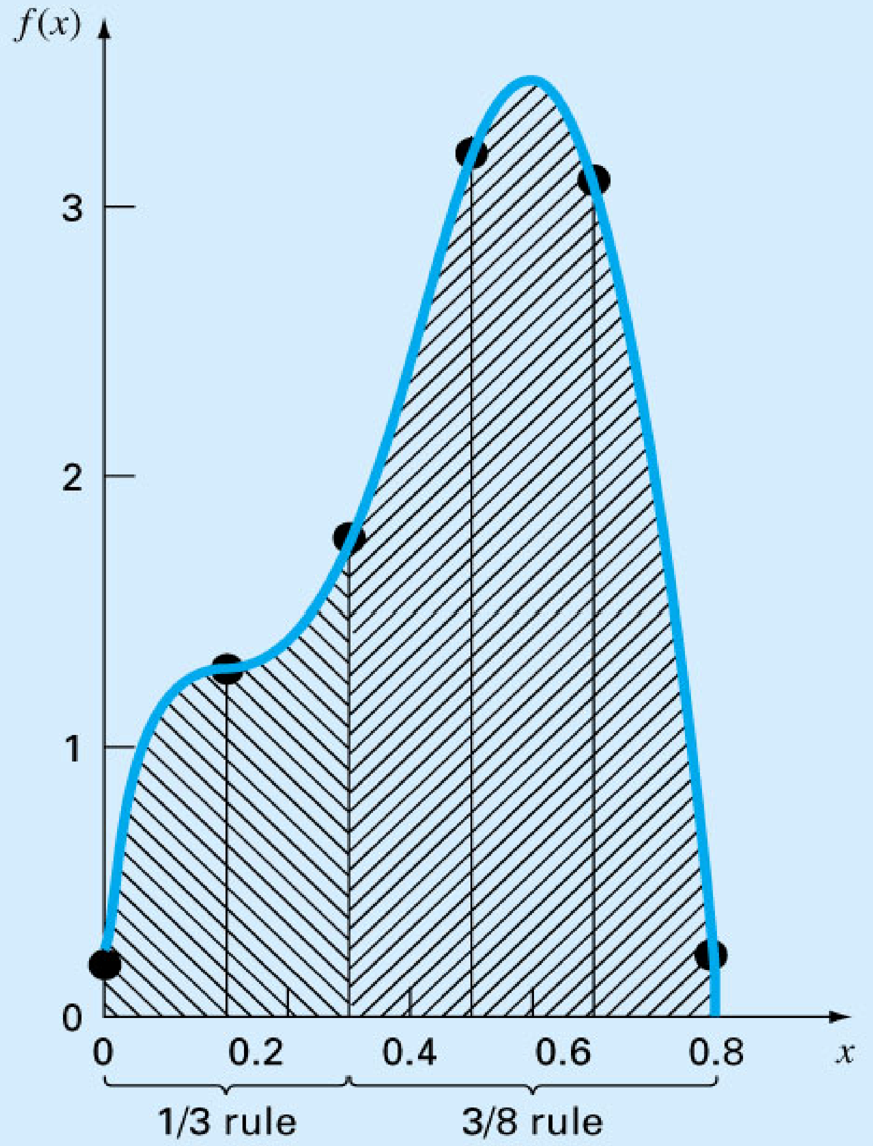



**FIGURE 21.12**
Illustration of how Simpson's 1/3 and 3/8 rules can be applied in tandem to handle multiple applications with odd numbers of intervals.

# Pseudocodes for Simpson's Rules:

(a)
```
FUNCTION Simp13 (h, f0, f1, f2)
  Simp13 = 2*h* (f0+4*f1+f2) / 6
END Simp13
```

(b)
```
FUNCTION Simp38 (h, f0, f1, f2, f3)
  Simp38 = 3*h* (f0+3*(f1+f2)+f3) / 8
END Simp38
```

(c)
```
FUNCTION Simp13m (h, n, f)
  sum = f(0)
  DOFOR i = 1, n - 2, 2
    sum = sum + 4 * f_i + 2 * f_(i+1)
  END DO
  sum = sum + 4 * f_(n-1) + f_n
  Simp13m = h * sum / 3
END 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
```

**FIGURE 21.13**
Pseudocode 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, $n$ must be $\geq 1$.

# Integration of Equations

## Chapter 22

- Functions to be integrated numerically are in two forms:
  - *A table of values*. We are limited by the number of points that are given.
  - *A function*. We can generate as many values of *f(x)* as needed to attain acceptable accuracy.
- Will focus on two techniques that are designed to analyze functions:
  - *Romberg integration*
  - *Gauss quadrature*

# Romberg Integration

- Is based on successive application of the trapezoidal rule to attain efficient numerical integrals of functions.

**Richardson's Extrapolation/**

- Uses two estimates of an integral to compute a third and more accurate approximation.

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

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

$$h = (b-a)/n$$

$$I(h_1) + E(h_1) = I(h_2) + E(h_2)$$

$$n = (b-a)/h$$

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

Assumed constant regardless of step size

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

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

*I* =exact value of integral

*I(h)* =the approximation from an *n* segment application of trapezoidal rule with step size *h*

*E(h)* =the truncation error

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

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

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

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

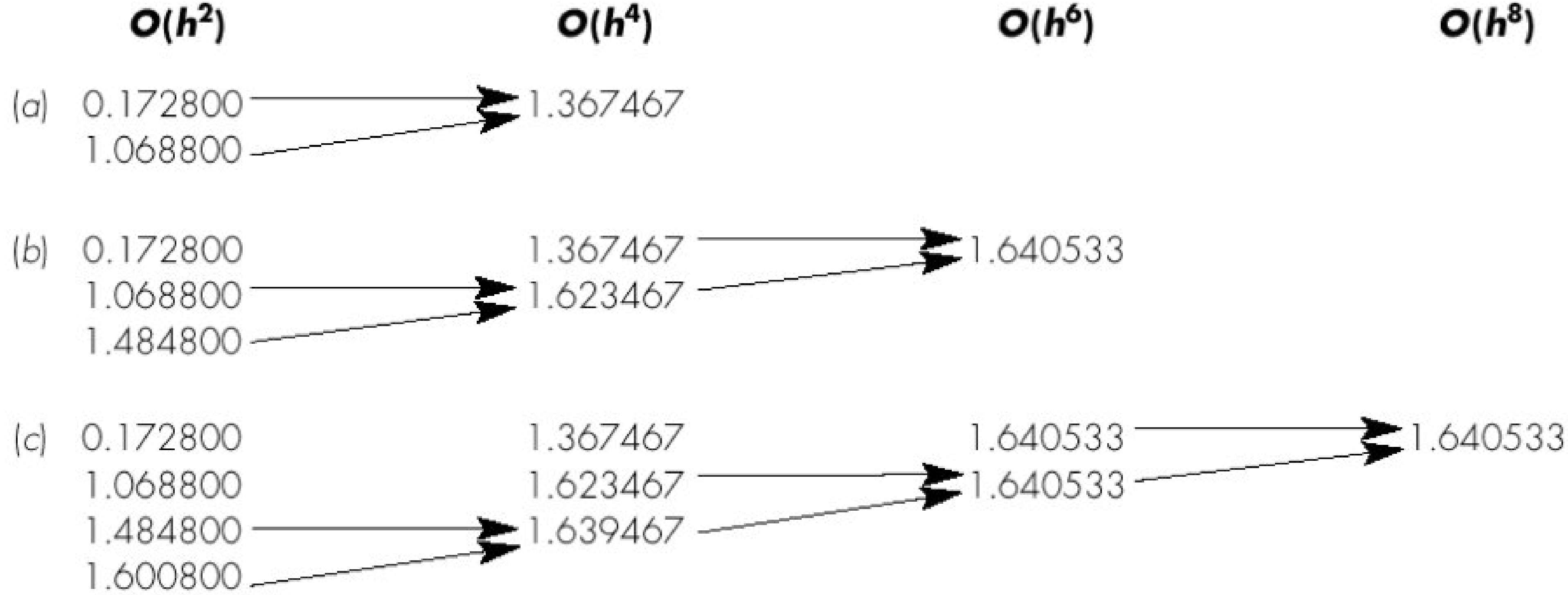
Improved estimate of the integral

# Romberg integration algorithm

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

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

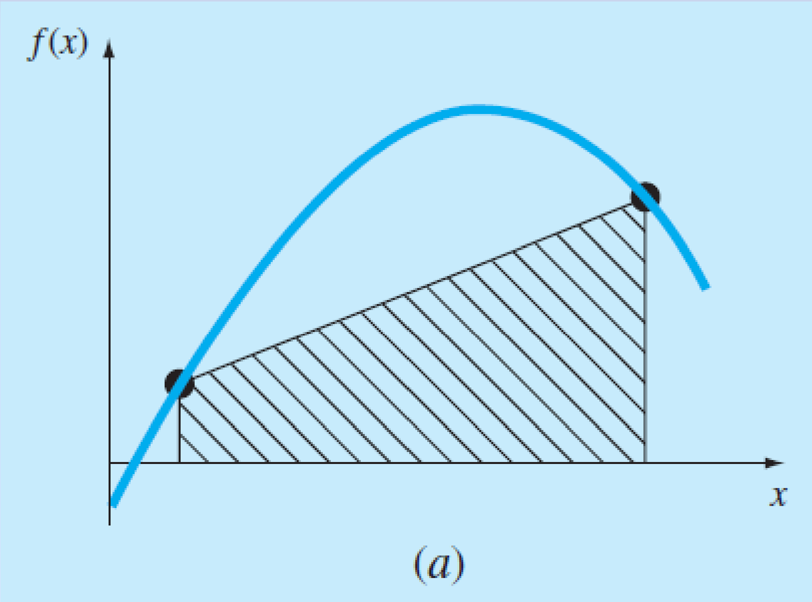
```
FUNCTION Romberg (a, b, maxit, es)
  LOCAL I(10, 10)
  n = 1
  I(1,1) = TrapEq(n, a, b)
  iter = 0
  DO
    iter = iter + 1
    n = 2^iter
    I(iter+1,1) = TrapEq(n, a, b)
    DOFOR k = 2, iter + 1
      j = 2 + iter − k
      I(j,k) = (4^(k−1) * I(j+1,k−1) − I(j,k−1)) / (4^(k−1) − 1)
    END DO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

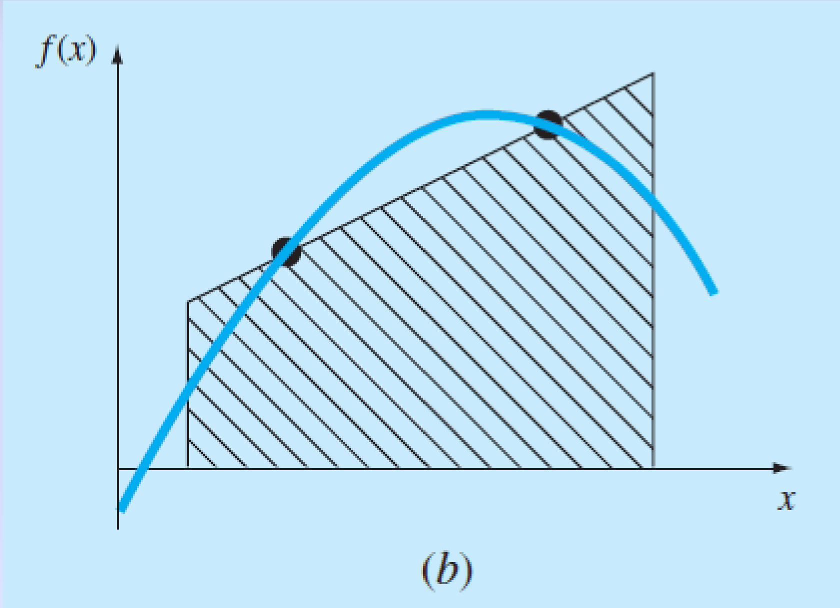



Graphical depiction of the sequence of integral estimates generated using Romberg integration.
(a) First iteration. (b) Second iteration. (c) Third iteration.

# Gauss Quadrature

- ***Gauss quadrature*** implements a strategy of positioning any two points on a curve to define a straight line that would balance the positive and negative errors.
- Hence the area evaluated under this straight line provides an improved estimate of the integral.




(a) Graphical depiction of the trapezoidal rule as the area under the straight line joining fixed end points.

(b) An improved integral estimate obtained by taking the area under the straight line passing through two intermediate points. By positioning these points wisely, the positive and negative errors are balanced, and an improved integral estimate results.

# Method of Undetermined Coefficients/

$$I \cong c_0 f(a) + c_1 f(b)$$

- The trapezoidal rule yields exact results when the function being integrated is a constant or a straight line, such as $y=1$ and $y=x$:

$$c_0 + c_1 = \int_{-(b-a)/2}^{(b-a)/2} 1\,dx$$

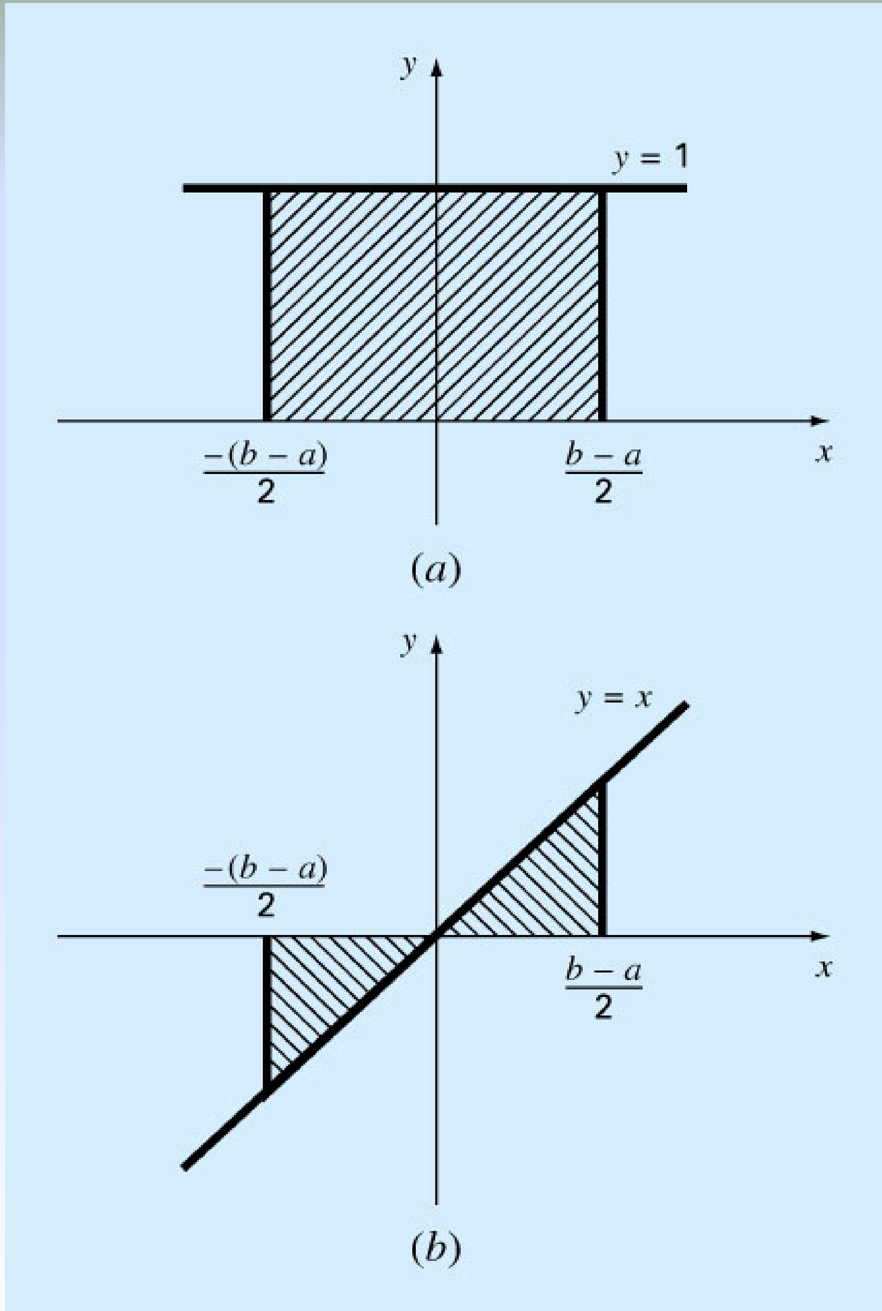
$$-c_0 \frac{b-a}{2} + c_1 \frac{b-a}{2} = \int_{-(b-a)/2}^{(b-a)/2} x\,dx$$

$$\left.\begin{aligned} c_0 + c_1 &= b-a \\ -c_0 \frac{b-a}{2} + c_1 \frac{b-a}{2} &= 0 \end{aligned}\right\} \text{Solve simultaneously}$$

$$c_0 = c_1 = \frac{b-a}{2}$$

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

Trapezoidal rule




Two integrals that should be evaluated exactly by the trapezoidal rule:
(a) a constant,
(b) a straight line.

## Derivation of the Two-Point Gauss-Legendre Formula

- The object of Gauss quadrature is to determine the equations of the form

$$I \cong c_0 f(x_0) + c_1 f(x_1)$$

- However, in contrast to trapezoidal rule that uses fixed end points *a* and *b*, the function arguments $x_0$ and $x_1$ are not fixed end points but unknowns.
- Thus, *four unknowns* to be evaluated require *four conditions*.
- First two conditions are obtained by assuming that the above eqn. for *I* fits the integral of a constant and a linear function exactly.
- The other two conditions are obtained by extending this reasoning to *a parabolic* and *a cubic* functions.

$$\left.\begin{aligned}
c_0 f(x_0) + c_1 f(x_1) &= \int_{-1}^{1} 1\, dx = 2 \\
c_0 f(x_0) + c_1 f(x_1) &= \int_{-1}^{1} x\, dx = 0 \\
c_0 f(x_0) + c_1 f(x_1) &= \int_{-1}^{1} x^2\, dx = \frac{2}{3} \\
c_0 f(x_0) + c_1 f(x_1) &= \int_{-1}^{1} x^3\, dx = 0
\end{aligned}\right\}$$

Solved simultaneously

$$c_0 = c_1 = 1$$

$$x_0 = -\frac{1}{\sqrt{3}} = -0.5773503\ldots$$

$$x_1 = \frac{1}{\sqrt{3}} = -0.5773503\ldots$$

$$\boxed{I \cong f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)}$$

Yields an integral estimate that is third order accurate

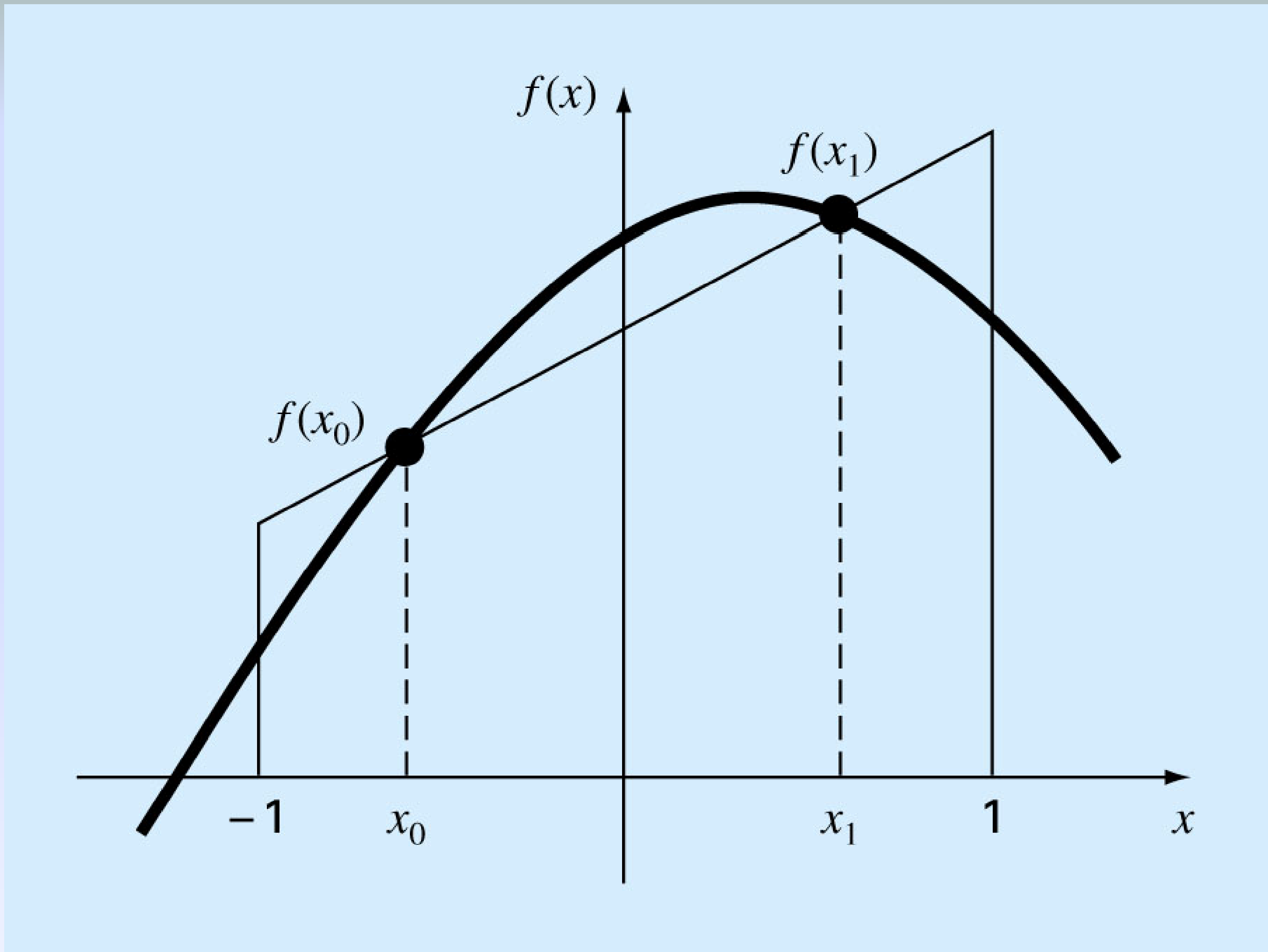



**FIGURE 22.8**
Graphical depiction of the unknown variables $x_0$ and $x_1$ for integration by Gauss quadrature.

- Notice that the integration limits are from −1 to 1. This was done for simplicity and make the formulation as general as possible.
- A simple change of variable is used to translate other limits of integration into this form.
- Provided that the higher order derivatives do not increase substantially with increasing number of points ($n$), Gauss quadrature is superior to Newton-Cotes formulas.

$$E_t = \frac{2^{2n+3}\left[(n=1)!\right]^4}{(2n+3)\left[(2n+2)!\right]^3} f^{(2n+2)}(\xi)$$

**Error for the Gauss-Legendre formulas**

# Improper Integrals

- Improper integrals can be evaluated by making a change of variable that transforms the infinite range to one that is finite,

$$\int_a^b f(x)dx = \int_{1/b}^{1/a} \frac{1}{t^2} f\left(\frac{1}{t}\right) dt \qquad ab \succ 0$$

$$\int_{-\infty}^{\infty} f(x)dx = \int_{-\infty}^{-A} f(x)dx + \int_{-A}^{b} f(x)dx$$

where $-A$ is chosen as a sufficiently large negative value so that the function has begun to approach zero asymptotically at least as fast as $1/x^2$.