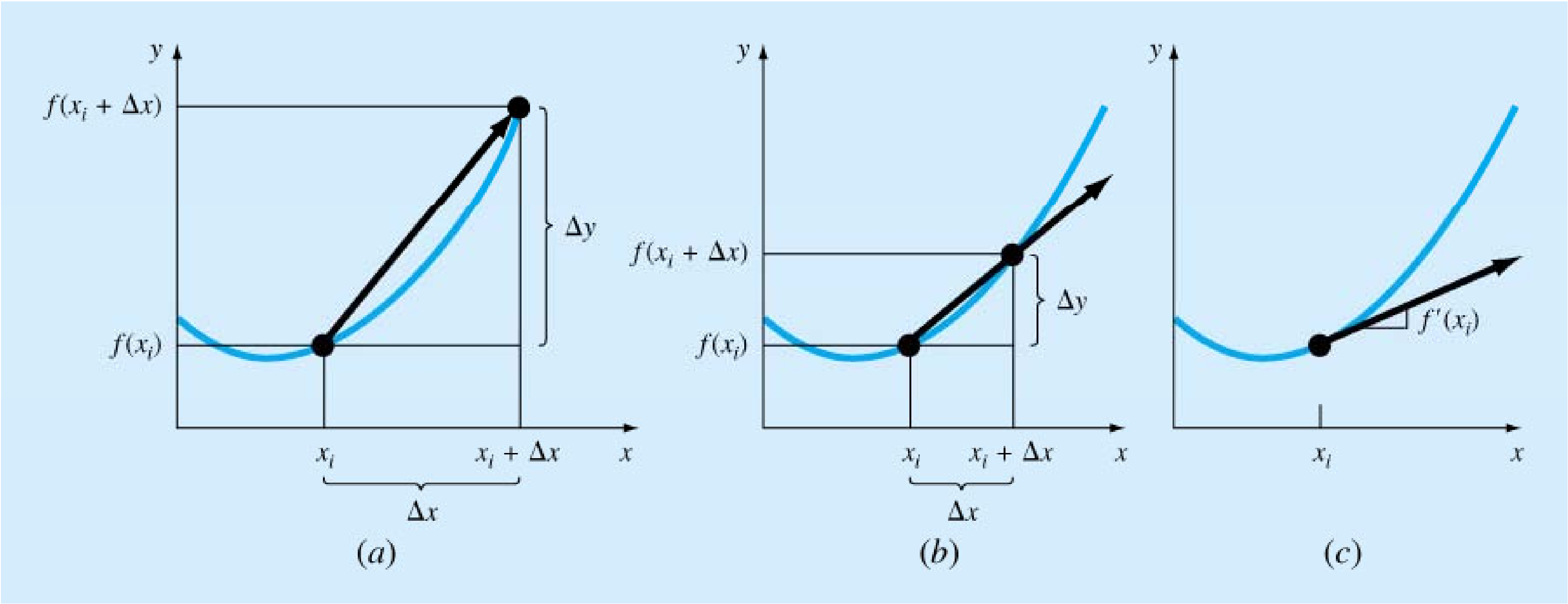
Numerical Differentiation and Integration

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

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

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

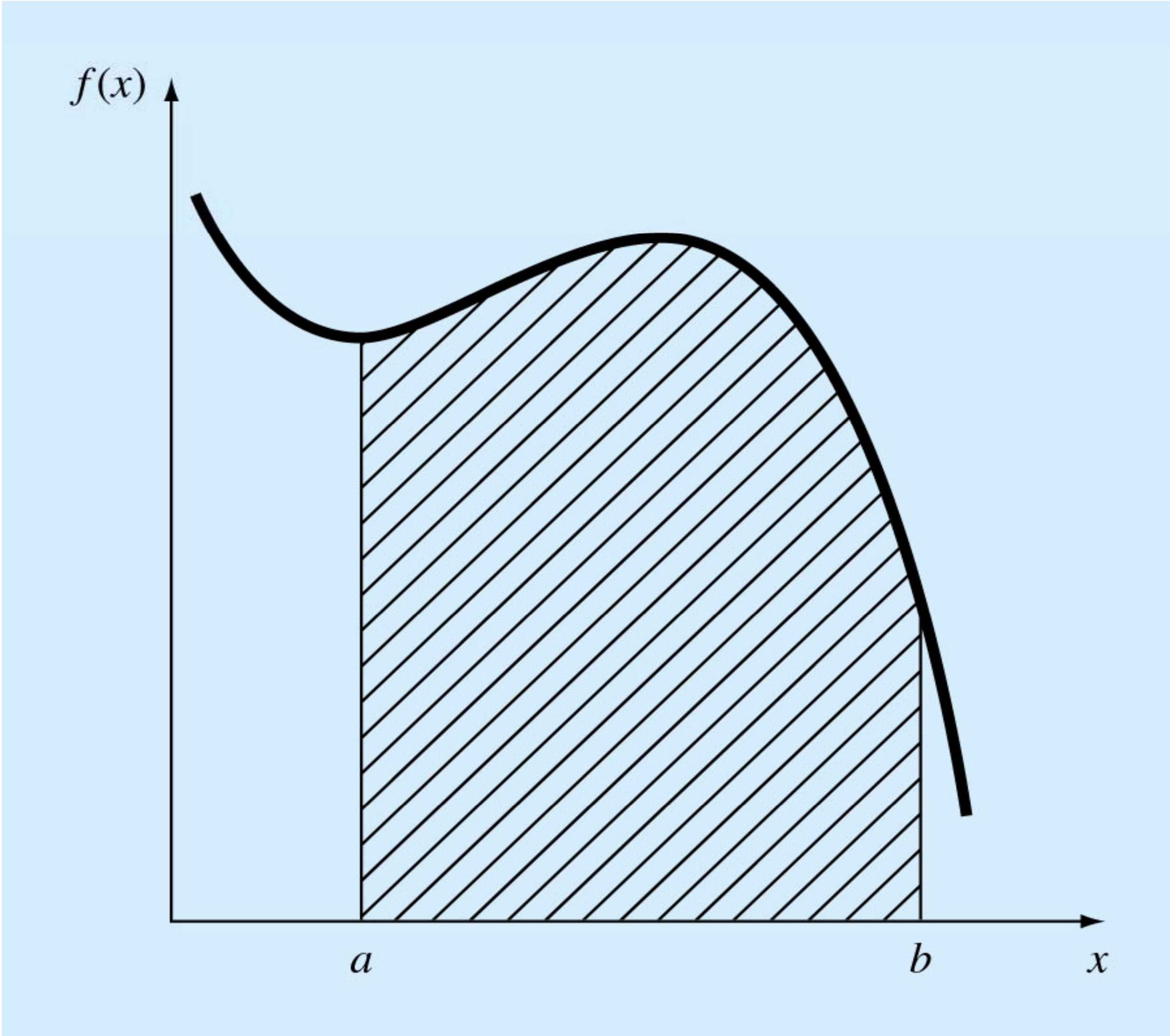
$$I = \int_a^b f(x)dx$$



y
f(x_i + Δx)
f(x_i)
Δy
x_i
x_i + Δx
x
Δx
(a)
y
f(x_i + Δx)
f(x_i)
Δy
x_i
x_i + Δx
x
Δx
(b)
y
f′(x_i)
x_i
x
(c)

Figure 4.1

Figure 4.2



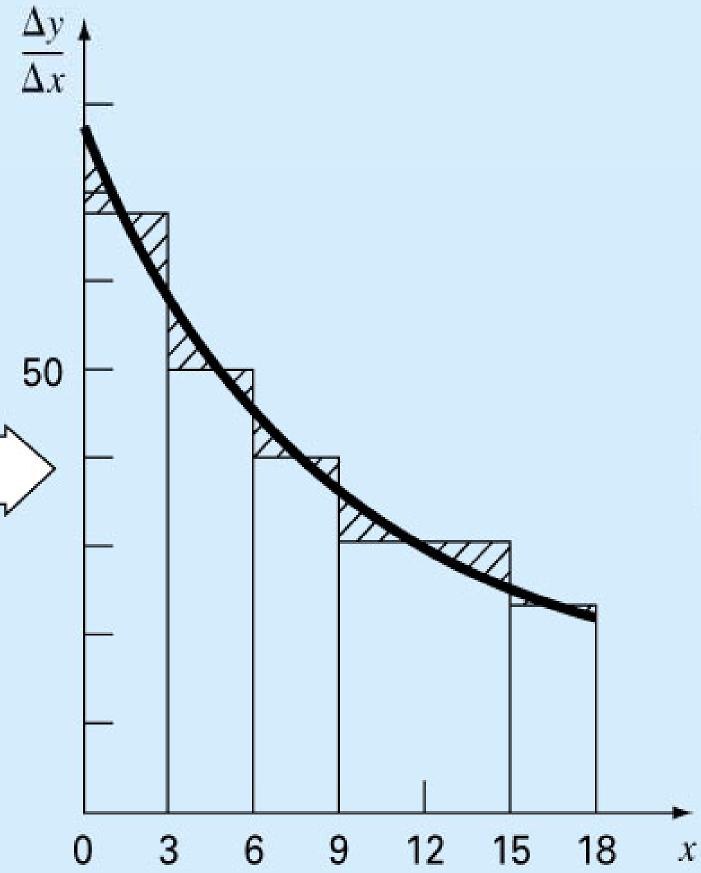
Noncomputer Methods for Differentiation and Integration

- 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 4.3

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*)

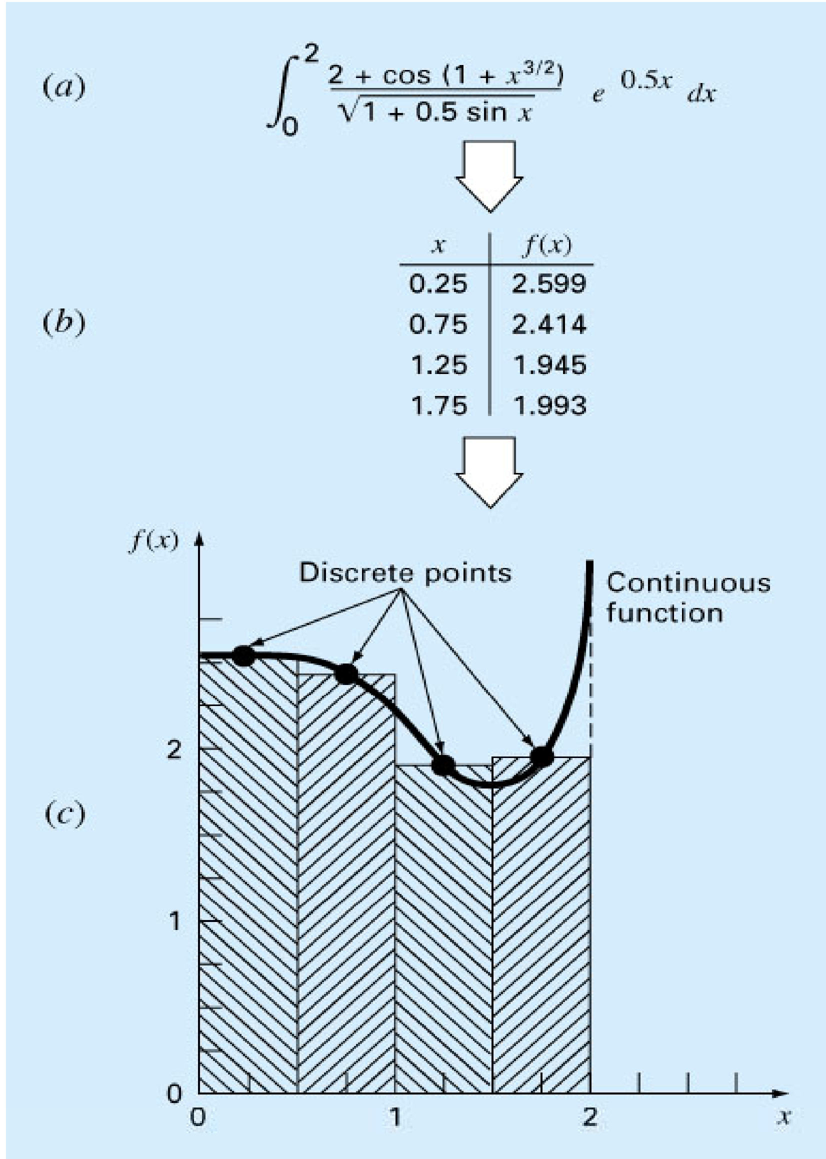


(*b*)

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

(*c*)

Figure 4.4



(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)
f(x)
Discrete points
Continuous function
0
1
2
0
1
2
x

Newton-Cotes Integration Formulas

- 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 4.5

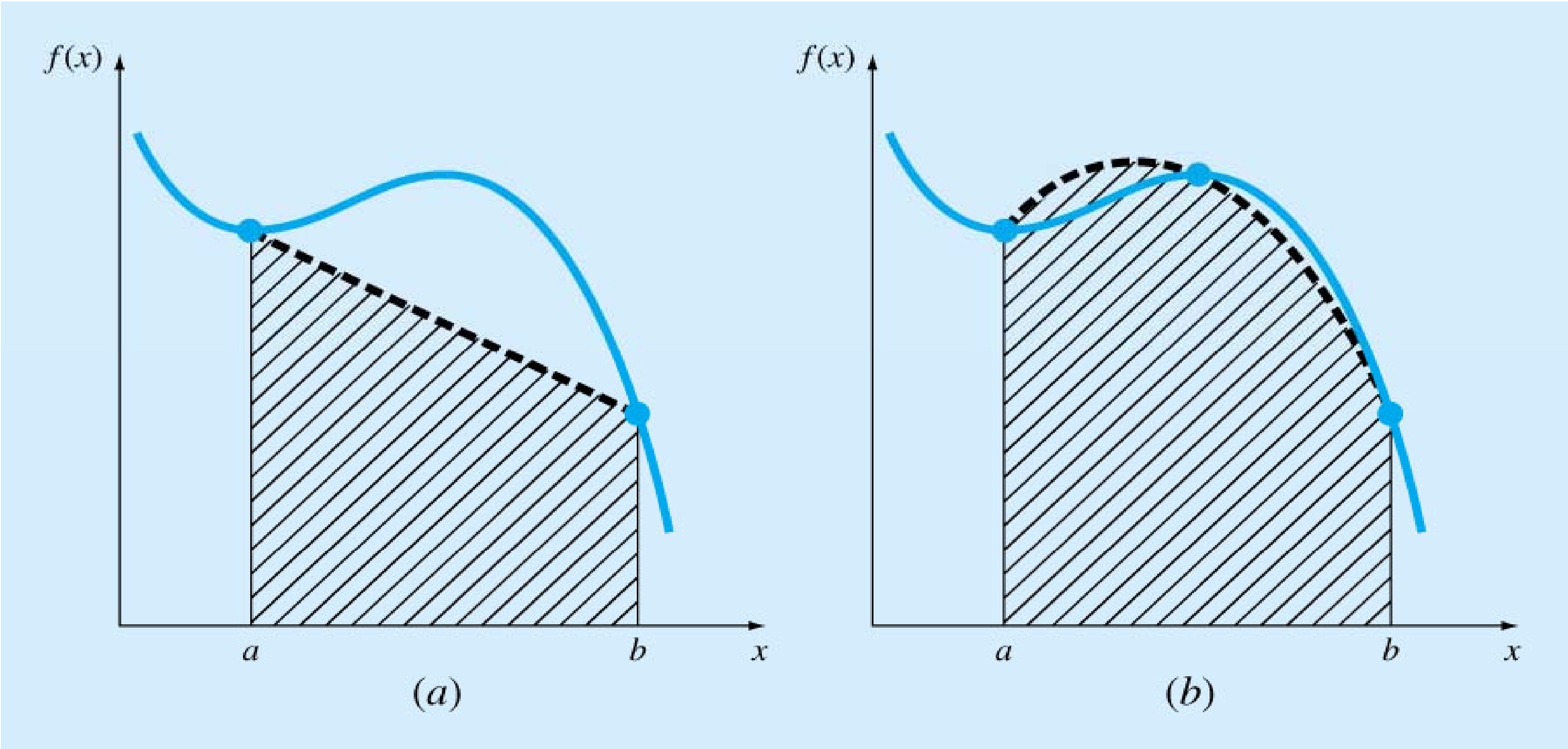
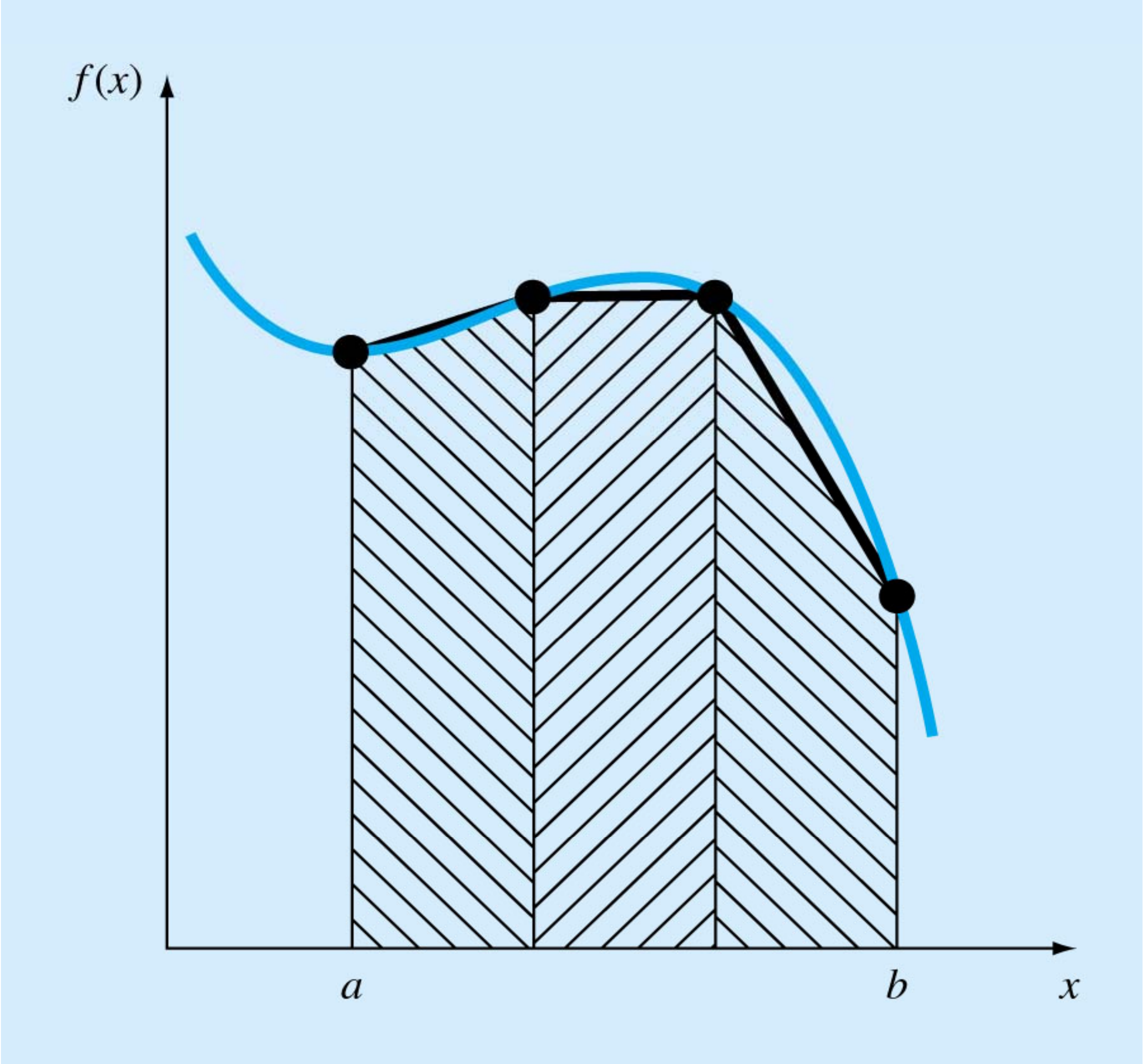


Figure 4.6



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:

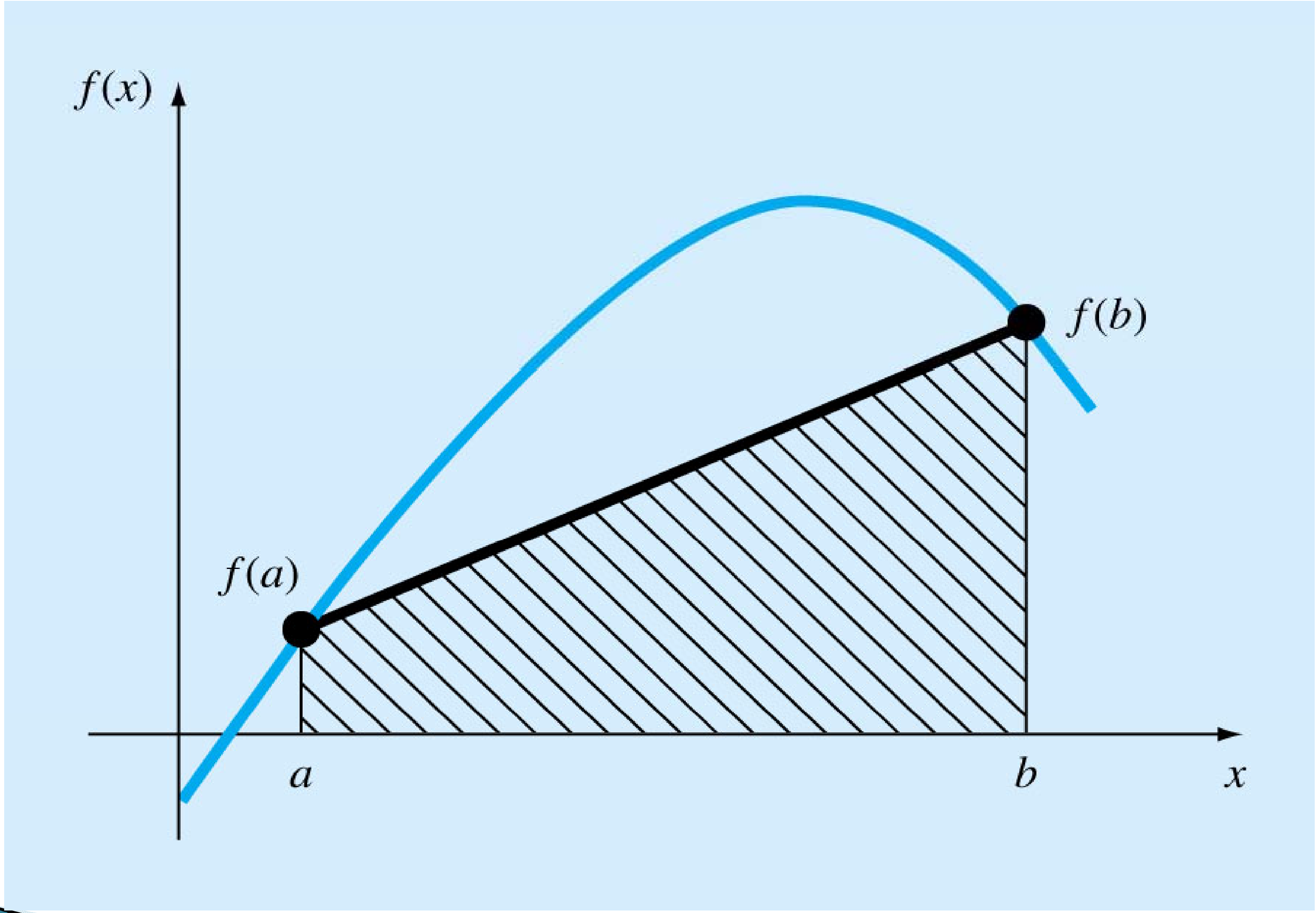
$$I = \int_a^b f(x)dx \cong \int_a^b f_1(x)dx$$

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

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

Trapezoidal rule

Figure 4.7



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*.

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.

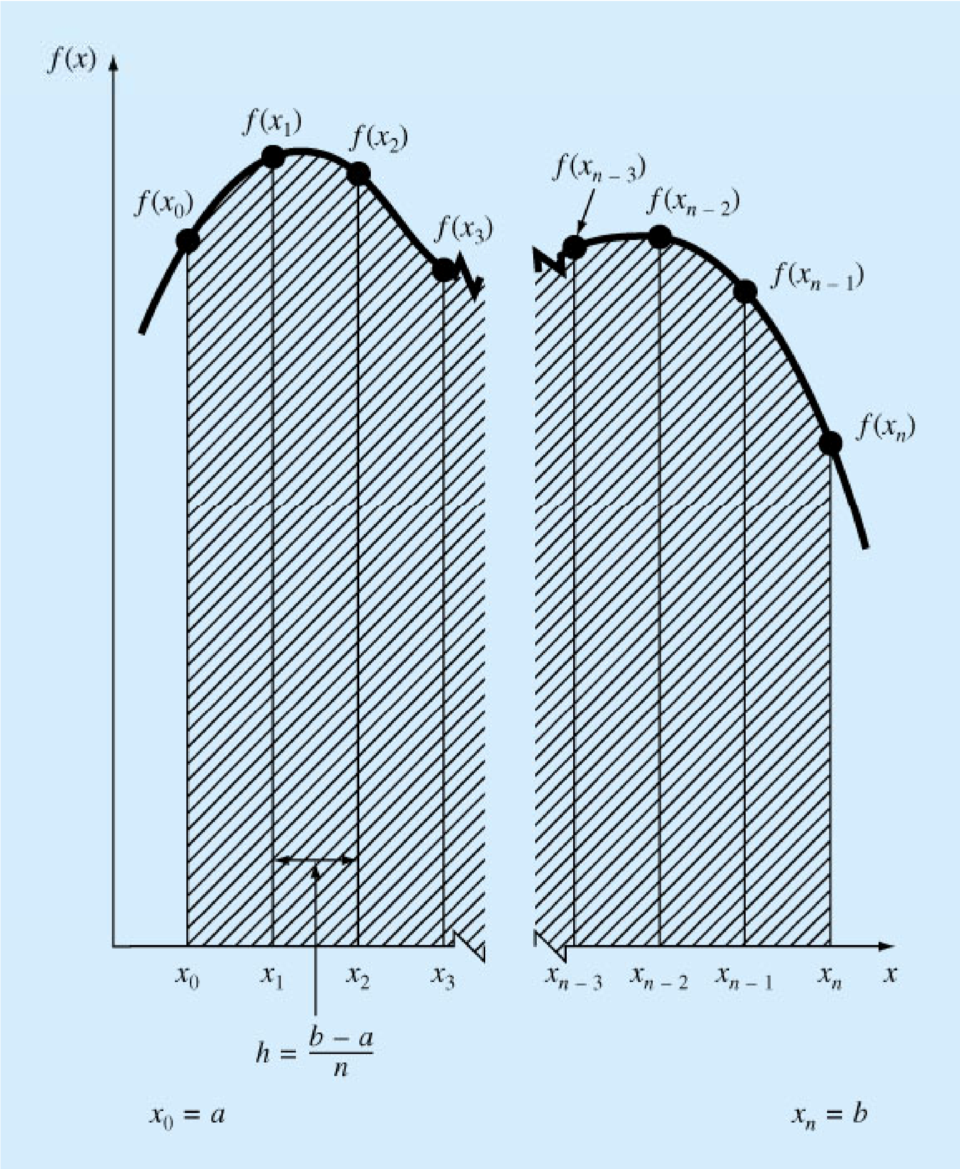
$$h = \frac{b-a}{n} \qquad a = x_0 \quad b = x_n$$

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

Substituting the trapezoidal rule for each integral yields:

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

Figure 4.8



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

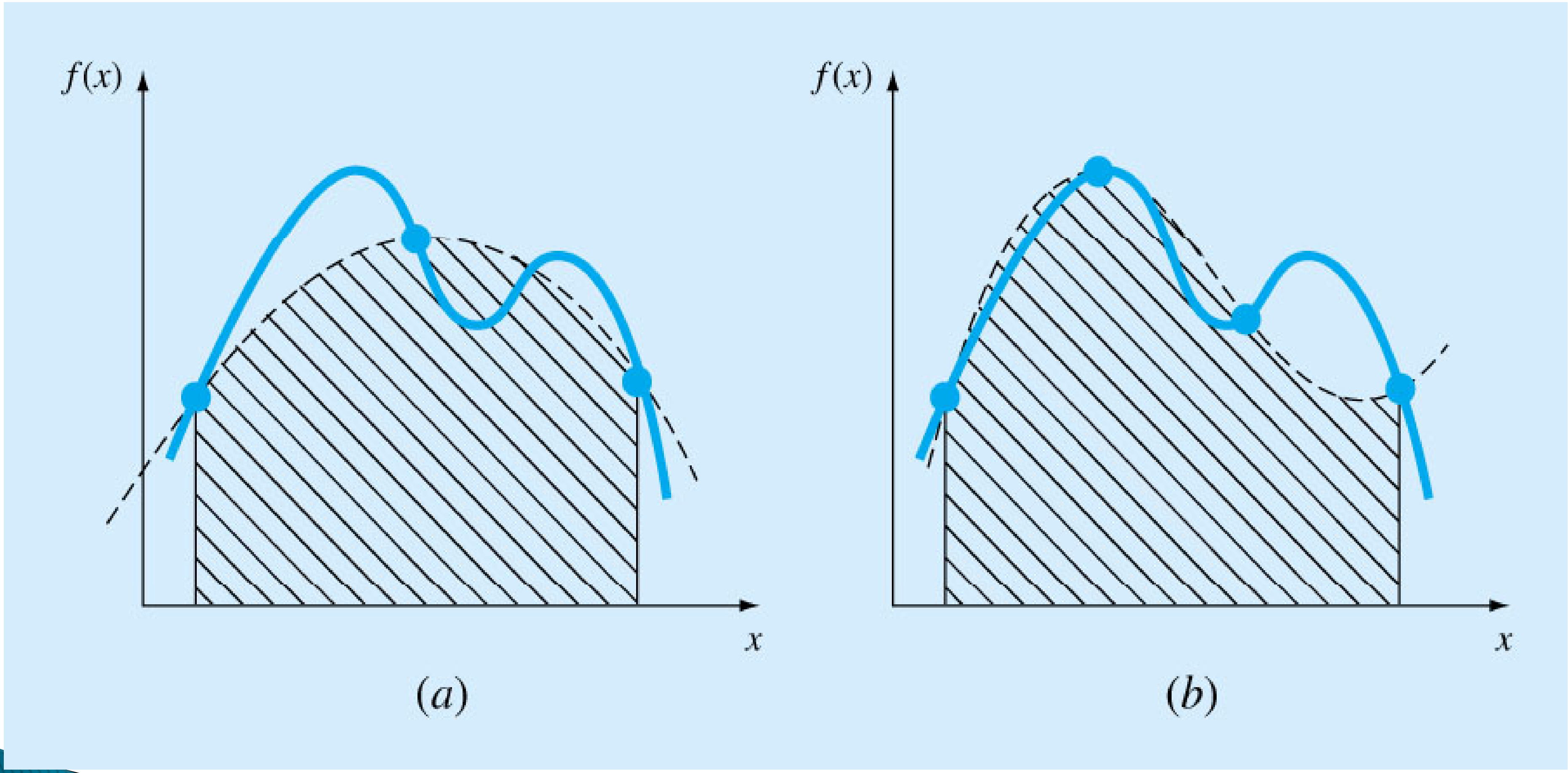
Simpson's Rules

- 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 4.9



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

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

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

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

Simpson's 1/3 Rule