Numerical Integration (and Differentiation)

Introduction to Numerical Problem Solving, Spring 2017

 Sakari Lukkarinen
Helsinki Metropolia University of Applied Sciences

All pictures and exercises from Chapra & Canale (2010). Numerical Methods for Engineers. Chapter

Motivation

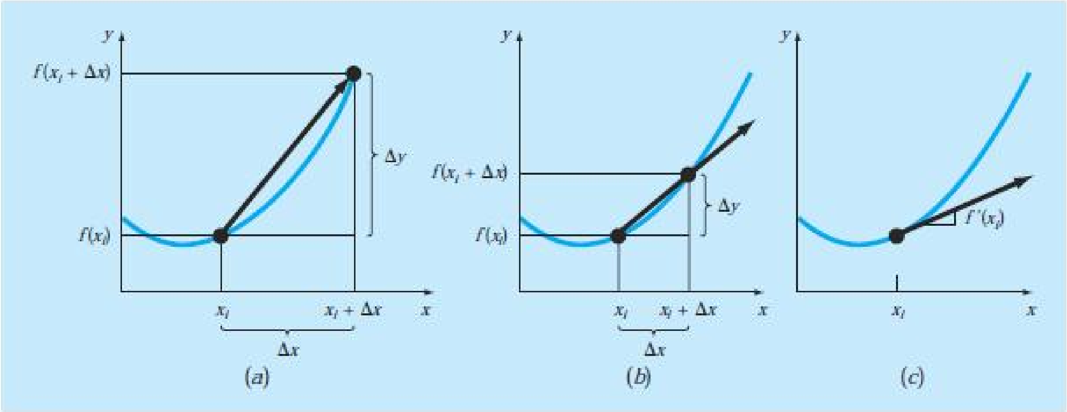


FIGURE PT6.1
The graphical definition of a derivative: as Δx approaches zero in going from (a) to (c), the difference approximation becomes a derivative.

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

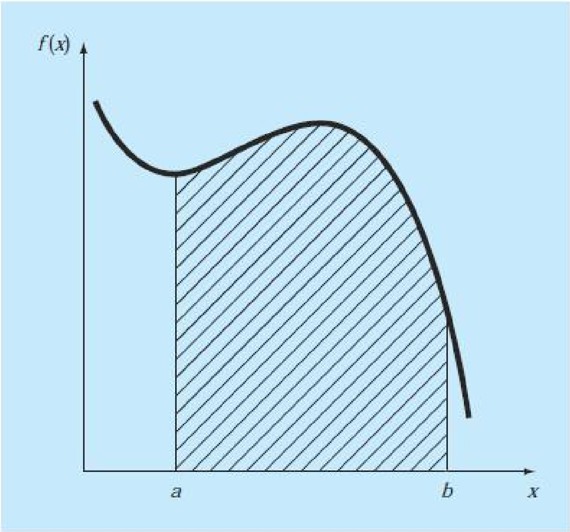


FIGURE PT6.2
Graphical representation of the integral of f(x) between the limits $x = a$ to b. The integral is equivalent to the area under the curve.

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

Non-computer Methods

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

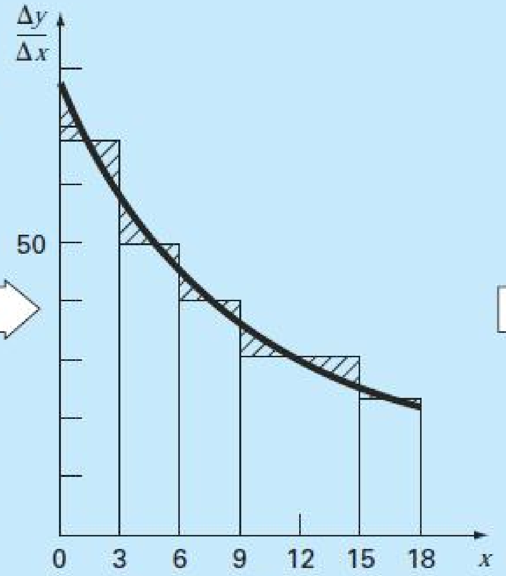
1. A simple continuous function such as a polynomial, an exponential, or a trigonometric function.
2. A complicated continuous function that is difficult or impossible to differentiate or integrate directly.
3. A tabulated function where values of x and $f(x)$ are given at a number of discrete points,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

Equal area differentiation

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.

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*)

Grid-based Integration

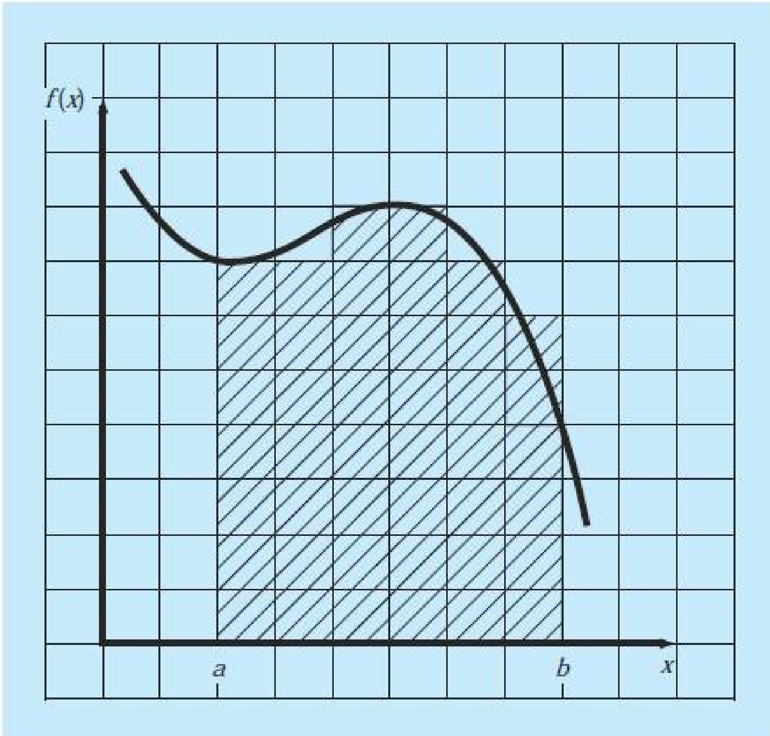


FIGURE PT6.5
The use of a grid to approximate an integral.

Strip-based Integration

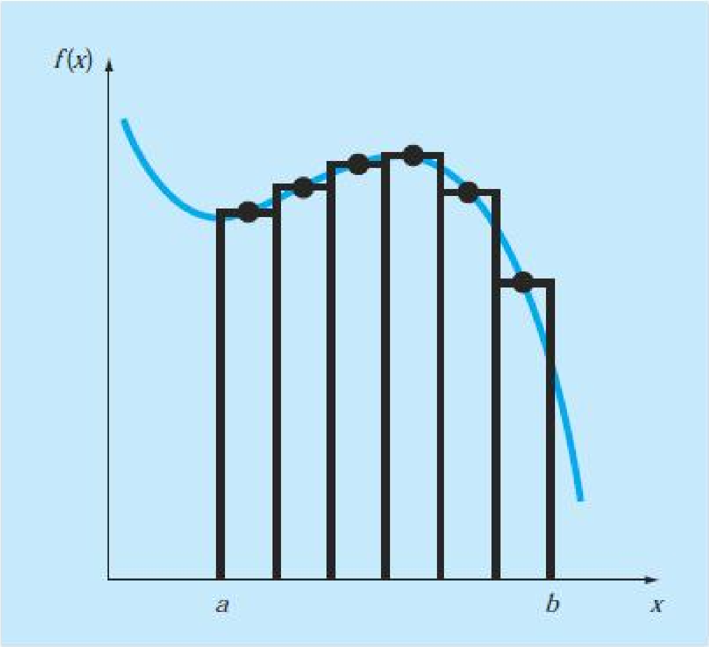


FIGURE PT6.6
The use of rectangles, or strips, to approximate the integral.

(*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*)

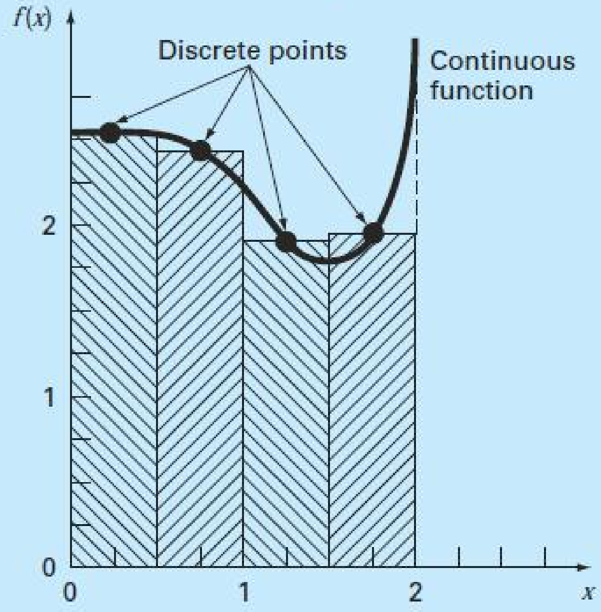
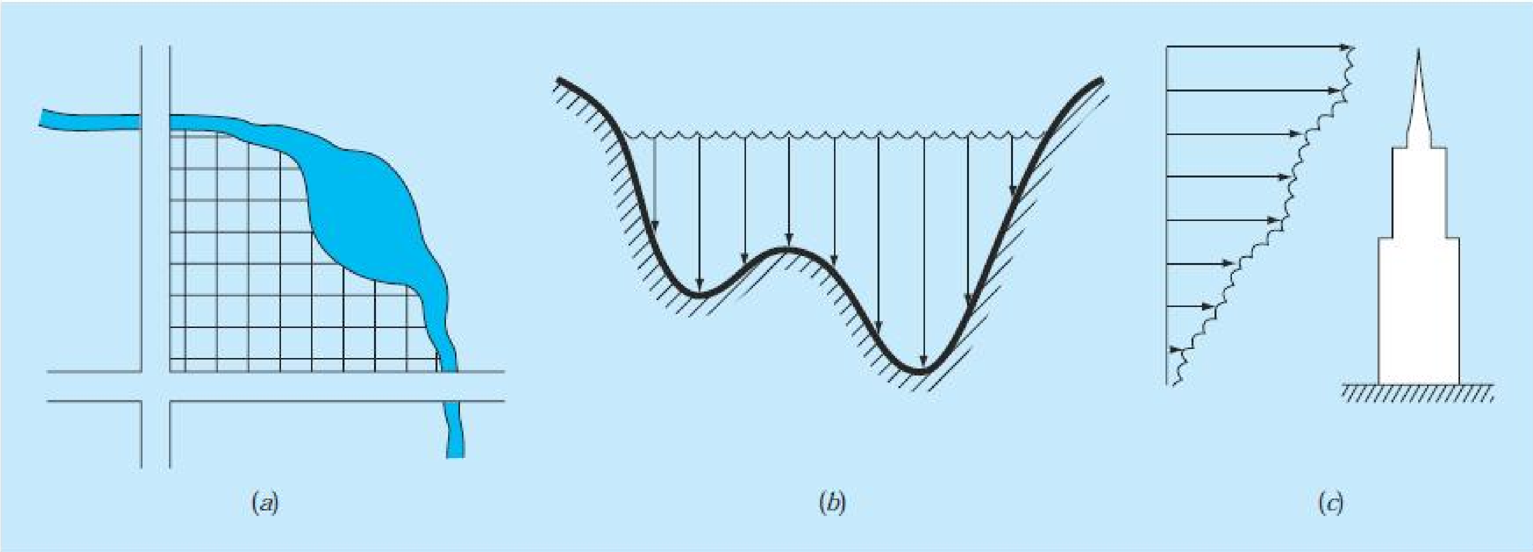


FIGURE PT6.7
Application of a numerical integration method: (*a*) A complicated, continuous function. (*b*) Table of discrete values of $f(x)$ generated from the function. (*c*) Use of a numerical method (the strip method here) to estimate the integral on the basis of the discrete points. For a tabulated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

Engineering examples

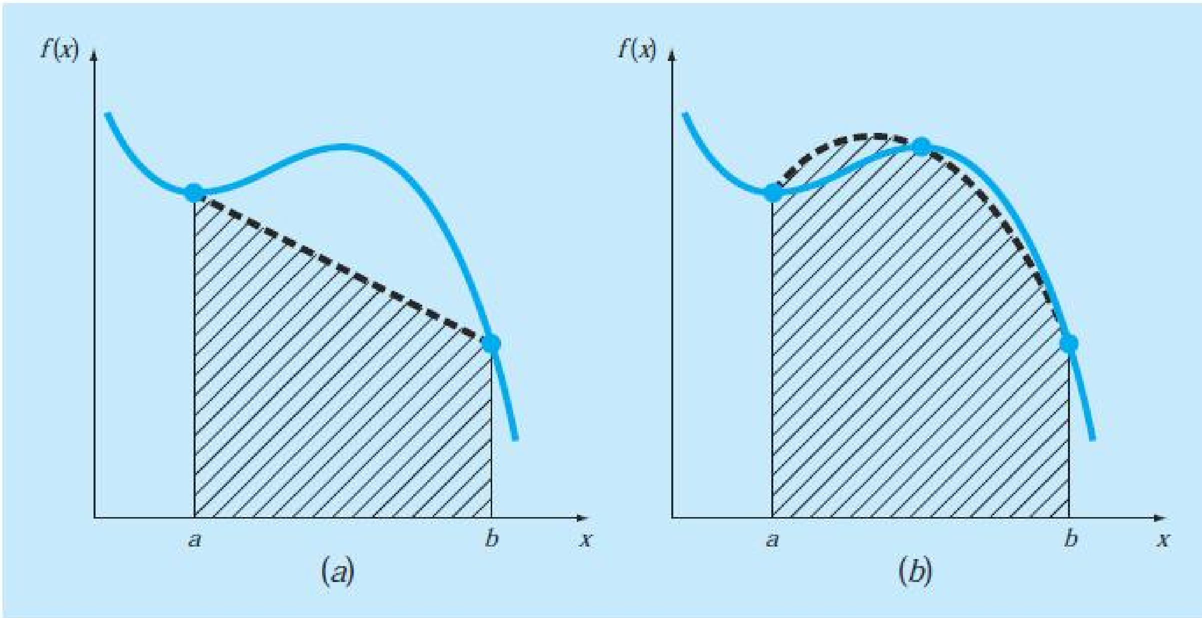
FIGURE PT6.8

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.



Newton-Cotes Integration Formulas

FIGURE 21.1
The approximation of an integral by the area under (a) a single straight line and (b) a single parabola.



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

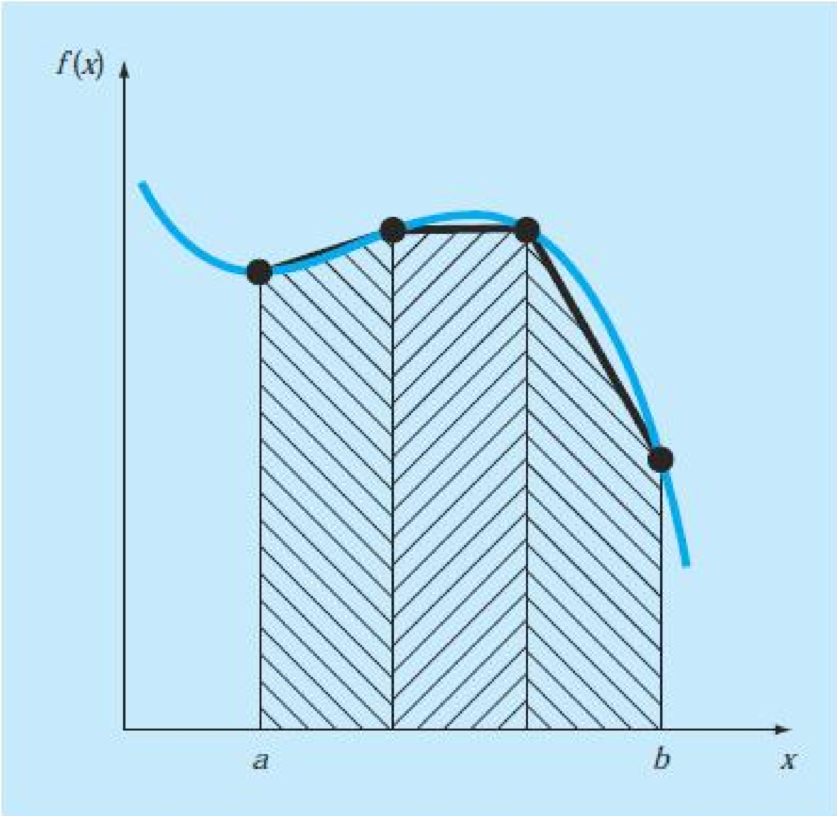
where $f_n(x)$ = a polynomial of the form

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

Trapezoidal rule

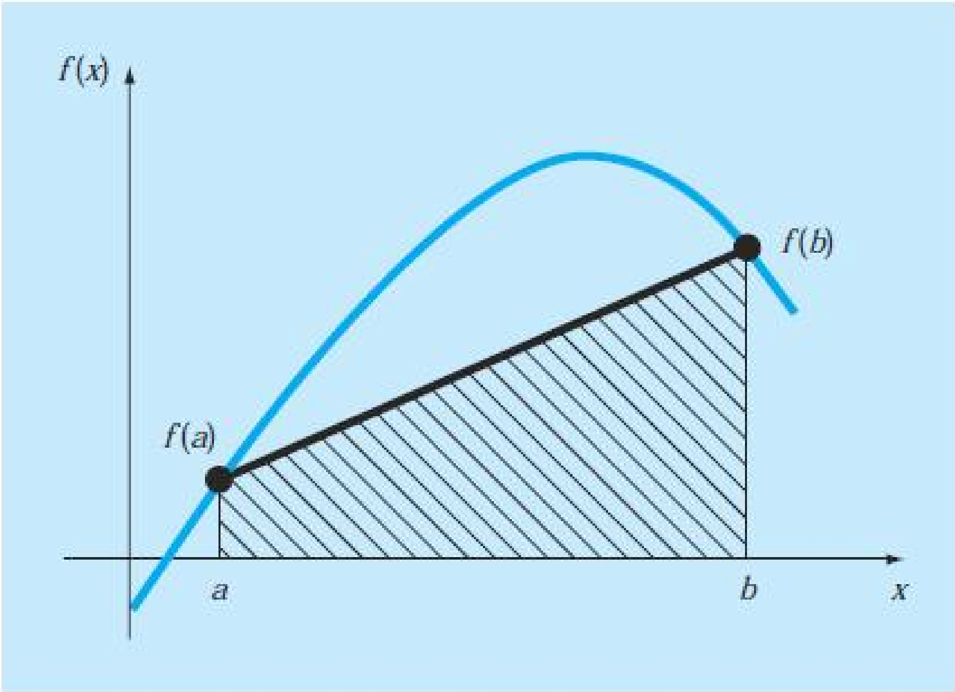
$$I = (b - a)\frac{f(a) + f(b)}{2}$$

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



Problems with Trapezoidals

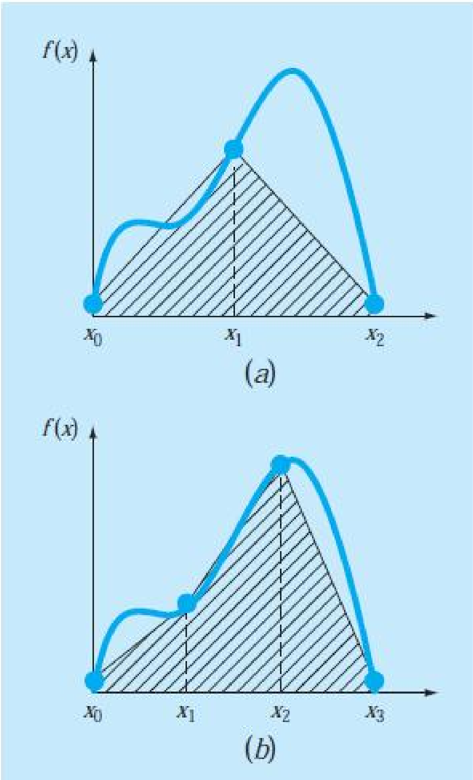
FIGURE 21.4
Graphical depiction of the trapezoidal rule.



Error estimate

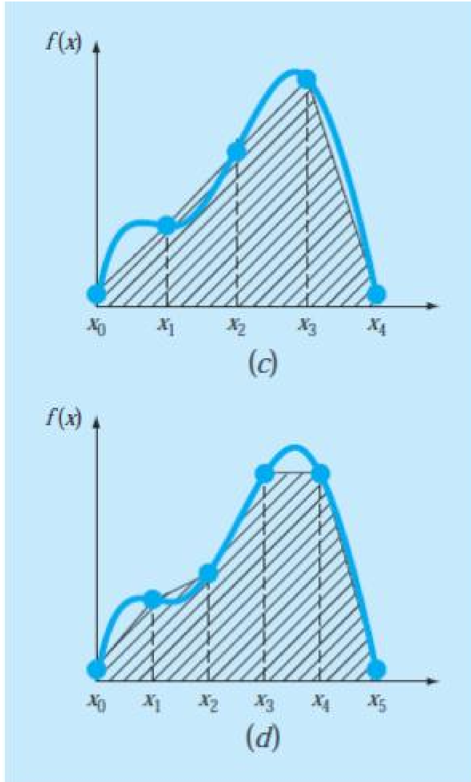
$$E_t = -\frac{1}{12} f''(\xi)(b-a)^3$$

Solution: Multiple Trapezoidals



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

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

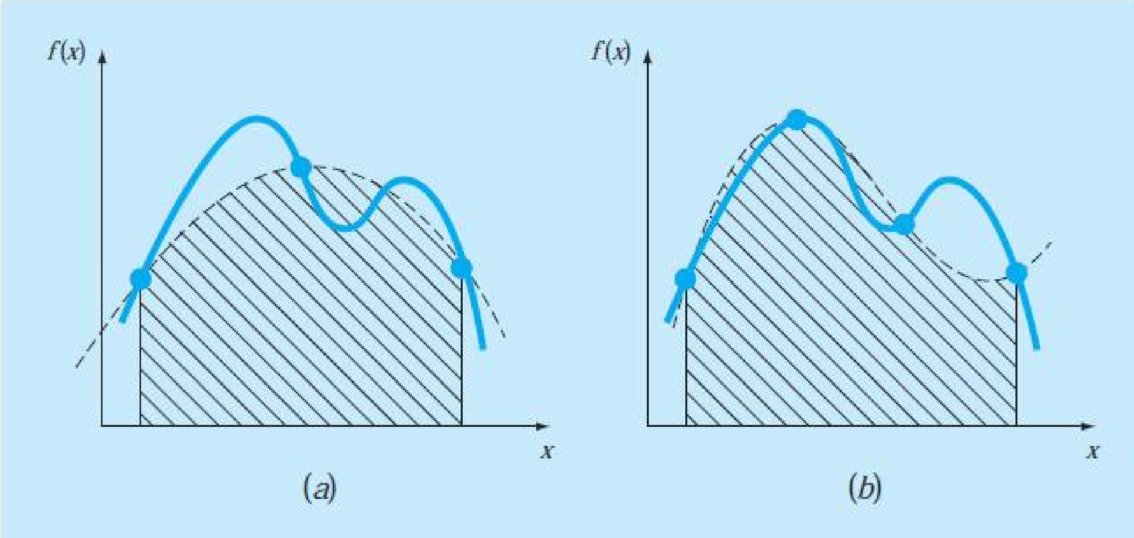


Simpson’s 1/3 rule

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

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

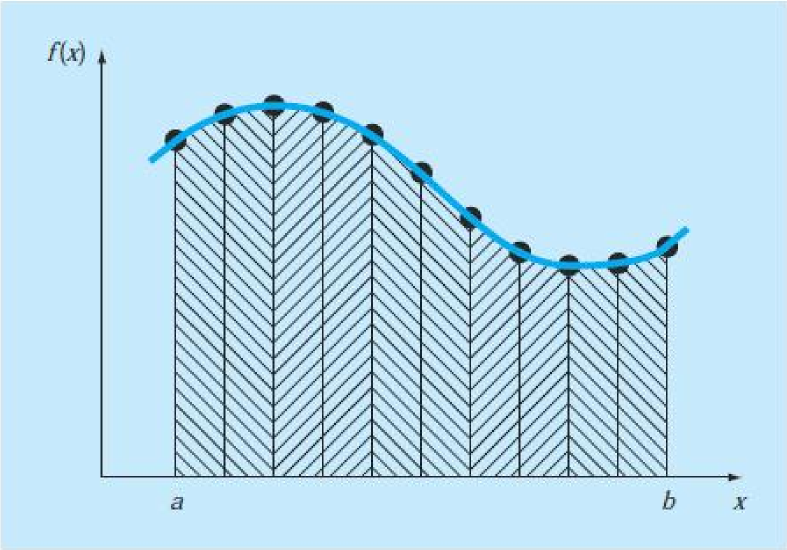
FIGURE 21.10
(*a*) Graphical depiction of Simpson’s 1/3 rule: It consists of taking the area under a parabola connecting three points. (*b*) Graphical depiction of Simpson’s 3/8 rule: It consists of taking the area under a cubic equation connecting four points.



Multiple 1/3 Simpsons

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

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.



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

Simpson's 3/8 rule

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

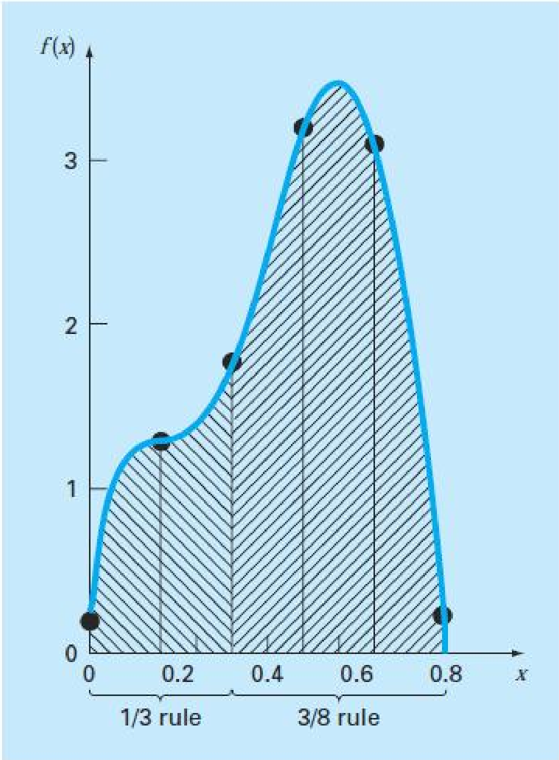


FIGURE 21.12
Illustration of how Simpson's 1/3 and 3/8 rules can be applied in tandem to handle multiple applications with odd numbers of intervals.

Integration (scipy.integrate)

The scipy.integrate sub-package provides several integration techniques including an ordinary differential equation integrator. An overview of the module is provided by the help command:

```
>>> help(integrate)
 Methods for Integrating Functions given function object.

   quad          -- General purpose integration.
   dblquad       -- General purpose double integration.
   tplquad       -- General purpose triple integration.
   fixed_quad    -- Integrate func(x) using Gaussian quadrature of order n.
   quadrature    -- Integrate with given tolerance using Gaussian quadrature.
   romberg       -- Integrate func using Romberg integration.

 Methods for Integrating Functions given fixed samples.

   trapz         -- Use trapezoidal rule to compute integral from samples.
   cumtrapz      -- Use trapezoidal rule to cumulatively compute integral.
   simps         -- Use Simpson's rule to compute integral from samples.
   romb          -- Use Romberg Integration to compute integral from
                    (2**k + 1) evenly-spaced samples.

   See the special module's orthogonal polynomials (special) for Gaussian
      quadrature roots and weights for other weighting factors and regions.

 Interface to numerical integrators of ODE systems.

   odeint        -- General integration of ordinary differential equations.
   ode           -- Integrate ODE using VODE and ZVODE routines.
```

21.1 Evaluate the following integral:

$$\int_0^{\pi/2} (8 + 4\cos x)\, dx$$

(a) analytically; **(b)** single application of the trapezoidal rule; **(c)** multiple-application trapezoidal rule, with $n = 2$ and 4; **(d)** single application of Simpson's 1/3 rule; **(e)** multiple-application Simpson's 1/3 rule, with $n = 4$; **(f)** single application of Simpson's 3/8 rule; and **(g)** multiple-application Simpson's rule, with $n = 5$. For each of the numerical estimates **(b)** through **(g)**, determine the percent relative error based on **(a)**.

21.4 Integrate the following function analytically and using the trapezoidal rule, with $n = 1, 2, 3$, and 4:

$$\int_1^2 (x + 1/x)^2\, dx$$

Use the analytical solution to compute true percent relative errors to evaluate the accuracy of the trapezoidal approximations.

21.5 Integrate the following function both analytically and using Simpson's rules, with $n = 4$ and 5. Discuss the results.

$$\int_{-3}^{5} (4x - 3)^3\, dx$$

21.2 Evaluate the following integral:

$$\int_0^3 (1 - e^{-x})\, dx$$

(a) analytically; **(b)** single application of the trapezoidal rule; **(c)** multiple-application trapezoidal rule, with $n = 2$ and 4; **(d)** single application of Simpson's 1/3 rule; **(e)** multiple-application Simpson's 1/3 rule, with $n = 4$; **(f)** single application of Simpson's 3/8 rule; and **(g)** multiple-application Simpson's rule, with $n = 5$. For each of the numerical estimates **(b)** through **(g)**, determine the percent relative error based on **(a)**.

21.3 Evaluate the following integral:

$$\int_{-2}^{4} (1 - x - 4x^3 + 2x^5)\, dx$$

(a) analytically; **(b)** single application of the trapezoidal rule; **(c)** composite trapezoidal rule, with $n = 2$ and 4; **(d)** single application of Simpson's 1/3 rule; **(e)** Simpson's 3/8 rule; and **(f)** Boole's rule. For each of the numerical estimates **(b)** through **(f)** determine the percent relative error based on **(a)**.