Numerical Integration Formulas

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Reference:

1. *Applied Numerical Methods with MATLAB for Engineers*, Chapter 19 & Teaching material

Chapter Objectives (1/2)

- Recognizing that Newton-Cotes integration formulas are based on the strategy of replacing a complicated function or tabulated data with a polynomial that is easy to integrate
- Knowing how to implement the following single application Newton-Cotes formulas:
  - Trapezoidal rule
  - Simpson's 1/3 rule
  - Simpson's 3/8 rule
- Knowing how to implement the following composite Newton-Cotes formulas:
  - Trapezoidal rule
  - Simpson's 1/3 rule

Chapter Objectives (2/2)

- Recognizing that even-segment-odd-point formulas like Simpson's 1/3 rule achieve higher than expected accuracy
- Knowing how to use the trapezoidal rule to integrate unequally spaced data
- Understanding the difference between open and closed integration formulas

Integration

- Integration:

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

is the total value, or summation, of $f(x)\,dx$ over the range from a to b:

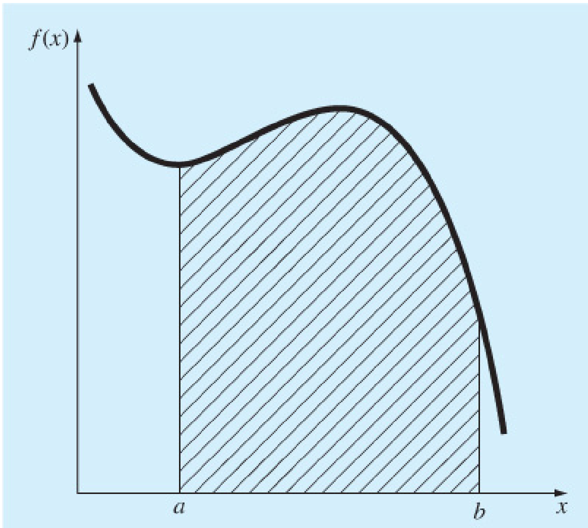


FIGURE 19.1
Graphical representation of the integral of $f(x)$ between the limits $x = a$ to b. The integral is equivalent to the area under the curve.

Newton-Cotes Formulas

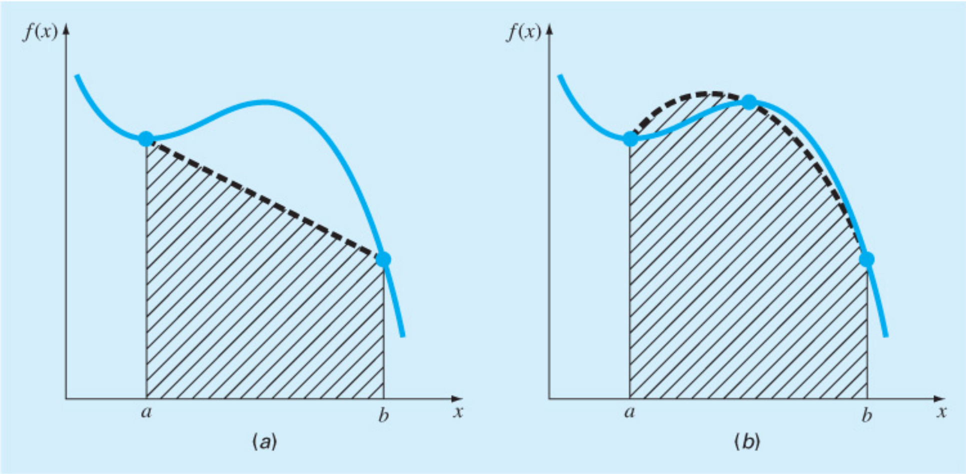
- The ***Newton-Cotes formulas*** are the most common numerical integration schemes
- Generally, they are based on replacing a complicated function or tabulated data with a polynomial that is easy to integrate:

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

  – where $f_n(x)$ is an n^{th} order interpolating polynomial

Newton-Cotes Examples

- The integrating function can be polynomials for any order - for example, (a) straight lines or (b) parabolas
- The integral can be approximated in one step or in a series of steps to improve accuracy



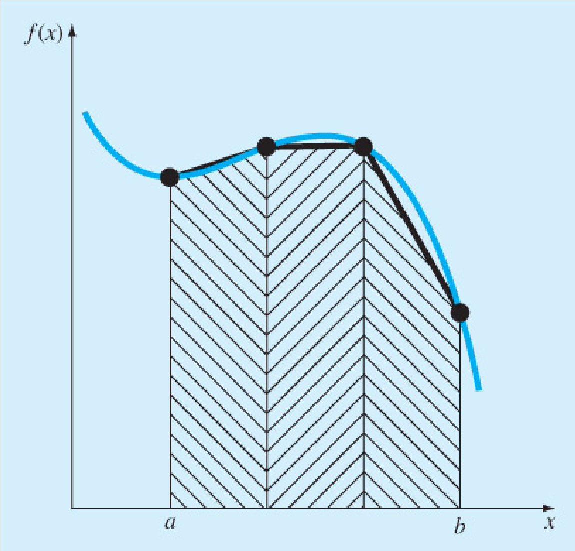


FIGURE 19.5
The approximation of an integral by the area under three straight-line segments.

The Trapezoidal Rule

- The ***trapezoidal rule*** is the first of the Newton-Cotes closed integration formulas; it uses a straight-line approximation for the function:

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

$$I = \int_a^b \left[f(a) + \frac{f(b) - f(a)}{b - a}(x - a) \right] dx$$

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

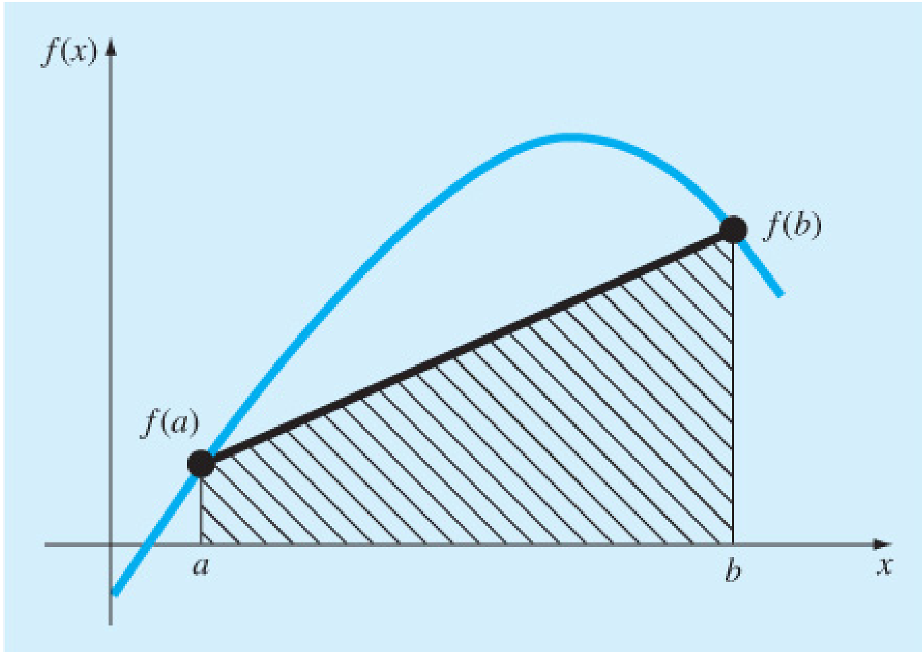


FIGURE 19.7
Graphical depiction of the trapezoidal rule.

Error of the Trapezoidal Rule

- An estimate for the local truncation error of a single application of the trapezoidal rule is:

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

  where ξ is somewhere between *a* and *b*
- This formula indicates that the error is dependent upon the curvature of the actual function as well as the distance between the points
- Error can thus be reduced by breaking the curve into parts

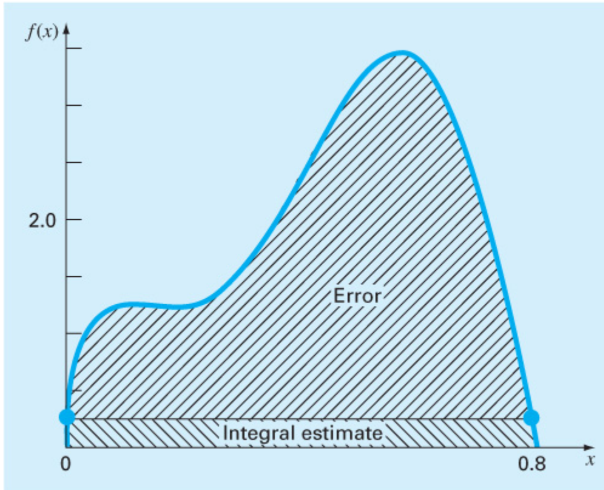


FIGURE 19.8
Graphical depiction of the use of a single application of the trapezoidal rule to approximate the integral of $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$ from $x = 0$ to 0.8.

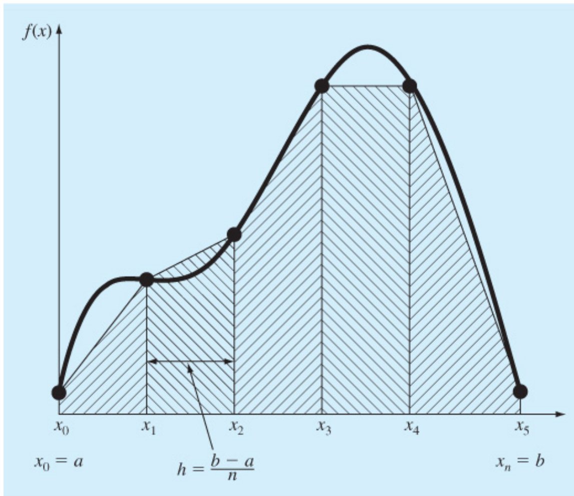


FIGURE 19.9
Composite trapezoidal rule.

Trapezoidal Rule: An Example

Single Application of the Trapezoidal Rule

Problem Statement. Use Eq. (19.11) to numerically integrate

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

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

Solution. The function values $f(0) = 0.2$ and $f(0.8) = 0.232$ can be substituted into Eq. (19.11) to yield

$$I = (0.8 - 0)\frac{0.2 + 0.232}{2} = 0.1728$$

which represents an error of $E_t = 1.640533 - 0.1728 = 1.467733$, which corresponds to a percent relative error of $\varepsilon_t = 89.5\%$. The reason for this large error is evident from the graphical depiction in Fig. 19.8. Notice that the area under the straight line neglects a significant portion of the integral lying above the line.

Example 19.1

Composite Trapezoidal Rule

- Assuming *n*+1 data points are evenly spaced, there will be *n* intervals over which to integrate
- The total integral can be calculated by integrating each subinterval and then adding them together:

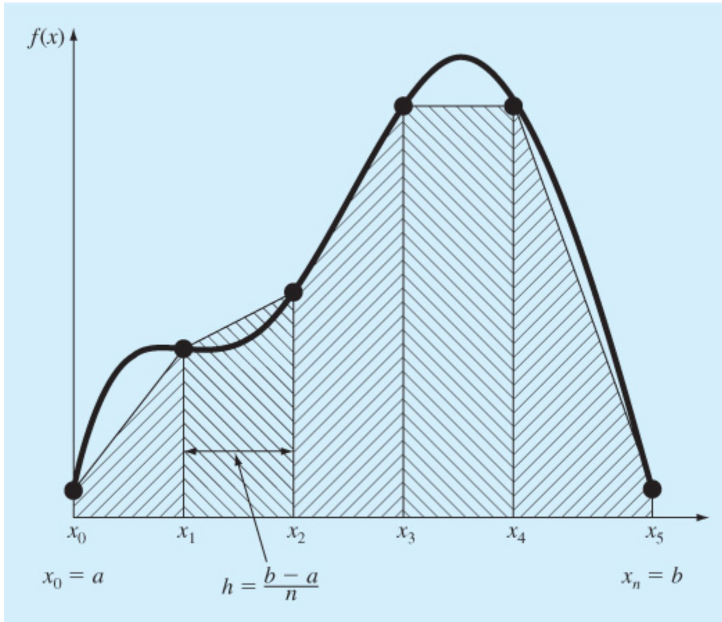


FIGURE 19.9
Composite trapezoidal rule.

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

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

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

Composite Trapezoidal Rule: An Example

Composite Application of the Trapezoidal Rule

Problem Statement. Use the two-segment trapezoidal rule to estimate the integral of

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

from $a = 0$ to $b = 0.8$. Employ Eq. (19.21) to estimate the error. Recall that the exact value of the integral is 1.640533.

Solution. For $n = 2$ ($h = 0.4$):

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

$$I = 0.8\frac{0.2 + 2(2.456) + 0.232}{4} = 1.0688$$

$$E_t = 1.640533 - 1.0688 = 0.57173 \qquad \varepsilon_t = 34.9\%$$

Example 19.2

MATLAB Program

```
function I = trap(func,a,b,n,varargin)
% trap: composite trapezoidal rule quadrature
%   I = trap(func,a,b,n,p1,p2,...):
%                   composite trapezoidal rule
% input:
%   func = name of function to be integrated
%   a, b = integration limits
%   n = number of segments (default = 100)
%   p1,p2,... = additional parameters used by func
% output:
%   I = integral estimate

if nargin<3,error('at least 3 input arguments required'),end
if ~(b>a),error('upper bound must be greater than lower'),end
if nargin<4|isempty(n),n=100;end
x = a; h = (b - a)/n;
s=func(a,varargin{:});
for i = 1 : n-1
  x = x + h;
  s = s + 2*func(x,varargin{:});
end
s = s + func(b,varargin{:});
I = (b - a) * s/(2*n);
```

FIGURE 19.10
M-file to implement the composite trapezoidal rule.

Simpson's Rules

- One drawback of the trapezoidal rule is that the error is related to the second derivative of the function
- More complicated approximation formulas can improve the accuracy for curves - these include using (a) 2nd and (b) 3rd order polynomials
- The formulas that result from taking the integrals under these polynomials are called ***Simpson's rules***

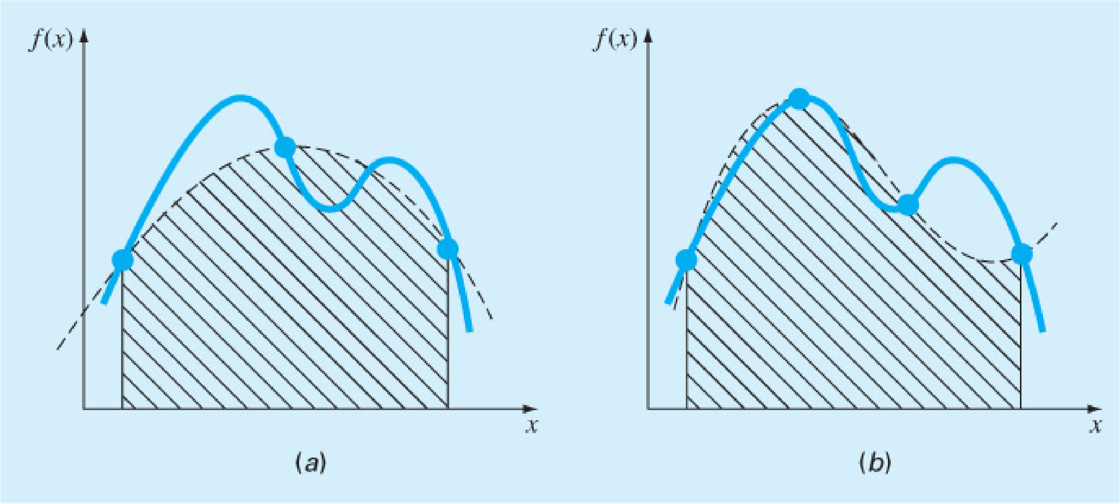


FIGURE 19.11
(*a*) Graphical depiction of Simpson's 1/3 rule: It consists of taking the area under a parabola connecting three points. (*b*) Graphical depiction of Simpson's 3/8 rule: It consists of taking the area under a cubic equation connecting four points.

Simpson's 1/3 Rule

- Simpson's 1/3 rule corresponds to using second-order polynomials. Using the **Lagrange form** for a quadratic fit of three points:

$$f_n(x)=\frac{(x-x_1)}{(x_0-x_1)}\frac{(x-x_2)}{(x_0-x_2)}f(x_0)+\frac{(x-x_0)}{(x_1-x_0)}\frac{(x-x_2)}{(x_1-x_2)}f(x_1)+\frac{(x-x_0)}{(x_2-x_0)}\frac{(x-x_1)}{(x_2-x_1)}f(x_2)$$

  – Integration over the three points simplifies to:

$$I=\int_{x0}^{x2} f_n(x)\,dx$$

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

$$=(b-a)\frac{f(x_0)+4f(x_1)+f(x_2)}{6}$$

$$h=\frac{b-a}{2}$$

Error of Simpson's 1/3 Rule

- An estimate for the local truncation error of a single application of Simpson's 1/3 rule is:

$$E_t = -\frac{1}{2880} f^{(4)}(\xi)(b-a)^5$$

  where again ξ is somewhere between *a* and *b*
- This formula indicates that the error is dependent upon the fourth-derivative of the actual function as well as the distance between the points
- Note that the error is dependent on the fifth power of the step size (rather than the third for the trapezoidal rule)
- Error can thus be reduced by breaking the curve into parts

Simpson's 1/3 Rule: An Example

Single Application of Simpson's 1/3 Rule

Problem Statement. Use Eq. (19.23) to integrate

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

from $a = 0$ to $b = 0.8$. Employ Eq. (19.24) to estimate the error. Recall that the exact integral is 1.640533.

Solution. $n = 2(h = 0.4)$:

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

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

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

which is approximately five times more accurate than for a single application of the trapezoidal rule (Example 19.1).

Example 19.3

Composite Simpson's 1/3 Rule

- Simpson's 1/3 rule can be used on a set of subintervals in much the same way the trapezoidal rule was, except there *must* be an odd number of points
- Because of the heavy weighting of the internal points, the formula is a little more complicated than for the trapezoidal rule:

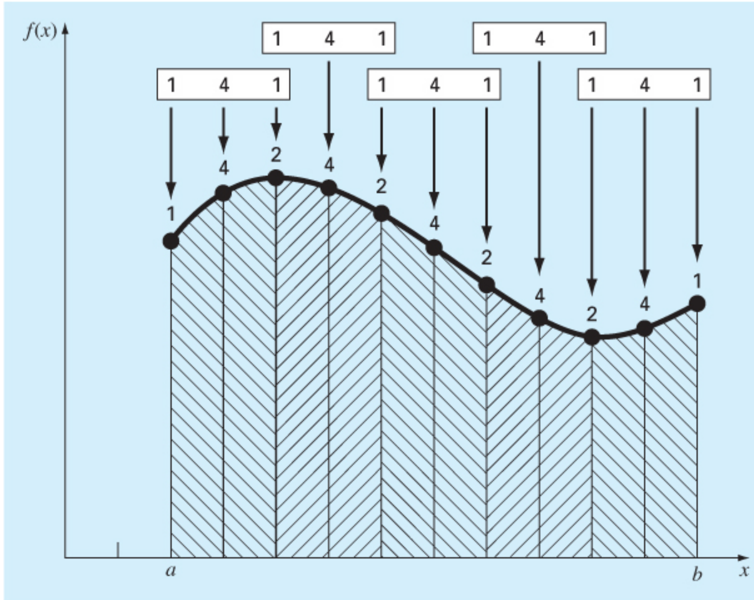


FIGURE 19.12
Composite Simpson's 1/3 rule. The relative weights are depicted above the function values. Note that the method can be employed only if the number of segments is even.

$$I = \int_{x0}^{xn} f_n(x)\,dx = \int_{x0}^{x2} f_n(x)\,dx + \int_{x2}^{x4} f_n(x)\,dx + \cdots + \int_{xn-2}^{xn} f_n(x)\,dx$$

$$\Rightarrow I = \frac{h}{3}\left[f(x_0) + 4f(x_1) + f(x_2)\right] + \frac{h}{3}\left[f(x_2) + 4f(x_3) + f(x_4)\right] + \cdots + \frac{h}{3}\left[f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)\right]$$

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

$$\Rightarrow I = \frac{h}{3}\left[f(x_0) + 4\sum_{\substack{i=1 \\ i,\,\text{odd}}}^{n-1} f(x_i) + 2\sum_{\substack{j=2 \\ j,\,\text{even}}}^{n-2} f(x_i) + f(x_n) \right] \Rightarrow I = (b-a)\frac{f(x_0) + 4\sum_{\substack{i=1 \\ i,\,\text{odd}}}^{n-1} f(x_i) + 2\sum_{\substack{j=2 \\ j,\,\text{even}}}^{n-2} f(x_i) + f(x_n)}{3n}$$

Composite Simpson's 1/3 Rule: An Example

Composite Simpson's 1/3 Rule

Problem Statement. Use Eq. (19.26) 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 $b = 0.8$. Employ Eq. (19.27) to estimate the error. 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. (19.26):

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

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

Example 19.4

Simpson's 3/8 Rule

- Simpson's 3/8 rule corresponds to using third-order polynomials to fit four points. Integration over the four points simplifies to:

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

$$I = \int_{x0}^{x3} f_n(x)\,dx$$

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

$$= (b-a)\frac{f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)}{8}$$

- Simpson's 3/8 rule is generally used in concert with Simpson's 1/3 rule when **the number of segments is odd**

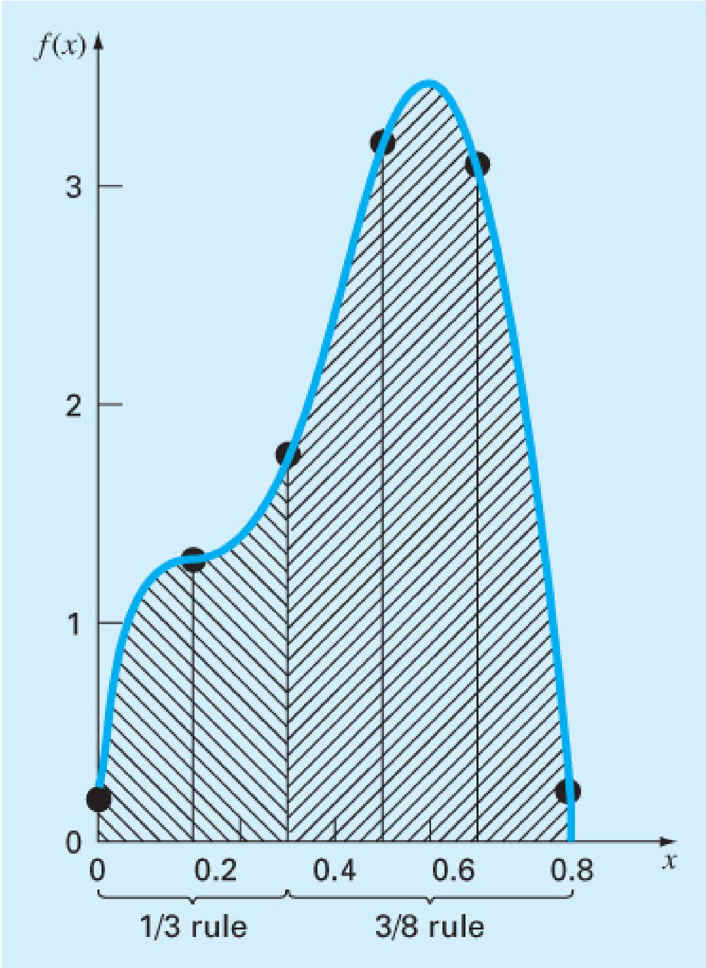


FIGURE 19.13
Illustration of how Simpson's 1/3 and 3/8 rules can be applied in tandem to handle multiple applications with odd numbers of intervals.

Simpson's 3/8 Rule: An Example (1/2)

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. (19.28):

$$I = 0.8\frac{0.2 + 3(1.432724 + 3.487177) + 0.232}{8} = 1.51970$$

Example 19.5

Simpson's 3/8 Rule: An Example (2/2)

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

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

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

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

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

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

The total integral is computed by summing the two results:

$$I = 0.3803237 + 1.264754 = 1.645077$$

Higher-Order Formulas

- Higher-order Newton-Cotes formulas may also be used - in general, the higher the order of the polynomial used, the higher the derivative of the function in the error estimate and the higher the power of the step size

- As in Simpson's 1/3 and 3/8 rule, the even-segment-odd-point formulas have truncation errors that are the same order as formulas adding one more point. For this reason, the even-segment-odd-point formulas are usually the methods of preference

Integration with Unequal Segments

- Previous formulas were simplified based on equispaced data points - though this is not always the case
- The trapezoidal rule may be used with data containing unequal segments:

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

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

Integration Code for Unequal Segments

```
function I = trapuneq(x,y)
% trapuneq: unequal spaced trapezoidal rule quadrature
%   I = trapuneq(x,y):
%   Applies the trapezoidal rule to determine the integral
%   for n data points (x, y) where x and y must be of the
%   same length and x must be monotonically ascending
% input:
%   x = vector of independent variables
%   y = vector of dependent variables
% output:
%   I = integral estimate

if nargin<2,error('at least 2 input arguments required'),end
if any(diff(x)<0),error('x not monotonically ascending'),end
n = length(x);
if length(y)~=n,error('x and y must be same length'); end
s = 0;
for k = 1:n-1
  s = s + (x(k+1)-x(k))*(y(k)+y(k+1))/2;
end
I = s;
```

FIGURE 19.14
M-file to implement the trapezoidal rule for unequally spaced data.

MATLAB Functions

- MATLAB has built-in functions to evaluate integrals based on the trapezoidal rule
- `z = trapz(y)`
  `z = trapz(x, y)`
  produces the integral of `y` with respect to `x`. If `x` is omitted, the program assumes *h*=1
- `z = cumtrapz(y)`
  `z = cumtrapz(x, y)`
  produces the cumulative integral of `y` with respect to `x`. If `x` is omitted, the program assumes *h*=1

Multiple Integrals

- Multiple integrals can be determined numerically by first integrating in one dimension, then a second, and so on for all dimensions of the problem

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

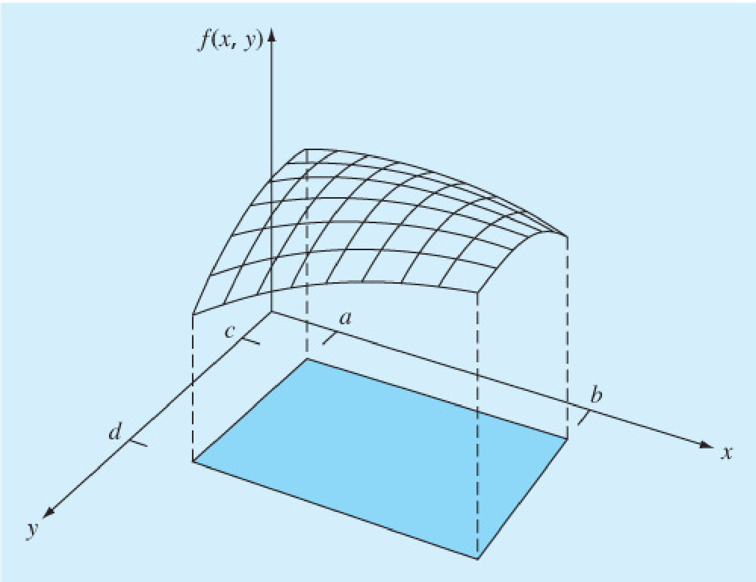


FIGURE 19.16
Double integral as the area under the function surface.

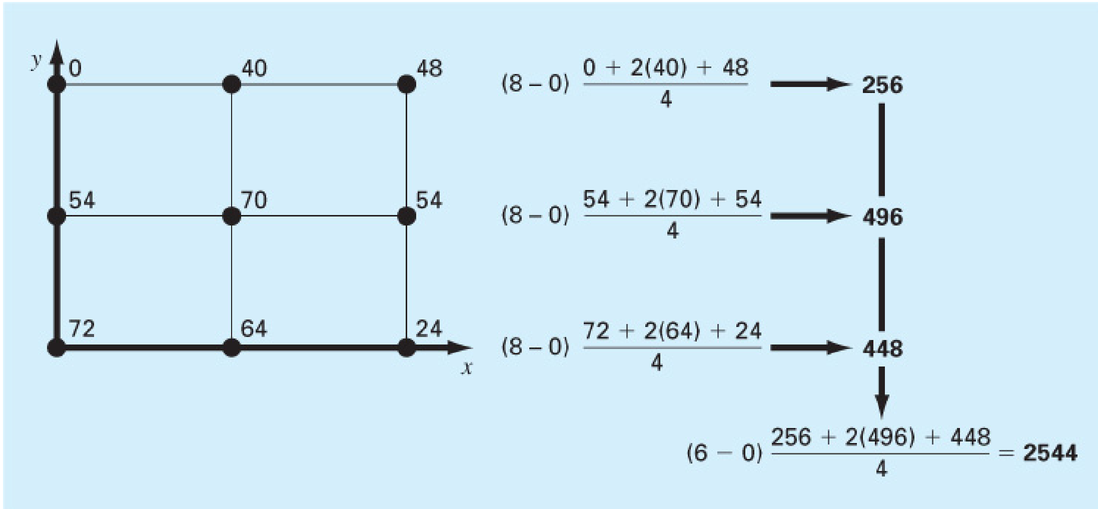


FIGURE 19.17
Numerical evaluation of a double integral using the two-segment trapezoidal rule.