Numerical Integration and Differentiation

CEE3804: Computer Apps for Civil and Environmental Engineering

Newton Cotes Integration Formulas

- **Replace function or tabulated data to be integrated with a simpler, easy to integrate approximating function**

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

- **where $f_n(x)$ is a polynomial of form**

$$f_n(x) = a_0 + a_1 x + a_2 x^2 + \ldots + a_n x^n$$

Trapezoid Rule

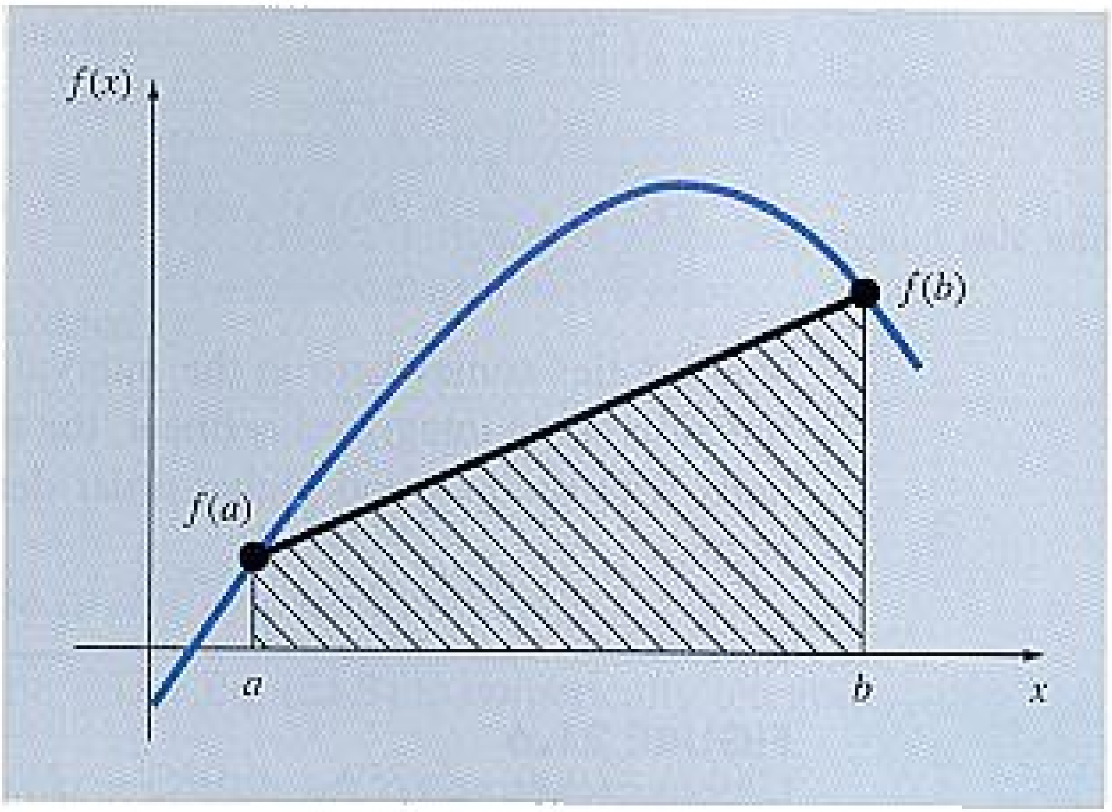
- **Newton-Cotes with n = 1**

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

- **where**

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

FIGURE 21.4
Graphical depiction of the trapezoidal rule.



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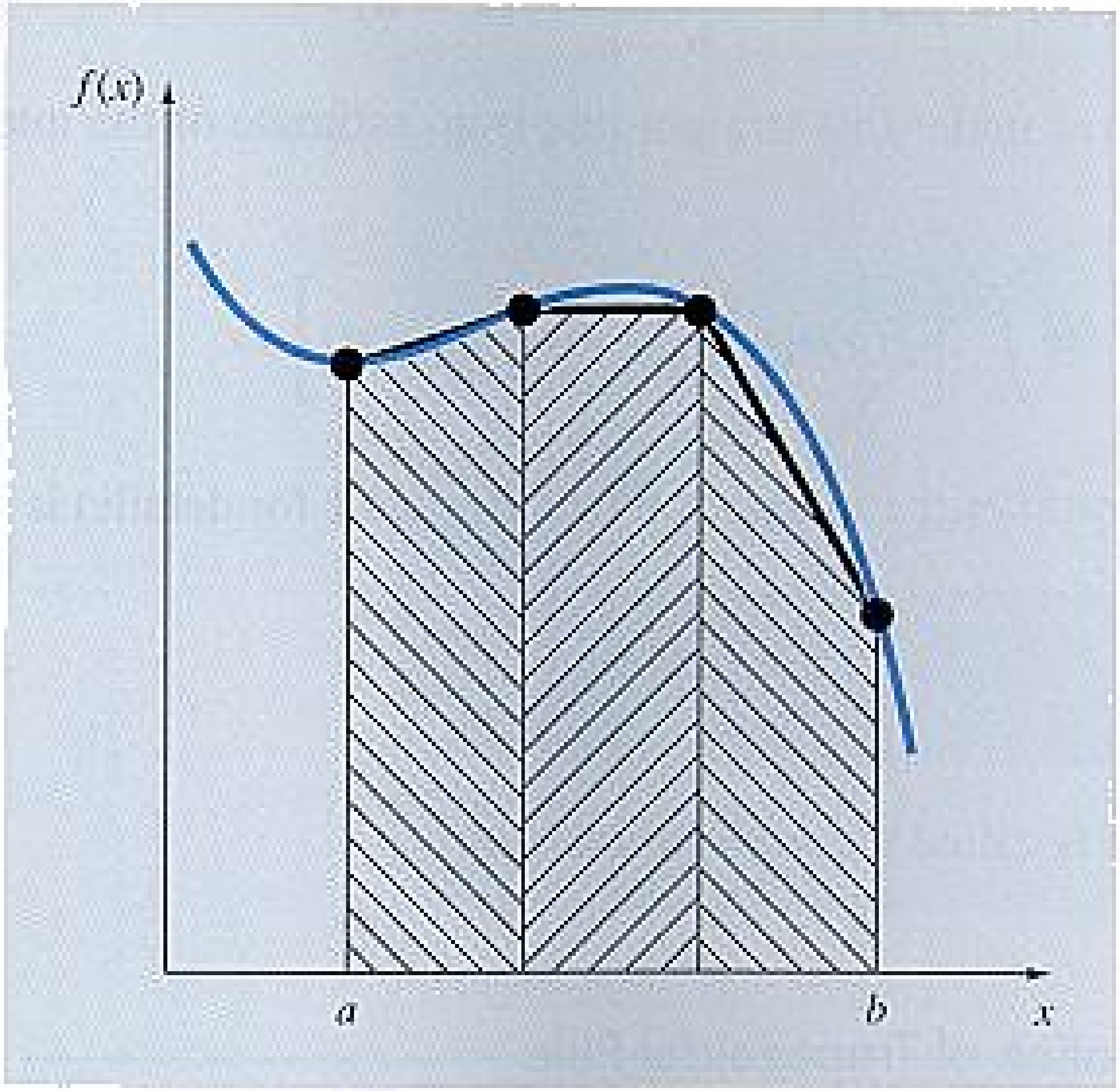
Trapezoid Rule, continued

- Substituting and integrating

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

- This is termed the trapezoid rule
- For all Newton-Cotes
  - I = width * average height
  - where the average height varies with n

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



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Trapezoid Rule, Comments

- Easy to implement
- Works with function or tabulated data
- For equally spaced data with n equally spaced points, formula can be simplified to
- $$I = \left(\frac{y_1 + y_n}{2} + \sum_{i=2}^{n-1} y_i \right) \Delta x$$
- Trapezoid has relatively poor accuracy compared to other techniques. Accuracy increases as use more points (i.e. delta x smaller)

Simpson’s 1/3 Rule

- **Set n= 2 in Newton-Cotes**
- **Pass parabola (quadratic) through 3 points**
- **Simple formula if even number of subintervals (i.e. number of data points is odd) and the data points are equally spaced**

$$I = \int_a^b y\,dx = \frac{1}{3}\left(y_1 + 4y_2 + 2y_3 + 4y_4 + 2y_5 + \ldots + 2y_{n-2} + 4y_{n-1} + y_n\right)\Delta x$$

- **Termed Simpson’s 1/3 Rule**

FIGURE 21.11
(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.

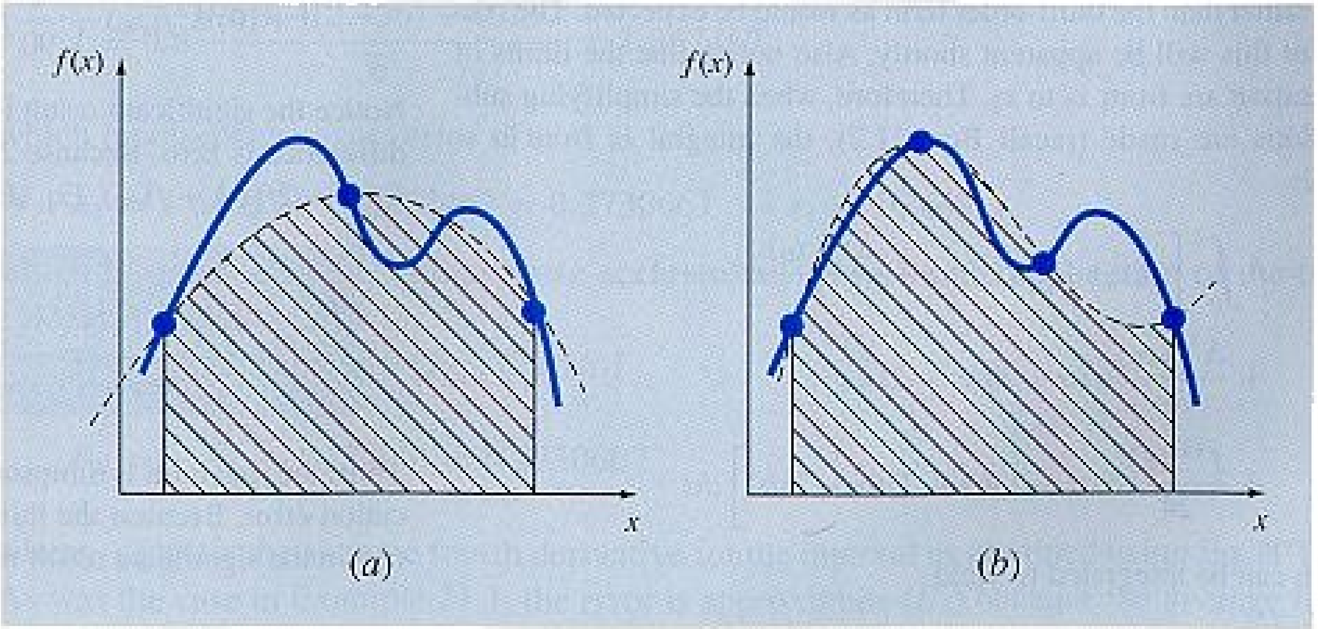

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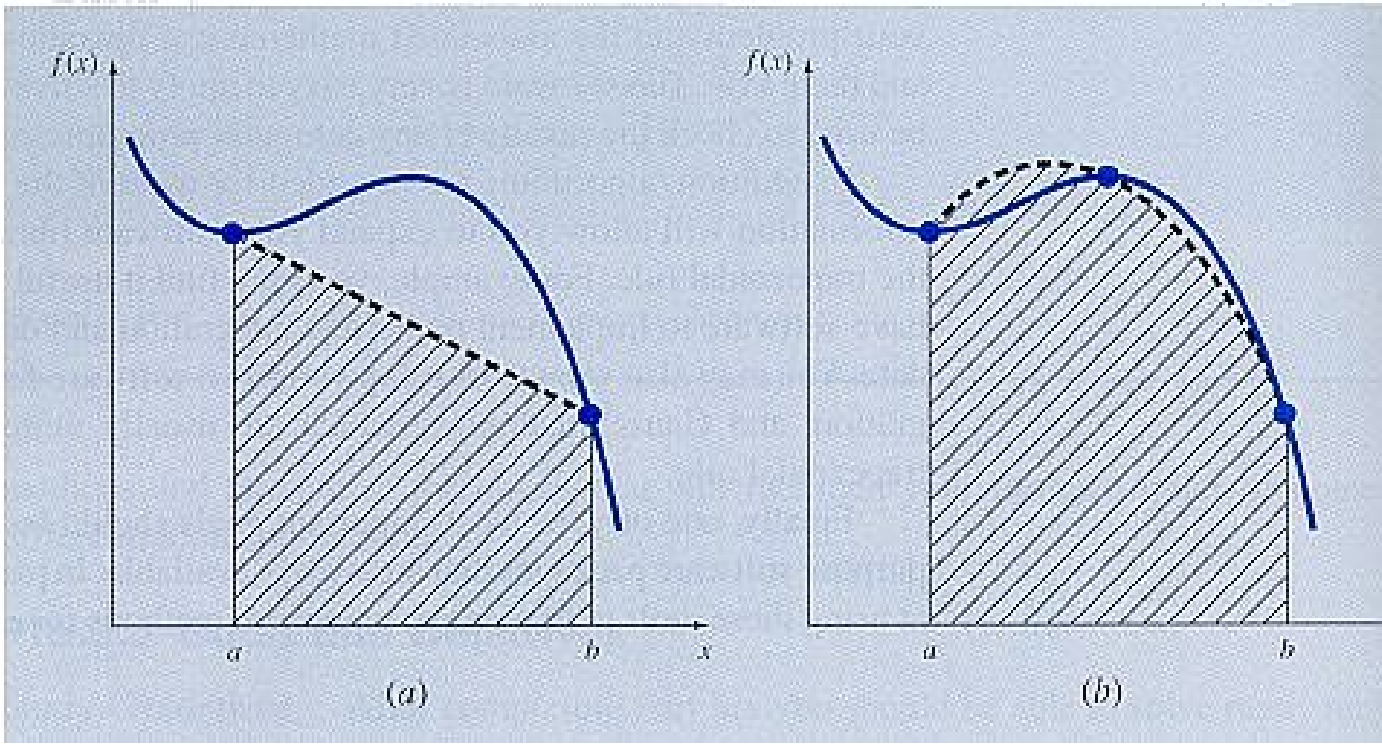
FIGURE 21.1
The approximation of an integral by the area under (*a*) a single straight line and (*b*) a single parabola.



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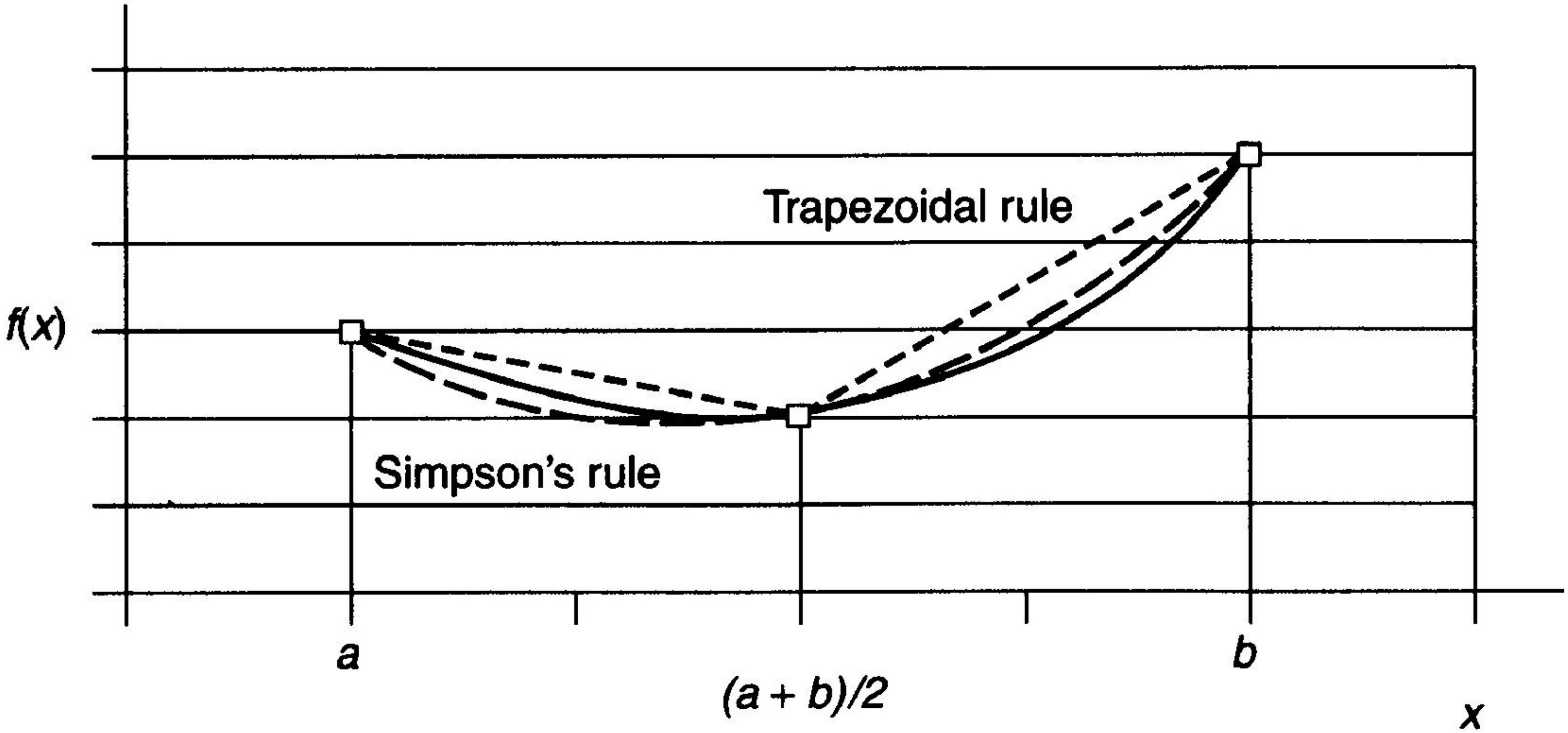

Figure 7-5 Simpson's Rule for Integration

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Simpson's 3/8 Rule

- If <u>even number of points</u> and odd number of segments, can use Simpson's 3/8 Rule

$$I = \frac{3}{8}\left(y_1 + 3y_2 + 3y_3 + y_4\right)\Delta x$$

- 3/8 rule is harder to apply than 1/3 rule because it needs 4 points instead of 3. Most common use is in conjunction with 1/3 rule. For odd number of segments, use 3/8 rule on last 3 segments, 1/3 rule on remaining

TABLE 21.2 Newton-Cotes closed integration formulas. The formulas are presented in the format of Eq. (21.5) so that the weighting of the data points to estimate the average height is apparent. The step size is given by $h = (b - a)/n$.

Segments (n)	Points	Name	Formula	Truncation Error
1	2	Trapezoidal rule	$(b-a)\dfrac{f(x_0)+f(x_1)}{2}$	$-(1/12)h^3 f''(\xi)$
2	3	Simpson's 1/3 rule	$(b-a)\dfrac{f(x_0)+4f(x_1)+f(x_2)}{6}$	$-(1/90)h^5 f^{(4)}(\xi)$
3	4	Simpson's 3/8 rule	$(b-a)\dfrac{f(x_0)+3f(x_1)+3f(x_2)+f(x_3)}{8}$	$-(3/80)h^5 f^{(4)}(\xi)$
4	5	Boole's rule	$(b-a)\dfrac{7f(x_0)+32f(x_1)+12f(x_2)+32f(x_3)+7f(x_4)}{90}$	$-(8/945)h^7 f^{(6)}(\xi)$
5	6		$(b-a)\dfrac{19f(x_0)+75f(x_1)+50f(x_2)+50f(x_3)+75f(x_4)+19f(x_5)}{288}$	$-(275/12{,}096)h^7 f^{(6)}(\xi)$

Overall Unequal spaced data

- Unequal trapezoid will always work, but can improve accuracy if any equally spaced segments are evaluated with Simpson's rule
  - If 2 adjacent segments are unequal, use trapezoid
  - if 2 adjacent segments are equal, use Simpson's 1/3
  - if 3 adjacent segments are equal, use Simpson's 3/8
  - if 4 adjacent segments are equal, use Simpson's 1/3 on first 2, remove the 1st segment from consideration, and continue

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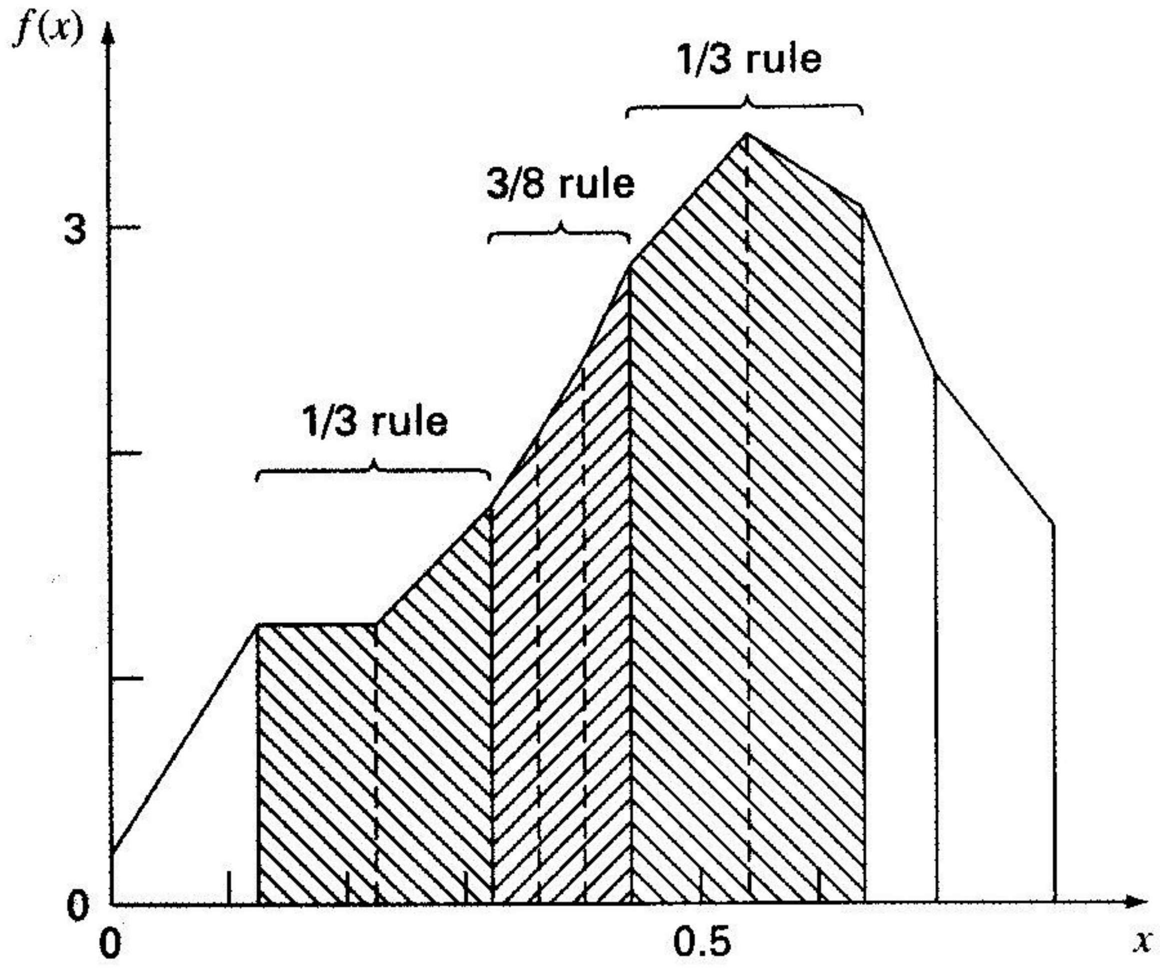


FIGURE 21.15

Use of the trapezoidal rule to determine the integral of unevenly spaced data. N
shaded segments could be evaluated with Simpson's rule to attain higher accurc

Numerical Differentiation

Numerical Differentiation
First Derivatives

Difference	Equation	Error
Forward	$f'(x_i)=\dfrac{f(x_{i+1})-f(x_i)}{h}$	O(h)
Backward	$f'(x_i)=\dfrac{f(x_i)-f(x_{i-1})}{h}$	O(h)
Central	$f'(x_i)=\dfrac{f(x_{i+1})-f(x_{i-1})}{2h}$	$O(h^2)$

Central more accurate than forward or backward, but requires more calculations

Numerical Differentiation
Accurate First Derivatives

Difference	Equation	Error
Forward	$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}$	$O(h^2)$
Backward	$f'(x_i) = \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h}$	$O(h^2)$
Central	$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h}$	$O(h^4)$

Numerical Differentiation
Second Derivatives

Second Derivative (central)

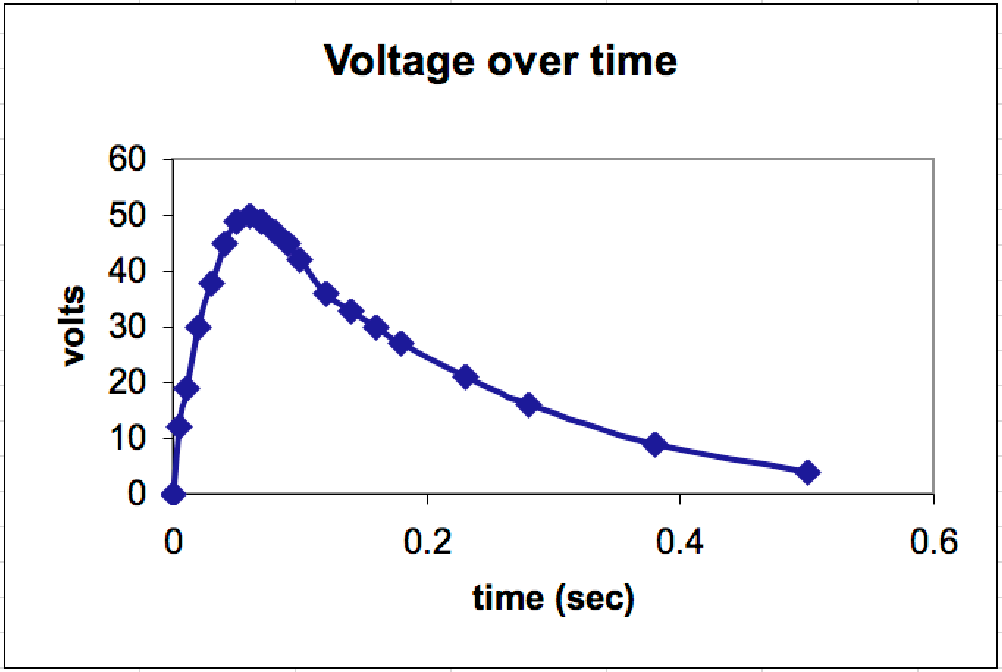
Difference	Equation	Error
standard	$f''(x_i)=\dfrac{f(x_{i+1})-2f(x_i)+f(x_{i-1})}{h^2}$	$O(h^2)$
more accurate	$f''(x_i)=\dfrac{-f(x_{i+2})+16f(x_{i-1})-30f(x_i)+16f(x_{i-1})-f(x_{i-2})}{12h^2}$	$O(h^4)$

Example of Numerical Integration

Numerical Integration using Trapeziod Rule wuth Unequally Spaced Data
Taken from Gottfried

t (sec)	v (volts)	delta t	avg v	area
0	0	0.005	6	0.03
0.005	12	0.005	15.5	0.0775
0.01	19	0.01	24.5	0.245
0.02	30	0.01	34	0.34
0.03	38	0.01	41.5	0.415
0.04	45	0.01	47	0.47
0.05	49	0.01	49.5	0.495
0.06	50	0.01	49.5	0.495
0.07	49	0.01	48	0.48
0.08	47	0.01	46	0.46
0.09	45	0.01	43.5	0.435
0.1	42	0.02	39	0.78
0.12	36	0.02	34.5	0.69
0.14	33	0.02	31.5	0.63
0.16	30	0.02	28.5	0.57
0.18	27	0.05	24	1.2
0.23	21	0.05	18.5	0.925
0.28	16	0.1	12.5	1.25
0.38	9	0.12	6.5	0.78
0.5	4			
			sum	10.7675

trapezoid 10.7675 using VBA trapezoid function



Example VBA Code (Trapezoidal)

```
Option Explicit

Public Function trapezoid(x As Range, y As Range) As Double
   Dim n As Integer, i As Integer
   Dim sum As Double
   sum = 0#
   n = x.Rows.Count
   For i = 2 To n
'      sum = sum + (x.Cells(i).Value - x.Cells(i - 1).Value) * (y.Cells(i).Value + y.Cells(i - 1).Value) / 2
      sum = sum + (x(i) - x(i - 1)) * (y(i) + y(i - 1)) / 2
   Next i
   trapezoid = sum
End Function

Private Function simp13(dx As Double, f1 As Double, f2 As Double, f3 As Double) As Double
   simp13 = 2 * dx * (f1 + 4 * f2 + f3) / 6
End Function

Private Function simp38(dx As Double, f1 As Double, f2 As Double, f3 As Double, f4 As Double) As Double
   simp38 = 3 * dx * (f1 + 3 * (f2 + f3) + f4) / 8
End Function
```

Few Things to Observe

- The variables in function Trapezoid are defined explicitly
- For example:
  - Dim = dimension statement in VBA (reserved to declare variables at the beginning of a program)
  - Double = double precision variable (reserves 8 bytes for each variable to carry 15 decimal places in calculations)
  - Integer = variable to contain integer numbers (saves memory space)
  - Range = a variable defines to contain multiple elements in a worksheet range

Other Things to Observe

- Statement n = x.Rows.Count
- Counts the number of elements in the variable x defined in function “trapezoid”
- “n” is used as a counter in the for-loop inside function trapezoid
- Variable “sum” is initialized to add the areas under each one of the intervals making up the numerical integration

Integrating Functions with Matlab

Main File (any name)

```
% Matlab quad function use

% Illustrates the use of the "quad" function in Matlab
% to perform numerical integration

% Function calls: fsim.m
%

integralArea = quad('fsim2',0,1.0);

fprintf('The value of the area under the curve is %15.8f\n',integralArea)
```

File = fsim2.m

```
% Function to be integrated using Matlab numerical in
%
% Programmer: A. Trani
% date: 03/12/07
%
function f=fsim2(x)

f= exp (- x .^ 2);
```