Part 5

Chapter 17

Numerical Integration Formulas

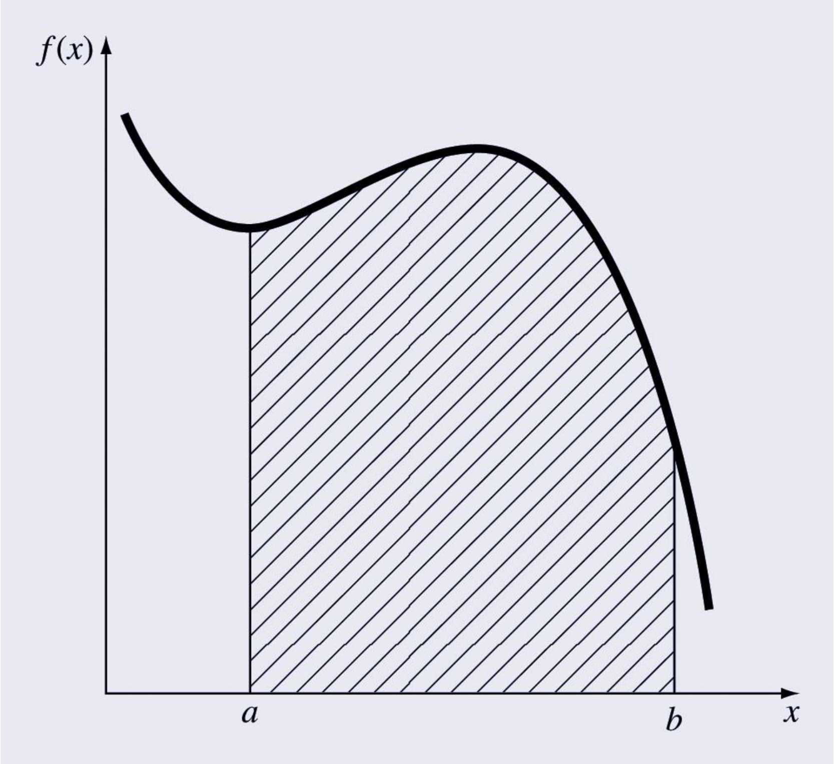
Chapter Objectives

- 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 3/8 rule
- 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:
- *I* represents the area under the curve f(x) between x= a and b.



Integration in Engineering and Science

- This integral can be evaluated over a line, an area, or a volume.
- For example the total mass of gas contained in a volume is given as the product of the density and the volume. However, suppose that the density varies from location to location within a volume, it is necessary to sum the product

$$mass = \sum_{i=1}^{n} \rho_i \Delta V_i$$

- For a continuous case, the integration is expressed by

$$mass = \iiint \rho(x, y, z)dxdydz \qquad mass = \iiint_V \rho(V)dV$$

- There is strong analogy between summation and integration

→ Basis of numerical integration

Newton-Cotes Formulas

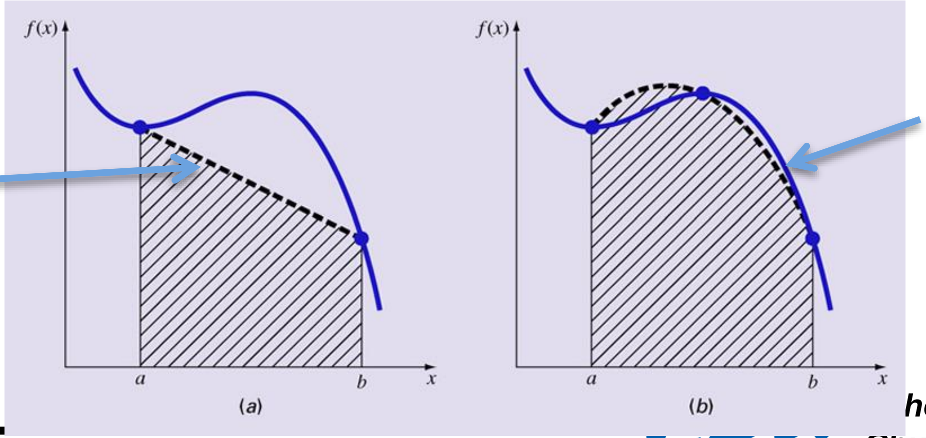
- The Newton-Cotes formulas are the most common numerical integration schemes.
- Generally, they are based on replacing a complicated function or tabulated data with a polynomial that is easy to integrate:

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

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

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

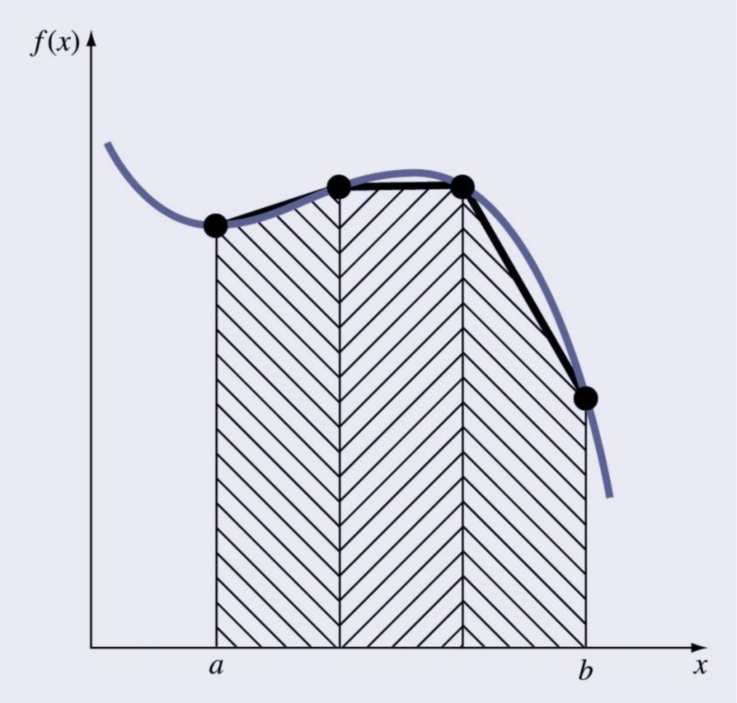
First-order polynomial (line)



Parabola

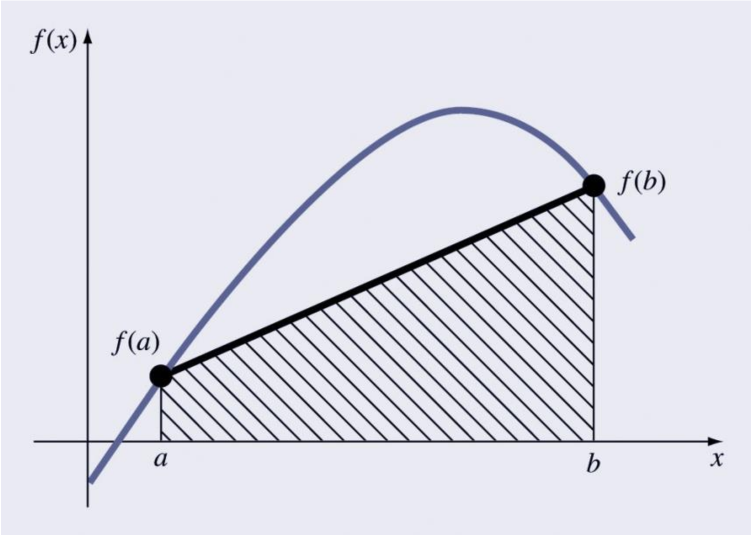
The Trapezoidal Rule

- The integral can be approximated using a series of polynomials applied piecewise to the function or data over segments of constant length.
- For example, three straight line segments are used to approximate the integral. Higher-order polynomial can be used for the same purpose.



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:



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

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

$$I = (b-a)\frac{f(a)+f(b)}{2} \rightarrow I = (b-a)(\text{average height})$$

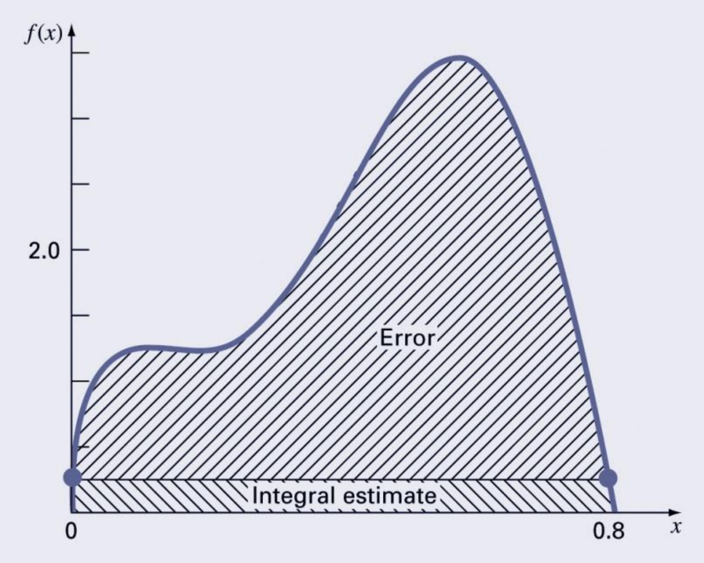
Error of the Trapezoidal Rule

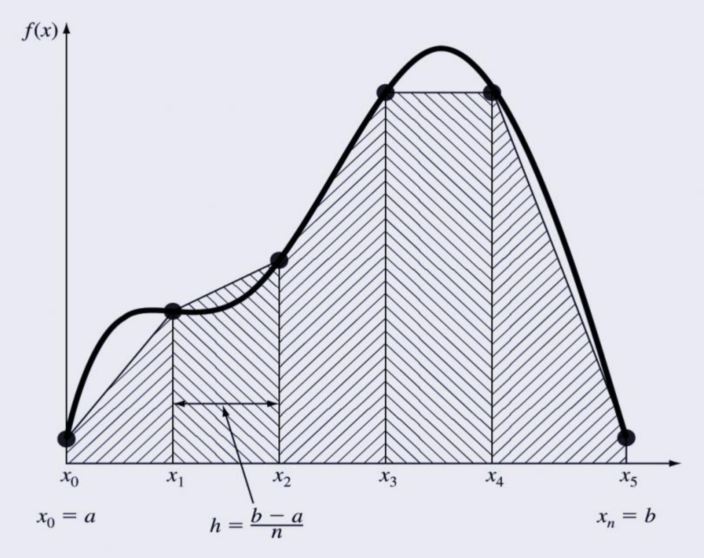
- An estimate for the local truncation error of a single application of the trapezoidal rule is:

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

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.





Example 17.1 (1/2)

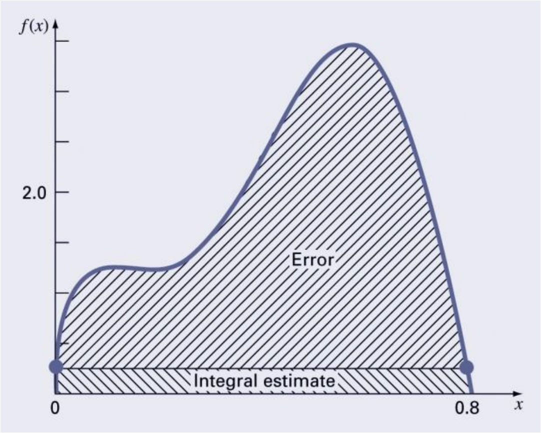
- Q. Use the trapezoidal rule to numerically integrate the following equation from a = 0 to b = 0.8. The true solution is 1.640533.

$$f(x) = 0.2 + 2.5x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

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

$\rightarrow E_t = 1.640533 - 0.1728 = 1.467733$

$\rightarrow \varepsilon_t = 89.5\%$



Example 17.1 (2/2)

Approximate error:

$$f''(x) = -400 + 4{,}050x - 10{,}800x^2 + 8{,}000x^3$$

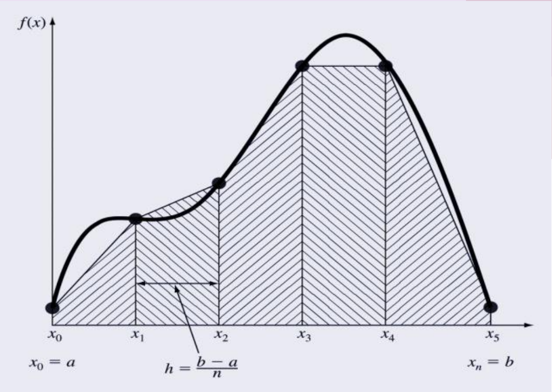
$$\bar{f}''(x) = \frac{\int_0^{0.8} (-400 + 4{,}050x - 10{,}800x^2 + 8{,}000x^3)dx}{0.8 - 0} = -60$$

$$E_a = -\frac{1}{12}(-60)(0.8)^3 = 2.56$$

note : this value is of the same order of magnitude and sign as the true error. Average second derivative is not an accurate approximation of f''(ξ), so a discrepancy exists and E_a rather E_t.

Composite Trapezoidal Rule

- One way to improve the accuracy is to divide the integration interval from a to b into a number of segments and apply the method to each segment.
- 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:



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

$$\sum_{i=1}^{n} f''(\xi_i) \cong n\bar{f}''$$

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

If the number of segments is doubled, the error will be quartered

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

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

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

MATLAB Program

```
function I = trap(func,a,b,n,varargin)
% trap: composite trapezoidal rule quadrature
%   I = trap(func,a,b,n,pl,p2,...):
%                     composite trapezoidal rule
% input:
%   func = name of function to be integrated
%   a, b = integration limits
%   n = number of segments (default = 100)
%   pl,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);
```

Example 17.2 (1/2)

- Q. Use the two-segment and composite trapezoidal rule to estimate the integral of the function from a = 0 to b = 0.8. The exact value is 1.640533.

$$f(x) = 0.2 + 2.5x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

Sol.

For $n = 2$ ($h = 0.4$)

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

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

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

$$E_a = -\frac{0.8^3}{12(2)^2}(-60) = 0.64$$

Example 17.2 (2/2)

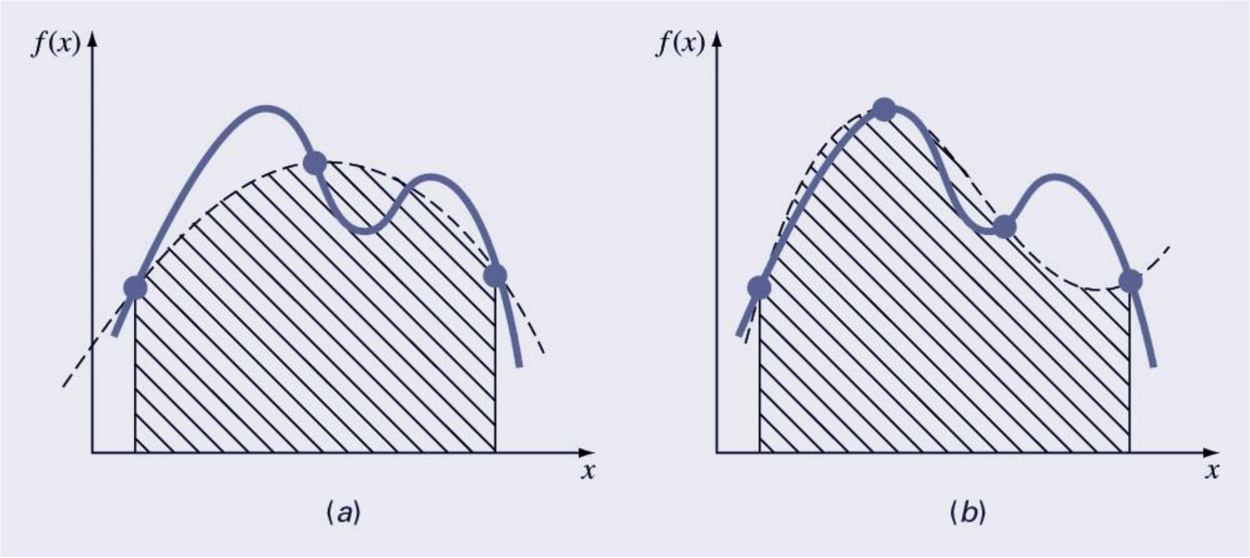
<Results for the composite trapezoidal rule to estimate the integral of $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4$ from $x = 0$ to 0.8. The exact value is 1.640533>

→ As the number of segments increases, the error decreases.

n	*h*	*I*	ε_t (%)
2	0.4	1.0688	34.9
3	0.2667	1.3695	16.5
4	0.2	1.4848	9.5
5	0.16	1.5399	6.1
6	0.1333	1.5703	4.3
7	0.1143	1.5887	3.2
8	0.1	1.6008	2.4
9	0.0889	1.6091	1.9
10	0.08	1.6150	1.6

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.



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:

$$I=\int_{x_0}^{x_2} f_n(x)\,dx$$

$$I=\frac{h}{3}\left[f(x_0)+4f(x_1)+f(x_2)\right]=I=(b-a)\frac{f(x_0)+4f(x_1)+f(x_2)}{6}$$

Where, $h=(b-a)/2$, $a=x_0$, $b=x_2$, and $x_1=(a+b)/2$

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.

Example 17.3

- Q. Use Simpson 1/3 rule to integrate the following equation from a = 0 to b = 0.8. Exact solution is 1.640533.

$$f(x) = 0.2 + 2.5x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

sol) for n = 2 (h = 0.4)에 대해서

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

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

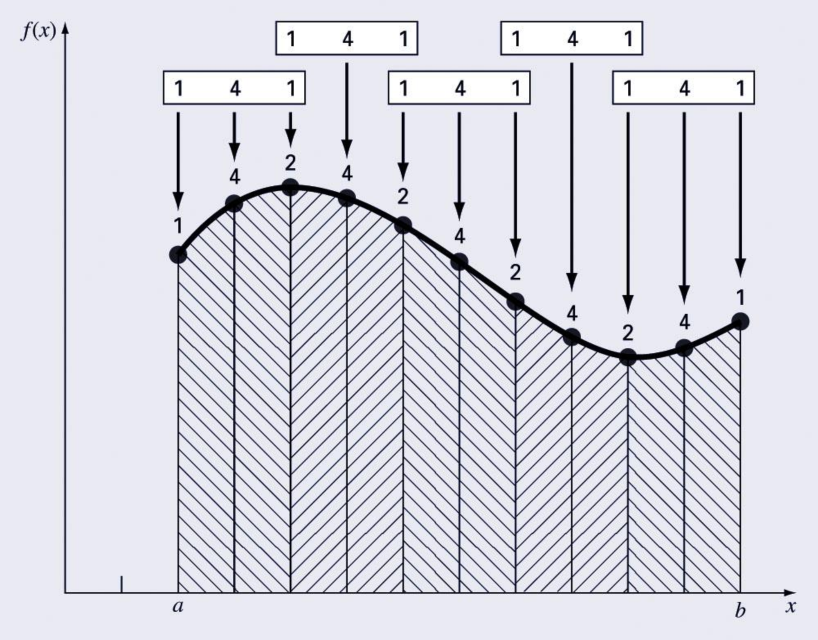
$\rightarrow$ This shows improved results compared to the trapezoidal rule.

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

$$E_a = -\frac{0.8^5}{2880}(-2400) = 0.2730667$$

Composite Simpson's 1/3 Rule

- For improved results, 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:



$$I=\int_{x_0}^{x_n} f_n(x)\,dx=\int_{x_0}^{x_2} f_n(x)\,dx+\int_{x_2}^{x_4} f_n(x)\,dx+\cdots+\int_{x_{n-2}}^{x_n} f_n(x)\,dx$$

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

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

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

Example 17.4

- Q. Use composite Simpson 1/3 rule to integrate the following equation from a = 0 to b = 0.8. Exact solution is 1.640533.

$$f(x) = 0.2 + 2.5x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

Sol.) for n = 4 (h = 0.2)

$$f(0) = 0.2 \qquad f(0.2) = 1.288$$
$$f(0.4) = 2.456 \qquad f(0.6) = 3.464$$
$$f(0.8) = 0.232$$

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

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

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

Example 17.4

- The composite version of Simpson 1/3 rule is superior to the trapezoidal rule for most applications.
- It is limited to cases where the values are equispaced., even number of segments, and odd number of points.
- Odd segment and even point formula is known as Simpson 3/8 formula.

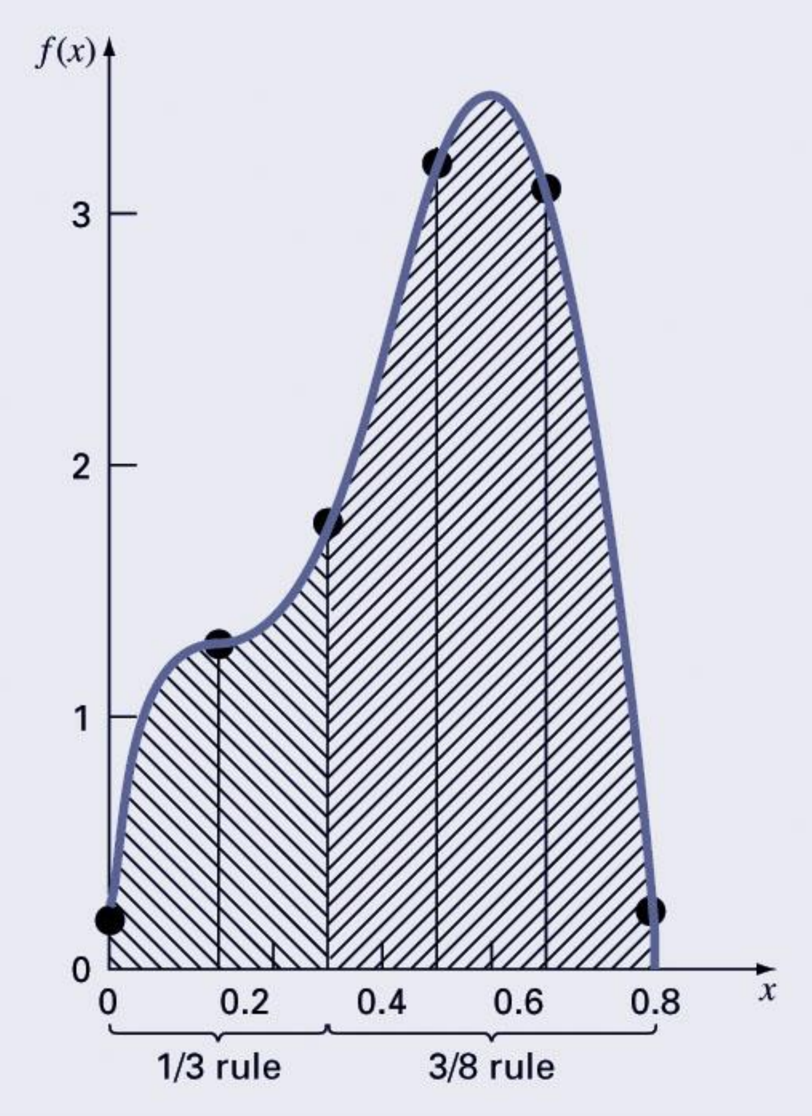
Simpson's 3/8 Rule

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

$$I = \int_{x_0}^{x_3} f_n(x)\,dx$$

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

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



Higher-Order Formulas

- Higher-order Newton-Cotes formulas may also be used

  - in general, the higher order of the polynomial used, the higher 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.

Example 17.5 (1/2)

- Q. (a) Use Simpson 3/8 to integrate from a = 0 to b = 0.8. (b) Use it in conjunction with Simpson 1/3 for five segment integration.

$$f(x) = 0.2 + 2.5x - 200x^2 + 675x^3 - 900x^4 + 400x^5$$

Sol.) (a) For n = 3 (h = 0.2667)

$$f(0) = 0.2 \qquad f(0.2667) = 1.432724$$

$$f(0.5333) = 3.487177 \qquad f(0.8) = 0.232$$

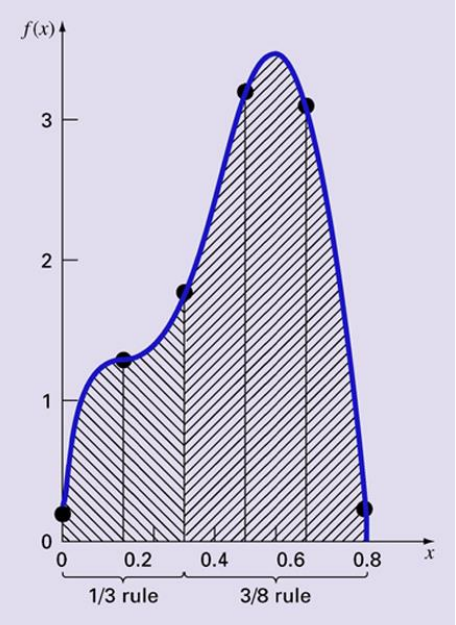
$$I = 0.8\frac{0.2 + 3(1.432724 + 3.487177) + 0.232}{8} = 1.51970$$

(b) For n = 5 (h = 0.16)

$$f(0) = 0.2 \qquad f(0.16) = 1.296919$$

$$f(0.32) = 1.743393 \qquad f(0.48) = 3.186015$$

$$f(0.64) = 3.181929 \qquad f(0.80) = 0.232$$



Example 17.5 (2/2)

The integral for the first two segments using Simpson 1/3

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

For the last three segments, the Simpson 3/8

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

The total integral is by summing the two results.

$$I = 0.3803237 + 1.264754 = 1.645077$$

Summary

<Newton-Cotes integration: h = (b − a)/n>

n	*points*	*name*	공 식	절단오차
1	2	Trapezoidal rull	$(b-a)\dfrac{f(x_0)+f(x_1)}{2}$	$-(1/12)h^3 f''(\xi)$
2	3	Simpson 1/3	$(b-a)\dfrac{f(x_0)+4f(x_1)+f(x_2)}{6}$	$-(1/90)h^5 f^{(4)}(\xi)$
3	4	Simpson 3/8	$(b-a)\dfrac{f(x_0)+3f(x_1)+3f(x_2)+f(x_3)}{8}$	$-(3/80)h^5 f^{(4)}(\xi)$
4	5	Boole's rull	$(b-a)\dfrac{7f(x_0)+32f(x_1)+12f(x_2)+32f(x_3)+7f(x_4)}{90}$	$-(8/945)h^7 f^{(6)}(\xi)$
5	6		$(b-a)\dfrac{19f(x_0)+75f(x_1)+50f(x_2)+50f(x_3)+75f(x_4)+19f(x_5)}{288}$	$-(275/12{,}096)h^7 f^{(6)}(\xi)$

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;
```

MATLAB Functions (option)

- 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.

```
>> x = [0 .12 .22 .32 .36 .4 .44 .54 .64 .7 .8];
>> y = 0.2 + 25*x - 200*x.^2 + 675*x.^3 - 900*x.^4 + 400*x.^5;
>> trapz(x,y)
ans =
            1.5948
```

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.