

CH204 CSL

Numerical Integration

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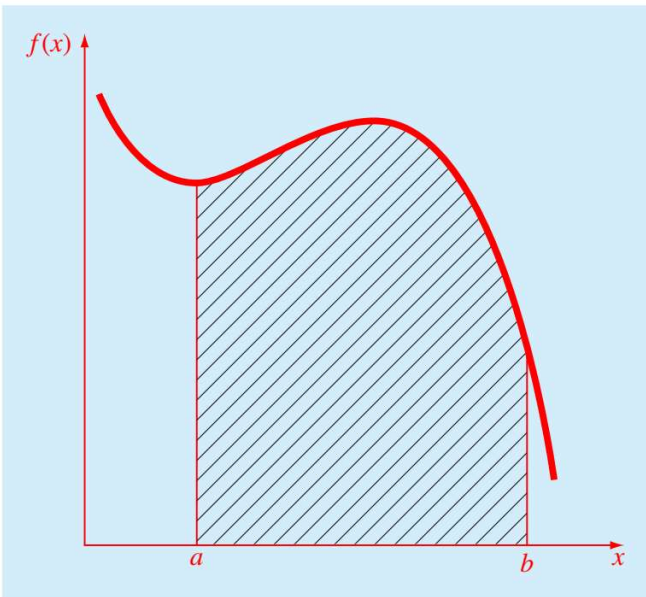
What Is Integration?

Mathematically, definite integration is represented by

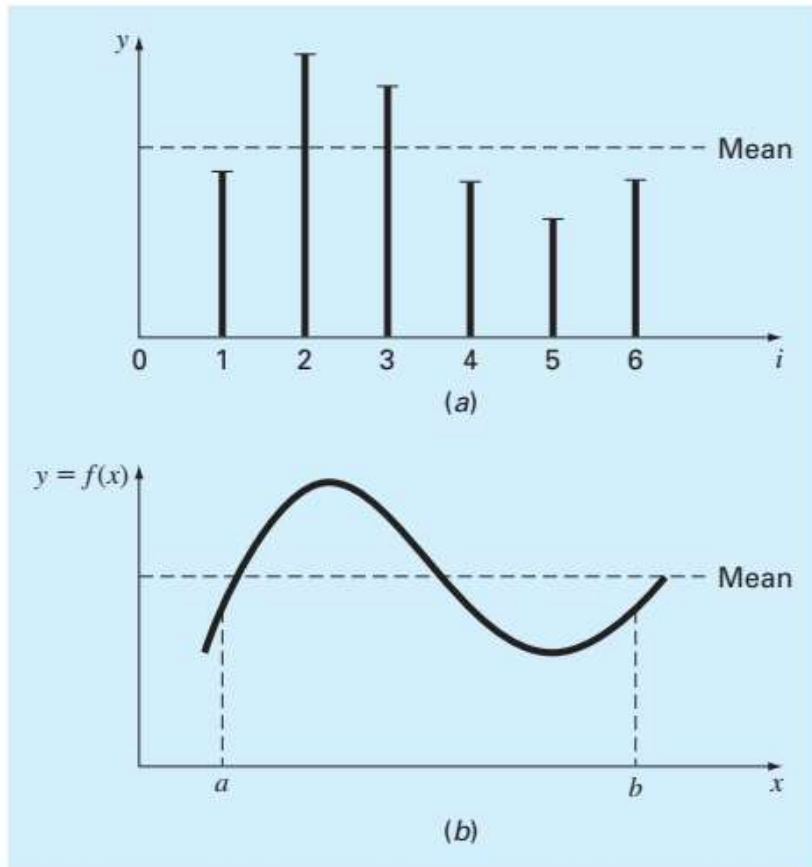
$$I = \int_a^b f(x) dx$$

which stands for the integral of the function $f(x)$ with respect to the independent variable x , evaluated between the limits $x = a$ to $x = b$.

I is basically the total value, or summation, of $f(x) dx$ over the range $x = a$ to b .



The integral expressed by I corresponds to the area under the curve of $f(x)$ between $x = a$ and b



The mean of n discrete data points can be calculated by

$$\text{Mean} = \frac{\sum_{i=1}^n y_i}{n}$$

where y_i are individual measurements.

Suppose that y is a continuous function of an independent variable x . For this case, there are an infinite number of values between a and b .

$$\text{Mean} = \frac{\int_a^b f(x) dx}{b - a}$$

A number of examples relate directly to the idea of the integral as the area under a curve.

The integral may be evaluated over a line, an area, or a volume. For example, the total mass of chemical contained in a reactor is given as the product of the concentration of chemical and the reactor volume, or

Mass = concentration $\times$ volume, where concentration has units of mass per volume. However, suppose that concentration varies from location to location within the reactor. In this case, it is necessary to sum the products of local concentrations c_i and corresponding elemental volumes ΔV_i :

$$\text{Mass} = \sum_{i=1}^n c_i \Delta V_i$$

where n is the number of discrete volumes.

For the continuous case, where $c(x, y, z)$ is a known function and x, y , and z are independent variables designating position in Cartesian coordinates, integration can be used for the same purpose:

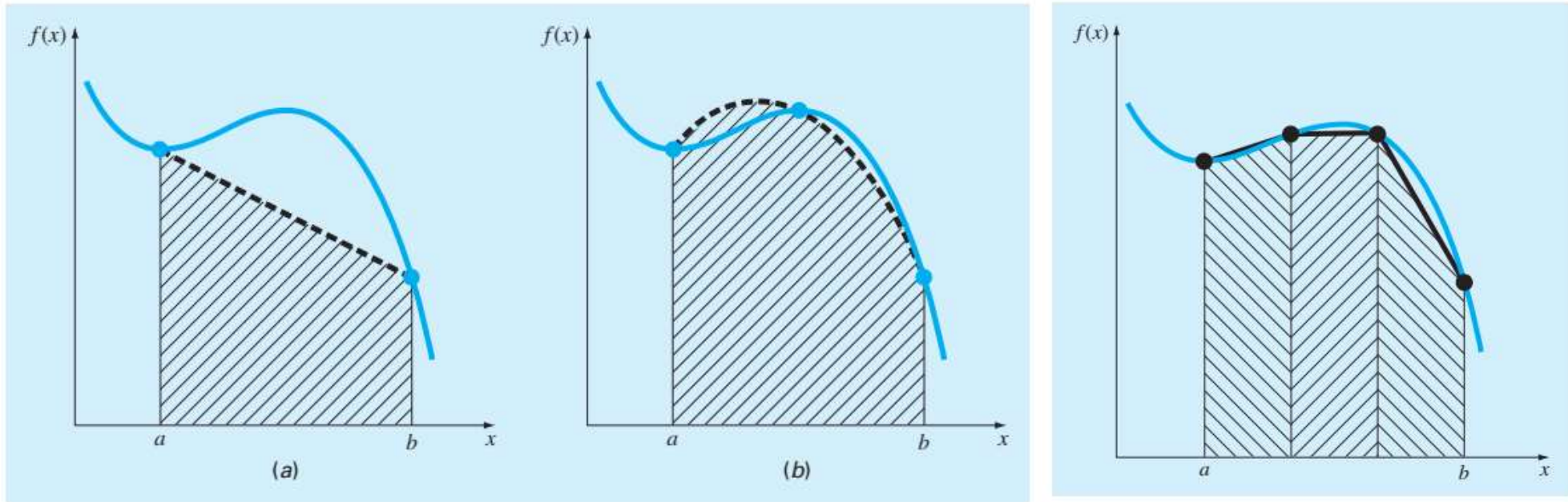
$$\text{Mass} = \iiint c(x, y, z) dx dy dz$$

$$\text{Mass} = \iiint_V c(V) dV$$

The total rate of energy transfer across a plane where the flux (in calories per square centimeter per second) is a function of position is given by

$$\text{Flux} = \iint_A u_x dA$$

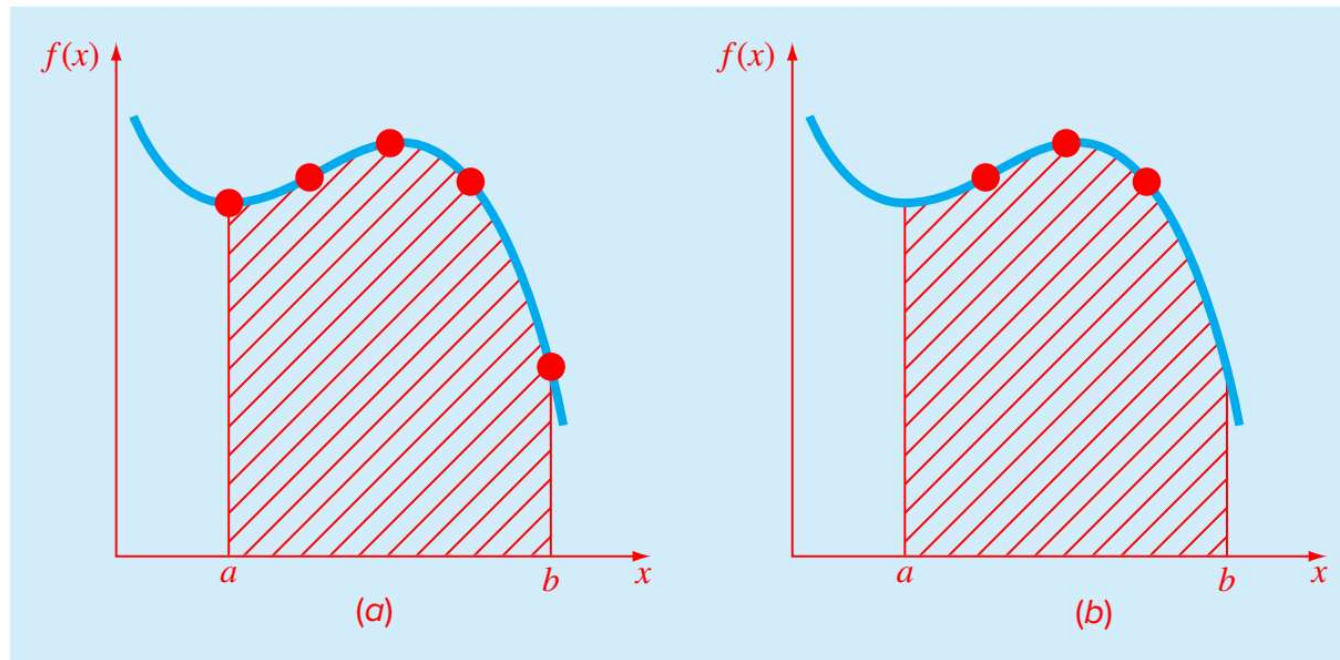
NEWTON-COTES FORMULAE



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 a polynomial that is easy to integrate:

$$I = \int_a^b f(x) dx \cong \int_a^b f_n(x) dx \quad \text{where } f_n(x) = \text{a polynomial of the form}$$

$$f_n(x) = a_0 + a_1x + \cdots + a_{n-1}x^{n-1} + a_nx^n \quad \text{where } n \text{ is the order of the polynomial.}$$



Closed and open forms of the Newton-Cotes formulas are available. The *closed forms* are those where the data points at the beginning and end of the limits of integration are known. The *open forms* have integration limits that extend beyond the range of the data.

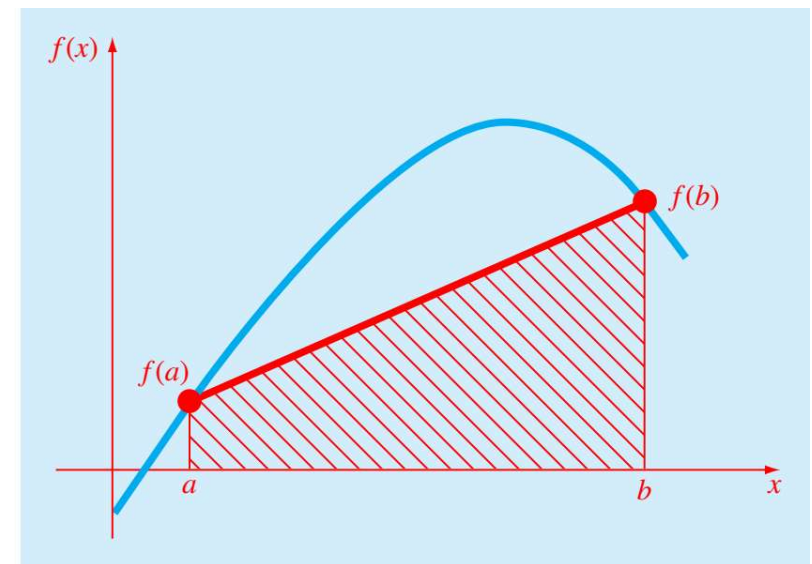
THE TRAPEZOIDAL RULE

The trapezoidal rule is the first of the Newton-Cotes closed integration formulas. It corresponds to the case where the polynomial is first-order:

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

The result of the integration is

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



Geometrically, the trapezoidal rule is equivalent to approximating the area of the trapezoid under the straight line connecting $f(a)$ and $f(b)$.

Error of the Trapezoidal Rule

When we employ the integral under a straight-line segment to approximate the integral under a curve, we obviously can incur an error that may be substantial. An estimate for the local truncation error of a single application of the trapezoidal rule is

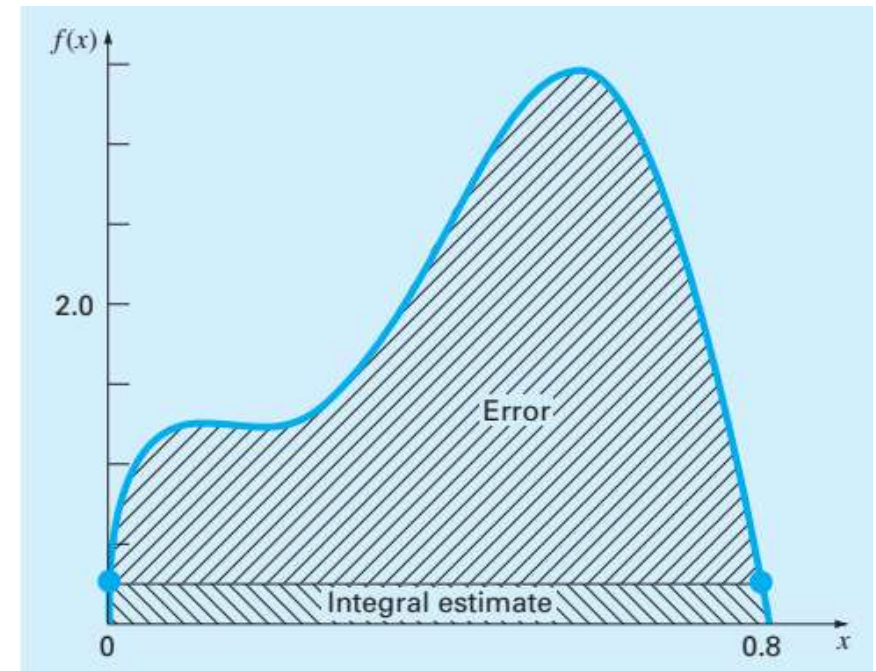
$$E_t = -\frac{1}{12}f''(\xi)(b-a)^3$$

where ξ lies somewhere in the interval from a to b . E_t indicates that if the function being integrated is linear, the trapezoidal rule will be exact because the second derivative of a straight line is zero. Otherwise, for functions with second- and higher-order derivatives (i.e., with curvature), some error can occur.

Note that the exact value of the integral can be determined analytically to be 1.640533.

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

which represents an error of $E_t = 1.640533 - 0.1728 = 1.467733$, which corresponds to a percent relative error of $\epsilon_t = 89.5\%$.



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

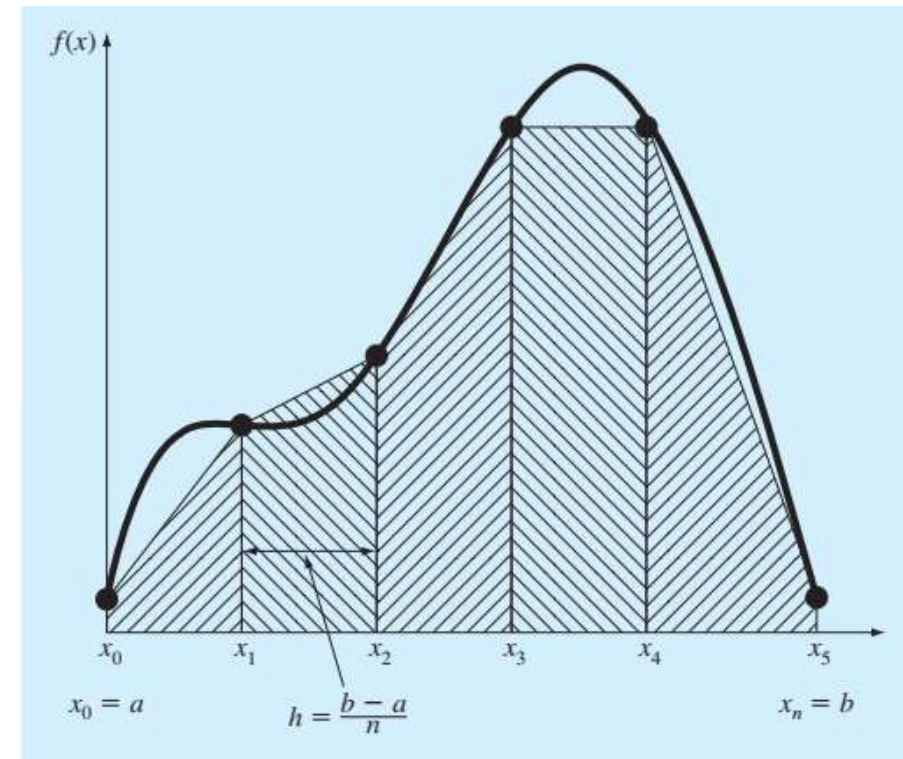
One way to improve the accuracy of the trapezoidal rule is to divide the integration interval from a to b into a number of segments and apply the method to each segment. The areas of individual segments can then be added to yield the integral for the entire interval. The resulting equations are called *composite*, or *multiple-segment*, *integration formulas*.

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

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

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

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



An error for the composite trapezoidal rule can be obtained by summing the individual errors for each segment to give

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

where $f''(\xi_i)$ is the second derivative at a point ξ_i located in segment i . This result can be simplified by estimating the mean or average value of the second derivative for the entire interval as

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

$$\text{Therefore } \sum f''(\xi_i) \cong n \bar{f}''$$

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

Thus, if the number of segments (n) is doubled, the truncation error will be quartered.

Results for the composite trapezoidal rule to estimate the integral of $f(x) = 0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5$ from $x = 0$ to 0.8 . The exact value is 1.640533 .

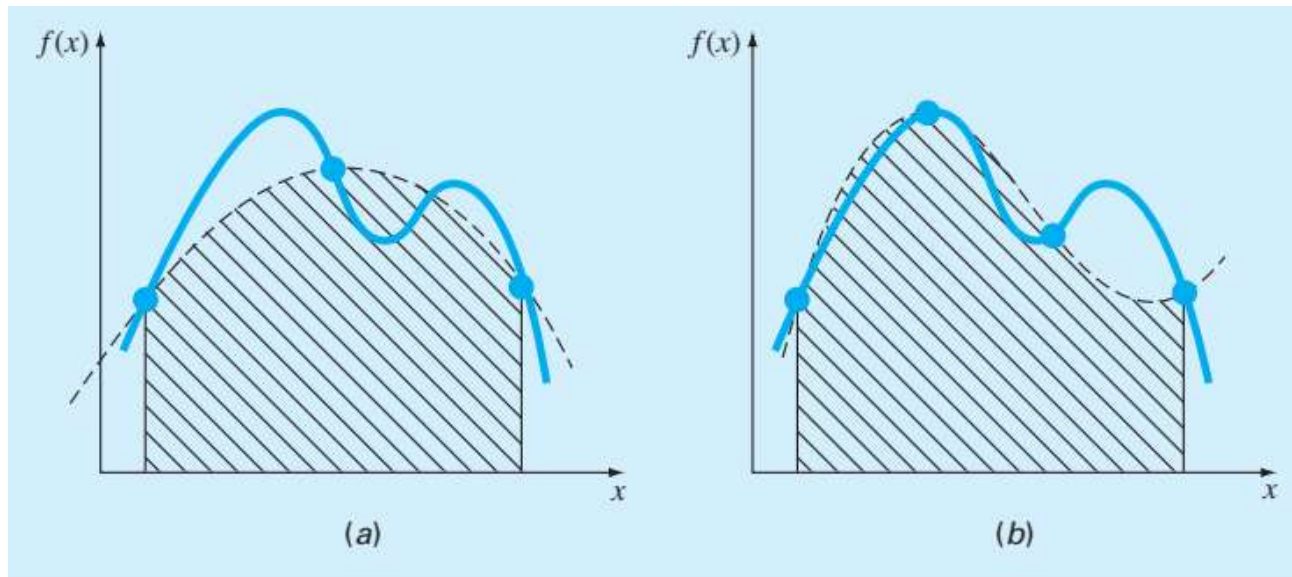
n	h	I	ϵ_t (%)
2	0.4	1.0688	34.9
3	0.2667	1.3695	16.5
4	0.2	1.4848	9.5
5	0.16	1.5399	6.1
6	0.1333	1.5703	4.3
7	0.1143	1.5887	3.2
8	0.1	1.6008	2.4
9	0.0889	1.6091	1.9
10	0.08	1.6150	1.6

SIMPSON'S RULES

Another way to obtain a more accurate estimate of an integral is to use higher-order polynomials to connect the points.

For example, if there is an extra point midway between $f(a)$ and $f(b)$, the three points can be connected with a parabola.

If there are two points equally spaced between $f(a)$ and $f(b)$, the four points can be connected with a third-order polynomial. 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 the case where the polynomial f_n is second order:

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

where a and b are designated as x_0 and x_2 , respectively. The result of the integration is

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

where, for this case, $h = (b - a)/2$. This equation is known as *Simpson's 1/3 rule*.

The label "1/3" stems from the fact that h is divided by 3

where $a = x_0$, $b = x_2$, and x_1 = the point midway between a and b , which is given by $(a + b)/2$.

The middle point is weighted by two thirds and the two end points by one-sixth

$$E_t = -\frac{1}{90}h^5 f^{(4)}(\xi)$$

or, because $h = (b - a)/2$:

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

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

where ξ lies somewhere in the interval from a to b . Thus, Simpson's 1/3 rule is more accurate than the trapezoidal rule.

Rather than being proportional to the third derivative, the error is proportional to the fourth derivative. Consequently, Simpson's 1/3 rule is third order accurate even though it is based on only three points. In other words, it yields exact results for cubic polynomials even though it is derived from a parabola!

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

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

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

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

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

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

which is approximately five times more accurate than for a single application of the trapezoidal rule

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

where -2400 is the average fourth derivative for the interval.

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

Simpson's rule can be improved by dividing the integration interval into a number of segments of equal width

$$\int_a^b f(x) dx = h/3 [(y_0 + y_n) + 4(y_1 + y_3 + y_5 + \dots + y_{n-1}) + 2(y_2 + y_4 + y_6 + \dots + y_{n-2})]$$

Substituting Simpson's 1/3 rule for each integral yields

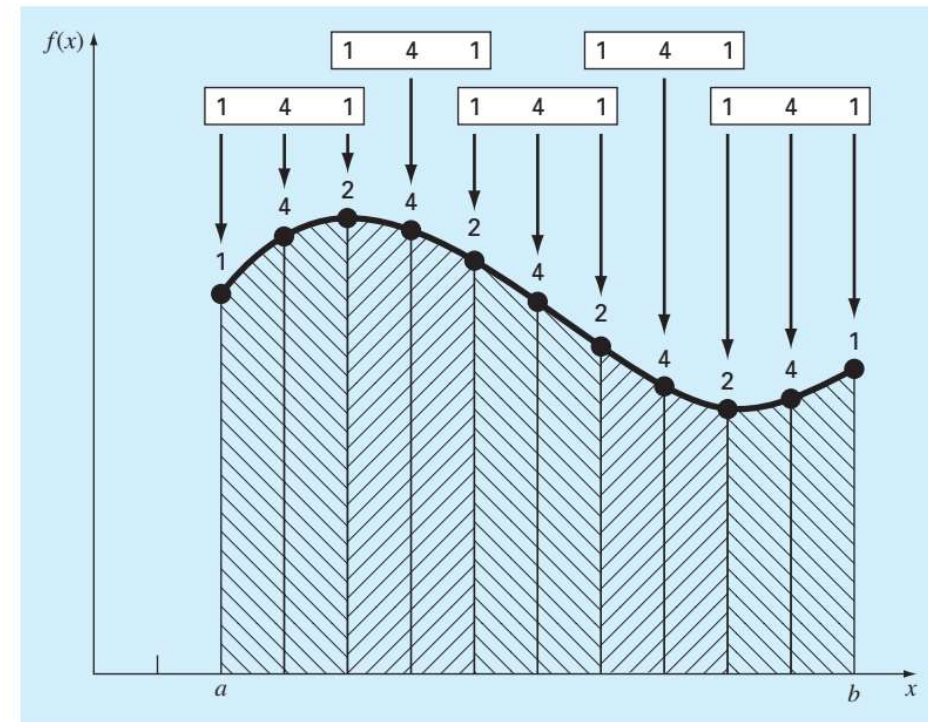
$$I = 2h \frac{f(x_0) + 4f(x_1) + f(x_2)}{6} + 2h \frac{f(x_2) + 4f(x_3) + f(x_4)}{6}$$

$$+ \cdots + 2h \frac{f(x_{n-2}) + 4f(x_{n-1}) + f(x_n)}{6}$$

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

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

where $f^{(4)}$ is the average fourth derivative for the interval.



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

from $a = 0$ to $b = 0.8$. Employ Eq. (19.27) to estimate the error. Recall that the exact integral is 1.640533.

Solution. $n = 4 (h = 0.2)$:

$$\begin{aligned} f(0) &= 0.2 & f(0.2) &= 1.288 \\ f(0.4) &= 2.456 & f(0.6) &= 3.464 \\ f(0.8) &= 0.232 \end{aligned}$$

From Eq. (19.26):

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

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

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

Simpson's 3/8 Rule

In a similar manner to the derivation of the trapezoidal and Simpson's 1/3 rule, a third order Lagrange polynomial can be fit to four points and integrated to yield

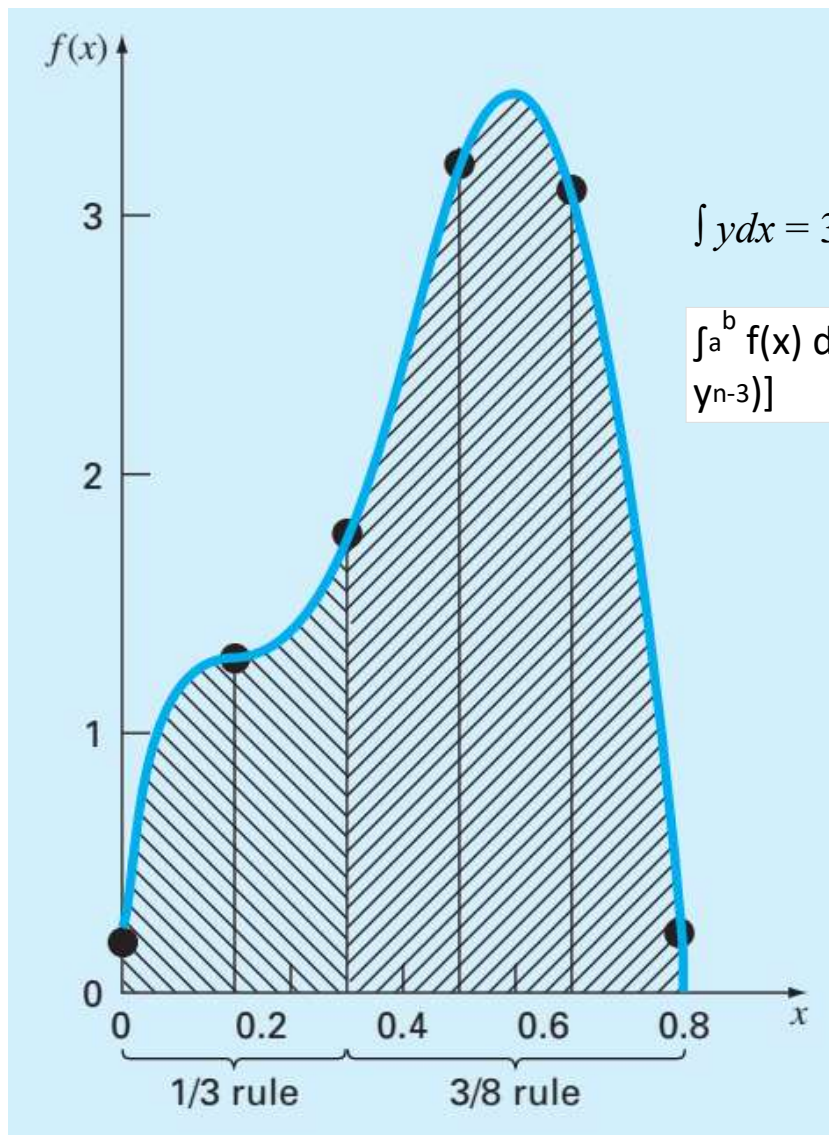
$$I = \frac{3h}{8} [f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)]$$

where $h = (b - a)/3$. This equation is known as *Simpsons 3/8 rule* because h is multiplied by 3/8.

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

Thus, the two interior points are given weights of three-eighths, whereas the end points are weighted with one-eighth. Simpson's 3/8 rule has an error of

$$E_t = -\frac{3}{80}h^5 f^{(4)}(\xi) \quad \text{or, because } h = (b - a)/3:$$
$$E_t = -\frac{(b - a)^5}{6480} f^{(4)}(\xi)$$



$$\int y dx = \frac{3h}{8} [y_0 + 2(y_3 + y_6 + \dots + y_{n-3}) + 3(y_1 + y_2 + y_4 + y_5 + \dots + y_{n-2} + y_{n-1}) + y_n]$$

$$\int_a^b f(x) dx = \frac{3h}{8} [(y_0 + y_n) + 3(y_1 + y_2 + y_4 + y_5 + \dots + y_{n-1}) + 2(y_3 + y_6 + y_9 + \dots + y_{n-3})]$$

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):

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

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

$$\begin{array}{ll} f(0) = 0.2 & f(0.16) = 1.296919 \\ f(0.32) = 1.743393 & f(0.48) = 3.186015 \\ f(0.64) = 3.181929 & f(0.80) = 0.232 \end{array}$$

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:

$$I = 0.3803237 + 1.264754 = 1.645077$$

$$h = (b - a)/n.$$

Segments

Segments (n)	Points	Name	Formula	Truncation Error
1	2	Trapezoidal rule	$(b - a) \frac{f(x_0) + f(x_1)}{2}$	$-(1/12)h^3 f''(\xi)$
2	3	Simpson's 1/3 rule	$(b - a) \frac{f(x_0) + 4f(x_1) + f(x_2)}{6}$	$-(1/90)h^5 f^{(4)}(\xi)$
3	4	Simpson's 3/8 rule	$(b - a) \frac{f(x_0) + 3f(x_1) + 3f(x_2) + f(x_3)}{8}$	$-(3/80)h^5 f^{(4)}(\xi)$

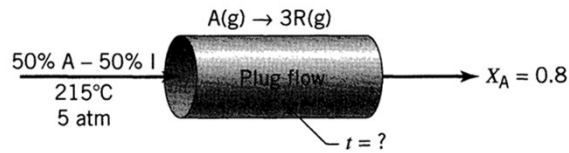
INTEGRATION WITH UNEQUAL SEGMENTS

Apply the trapezoidal rule to each segment and sum the results:

x	$f(x)$	x	$f(x)$
0.00	0.200000	0.44	2.842985
0.12	1.309729	0.54	3.507297
0.22	1.305241	0.64	3.181929
0.32	1.743393	0.70	2.363000
0.36	2.074903	0.80	0.232000
0.40	2.456000		

$$I = 0.12 \frac{0.2 + 1.309729}{2} + 0.10 \frac{1.309729 + 1.305241}{2} \\ + \dots + 0.10 \frac{2.363 + 0.232}{2} = 1.594801$$

which represents an absolute percent relative error of $\varepsilon_t = 2.8\%$.



A homogeneous gas reaction $A \rightarrow 3R$ has a reported rate at temperature 215°C $-r_A = 10^{-2} \sqrt{C_A}$, [mol/(liter.s)] where C_A is the concentration of A in the reaction mixture. The concentration of A in the feed is $C_{A0} = 0.0625$ mol/liter.

Find the space-time needed for achieving 80% conversion of a 50% A-50% inert feed to a plug flow reactor (PFR) operating at 215°C and 5 atm.

Note that the reactant concentration C_A continuously decreases (as it is consumed by reaction when it flows along the reactor) and therefore, the rate of reaction continuously changes with respect to the length of the reactor.

$C_A = C_{A0} \frac{(1-X_A)}{(1+\epsilon_A X_A)}$ where X_A is the fractional conversion achieved at a fixed axial distance from the inlet of the reactor and ϵ_A is the fractional change in volume of the reaction mixture between no conversion and complete conversion of reactant A ($\epsilon_A = 1$).

The space time can be determined from the performance equation of PFR

$$\tau = C_{A0} \int_0^{X_A} \frac{1}{(-r_A)} dX_A$$

Use trapezoidal and Simpson's rules.