Chapter 2

Numerical Integration Formulas

2.1 Introduction and Background

According to the dictionary definition, to integrate means "to bring together, as parts, into a whole; to unite; to indicate the total amount. . . ." 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 $x = b$.

The "meaning" of the equation is the total value, or summation, of $f(x)dx$ over the range $x = a$ to b. In fact, the symbol ∫ is actually a stylized capital S that is intended to signify the close connection between integration and summation.

Figure 1 shows 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.

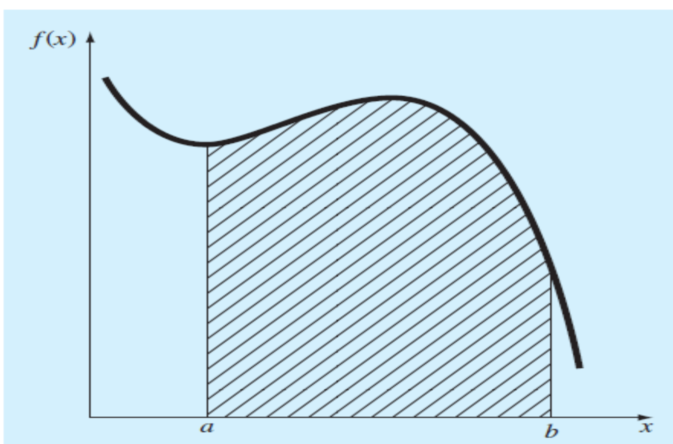

Figure 1 shows graphical representation of the integral of $f(x)$

2.2 Newton-Cotes Formulas

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:

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

$$f_n(x) = a_0 + a_1x + \cdots + a_{n-1}x^{n-1} + a_nx^n$$

where n is the order of the polynomial.

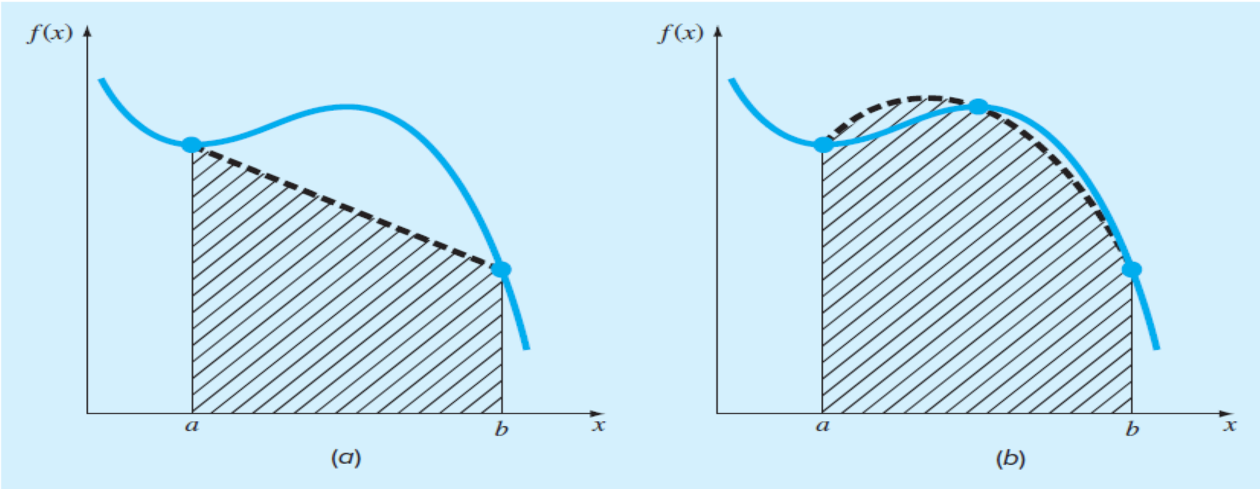

Figure 2: the approximation of an integral by the area under (*a*) a straight line and (*b*) a parabola

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

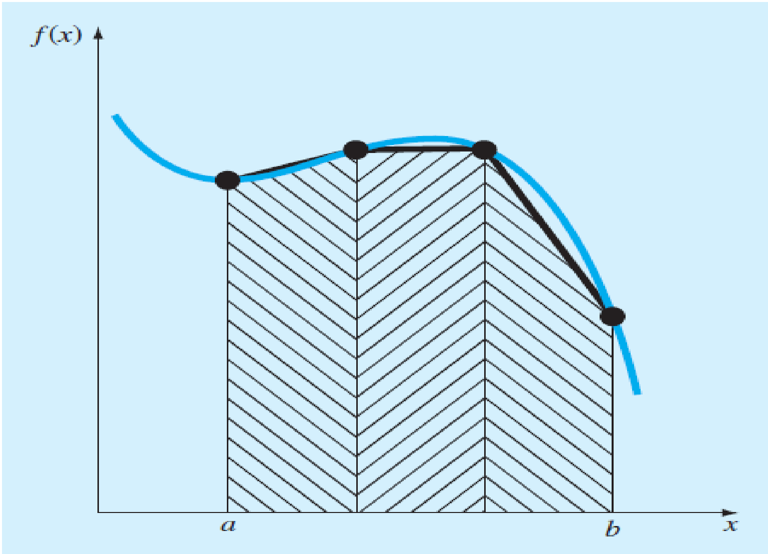

Figure 3: the approximation of an integral by the area under three straight-line segments

The difference between (a) closed and (b) open integration formulas

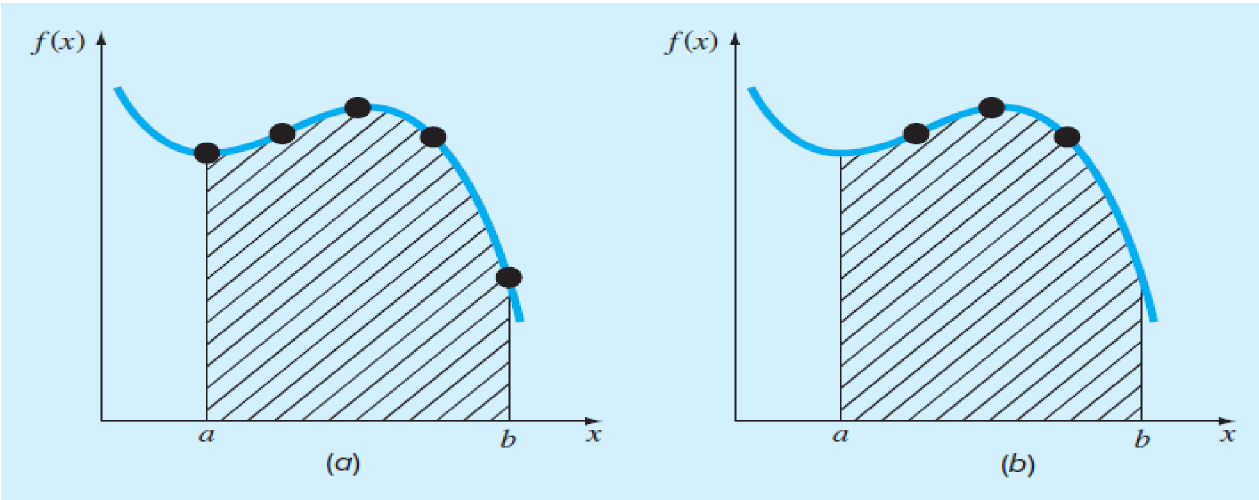

Figure 4: The difference between (a) closed and (b) open integration formulas

The closed forms are those where the data points at the beginning and end of the limits of integration are known (Fig. 4a). The open forms have integration limits that extend beyond the range of the data (Fig. 4b).

2.3 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 trapezoidal rule integration is

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

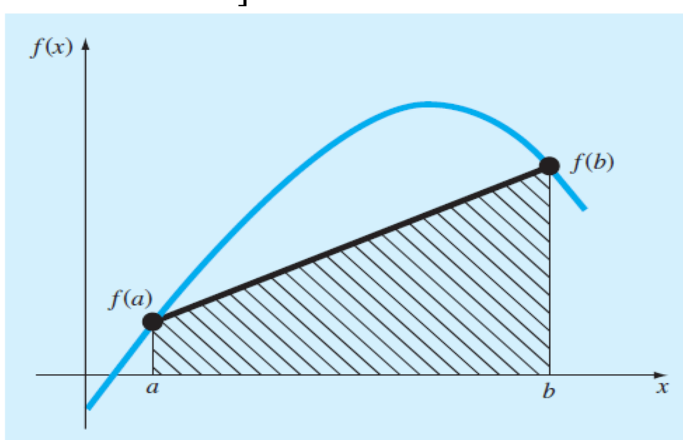

Figure 5: The trapezoidal rule integration

Example 1: Use trapezoidal rule 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

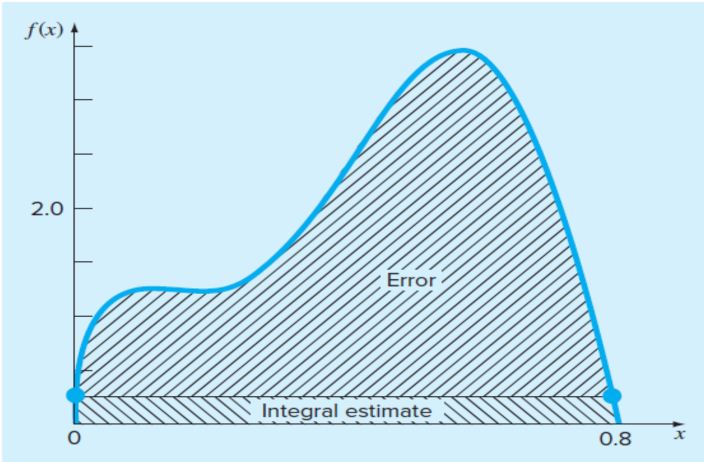

Figure 6: Graphical depiction of the use of a single application of the trapezoidal rule to approximate the integral of example 1

Solution: $f(0) = 0.2\ and\ f(0.8) = 0.232$

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

The percent relative error of ε_t = 89.5%.

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.

From Figure 7, there are $n + 1$ equally spaced base points$(x_0, x_1, \cdots, x_n)$. Consequently, there are n segments of equal width:

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

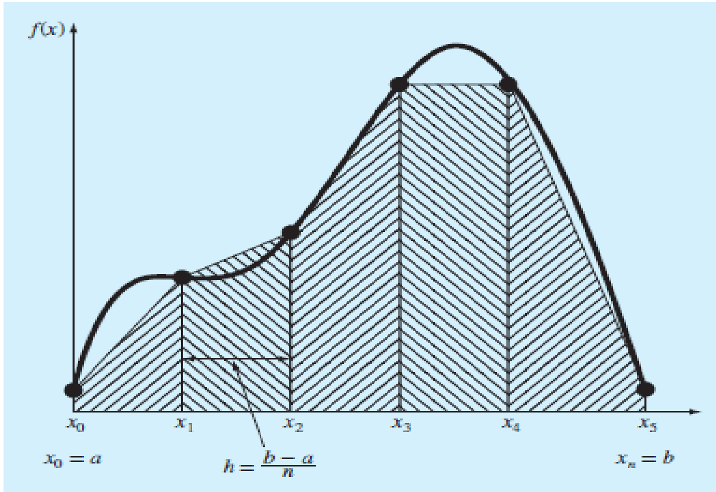

Figure 7: Composite trapezoidal rule.

If a and b are designated as x_0, and x_n, respectively, the total integral can be represented as

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

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

Example 2: Use the two segment trapezoidal rule to estimate the integral from $a = 0$ to $b = 0.8$ of

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

Solution:

$$n = 2$$

$$h = \frac{0.8 - 0}{2} = 0.4$$

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

$$I = \frac{0.4}{2}[0.2 + 2(2.456) + 0.232] = 1.0688$$

The percent of error is 34.9%

2.4 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.

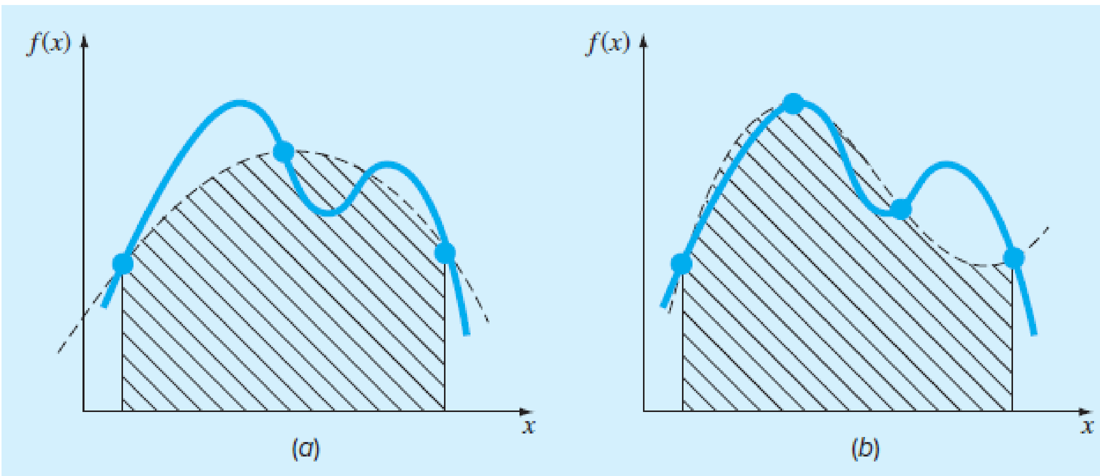

Figure 8 (a) Graphical depiction of Simpson's 1⁄3 rule: It consists of taking the area under a parabola connecting three points. (b) Graphical depiction of Simpson's 3⁄8 rule: It consists of taking the area under a cubic equation connecting four points.

2.4.1Simpson's 1⁄3 Rule

Simpson's 1⁄3 rule corresponds to the case where the polynomial is second order:

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

The result of the integration is

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

Where for this case,

$$h = \frac{b-a}{2}, a = x_0, b = x_2 \; and$$

$$x_1 = the\ point\ midway\ between\ a\ and\ b, which\ is\ given\ by \frac{a+b}{2}$$

Example 3: Use Simpson's 1⁄3 rule to estimate the integral from $a = 0$ to $b = 0.8$ of

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

$$h = \frac{0.8 - 0}{2} = 0.4$$

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

$$I = \frac{0.4}{3}[0.2 + 4(2.456) + 0.232] = 1.3674$$

The percent of error is 16.6%

Simpson's rule can be improved by dividing the integration interval into a number of segments of equal width. The total integral can be represented as

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

The following Figure shows composite Simpson's 1⁄3 rule and the relative weights are depicted above the function values. Note that the method can be employed only if the number of segments is even.

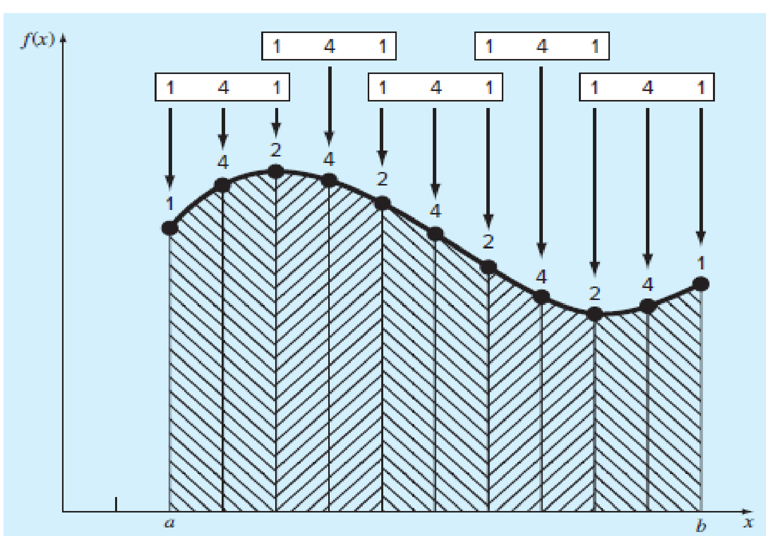

Figure 9: Composite Simpson's 1⁄3 rule.

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

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

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

Example 4: Use the four segment Simpson's 1⁄3 rule to estimate the integral from $a = 0$ to $b = 0.8$ of

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

$$h = \frac{0.8 - 0}{4} = 0.2$$

$$f(0) = 0.2 \quad f(0.2) = 1.288$$

$$f(0.4) = 2.456 \quad f(0.6) = 3.464$$

$$f(0.8) = 0.232$$

$$I = \frac{0.2}{3}[0.2 + 4(1.288 + 3.464) + 2(2.456) + 0.232] = 1.623467$$

1.04% is the error percentage

2.4.2 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

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

The 3⁄8 rule has utility when the number of segments is odd. An alternative would be to apply Simpson's 1⁄3 rule to the first two segments and Simpson's 3⁄8 rule to the last three.

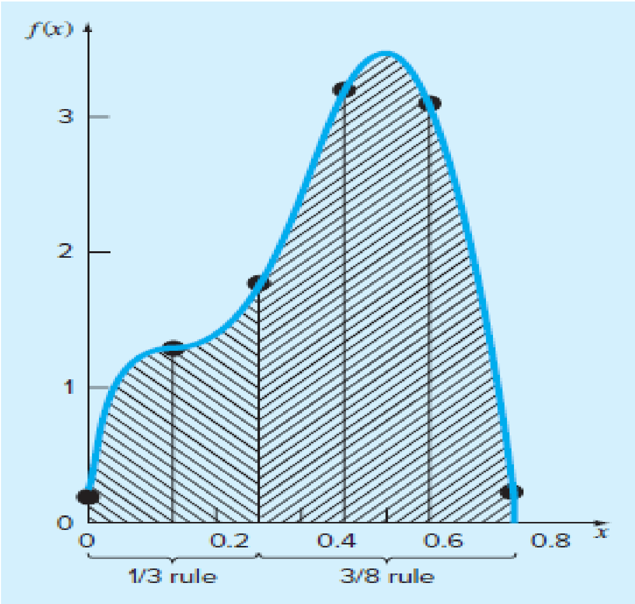

Figure 10: an illustration of how Simpson's 1⁄3 and 3⁄8 rules can be applied in tandem to handle multiple applications with odd numbers of intervals

Example 5: (a) Use Simpson's 3⁄8 rule to estimate the integral from $a = 0$ to $b = 0.8$ of

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

$$h = \frac{0.8 - 0}{3} = 0.266$$

$$f(0) = 0.2 \quad f(0.2667) = 1.4327$$

$$f(0.5333) = 3.4871 \quad f(0.8) = 0.232$$

$$I = \frac{3(0.2667)}{8}[0.2 + 3(1.4327) + 3(3.4871) + 0.232] = 1.51917$$

(b) Use it in conjunction with Simpson's 1⁄3 rule to integrate the same function for five segments.

$$h = \frac{0.8 - 0}{5} = 0.16$$

$$f(0) = 0.2 \quad f(0.16) = 1.2969$$

$$f(0.32) = 1.7433 \quad f(0.48) = 3.186$$

$$f(0.64) = 3.1819 \quad f(0.8) = 0.232$$

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

$$I = \frac{0.16}{3}[0.2 + 4(1.2969) + 1.74339] = 0.38032$$

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

$$I = \frac{3(0.16)}{8}[1.74339 + 3(3.186) + 3(3.1819) + 0.232] = 1.264754$$

The total integral is computed by summing the two results:

$$I = 0.38032 + 1.264754 = 1.645$$

2.6 Multiple Integrals

Multiple integrals are widely used in engineering and science. For example, a general equation to compute the average of a two-dimensional function can be written as

$$\bar{f} = \frac{\int_c^d \left(\int_a^b f(x,y)\, dx\right)}{(d-c)(b-a)}$$

The numerator is called a *double integral*. Such integrals can be computed as iterated integral. Thus, the integral in one of the dimensions is evaluated first. The result of this first integration is integrated in the second dimension. The order of integration is not important.

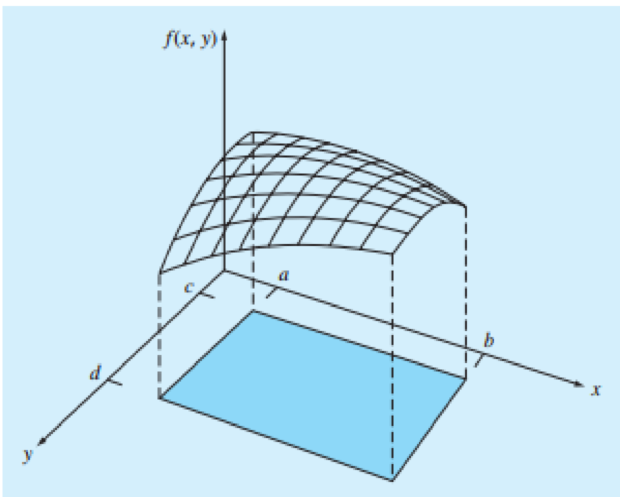

Figure 11: Double integral as the area under the function surface

A numerical double integral would be based on the same idea. First, methods such as the composite trapezoidal or Simpson's rule would be applied in the first dimension with each value of the second dimension held constant. Then the method would be applied to integrate the second dimension. The approach is illustrated in the following example.

$$\int_c^d \left(\int_a^b f(x,y)\, dx \right) dy = \int_a^b \left(\int_c^d f(x,y)\, dy \right) dx$$

Example 5: Suppose that the temperature of a rectangular heated plate is described by the following function:

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

If the plate is 8 m long (x dimension) and 6 m wide (y dimension), compute the average temperature.

Solution. First, use two-segment applications of the trapezoidal rule in each dimension. The temperatures at the necessary x and y values are depicted in the following Figure. The function can also be evaluated analytically to yield a result of 58.66667.

The trapezoidal rule is first implemented along the x dimension for each y value. These values are then integrated along the y dimension to give the final result of 2544. Dividing this by the area yields the average temperature as $2544/(6 \times 8) = 53$.

When apply a single-segment Simpson's 1/3 rule in the same fashion. This results in an integral of 2816 and an average of 58.66667, which is exact.

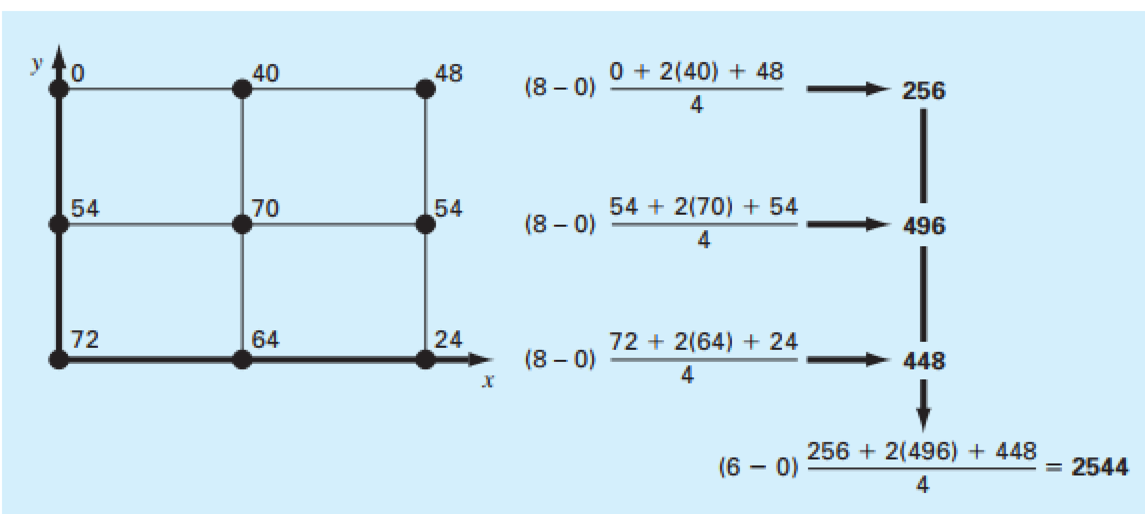

Figure 12: Numerical evaluation of a double integral using the two-segment trapezoidal rule

2.5 Gauss Quadrature

Gauss quadrature is the name for a class of techniques to implement a strategy to evaluate the area under a straight line that joining any two points on the curve as shown in Figure 13

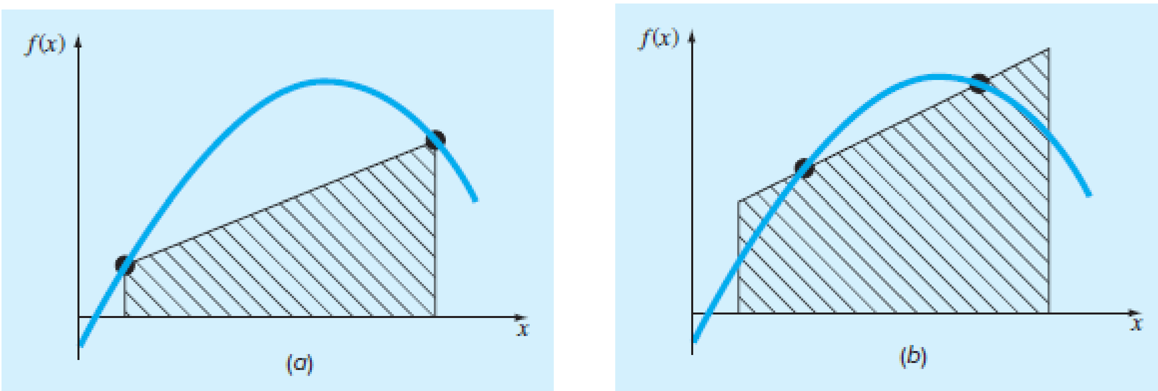

Figure 13 (*a*) Graphical depiction of the trapezoidal rule as the area under the straight line joining fixed end points. (*b*) An improved integral estimate obtained by taking the area under the straight line passing through two intermediate points. By positioning these points wisely, the positive and negative errors are better balanced, and an improved integral estimate results.

The object of Gauss quadrature is to determine the coefficients of an equation of the form

$$I \cong c_0 f(x_0) + c_1 f(x_1)$$

where the *c*'s = the unknown coefficients and the function arguments x_0 and x_1 are not fixed at the end points, but are unknowns as shown in Figure 14. Thus, require four conditions to determine a total of four unknowns

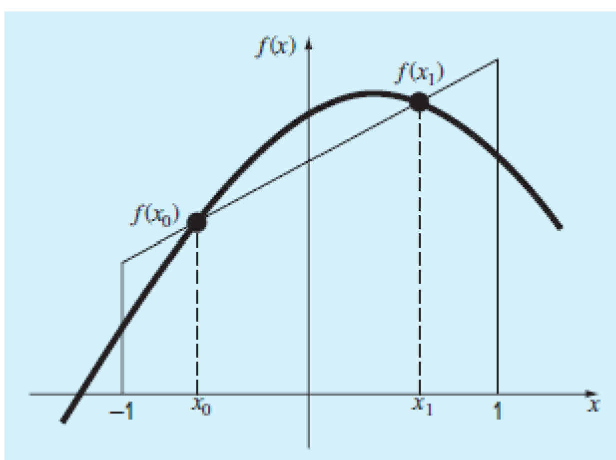

Figure 14: Graphical depiction of the unknown variables *x*0 and *x*1 for integration by Gauss quadrature

These conditions is obtained by assuming that the equation I fits the integral of a constant and a linear function and it also fits the integral of a parabolic ($y = x^2$) and a cubic ($y = x^3$) function. Note that the integration limits in above integrals are from −1 to 1.

Therefore, the two-point Gauss-Legendre formula is

$$I = f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right)$$

In the equation to be integrated, a simple change of variable can be used to translate other limits of integration into form -1,1. This is accomplished by assuming that a new variable x_d is related to the original variable x in a linear fashion, as in

$$x = \frac{(b+a) + (b-a)x_d}{2}$$

$$dx = \frac{(b-a)}{2} dx_d$$

Example 6: Use the two-point Gauss-Legendre formula to evaluate the integral from $a = 0$ to $b = 0.8$ of

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

$$x = 0.4 + 0.4x_d$$

$$dx = 0.4\, dx_d$$

Both of these can be substituted into the original equation to yield

$$\int_0^{0.8} (0.2 + 25x - 200x^2 + 675x^3 - 900x^4 + 400x^5) dx$$

$$= \int_{-1}^{1} [0.2 + 25(0.4 + 0.4x_d) - 200(0.4 + 0.4x_d)^2 + 675(0.4 + 0.4x_d)^3 - 900(0.4 + 0.4x_d)^4 + 400(0.4 + 0.4x_d)^5] 0.4 dx_d$$

$$I = f\left(\frac{-1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) = 0.516741 + 1.305837 = 1.82257$$

Exercises:

1. 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)** determine the true percent relative error.

2. Evaluate the double integral

$$\int_{-2}^{2}\int_{0}^{4}(x^2 - 3y^2 + xy^3)\,dxdy$$

(a) analytically, **(b)** using the composite trapezoidal rule with *n* = 2, and **(c)** using single applications of Simpson's 1/3 rule. For **(b)** and **(c)**, compute the percent relative error.

3. Evaluate the following integral with the two-point Gauss quadrature formula

$$\int_{0}^{3} xe^{2x}dx$$