



# Integration



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## Topic: Gauss Quadrature Rule of Integration

Major: Chemical Engineering

# What is Integration?

## Integration

The process of measuring the area under a curve.

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

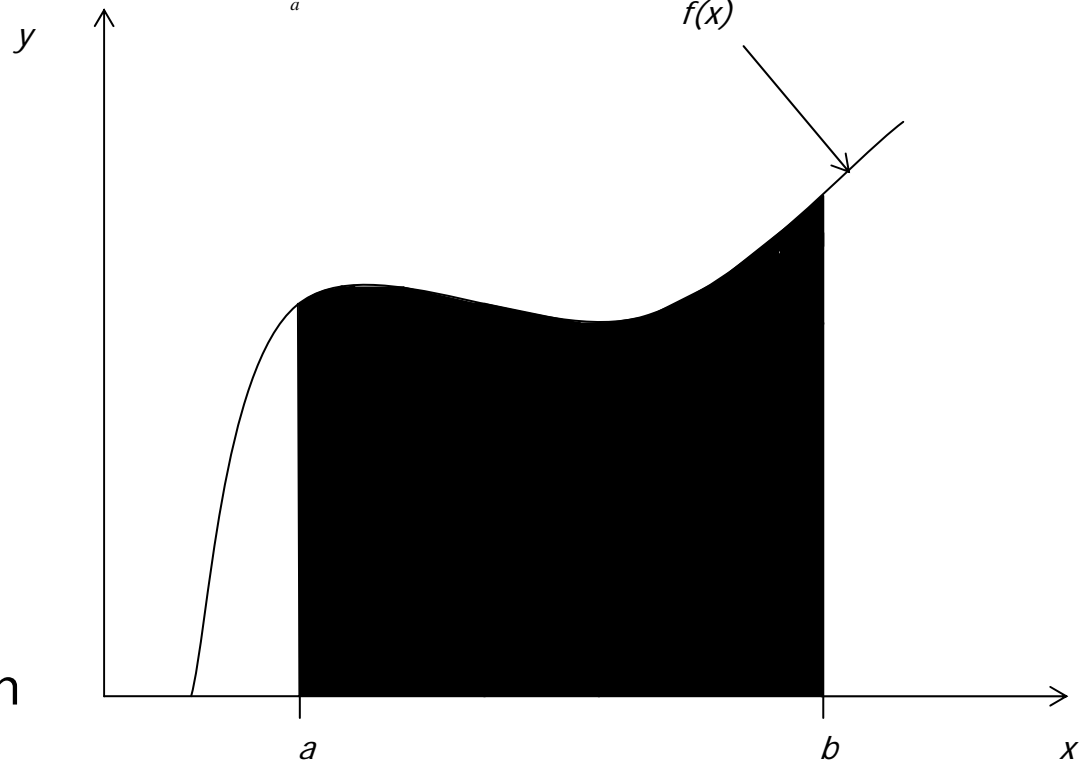
Where:

$f(x)$  is the integrand

$a$  = lower limit of integration

$b$  = upper limit of integration

$$\blacksquare \int_a^b f(x) dx$$





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# Two-Point Gaussian Quadrature Rule



# Basis of the Gaussian Quadrature Rule

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Previously, the Trapezoidal Rule was developed by the method of undetermined coefficients. The result of that development is summarized below.

$$\int_a^b f(x) dx \cong c_1 f(a) + c_2 f(b)$$
$$= \frac{b-a}{2} f(a) + \frac{b-a}{2} f(b)$$



# Basis of the Gaussian Quadrature Rule

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The two-point Gauss Quadrature Rule is an extension of the Trapezoidal Rule approximation where the arguments of the function are not predetermined as  $a$  and  $b$  but as unknowns  $x_1$  and  $x_2$ . In the two-point Gauss Quadrature Rule, the integral is approximated as

$$I = \int_a^b f(x) dx \approx c_1 f(x_1) + c_2 f(x_2)$$



# Basis of the Gaussian Quadrature Rule

The four unknowns  $x_1$ ,  $x_2$ ,  $c_1$  and  $c_2$  are found by assuming that the formula gives exact results for integrating a general third order polynomial,  $f(x) = a_0 + a_1x + a_2x^2 + a_3x^3$ .

Hence

$$\begin{aligned}\int_a^b f(x) dx &= \int_a^b (a_0 + a_1x + a_2x^2 + a_3x^3) dx \\ &= \left[ a_0x + a_1 \frac{x^2}{2} + a_2 \frac{x^3}{3} + a_3 \frac{x^4}{4} \right]_a^b \\ &= a_0(b-a) + a_1 \left( \frac{b^2 - a^2}{2} \right) + a_2 \left( \frac{b^3 - a^3}{3} \right) + a_3 \left( \frac{b^4 - a^4}{4} \right)\end{aligned}$$



# Basis of the Gaussian Quadrature Rule

It follows that

$$\int_a^b f(x) dx = c_1(a_0 + a_1x_1 + a_2x_1^2 + a_3x_1^3) + c_2(a_0 + a_1x_2 + a_2x_2^2 + a_3x_2^3)$$

Equating Equations the two previous two expressions yield

$$\begin{aligned} & a_0(b-a) + a_1\left(\frac{b^2 - a^2}{2}\right) + a_2\left(\frac{b^3 - a^3}{3}\right) + a_3\left(\frac{b^4 - a^4}{4}\right) \\ &= c_1(a_0 + a_1x_1 + a_2x_1^2 + a_3x_1^3) + c_2(a_0 + a_1x_2 + a_2x_2^2 + a_3x_2^3) \\ &= a_0(c_1 + c_2) + a_1(c_1x_1 + c_2x_2) + a_2(c_1x_1^2 + c_2x_2^2) + a_3(c_1x_1^3 + c_2x_2^3) \end{aligned}$$



# Basis of the Gaussian Quadrature Rule

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Since the constants  $a_0, a_1, a_2, a_3$  are arbitrary

$$b - a = c_1 + c_2$$

$$\frac{b^2 - a^2}{2} = c_1 x_1 + c_2 x_2$$

$$\frac{b^3 - a^3}{3} = c_1 x_1^2 + c_2 x_2^2$$

$$\frac{b^4 - a^4}{4} = c_1 x_1^3 + c_2 x_2^3$$



# Basis of Gauss Quadrature

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The previous four simultaneous nonlinear Equations have only one acceptable solution,

$$x_1 = \left(\frac{b-a}{2}\right)\left(-\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2}$$

$$x_2 = \left(\frac{b-a}{2}\right)\left(\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2}$$

$$c_1 = \frac{b-a}{2}$$

$$c_2 = \frac{b-a}{2}$$



# Basis of Gauss Quadrature

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Hence Two-Point Gaussian Quadrature Rule

$$\int_a^b f(x) dx \approx$$

$$c_1 f(x_1) + c_2 f(x_2) \frac{b-a}{2} f\left(\frac{b-a}{2}\left(-\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2}\right) + \frac{b-a}{2} f\left(\frac{b-a}{2}\left(\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2}\right)$$



# Higher Point Gaussian Quadrature Formulas



# Higher Point Gaussian Quadrature Formulas

$$\int_a^b f(x) dx \cong c_1 f(x_1) + c_2 f(x_2) + c_3 f(x_3)$$

is called the three-point Gauss Quadrature Rule.

The coefficients  $c_1$ ,  $c_2$ , and  $c_3$ , and the functional arguments  $x_1$ ,  $x_2$ , and  $x_3$  are calculated by assuming the formula gives exact expressions for integrating a fifth order polynomial

$$\int_a^b (a_0 + a_1 x + a_2 x^2 + a_3 x^3 + a_4 x^4 + a_5 x^5) dx$$

General n-point rules would approximate the integral

$$\int_a^b f(x) dx \approx c_1 f(x_1) + c_2 f(x_2) + \dots + c_n f(x_n)$$

# Arguments and Weighing Factors for n-point Gauss Quadrature Formulas

In handbooks, coefficients and arguments given for n-point Gauss Quadrature Rule are given for integrals

$$\int_{-1}^1 g(x) dx \cong \sum_{i=1}^n c_i g(x_i)$$

as shown in Table 1.

**Table 1: Weighting factors c and function arguments x used in Gauss Quadrature Formulas.**

Points	Weighting Factors	Function Arguments
2	$c_1 = 1.000000000$ $c_2 = 1.000000000$	$x_1 = -0.577350269$ $x_2 = 0.577350269$
3	$c_1 = 0.555555556$ $c_2 = 0.888888889$ $c_3 = 0.555555556$	$x_1 = -0.774596669$ $x_2 = 0.000000000$ $x_3 = 0.774596669$
4	$c_1 = 0.347854845$ $c_2 = 0.652145155$ $c_3 = 0.652145155$ $c_4 = 0.347854845$	$x_1 = -0.861136312$ $x_2 = -0.339981044$ $x_3 = 0.339981044$ $x_4 = 0.861136312$

# Arguments and Weighing Factors for n-point Gauss Quadrature Formulas

Table 1 (cont.) : Weighting factors  $c$  and function arguments  $x$  used in Gauss Quadrature Formulas.

Points	Weighting Factors	Function Arguments
5	$c_1 = 0.236926885$ $c_2 = 0.478628670$ $c_3 = 0.568888889$ $c_4 = 0.478628670$ $c_5 = 0.236926885$	$x_1 = -0.906179846$ $x_2 = -0.538469310$ $x_3 = 0.000000000$ $x_4 = 0.538469310$ $x_5 = 0.906179846$
6	$c_1 = 0.171324492$ $c_2 = 0.360761573$ $c_3 = 0.467913935$ $c_4 = 0.467913935$ $c_5 = 0.360761573$ $c_6 = 0.171324492$	$x_1 = -0.932469514$ $x_2 = -0.661209386$ $x_3 = -0.2386191860$ $x_4 = 0.2386191860$ $x_5 = 0.661209386$ $x_6 = 0.932469514$

# Arguments and Weighing Factors for n-point Gauss Quadrature Formulas

So if the table is given for  $\int_{-1}^1 g(x) dx$  integrals, how does one solve  $\int_a^b f(x) dx$ ? The answer lies in that any integral with limits of  $[a, b]$  can be converted into an integral with limits  $[-1, 1]$  Let

$$x = mt + c$$

$$\text{If } x = a, \quad \text{then } t = -1$$

$$\text{If } x = b, \quad \text{then } t = 1$$

Such that:

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

# Arguments and Weighing Factors for n-point Gauss Quadrature Formulas

Then  $c = \frac{b+a}{2}$  Hence

$$x = \frac{b-a}{2}t + \frac{b+a}{2} \quad dx = \frac{b-a}{2}dt$$

Substituting our values of  $x$ , and  $dx$  into the integral gives us

$$\int_a^b f(x)dx = \int_{-1}^1 f\left(\frac{b-a}{2}x + \frac{b+a}{2}\right)\frac{b-a}{2}dx$$



# Example 1

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For an integral  $\int_a^b f(x) dx$ , derive the one-point Gaussian Quadrature Rule.

## Solution

The one-point Gaussian Quadrature Rule is

$$\int_a^b f(x) dx \approx c_1 f(x_1)$$



# Solution

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Assuming the formula gives exact values for integrals

$$\int_{-1}^1 1 dx, \quad \text{and} \quad \int_{-1}^1 x dx,$$

$$\int_a^b 1 dx = b - a = c_1 \quad \int_a^b x dx = \frac{b^2 - a^2}{2} = c_1 x_1$$

Since  $c_1 = b - a$ , the other equation becomes

$$(b - a)x_1 = \frac{b^2 - a^2}{2} \quad x_1 = \frac{b + a}{2}$$



# Solution (cont.)

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Therefore, one-point Gauss Quadrature Rule can be expressed as

$$\int_a^b f(x) dx \approx (b - a) f\left(\frac{b + a}{2}\right)$$



## Example 2

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In an attempt to understand the mechanism of the depolarization process in a fuel cell, an electro-kinetic model for mixed oxygen-methanol current on platinum was developed in the laboratory at FAMU. A very simplified model of the reaction developed suggests a functional relation in an integral form. To find the time required for 50% of the oxygen to be consumed, the time,  $T$  (s) is given by

$$T = - \int_{1.22 \times 10^{-6}}^{0.61 \times 10^{-6}} \left( \frac{6.73 x + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} x} \right) dx$$

- Use two-point Gauss Quadrature Rule to find the time required for 50% of the oxygen to be consumed.
- Find the true error,  $E_t$  for part (a).
- Also, find the absolute relative true error,  $|\varepsilon_a|$  for part (a).



# Solution

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- a) First, change the limits of integration from  $[1.22 \times 10^{-6}, 0.61 \times 10^{-6}]$  to  $[-1, 1]$  by previous relations as follows

$$\int_{1.22 \times 10^{-6}}^{0.61 \times 10^{-6}} f(x) dx = \frac{0.61 \times 10^{-6} - 1.22 \times 10^{-6}}{2} \int_{-1}^1 f\left(\frac{0.61 \times 10^{-6} - 1.22 \times 10^{-6}}{2} x + \frac{0.61 \times 10^{-6} + 1.22 \times 10^{-6}}{2}\right) dx$$
$$= -0.305 \times 10^{-6} \int_{-1}^1 f(-3.05 \times 10^{-6} x + 0.915 \times 10^{-6}) dx$$



# Solution (cont)

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Next, get weighting factors and function argument values from Table 1 for the two point rule,

$$c_1 = 1.000000000$$

$$x_1 = -0.577350269$$

$$c_2 = 1.000000000$$

$$x_2 = 0.577350269$$



# Solution (cont.)

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Now we can use the Gauss Quadrature formula

$$\begin{aligned} -0.305 \times 10^{-6} \int_{-1}^1 f(-0.305 \times 10^{-6} x + 0.915 \times 10^{-6}) dx &\approx -0.305 \times 10^{-6} \left[ c_1 f(-0.305 \times 10^{-6} x_1 + 0.915 \times 10^{-6}) \right. \\ &\quad \left. + c_2 f(-0.305 \times 10^{-6} x_2 + 0.915 \times 10^{-6}) \right] \\ &= -0.305 \times 10^{-6} \left[ f(-0.305 \times 10^{-6} (-0.57735) + 0.915 \times 10^{-6}) + f(-0.305 \times 10^{-6} (0.57735) + 0.915 \times 10^{-6}) \right] \\ &= -0.305 \times 10^{-6} \left[ f(1.0911 \times 10^{-6}) + f(0.73891 \times 10^{-6}) \right] \\ &= -0.305 \times 10^{-6} \left[ (-3.0761 \times 10^{11}) + (-3.1573 \times 10^{11}) \right] \\ &= 190119s \end{aligned}$$



# Solution (cont)

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since

$$f(1.0911 \times 10^{-6}) = - \left[ \frac{6.73(1.0911 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} (1.0911 \times 10^{-6})} \right] = -3.0761 \times 10^{11}$$

$$f(0.73891 \times 10^{-6}) = - \left[ \frac{6.73(0.73891 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} (0.73891 \times 10^{-6})} \right] = -3.1573 \times 10^{11}$$



# Solution (cont)

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b) The true error,  $E_t$ , is

$$E_t = \text{True Value} - \text{Approximate Value}$$

$$= 1.90135 \times 10^5 - 1.90119 \times 10^5$$

$$= 16.000$$

c) The absolute relative true error,  $|\epsilon_t|$ , is (Exact value = 190135s)

$$|\epsilon_t| = \left| \frac{1.90135 \times 10^5 - 190119}{1.90135 \times 10^5} \right| \times 100$$

$$= 0.0085729\%$$