

Chapter 07.05

Gauss Quadrature Rule of Integration

After reading this chapter, you should be able to:

- 1. derive the Gauss quadrature method for integration and be able to use it to solve problems, and*
- 2. use Gauss quadrature method to solve examples of approximate integrals.*

What is integration?

Integration is the process of measuring the area under a function plotted on a graph. Why would we want to integrate a function? Among the most common examples are finding the velocity of a body from an acceleration function, and displacement of a body from a velocity function. Throughout many engineering fields, there are (what sometimes seems like) countless applications for integral calculus. You can read about some of these applications in Chapters 07.00A-07.00G.

Sometimes, the evaluation of expressions involving these integrals can become daunting, if not indeterminate. For this reason, a wide variety of numerical methods has been developed to simplify the integral.

Here, we will discuss the Gauss quadrature rule of approximating integrals of the form

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

where

- $f(x)$ is called the integrand,
- a = lower limit of integration
- b = upper limit of integration

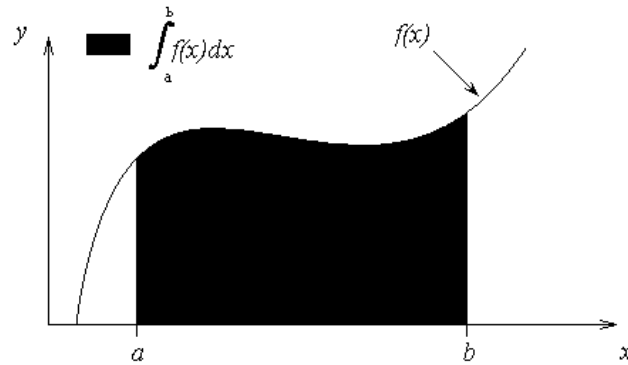


Figure 1 Integration of a function.

Gauss Quadrature Rule

Background:

To derive the trapezoidal rule from the method of undetermined coefficients, we approximated

$$\int_a^b f(x) dx \approx c_1 f(a) + c_2 f(b) \quad (1)$$

Let the right hand side be exact for integrals of a straight line, that is, for an integrated form of

$$\int_a^b (a_0 + a_1 x) dx$$

So

$$\begin{aligned} \int_a^b (a_0 + a_1 x) dx &= \left[a_0 x + a_1 \frac{x^2}{2} \right]_a^b \\ &= a_0 (b - a) + a_1 \left(\frac{b^2 - a^2}{2} \right) \end{aligned} \quad (2)$$

But from Equation (1), we want

$$\int_a^b (a_0 + a_1 x) dx = c_1 f(a) + c_2 f(b) \quad (3)$$

to give the same result as Equation (2) for $f(x) = a_0 + a_1 x$.

$$\begin{aligned} \int_a^b (a_0 + a_1 x) dx &= c_1 (a_0 + a_1 a) + c_2 (a_0 + a_1 b) \\ &= a_0 (c_1 + c_2) + a_1 (c_1 a + c_2 b) \end{aligned} \quad (4)$$

Hence from Equations (2) and (4),

$$a_0 (b - a) + a_1 \left(\frac{b^2 - a^2}{2} \right) = a_0 (c_1 + c_2) + a_1 (c_1 a + c_2 b)$$

Since a_0 and a_1 are arbitrary constants for a general straight line

$$c_1 + c_2 = b - a \quad (5a)$$

$$c_1 a + c_2 b = \frac{b^2 - a^2}{2} \quad (5b)$$

Multiplying Equation (5a) by a and subtracting from Equation (5b) gives

$$c_2 = \frac{b - a}{2} \quad (6a)$$

Substituting the above found value of c_2 in Equation (5a) gives

$$c_1 = \frac{b - a}{2} \quad (6b)$$

Therefore

$$\begin{aligned} \int_a^b f(x) dx &\approx c_1 f(a) + c_2 f(b) \\ &= \frac{b - a}{2} f(a) + \frac{b - a}{2} f(b) \end{aligned} \quad (7)$$

Derivation of two-point Gauss quadrature rule

Method 1:

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 . So in the two-point Gauss quadrature rule, the integral is approximated as

$$\begin{aligned} I &= \int_a^b f(x) dx \\ &\approx c_1 f(x_1) + c_2 f(x_2) \end{aligned}$$

There are four unknowns x_1 , x_2 , c_1 and c_2 . These are found by assuming that the formula gives exact results for integrating a general third order polynomial, $f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$. Hence

$$\begin{aligned} \int_a^b f(x) dx &= \int_a^b (a_0 + a_1 x + a_2 x^2 + a_3 x^3) dx \\ &= \left[a_0 x + a_1 \frac{x^2}{2} + a_2 \frac{x^3}{3} + a_3 \frac{x^4}{4} \right]_a^b \\ &= a_0 (b - a) + a_1 \left(\frac{b^2 - a^2}{2} \right) + a_2 \left(\frac{b^3 - a^3}{3} \right) + a_3 \left(\frac{b^4 - a^4}{4} \right) \end{aligned} \quad (8)$$

The formula would then give

$$\begin{aligned} \int_a^b f(x) dx &\approx c_1 f(x_1) + c_2 f(x_2) = \\ &c_1 (a_0 + a_1 x_1 + a_2 x_1^2 + a_3 x_1^3) + c_2 (a_0 + a_1 x_2 + a_2 x_2^2 + a_3 x_2^3) \end{aligned} \quad (9)$$

Equating Equations (8) and (9) gives

$$\begin{aligned}
 & a_0(b-a) + a_1\left(\frac{b^2-a^2}{2}\right) + a_2\left(\frac{b^3-a^3}{3}\right) + a_3\left(\frac{b^4-a^4}{4}\right) \\
 &= c_1(a_0 + a_1x_1 + a_2x_1^2 + a_3x_1^3) + c_2(a_0 + a_1x_2 + a_2x_2^2 + a_3x_2^3) \\
 &= a_0(c_1 + c_2) + a_1(c_1x_1 + c_2x_2) + a_2(c_1x_1^2 + c_2x_2^2) + a_3(c_1x_1^3 + c_2x_2^3)
 \end{aligned} \tag{10}$$

Since in Equation (10), the constants a_0 , a_1 , a_2 , and a_3 are arbitrary, the coefficients of a_0 , a_1 , a_2 , and a_3 are equal. This gives us four equations as follows.

$$\begin{aligned}
 b-a &= c_1 + c_2 \\
 \frac{b^2-a^2}{2} &= c_1x_1 + c_2x_2 \\
 \frac{b^3-a^3}{3} &= c_1x_1^2 + c_2x_2^2 \\
 \frac{b^4-a^4}{4} &= c_1x_1^3 + c_2x_2^3
 \end{aligned} \tag{11}$$

Without proof (see Example 1 for proof of a related problem), we can find that the above four simultaneous nonlinear equations have only one acceptable solution

$$\begin{aligned}
 c_1 &= \frac{b-a}{2} \\
 c_2 &= \frac{b-a}{2} \\
 x_1 &= \left(\frac{b-a}{2}\right)\left(-\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2} \\
 x_2 &= \left(\frac{b-a}{2}\right)\left(\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2}
 \end{aligned} \tag{12}$$

Hence

$$\begin{aligned}
 \int_a^b f(x)dx &\approx c_1f(x_1) + c_2f(x_2) \\
 &= \frac{b-a}{2}f\left(\frac{b-a}{2}\left(-\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2}\right) + \frac{b-a}{2}f\left(\frac{b-a}{2}\left(\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2}\right)
 \end{aligned} \tag{13}$$

Method 2:

We can derive the same formula by assuming that the expression gives exact values for the individual integrals of $\int_a^b 1dx$, $\int_a^b xdx$, $\int_a^b x^2dx$, and $\int_a^b x^3dx$. The reason the formula can also be

derived using this method is that the linear combination of the above integrands is a general third order polynomial given by $f(x) = a_0 + a_1x + a_2x^2 + a_3x^3$.

These will give four equations as follows

$$\begin{aligned}\int_a^b 1 dx &= b - a = c_1 + c_2 \\ \int_a^b x dx &= \frac{b^2 - a^2}{2} = c_1x_1 + c_2x_2 \\ \int_a^b x^2 dx &= \frac{b^3 - a^3}{3} = c_1x_1^2 + c_2x_2^2 \\ \int_a^b x^3 dx &= \frac{b^4 - a^4}{4} = c_1x_1^3 + c_2x_2^3\end{aligned}\quad (14)$$

These four simultaneous nonlinear equations can be solved to give a single acceptable solution

$$\begin{aligned}c_1 &= \frac{b-a}{2} \\ c_2 &= \frac{b-a}{2} \\ x_1 &= \left(\frac{b-a}{2}\right)\left(-\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2} \\ x_2 &= \left(\frac{b-a}{2}\right)\left(\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2}\end{aligned}\quad (15)$$

Hence

$$\int_a^b f(x) dx \approx \frac{b-a}{2} f\left(\frac{b-a}{2}\left(-\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2}\right) + \frac{b-a}{2} f\left(\frac{b-a}{2}\left(\frac{1}{\sqrt{3}}\right) + \frac{b+a}{2}\right)\quad (16)$$

Since two points are chosen, it is called the two-point Gauss quadrature rule. Higher point versions can also be developed.

Higher point Gauss quadrature formulas

For example

$$\int_a^b f(x) dx \approx c_1f(x_1) + c_2f(x_2) + c_3f(x_3)\quad (17)$$

is called the three-point Gauss quadrature rule. The coefficients c_1 , c_2 and c_3 , and the function arguments x_1 , x_2 and x_3 are calculated by assuming the formula gives exact expressions for integrating a fifth order polynomial

$$\int_a^b (a_0 + a_1x + a_2x^2 + a_3x^3 + a_4x^4 + a_5x^5) dx.$$

General n -point rules would approximate the integral

$$\int_a^b f(x)dx \approx c_1f(x_1) + c_2f(x_2) + \dots + c_nf(x_n) \quad (18)$$

Arguments and weighing factors for n -point Gauss quadrature rules

In handbooks (see Table 1), coefficients and arguments given for n -point Gauss quadrature rule are given for integrals of the form

$$\int_{-1}^1 g(x)dx \approx \sum_{i=1}^n c_i g(x_i) \quad (19)$$

Table 1 Weighting factors c and function arguments x used in Gauss quadrature formulas

Points	Weighting Factors	Function Arguments
2	$c_1 = 1.000000000$	$x_1 = -0.577350269$
	$c_2 = 1.000000000$	$x_2 = 0.577350269$
3	$c_1 = 0.555555556$	$x_1 = -0.774596669$
	$c_2 = 0.888888889$	$x_2 = 0.000000000$
	$c_3 = 0.555555556$	$x_3 = 0.774596669$
4	$c_1 = 0.347854845$	$x_1 = -0.861136312$
	$c_2 = 0.652145155$	$x_2 = -0.339981044$
	$c_3 = 0.652145155$	$x_3 = 0.339981044$
	$c_4 = 0.347854845$	$x_4 = 0.861136312$
5	$c_1 = 0.236926885$	$x_1 = -0.906179846$
	$c_2 = 0.478628670$	$x_2 = -0.538469310$
	$c_3 = 0.568888889$	$x_3 = 0.000000000$
	$c_4 = 0.478628670$	$x_4 = 0.538469310$
	$c_5 = 0.236926885$	$x_5 = 0.906179846$
6	$c_1 = 0.171324492$	$x_1 = -0.932469514$
	$c_2 = 0.360761573$	$x_2 = -0.661209386$
	$c_3 = 0.467913935$	$x_3 = -0.238619186$
	$c_4 = 0.467913935$	$x_4 = 0.238619186$

$c_5 = 0.360761573$	$x_5 = 0.661209386$
$c_6 = 0.171324492$	$x_6 = 0.932469514$

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

$$x = mt + c \quad (20)$$

If $x = a$, then $t = -1$

If $x = b$, then $t = +1$

such that

$$a = m(-1) + c$$

$$b = m(1) + c \quad (21)$$

Solving the two Equations (21) simultaneously gives

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

$$c = \frac{b+a}{2} \quad (22)$$

Hence

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

$$dx = \frac{b-a}{2}dt$$

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

$$\int_a^b f(x)dx = \int_{-1}^1 f\left(\frac{b-a}{2}x + \frac{b+a}{2}\right) \frac{b-a}{2} dx \quad (23)$$

Example 1

For an integral $\int_{-1}^1 f(x)dx$, show that the two-point Gauss quadrature rule approximates to

$$\int_{-1}^1 f(x)dx \approx c_1 f(x_1) + c_2 f(x_2)$$

where

$$c_1 = 1$$

$$c_2 = 1$$

$$x_1 = -\frac{1}{\sqrt{3}}$$

$$x_2 = \frac{1}{\sqrt{3}}$$

Solution

Assuming the formula

$$\int_{-1}^1 f(x)dx = c_1 f(x_1) + c_2 f(x_2) \quad (\text{E1.1})$$

gives exact values for integrals $\int_{-1}^1 1dx$, $\int_{-1}^1 xdx$, $\int_{-1}^1 x^2 dx$, and $\int_{-1}^1 x^3 dx$. Then

$$\int_{-1}^1 1dx = 2 = c_1 + c_2 \quad (\text{E1.2})$$

$$\int_{-1}^1 xdx = 0 = c_1 x_1 + c_2 x_2 \quad (\text{E1.3})$$

$$\int_{-1}^1 x^2 dx = \frac{2}{3} = c_1 x_1^2 + c_2 x_2^2 \quad (\text{E1.4})$$

$$\int_{-1}^1 x^3 dx = 0 = c_1 x_1^3 + c_2 x_2^3 \quad (\text{E1.5})$$

Multiplying Equation (E1.3) by x_1^2 and subtracting from Equation (E1.5) gives

$$c_2 x_2 (x_1^2 - x_2^2) = 0 \quad (\text{E1.6})$$

The solution to the above equation is

$$c_2 = 0, \text{ or/and}$$

$$x_2 = 0, \text{ or/and}$$

$$x_1 = x_2, \text{ or/and}$$

$$x_1 = -x_2.$$

- I. $c_2 = 0$ is not acceptable as Equations (E1.2-E1.5) reduce to $c_1 = 2$, $c_1 x_1 = 0$, $c_1 x_1^2 = \frac{2}{3}$, and $c_1 x_1^3 = 0$. But since $c_1 = 2$, then $x_1 = 0$ from $c_1 x_1 = 0$, but $x_1 = 0$ conflicts with $c_1 x_1^2 = \frac{2}{3}$.
- II. $x_2 = 0$ is not acceptable as Equations (E1.2-E1.5) reduce to $c_1 + c_2 = 2$, $c_1 x_1 = 0$, $c_1 x_1^2 = \frac{2}{3}$, and $c_1 x_1^3 = 0$. Since $c_1 x_1 = 0$, then c_1 or x_1 has to be zero but this violates $c_1 x_1^2 = \frac{2}{3} \neq 0$.
- III. $x_1 = x_2$ is not acceptable as Equations (E1.2-E1.5) reduce to $c_1 + c_2 = 2$, $c_1 x_1 + c_2 x_1 = 0$, $c_1 x_1^2 + c_2 x_1^2 = \frac{2}{3}$, and $c_1 x_1^3 + c_2 x_1^3 = 0$. If $x_1 \neq 0$, then $c_1 x_1 + c_2 x_1 = 0$

gives $c_1 + c_2 = 0$ and that violates $c_1 + c_2 = 2$. If $x_1 = 0$, then that violates $c_1 x_1^2 + c_2 x_1^2 = \frac{2}{3} \neq 0$.

That leaves the solution of $x_1 = -x_2$ as the only possible acceptable solution and in fact, it does not have violations (see it for yourself)

$$x_1 = -x_2 \quad (\text{E1.7})$$

Substituting (E1.7) in Equation (E1.3) gives

$$c_1 = c_2 \quad (\text{E1.8})$$

From Equations (E1.2) and (E1.8),

$$c_1 = c_2 = 1 \quad (\text{E1.9})$$

Equations (E1.4) and (E1.9) gives

$$x_1^2 + x_2^2 = \frac{2}{3} \quad (\text{E1.10})$$

Since Equation (E1.7) requires that the two results be of opposite sign, we get

$$x_1 = -\frac{1}{\sqrt{3}}$$

$$x_2 = \frac{1}{\sqrt{3}}$$

Hence

$$\begin{aligned} \int_{-1}^1 f(x) dx &= c_1 f(x_1) + c_2 f(x_2) \\ &= f\left(-\frac{1}{\sqrt{3}}\right) + f\left(\frac{1}{\sqrt{3}}\right) \end{aligned} \quad (\text{E1.11})$$

Example 2

For an integral $\int_a^b f(x) dx$, derive the one-point Gauss quadrature rule.

Solution

The one-point Gauss quadrature rule is

$$\int_a^b f(x) dx \approx c_1 f(x_1) \quad (\text{E2.1})$$

Assuming the formula gives exact values for integrals $\int_{-1}^1 1 dx$, and $\int_{-1}^1 x dx$

$$\begin{aligned} \int_a^b 1 dx &= b - a = c_1 \\ \int_a^b x dx &= \frac{b^2 - a^2}{2} = c_1 x_1 \end{aligned} \quad (\text{E2.2})$$

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

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

$$x_1 = \frac{b+a}{2} \quad (\text{E2.3})$$

Therefore, one-point Gauss quadrature rule can be expressed as

$$\int_a^b f(x)dx \approx (b-a)f\left(\frac{b+a}{2}\right) \quad (\text{E2.4})$$

Example 3

What would be the formula for

$$\int_a^b f(x)dx = c_1 f(a) + c_2 f(b)$$

if you want the above formula to give you exact values of $\int_a^b (a_0 x + b_0 x^2) dx$, that is, a linear combination of x and x^2 .

Solution

If the formula is exact for a linear combination of x and x^2 , then

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

$$\int_a^b x^2 dx = \frac{b^3 - a^3}{3} = c_1 a^2 + c_2 b^2 \quad (\text{E3.1})$$

Solving the two Equations (E3.1) simultaneously gives

$$\begin{bmatrix} a & b \\ a^2 & b^2 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = \begin{bmatrix} \frac{b^2 - a^2}{2} \\ \frac{b^3 - a^3}{3} \end{bmatrix}$$

$$c_1 = -\frac{1 - ab - b^2 + 2a^2}{6a}$$

$$c_2 = -\frac{1 a^2 + ab - 2b^2}{6b} \quad (\text{E3.2})$$

So

$$\int_a^b f(x)dx = -\frac{1 - ab - b^2 + 2a^2}{6a} f(a) - \frac{1 a^2 + ab - 2b^2}{6b} f(b) \quad (\text{E3.3})$$

Let us see if the formula works.

Evaluate $\int_2^5 (2x^2 - 3x) dx$ using Equation(E3.3)

$$\begin{aligned} \int_2^5 (2x^2 - 3x) dx &\approx c_1 f(a) + c_2 f(b) \\ &= -\frac{1 - (2)(5) - 5^2 + 2(2)^2}{6} [2(2)^2 - 3(2)] - \frac{1 \cdot 2^2 + 2(5) - 2(5)^2}{6 \cdot 5} [2(5)^2 - 3(5)] \\ &= 46.5 \end{aligned}$$

The exact value of $\int_2^5 (2x^2 - 3x) dx$ is given by

$$\begin{aligned} \int_2^5 (2x^2 - 3x) dx &= \left[\frac{2x^3}{3} - \frac{3x^2}{2} \right]_2^5 \\ &= 46.5 \end{aligned}$$

Any surprises?

Now evaluate $\int_2^5 3dx$ using Equation (E3.3)

$$\begin{aligned} \int_2^5 3dx &\approx c_1 f(a) + c_2 f(b) \\ &= -\frac{1 - 2(5) - 5^2 + 2(2)^2}{6} (3) - \frac{1 \cdot 2^2 + 2(5) - 2(5)^2}{6 \cdot 5} (3) \\ &= 10.35 \end{aligned}$$

The exact value of $\int_2^5 3dx$ is given by

$$\begin{aligned} \int_2^5 3dx &= [3x]_2^5 \\ &= 9 \end{aligned}$$

Because the formula will only give exact values for linear combinations of x and x^2 , it does not work exactly even for a simple integral of $\int_2^5 3dx$.

Do you see now why we choose $a_0 + a_1x$ as the integrand for which the formula

$$\int_a^b f(x) dx \approx c_1 f(a) + c_2 f(b)$$

gives us exact values?

Example 4

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

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

Use two-point Gauss quadrature rule to find the time required for 50 % of the oxygen to be consumed. Also, find the absolute relative true error.

Solution

First, change the limits of integration from $[1.22 \times 10^{-6}, 0.61 \times 10^{-6}]$ to $[-1, 1]$ using

$$a = 1.22 \times 10^{-6}$$

$$b = 0.61 \times 10^{-6}$$

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

gives

$$\begin{aligned} \int_{1.22 \times 10^{-6}}^{0.61 \times 10^{-6}} f(x) dx &= \frac{0.61 \times 10^{-6} - 1.22 \times 10^{-6}}{2} \int_{-1}^1 f\left(\frac{0.61 \times 10^{-6} - 1.22 \times 10^{-6}}{2}x + \frac{0.61 \times 10^{-6} + 1.22 \times 10^{-6}}{2}\right) dx \\ &= -0.305 \times 10^{-6} \int_{-1}^1 f(-0.305 \times 10^{-6}x + 0.91500 \times 10^{-6}) dx \end{aligned}$$

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

$$c_1 = 1.0000$$

$$x_1 = -0.57735$$

$$c_2 = 1.0000$$

$$x_2 = 0.57735$$

Now we can use the Gauss Quadrature formula

$$\begin{aligned} &-0.305 \times 10^{-6} \int_{-1}^1 f(-0.305 \times 10^{-6}x + 0.915 \times 10^{-6}) dx \\ &\approx -0.305 \times 10^{-6} \left[c_1 f(-0.305 \times 10^{-6}x_1 + 0.915 \times 10^{-6}) \right. \\ &\quad \left. + c_2 f(-0.305 \times 10^{-6}x_2 + 0.915 \times 10^{-6}) \right] \\ &\approx -0.305 \times 10^{-6} \left[f(-0.305 \times 10^{-6}(-0.57735) + 0.915 \times 10^{-6}) \right. \\ &\quad \left. + f(-0.305 \times 10^{-6}(0.57735) + 0.915 \times 10^{-6}) \right] \\ &\approx -0.305 \times 10^{-6} \left[f(1.0911 \times 10^{-6}) + f(0.73891 \times 10^{-6}) \right] \\ &\approx -0.305 \times 10^{-6} \left[(-3.0761 \times 10^{11}) + (-3.1573 \times 10^{11}) \right] \\ &\approx 190120 \text{ s} \end{aligned}$$

since

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

$$\begin{aligned}
 &= -3.0761 \times 10^{11} \\
 f(0.73891 \times 10^{-6}) &= - \left[\frac{6.73(0.73891 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11} (0.73891 \times 10^{-6})} \right] \\
 &= -3.1573 \times 10^{11}
 \end{aligned}$$

The absolute relative true error, $|\epsilon_i|$, is (Exact value = 190140 s)

$$\begin{aligned}
 |\epsilon_i| &= \left| \frac{1.90140 \times 10^5 - 190140}{1.90140 \times 10^5} \right| \times 100 \% \\
 &= 0.0082023 \%
 \end{aligned}$$

Example 5

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

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

Use three-point Gauss quadrature rule to find the time required for 50 % of the oxygen to be consumed. Also, find the absolute relative true error.

Solution

First, change the limits of integration from $[1.22 \times 10^{-6}, 0.61 \times 10^{-6}]$ to $[-1, 1]$ using

$$a = 1.22 \times 10^{-6}$$

$$b = 0.61 \times 10^{-6}$$

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

gives

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

The weighting factors and function argument values are

$$c_1 = 0.55556$$

$$x_1 = -0.77460$$

$$\begin{aligned}
 c_2 &= 0.88889 \\
 x_2 &= 0.0000 \\
 c_3 &= 0.55556 \\
 x_3 &= 0.77460
 \end{aligned}$$

and the formula is

$$\begin{aligned}
 & -0.305 \times 10^{-6} \int_{-1}^1 f(-0.305 \times 10^{-6} x + 0.915 \times 10^{-6}) dx \\
 & \approx -0.305 \times 10^{-6} \left[\begin{aligned} & c_1 f(-0.305 \times 10^{-6} x_1 + 0.915 \times 10^{-6}) \\ & + c_2 f(-0.305 \times 10^{-6} x_2 + 0.915 \times 10^{-6}) \\ & + c_3 f(-0.305 \times 10^{-6} x_3 + 0.915 \times 10^{-6}) \end{aligned} \right] \\
 & \approx -0.305 \times 10^{-6} \left[\begin{aligned} & 0.55556 f(-0.305 \times 10^{-6}(-0.77456) + 0.915 \times 10^{-6}) \\ & + 0.88889 f(-0.305 \times 10^{-6}(0.0000) + 0.915 \times 10^{-6}) \\ & + 0.55556 f(-0.305 \times 10^{-6}(0.77456) + 0.915 \times 10^{-6}) \end{aligned} \right] \\
 & \approx -0.305 \times 10^{-6} \left[\begin{aligned} & 0.55556 f(1.1512 \times 10^{-6}) + 0.88889 f(0.915 \times 10^{-6}) \\ & + 0.55556 f(0.67876 \times 10^{-6}) \end{aligned} \right] \\
 & \approx -0.305 \times 10^{-6} \left[\begin{aligned} & 0.55556(-3.0673 \times 10^{11}) + 0.88889(-3.1098 \times 10^{11}) \\ & + 0.55556(-3.1796 \times 10^{11}) \end{aligned} \right] \\
 & \approx 190140 \text{ s}
 \end{aligned}$$

since

$$\begin{aligned}
 f(1.1512 \times 10^{-6}) &= - \left[\frac{6.73(1.1512 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11}(1.1512 \times 10^{-6})} \right] \\
 &= -3.0672 \times 10^{11} \\
 f(0.915 \times 10^{-6}) &= - \left[\frac{6.73(0.915 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11}(0.915 \times 10^{-6})} \right] \\
 &= -3.1089 \times 10^{11} \\
 f(0.67876 \times 10^{-6}) &= - \left[\frac{6.73(0.67876 \times 10^{-6}) + 4.3025 \times 10^{-7}}{2.316 \times 10^{-11}(0.67876 \times 10^{-6})} \right] \\
 &= -3.1796 \times 10^{11}
 \end{aligned}$$

The absolute relative true error, $|\epsilon_t|$, is (Exact value = 190140 s)

$$\begin{aligned}
 |\epsilon_t| &= \left| \frac{190140 - (190140)}{190140} \right| \times 100 \% \\
 &= 0.00024868 \%
 \end{aligned}$$

INTEGRATION

Topic	Gauss quadrature rule
Summary	These are textbook notes of Gauss quadrature rule
Major	Chemical Engineering
Authors	Autar Kaw, Michael Keteltas
Date	August 27, 2009
Web Site	http://numericalmethods.eng.usf.edu
