5.1 Introduction

Multidimensional integration appears in many mathematical models and can seldom be calculated analytically. The numerical approximation of such integrals is a challenging work in numerical analysis, as many such integrals appear in the fields of finite element method (to calculate the stiffness matrix), in computer graphics (to solve integral equations), in financial mathematics (to determine the value of sophisticated financial derivatives, such as exotic options and to determine the value at risk) and in many other fields.

The cubature formulae for integration of higher dimensional integrals are typically derived by solving very complicated systems of non-linear equations. The integration rule proposed in this chapter does not require solving non-linear systems of equations, as a product formula is derived using the one-dimensional quadrature points given in Ma et.al (1996). It is true that, by using a product formula, the number of function evaluations increases geometrically with the increase in dimension. But this does not become a drawback as the present high speed computers can handle this in very few seconds, even up to ten dimensions. Moreover, the accuracy of the results are too good here that the issue with the function evaluations can be overlooked.

In this chapter, initially, an attempt is made to extend the approach in two-dimension (Chapter 3) and three-dimension (Chapter 4) to derive a general numerical integration formula to evaluate multiple integrals of the form:

\[ \int \ldots \int f(x_1, x_2, \ldots, x_n) \, dx_1 \ldots dx_n \]

Few results obtained in Chapter 5 is published in an international journal [3] (see page 204) and some more results have been communicated to an international journal (see page 205).
\[
I = \int_a^b \int_{g_1(x_1)}^{h_1(x_1)} \int_{g_2(x_2)}^{h_2(x_1,x_2)} \ldots \int_{g_{n-1}(x_1,x_2,\ldots,x_{n-1})}^{h_{n-1}(x_1,x_2,\ldots,x_{n-1})} f(\mathbf{x}) \ dx_n \ dx_{n-1} \ldots \ dx_1
\]

(5.1)

Few examples of integrals of four, five and six dimensions are chosen in order to show the working of the derived formula, in section 5.2. Later in section 5.3 and 5.4, the numerical integration formula over an n-dimensional cube and n-dimensional simplex is provided as special cases of the formula derived in section 5.2. In section 5.5, a numerical integration method for integration over n-dimensional balls using a different transformation technique is derived and in section 5.6, the derivation of integration over irregular domains in two-dimension (section 3.5) and three-dimension (4.6) is also extended to n-dimensions.

5.2 Derivation of the numerical integration method to evaluate multiple integrals

Let \( \Omega = \{(x,y,z) \mid a \leq x_1 \leq b, g_1(x_1) \leq x_2 \leq h_1(x_1), g_2(x_1, x_2) \leq x_3 \leq h_2(x_1, x_2) \ldots g_{n-1}(x_1, x_2, \ldots, x_{n-1}) \leq x_n \leq h_{n-1}(x_1, x_2, \ldots, x_{n-1})\} \)

To derive a numerical integration method to evaluate the integral in Eq. (5.1), the domain of integration, \( \Omega \) is transformed into a zero-one n-cube,

\[ C_n^* = \{(\xi_1, \xi_2, \ldots, \xi_n) \mid 0 \leq \xi_i \leq 1, i = 1, 2, \ldots, n\} \]

using the transformation,

\[
x_1 = (b-a)\xi_1 + a \\
x_2 = [h_1(x_1(\xi_1)) - g_1(x_1(\xi_1))]\xi_2 + g_1(x_1(\xi_1)) \\
x_3 = [h_2(x_1(\xi_1),x_2(\xi_1, \xi_2)) - g_2(x_1(\xi_1), x_2(\xi_1, \xi_2))]\xi_3 + g_2(x_1(\xi_1), x_2(\xi_1, \xi_2)) \\
\ldots \\
x_n = [h_{n-1}(\bar{x}(\xi_1, \xi_2, \ldots, \xi_{n-1})) - g_{n-1}(\bar{x}(\xi_1, \xi_2, \ldots, \xi_{n-1}))]\xi_n + g_{n-1}(\bar{x}(\xi_1, \xi_2, \ldots, \xi_{n-1}))
\]

where \( \bar{x} = (x_1, x_2, \ldots, x_{n-1}) \)

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Here, \( x_1 \) is a function of \( \xi_1 \), \( x_2 \) is a function of \( \xi_1, \xi_2 \), \( x_3 \) is a function of \( \xi_1, \xi_2, \xi_3 \) and so on.

The Jacobian of the transformation is

\[
|J| = (b - a) (g_1 - h_1) (g_2 - h_2) \ldots (g_{n-1} - h_{n-1}).
\]

After transformation of the integral region to a zero-one \( n \)-cube and then applying the generalized Gaussian quadrature formulae for each integral, the numerical integration rule for the integral in Eq. (5.1) is derived, in the following way:

\[
I = \int_a^b \int_{g_1(x_1)}^{h_1(x_1)} \int_{g_2(x_1,x_2)}^{h_2(x_1,x_2)} \ldots \int_{g_{n-1}(x_1,x_2,...,x_{n-1})}^{h_{n-1}(x_1,x_2,...,x_{n-1})} f(\vec{\xi}) \, dx_n \, dx_{n-1} \ldots dx_1
\]

\[
= \int_{\xi_1=0}^{1} \int_{\xi_2=0}^{1} \ldots \int_{\xi_n=0}^{1} f(\vec{\xi}(\xi_1,\xi_2,\ldots,\xi_{n-1},\xi_n)) \, |J| \, d\xi_n \ldots d\xi_2 \, d\xi_1
\]

where \( \vec{\xi} = (x_1,x_2,...,x_n) \)

\[
\approx \sum_{i_1=1}^{N} \sum_{i_2=1}^{N} \ldots \sum_{i_n=1}^{N} w_1^{i_1} w_2^{i_2} \ldots w_n^{i_n} f(\vec{\xi}(\xi_1^{i_1},\xi_2^{i_2},\ldots,\xi_{n-1}^{i_{n-1}},\xi_n^{i_n})) \, |J|
\]

\[
\approx \sum_{m=1}^{N^n} c_m f(x_{1m},x_{2m},\ldots,x_{nm})
\]

(5.2)

where,

\[
x_{1m} = (b - a) \xi_1^{i_1} + a;
\]

\[
x_{2m} = \left[ h_1 \left( (b - a) \xi_1^{i_1} + a \right) - g_1 \left( (b - a) \xi_1^{i_1} + a \right) \right] \xi_2^{i_2} + g_1 \left( (b - a) \xi_1^{i_1} + a \right);
\]

\[
x_{3m} = \left[ h_2 \left( x_{1m},x_2^{i_2} \right) - g_2 \left( x_{1m},x_2^{i_2} \right) \right] \xi_3^{i_3} + g_2 \left( x_{1m},x_2^{i_2} \right);
\]

\[
\ldots
\]

\[
x_{n-1m} = \left[ h_{n-2} \left( x_{1m},x_2^{i_2},\ldots,x_{n-2m} \right) - g_{n-2} \left( x_{1m},x_2^{i_2},\ldots,x_{n-2m} \right) \right] \xi_{n-1}^{i_{n-1}} + g_{n-2} \left( x_{1m},x_2^{i_2},\ldots,x_{n-2m} \right);
\]

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Here, $x_{nm} = \left[ h_{n-1}(x_{1m}, x_{2m}, ..., x_{n-1m}) - g_{n-1}(x_{1m}, x_{2m}, ..., x_{n-1m}) \right] \xi_n^i + g_{n-1}(x_{1m}, x_{2m}, ..., x_{n-1m})$; \hspace{1cm} (5.2a)

$c_m = (b - a) \left[ h_1(x_{1m}) - g_1(x_{1m}) \right] \left[ h_2(x_{1m}, x_{2m}) - g_2(x_{1m}, x_{2m}) \right] \ldots \left[ h_{n-1}(x_{1m}, x_{2m}, ..., x_{n-1m}) - g_{n-1}(x_{1m}, x_{2m}, ..., x_{n-1m}) \right] w_1^{i_1} w_2^{i_2} \ldots w_n^{i_n}$ \hspace{1cm} (5.2b)

Here, $\xi_{1}^{i_1}, \xi_{2}^{i_2}, \ldots, \xi_{n}^{i_n}$ are the node points in (0, 1) and $w_1^{i_1}, w_2^{i_2}, \ldots, w_n^{i_n}$ are their corresponding weights in one dimension. The generalized Gaussian quadrature nodes and weights for product of polynomials and logarithmic function given in Ma et. al. (1996) are used for evaluating the results.

The equations in (5.2a) gives the nodes $(x_{1m}, x_{2m}, ..., x_{n_{m}})$ for integrating any function over the integration domain $\Omega$ and Eq. (5.2b) is used to obtain the corresponding weights $c_m$ for these nodal points. After procuring $(c_m, x_{1m}, x_{2m}, ..., x_{n_{m}})$ for $\Omega$, one can obtain the integral of any function $f(\mathbf{x})$ numerically using Eq. (5.2) over the domain $\Omega$.

Five examples of integrals of four, five and six dimensions are chosen in order to show the functioning of the method. The integration rule for each of these integrals is given below and their numerical results are tabulated in Table 5.1.

**Example 1:**

$I_1 = \int_{0}^{1} \int_{0}^{x_1+x_2+x_3} \int_{0}^{x_4} (x_1 + x_2 + x_3 + x_4) \, dx_4 dx_3 dx_2 dx_1$

Exact value of $I_1 = 3.75$

Integration rule for $I_1$:

$I_1 \approx \sum_{m=1}^{N^n} c_m (x_{1m} + x_{2m} + x_{3m} + x_{4m})$

where,
\[ x_{1m} = \xi_1^{i_1}, \quad x_{2m} = \xi_2^{i_2}, \quad x_{3m} = \xi_3^{i_3}; \]
\[ x_{4m} = (\xi_1^{i_1} + \xi_2^{i_2} + \xi_3^{i_3})\xi_4^{i_4}; \]
\[ c_m = (\xi_1^{i_1} + \xi_2^{i_2} + \xi_3^{i_3})w_1^{i_1}w_2^{i_2}w_3^{i_3}w_4^{i_4}. \]

**Example 2:**

\[
I_2 = \int \int \int \int_{0 \times 0 \times 0 \times 0} (x_1 + x_2 + x_3 + x_4) \, dx_4 dx_3 dx_2 dx_1
\]

Exact value of \( I_2 = 0.083333333333333 \)

Integration rule for \( I_2 \):

\[
I_2 \approx \sum_{m=1}^{N^n} c_m (x_{1m} + x_{2m} + x_{3m} + x_{4m})
\]

where,

\[
x_{1m} = \xi_1^{i_1}, \quad x_{2m} = \xi_1^{i_1} \xi_2^{i_2}, \quad x_{3m} = \xi_1^{i_1} \xi_2^{i_2} \xi_3^{i_3}, \]
\[
x_{4m} = \xi_1^{i_1} \xi_2^{i_2} \xi_3^{i_3} \xi_4^{i_4}; \]
\[
c_m = (\xi_1^{i_1})^2 (\xi_2^{i_2})^2 \xi_3^{i_3} w_1^{i_1} w_2^{i_2} w_3^{i_3} w_4^{i_4}. \]

**Example 3:**

\[
I_3 = \int \int \int \int_{0 \times 0 \times 0 \times 0} (x_1^2 + x_2^2 + x_3^2 + x_4^2 + x_5^2) \, dx_5 dx_4 dx_3 dx_2 dx_1
\]

Exact value of \( I_3 = 0.013888888888888 \)

Integration rule for \( I_3 \):

\[
I_3 \approx \sum_{m=1}^{N^n} c_m (x_{1m}^2 + x_{2m}^2 + x_{3m}^2 + x_{4m}^2 + x_{5m}^2)
\]

where,

\[
x_{1m} = \xi_1^{i_1}, \quad x_{2m} = \xi_1^{i_1} \xi_2^{i_2}, \quad x_{3m} = \xi_1^{i_1} \xi_2^{i_2} \xi_3^{i_3}; \]

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$$x_4 = \xi_1 \xi_2 \xi_3 \xi_4$$, \quad x_5 = \xi_1 \xi_2 \xi_3 \xi_4 \xi_5$$

$$c_m = (\xi_1)^4 (\xi_2)^3 (\xi_3)^2 (\xi_4)^1 (\xi_5)^0 w_1 w_2 w_3 w_4 w_5$$

**Example 4:**

$$I_4 = \int_{0}^{1} \int_{0}^{2} \int_{0}^{3} \int_{0}^{4} \int_{0}^{0} e^{(x_1 + x_2 + x_3 + x_4)} (0.0001) \, dx_5 \, dx_4 \, dx_3 \, dx_2 \, dx_1$$

Exact value of \(I_4 = 1.1230142860467367\)

Integration rule for \(I_4\):

$$I_4 \approx \sum_{m=1}^{N^n} c_m (0.0001)$$

where,

$$c_m = 24e^{(\xi_1 + 2\xi_2 + 3\xi_3 + 4\xi_4)} w_1 i_1 w_2 i_2 w_3 i_3 w_4 i_4 w_5$$

**Example 5:**

$$I_5 = \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} \int_{0}^{x_1} \int_{0}^{x_2} \int_{0}^{x_3} \int_{0}^{x_4} \int_{0}^{x_5} (x_1 + x_2 + x_3 + x_4 + x_5 + x_6) dx_6 \, dx_5 \, dx_4 \, dx_3 \, dx_2 \, dx_1$$

Exact value of \(I_5 = 0.527777777777778\)

Integration rule for \(I_5\):

$$I_5 \approx \sum_{m=1}^{N^n} c_m (x_1 + x_2 + x_3 + x_4 + x_5 + x_6)$$

where,

- \(x_1 = \xi_1\), \(x_2 = \xi_2\), \(x_3 = \xi_3\),
- \(x_4 = \xi_4\), \(x_5 = \xi_5\), \(x_6 = (\xi_1 \xi_4 + \xi_2 \xi_5)\xi_6\).
\[ c_m = (\xi_1^i \xi_4^i + \xi_2^i \xi_5^i) \xi_1^i \xi_2^i w_1^i w_2^i w_3^i w_4^i w_5^i w_6^i \]

**Table 5.1: Integral values of the integrals in examples given in section 5.2**

<table>
<thead>
<tr>
<th>Integral</th>
<th>Computed value for N=5</th>
<th>Abs. Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>( I_1 )</td>
<td>3.750000000000008</td>
<td>7.99E-14</td>
</tr>
<tr>
<td>( I_2 )</td>
<td>0.083333333333333</td>
<td>0</td>
</tr>
<tr>
<td>( I_3 )</td>
<td>0.013888888888888</td>
<td>2.58E-15</td>
</tr>
<tr>
<td>( I_4 )</td>
<td>1.12301428599048</td>
<td>5.62E-11</td>
</tr>
<tr>
<td>( I_5 )</td>
<td>0.527777777777773</td>
<td>4.47E-14</td>
</tr>
</tbody>
</table>

### 5.3 Numerical integration formula over an n-dimensional cube

An n-dimensional cube is given by

\[ C_n = \{(x_1, x_2, \ldots, x_n) \mid a_1 \leq x_1 \leq b_1, a_2 \leq x_2 \leq b_2, \ldots, a_n \leq x_n \leq b_n\} \]

where \( n \) represents the dimension of the cube \( C_n \). A zero-one n-cube is the unit cube in the first orthant, \( C_n^* = \{(x_1, x_2, \ldots, x_n) \mid 0 \leq x_1 \leq 1, 0 \leq x_2 \leq 1, \ldots, 0 \leq x_n \leq 1\} \).

A two-dimensional cube, \( C_2 \) is a rectangle and a three-dimensional cube, \( C_3 \) is a cuboid.

The integration formula to evaluate the integral over an n-dimensional cube can be obtained from Eq. (5.2), by substituting the integration limits, \( a = a_1, b = b_1, g_1 = a_2, h_1 = b_2 \), \( \ldots, g_{n-1} = a_n, h_{n-1} = b_n \) in Eq. (5.2).
\[
 l = \int_{c_n} f(\vec{x}) \, dC_n = \int_{a_1}^{b_1} \int_{a_2}^{b_2} \ldots \int_{a_n}^{b_n} f(\vec{x}) \, dx_n \, dx_{n-1} \ldots dx_1
\]

\[
 l \approx \sum_{m=1}^{N^n} c_m f(x_{1m}, x_{2m}, \ldots, x_{nm})
\]

(5.3)

where \( c_m = w_1^{i_1}w_2^{i_2} \ldots w_n^{i_n}(b_1 - a_1)(b_2 - a_2) \ldots (b_n - a_n); \)

\[
x_{1m} = (b_1 - a_1) \xi_1^{i_1} + a_1;
\]

\[
x_{2m} = (b_2 - a_2) \xi_2^{i_2} + a_2;
\]

\[
\ldots
\]

\[
x_{nm} = (b_n - a_n)\xi_n^{i_n} + a_n
\]

(5.3a)

Eq. (5.3a) gives the weights and nodes \((c_m, x_{1m}, x_{2m}, \ldots, x_{nm})\) for integrating any function over the n-dimensional cube \(C_n\) and Eq. (5.3) estimates the integral value of any function \(f(\vec{x})\) over \(C_n\).

The nodes and weights \((c_m, x_{1m}, x_{2m}, x_{3m}, x_{4m})\) for a four-dimensional zero-one cube, \(C_4^* = \{(x_1, x_2, x_3, x_4) \mid 0 \leq x_1 \leq 1, 0 \leq x_2 \leq 1, 0 \leq x_3 \leq 1, 0 \leq x_4 \leq 1\}\) obtained using Eq. (5.3a), for \(N=5\), are listed in Appendix A.

A comparative study is made on the integration results of some functions obtained using the proposed method with that of the results given in Dooren and Ridder (1976) (Table 5.2). The variety of functions which are considered, for comparison of errors and the number of function evaluations (NUM), in Table 5.2 are:
Simple Integrands:

\[ I_6 = \int_0^1 \int_0^1 \int_0^1 \frac{8(1 + 2(x + y + z))^{-1}}{dx dy dz} = 2.152142832595894 \]

\[ I_7 = \int_0^2 \int_0^1 \int_0^1 x_3^2 x_4 \exp(x_3 x_4) (x_1 + x_2 + 1)^{-2} \, dx_1 dx_2 dx_3 dx_4 \]

\[ = 0.5753641449035616 \]

\[ I_8 = \int_{-1}^1 \int_{-1}^{\pi/2} \int_{-1}^0 \int_0^2 x_1 x_2^2 \sin(x_3) (4 + x_4 + x_5 + x_6)^{-1} \, dx_1 \ldots dx_6 \]

\[ = 1.434761888397263 \]

Oscillating Integrands:

\[ I_9 = \int_0^{3\pi} \int_0^{3\pi} \cos(x + y) \, dx dy = -4 \]

\[ I_{10} = \int_0^1 \int_0^1 \int_0^1 \int_0^1 \sin(10x_1) \, dx_1 dx_2 dx_3 dx_4 = 0.1839071529076452 \]

\[ I_{11} = \int_0^{\pi/2} \int_0^{\pi} \int_0^{\pi} \int_0^{\pi} \cos(x_1 + x_2 + x_3 + x_4 + x_5) \, dx_1 dx_2 dx_3 dx_4 dx_5 = 16 \]

Integrand with a peak:

\[ I_{12} = \int_0^1 \int_0^1 \left[ (x^2 + 0.0001) \left( (y + 0.25)^2 + 0.0001 \right) \right]^{-1} \, dx dy \]

\[ = 499.1249442241215 \]

Integrand with end-point singularities

\[ I_{13} = \int_0^1 \int_0^1 \int_0^1 (x + y + z)^{-2} \, dx dy dz = 0.8630462173553432 \]
Table 5.2: Comparison of integration results by the proposed method with the results in Dooren and Ridder (1976) over n-dimensional cubes

<table>
<thead>
<tr>
<th>Integral</th>
<th>Results in Dooren and Ridder (1976)</th>
<th>Results using the proposed method</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Abs. Error</td>
<td>NUM</td>
</tr>
<tr>
<td>$I_6$</td>
<td>0.13 E-4</td>
<td>495</td>
</tr>
<tr>
<td>$I_7$</td>
<td>0.84 E-4</td>
<td>1843</td>
</tr>
<tr>
<td>$I_8$</td>
<td>0.50 E-5</td>
<td>7967</td>
</tr>
<tr>
<td>$I_9$</td>
<td>0.25 E-5</td>
<td>1003</td>
</tr>
<tr>
<td>$I_{10}$</td>
<td>0.17 E-6</td>
<td>1261</td>
</tr>
<tr>
<td>$I_{11}$</td>
<td>0.24 E-5</td>
<td>29747</td>
</tr>
<tr>
<td>$I_{12}$</td>
<td>0.79 E-5</td>
<td>901</td>
</tr>
<tr>
<td>$I_{13}$</td>
<td>0.89 E-4</td>
<td>9945</td>
</tr>
</tbody>
</table>

It can be observed from Table 5.2 that the proposed method is ideal for integrating all type of functions. Using the current method better accuracy is acquired with lesser number of function evaluations for integration of $I_6$, $I_7$, $I_9$ and $I_{13}$. In the remaining integral evaluations even though the function evaluations are more, the accuracy has improved.

Some functions given in Sag and Szekeras (1964) are also tested over different dimensional cubes. The results of integration (computed value, absolute error and the number of function evaluations required to get the value) of two functions $\frac{1}{2^n}$ and $\sum_{i=1}^{n} x_i^2$, for $n = 2$, 3, 4, 5 and 6 over an n-dimensional cube are presented in Tables 5.3 and 5.4, respectively.

The integrals evaluated in Table 5.3 and Table 5.4 and its exact value are as follows:
\[
\int_{-1}^{1} \int_{-1}^{1} \ldots \int_{-1}^{1} \frac{1}{2^n} dx_1 dx_2 \ldots dx_n = 1
\]

and

\[
\int_{-1}^{1} \int_{-1}^{1} \ldots \int_{-1}^{1} \sum_{i=1}^{n} x_i^2 \ dx_1 dx_2 \ldots dx_n = \frac{1}{3} \sum_{i=1}^{n} i \ 2^i
\]

Table 5.3: Numerical results to evaluate: \( \int_{-1}^{1} \int_{-1}^{1} \ldots \int_{-1}^{1} \frac{1}{2^n} dx_1 dx_2 \ldots dx_n = 1 \)

<table>
<thead>
<tr>
<th>n</th>
<th>Computed value</th>
<th>Abs. Error</th>
<th>No. of computations</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>1.0000000000000000000</td>
<td>0</td>
<td>25</td>
</tr>
<tr>
<td>3</td>
<td>1.0000000000000000001</td>
<td>0.99E-16</td>
<td>125</td>
</tr>
<tr>
<td>4</td>
<td>1.0000000000000000001</td>
<td>0.99E-16</td>
<td>625</td>
</tr>
<tr>
<td>5</td>
<td>1.0000000000000000001</td>
<td>0.99E-16</td>
<td>3125</td>
</tr>
<tr>
<td>6</td>
<td>0.9999999999999444444</td>
<td>0.55E-14</td>
<td>15625</td>
</tr>
</tbody>
</table>

Table 5.4: Numerical results to evaluate: \( \int_{-1}^{1} \int_{-1}^{1} \ldots \int_{-1}^{1} \sum_{i=1}^{n} x_i^2 \ dx_1 dx_2 \ldots dx_n = \frac{1}{3} \sum_{i=1}^{n} i \ 2^i \)

<table>
<thead>
<tr>
<th>n</th>
<th>Computed value</th>
<th>Abs. Error</th>
<th>No. of computations</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>2.66666666666666669</td>
<td>0.23E-15</td>
<td>25</td>
</tr>
<tr>
<td>3</td>
<td>8.000000000000007</td>
<td>0.69E-15</td>
<td>125</td>
</tr>
<tr>
<td>4</td>
<td>21.3333333333319</td>
<td>0.14E-13</td>
<td>625</td>
</tr>
<tr>
<td>5</td>
<td>53.3333333333560</td>
<td>0.22E-12</td>
<td>3125</td>
</tr>
<tr>
<td>6</td>
<td>127.9999999999874</td>
<td>0.12E-11</td>
<td>15625</td>
</tr>
</tbody>
</table>
5.4 Numerical integration formula over an n-dimensional simplex

An n-simplex in the positive orthant, \( \mathbb{R}^n^+ \), with the origin as one of the corners is given by

\[
X_n = \left\{(x_1, x_2, \ldots, x_n) \mid \sum_{i=1}^{n} x_i \leq a, x_i \geq 0\right\}
\]

Here \( n \) represents the dimension of the simplex, \( X_n \).

A two-simplex is the triangle, whereas a three-simplex is a tetrahedron.

Consider the integral of a function \( f(\vec{x}) \) over the n-simplex,

\[
I = \int_{X_n} f(\vec{x}) dX_n = \int_0^a \int_0^{a-x_1} \cdots \int_0^{a-x_1-\cdots-x_{n-1}} f(x_1, x_2, \ldots, x_n) \, dx_n \cdots dx_2 \, dx_1
\]

(5.4)

By substituting the integration limits of the integral in Eq. (5.4) in Eq. (5.2), the integration formula to evaluate the integral in Eq. (5.4) numerically can be attained, which will be,

\[
I \approx \sum_{m=1}^{N^n} c_m f(x_{1m}, x_{2m}, \ldots, x_{nm})
\]

(5.5)

where,

\[
c_m = a^n \left(1 - \xi_1^{i_1}\right)^{n-1} \left(1 - \xi_2^{i_2}\right)^{n-2} \cdots \left(1 - \xi_{n-1}^{i_{n-1}}\right)^2 \left(1 - \xi_n^{i_n}\right) w_1^{i_1} w_2^{i_2} \cdots w_n^{i_n}
\]

\[
x_{1m} = a \xi_1^{i_1};
\]

\[
x_{2m} = a \left(1 - \xi_1^{i_1}\right) \xi_2^{i_2};
\]

\[
x_{3m} = a \left(1 - \xi_1^{i_1}\right) \left(1 - \xi_2^{i_2}\right) \xi_3^{i_3};
\]

\[
\ldots
\]

\[
x_{nm} = a \left(1 - \xi_1^{i_1}\right) \left(1 - \xi_2^{i_2}\right) \cdots \left(1 - \xi_{n-1}^{i_{n-1}}\right) \xi_n^{i_n}
\]
Applying the generalized Gaussian quadrature points $\xi^l_1, \xi^l_2, \ldots, \xi^l_n$ and their corresponding weights $w^l_1, w^l_2, \ldots, w^l_n$ (given in Ma et al. (1996)), in Eqs. (5.5a), the weights $c_m$ and the nodal points $(x_{1m}, x_{2m}, \ldots, x_{nm})$ for the simplex $X_n$ can be achieved. With these weights and nodes, one will be able to evaluate the integral value of a function over the simplex using Eq. (5.5).

The nodes and weights $(c_m, x_{1m}, x_{2m}, x_{3m}, x_{4m})$ for a four-dimensional simplex,

$$X_4 = \left\{ (x_1, x_2, x_3, x_4) \left| \sum_{i=1}^{4} x_i \leq 1, x_i \geq 0 \right. \right\}$$

obtained using Eq. (5.5a), taking $N=5$, are listed in Appendix B.

Table 5.5, 5.6 and 5.7 gives the results of integration of three functions

(i) $f_1(x, y) = 1$
(ii) $f_2(x, y) = \sqrt{\sum_{i=1}^{n} x_i}$
(iii) $f_3(x, y) = \frac{1}{\sqrt{\sum_{i=1}^{n} x_i}}$

over the simplex $X_n$ (with $a = 1$) for different dimensions

<table>
<thead>
<tr>
<th>n</th>
<th>Exact integral value</th>
<th>Computed value</th>
<th>Abs. Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.500000000000001</td>
<td>0.500000000000001</td>
<td>9.9E-16</td>
</tr>
<tr>
<td>3</td>
<td>0.166666666666667</td>
<td>0.166666666666664</td>
<td>2.7E-14</td>
</tr>
<tr>
<td>4</td>
<td>0.041666666666667</td>
<td>0.0416666666666652</td>
<td>1.5E-14</td>
</tr>
<tr>
<td>5</td>
<td>0.0083333333333333</td>
<td>0.008333333333330</td>
<td>2.8E-15</td>
</tr>
<tr>
<td>6</td>
<td>0.00138888888888889</td>
<td>0.001388924172021</td>
<td>3.52E-08</td>
</tr>
</tbody>
</table>
Table 5.6: Numerical value of the integral: $\int_0^1 \int_0^{1-x_1} \cdots \int_0^{1-x_1-x_2-\cdots-x_{n-1}} \frac{1}{\sqrt{\sum_{i=1}^n x_i^2}} \, dx_n \, dx_{n-1} \cdots \, dx_1$ for different $n$

<table>
<thead>
<tr>
<th>$n$</th>
<th>Exact integral value</th>
<th>Computed value</th>
<th>Abs. Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.4</td>
<td>0.399999999999480</td>
<td>5.2E-13</td>
</tr>
<tr>
<td>3</td>
<td>0.142857142857143</td>
<td>0.142857142857151</td>
<td>8.0E-15</td>
</tr>
<tr>
<td>4</td>
<td>0.0370370370370370</td>
<td>0.0370370370370237</td>
<td>1.3E-14</td>
</tr>
<tr>
<td>5</td>
<td>0.0075757575757575</td>
<td>0.00757575757575657</td>
<td>1.0E-15</td>
</tr>
<tr>
<td>6</td>
<td>0.00128205128205128</td>
<td>0.00128210079066106</td>
<td>4.95E-08</td>
</tr>
</tbody>
</table>

Table 5.7: Numerical value of the integral: $\int_0^1 \int_0^{1-x_1} \cdots \int_0^{1-x_1-x_2-\cdots-x_{n-1}} (\sum_{i=1}^n x_i)^{-0.5} \, dx_n \, dx_{n-1} \cdots \, dx_1$ for different $n$

<table>
<thead>
<tr>
<th>$n$</th>
<th>Exact integral value</th>
<th>Computed value</th>
<th>Abs. Error</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.6666666666666666</td>
<td>0.666666666673585</td>
<td>1.0E-09</td>
</tr>
<tr>
<td>3</td>
<td>0.2</td>
<td>0.200000000004725</td>
<td>4.7E-12</td>
</tr>
<tr>
<td>4</td>
<td>0.0476190476190476</td>
<td>0.047619047619046</td>
<td>1.4E-15</td>
</tr>
<tr>
<td>5</td>
<td>0.0092592592592926</td>
<td>0.0092592592592911</td>
<td>3.1E-14</td>
</tr>
<tr>
<td>6</td>
<td>0.00151515151515152</td>
<td>0.0015151676690702</td>
<td>1.61E-08</td>
</tr>
</tbody>
</table>

5.5 Numerical integration formula over an $n$-dimensional ball

An $n$-dimensional ball with origin as the centre and radius $a$, is given by

$$B_n = \left\{ (x_1, x_2, \ldots, x_n) \left| \sum_{i=1}^n x_i^2 \leq a^2 \right. \right\}$$

where $n$ represents the dimension of the ball $B_n$. 
A two-dimensional ball, $B_2$ is a circular disc $x_1^2 + x_2^2 \leq a^2$ and a three-dimensional ball, $B_3$ represents a sphere, $x_1^2 + x_2^2 + x_3^2 \leq a^2$.

In section 3.4, an optimal numerical integration formula for integration over a circular disc (2-ball) is derived and in section 4.5, such a formula for integration over a sphere (3-ball) is presented. Here those derivations are extended to develop an integration rule to integrate a function over an n-dimensional ball, i.e., to derive an integration formula to evaluate,

$$l = \int_{B_n} f(x_1, x_2, \ldots, x_n) \, dx_n \, dx_{n-1} \ldots dx_1$$

$$= \int_{-a}^{a} \int_{-a}^{\sqrt{a^2-x_1^2}} \ldots \int_{-a}^{\sqrt{a^2-x_1^2-x_2^2-\ldots-x_{n-1}^2}} f(x_1, x_2, \ldots, x_n) \, dx_n \, dx_2 \, dx_1$$

(5.6)

In order to derive the integration rule, initially $B_n$ is transformed to an n-dimensional cube,

$$C_n = \{ (x_1, x_2, \ldots, x_n) \mid 0 < r < a, 0 < \varphi_1 < \pi, 0 < \varphi_2 < \pi, \ldots, 0 < \varphi_{n-1} < \pi, \quad 0 < \varphi_n < 2\pi \}$$

using the transformation,

$$x_1 = r \cos \varphi_1$$

$$x_2 = r \sin \varphi_1 \cos \varphi_2$$

$$x_3 = r \sin \varphi_1 \sin \varphi_2 \cos \varphi_3$$

$$\ldots$$

$$x_{n-1} = r \sin \varphi_1 \sin \varphi_2 \sin \varphi_3 \ldots \sin \varphi_{n-2} \cos \varphi_{n-1}$$

$$x_n = r \sin \varphi_1 \sin \varphi_2 \sin \varphi_3 \ldots \sin \varphi_{n-2} \sin \varphi_{n-1}$$

The Jacobian of this transformation is

$$|J_1| = r^{n-1} \sin^{n-2} \varphi_1 \sin^{n-3} \varphi_2 \ldots \sin \varphi_{n-2}$$

Hence, the integral in Eq. (5.6) would be
A linear transformation is next applied,

\[ r = a_1 \xi_1, \quad \varphi = \pi \xi_2, \quad \varphi_2 = \pi \xi_3, \ldots, \varphi_{n-2} = \pi \xi_{n-1}, \quad \varphi_{n-1} = 2\pi \xi_n, \]

to transform \( C_n \) to a zero-one n-cube,

\[ C_n^* = \{(\xi_1, \xi_2, \ldots, \xi_n) \mid 0 \leq \xi_i \leq 1, i = 1, 2, \ldots, n\}. \]

The Jacobian of this transformation is \( |J_2| = 2\pi^{n-1} a \).

Now, the integral will be

\[
I = \int_{0}^{1} \int_{0}^{1} \cdots \int_{0}^{1} f(\bar{x}(a_{1\xi_1}, \pi \xi_2, \pi \xi_3, \ldots, \pi \xi_{n-1}, 2\pi \xi_n)) \mid J_1 \mid \mid J_2 \mid \, d\xi_2 \cdots d\xi_1
\]

Taking \( N_1, N_2, \ldots, N_n \) quadrature points along the \( \xi_1, \xi_2, \ldots, \xi_n \) directions respectively, the integral will be obtained as,

\[
I \approx \sum_{i_1=1}^{N_1} \sum_{i_2=1}^{N_2} \cdots \sum_{i_n=1}^{N_n} w_{1}^{i_1} w_{2}^{i_2} \cdots w_{n}^{i_n} f(\bar{x}(a_{1\xi_1}, \pi \xi_2, \pi \xi_3, \ldots, \pi \xi_{n-1}, 2\pi \xi_n)) \mid J_1 \mid \mid J_2 \mid
\]

where \( \bar{x} = (x_1, x_2, \ldots, x_n) \)

\[
\therefore I \approx \sum_{m=1}^{N_1 N_2 \cdots N_n} c_m f(x_{1m}, x_{2m}, \ldots, x_{nm})
\]

\[
(5.7)
\]

where,

\[
c_m = 2 a^n (\pi \xi_1^{i_1})^{n-1} \sin^{n-2}(\pi \xi_2^{i_2}) \sin^{n-3}(\pi \xi_3^{i_3}) \cdots \sin(\pi \xi_{n-1}^{i_{n-1}}) w_{1}^{i_1} w_{2}^{i_2} \cdots w_{n}^{i_n};
\]

\[
x_{1m} = a \xi_1^{i_1} \cos(\pi \xi_2^{i_2});
\]

\[
x_{2m} = a \xi_1^{i_1} \sin(\pi \xi_2^{i_2}) \cos(\pi \xi_3^{i_3});
\]

\[
x_{3m} = a \xi_1^{i_1} \sin(\pi \xi_2^{i_2}) \sin(\pi \xi_3^{i_3}) \cos(\pi \xi_4^{i_4});
\]

\[ \ldots \]
The set of equations in (5.7a) gives the weights and nodes required for integration of any function \( f(x_1, x_2, \ldots, x_n) \) over an n-dimensional ball using Eq. (5.7).

**Appendix C** lists the nodes and weights, \((c_m, x_{1m}, x_{2m}, x_{3m}, x_{4m})\) required for integration over a unit four-dimensional ball centred at the origin,

\[
B_4 = \left\{ (x_1, x_2, x_3, x_4) \left| \sum_{i=1}^{4} x_i^2 \leq 1 \right. \right\}.
\]

Table 5.8 gives the numerical results of integration of the constant test function given in Sag and Szekeras (1964), \( f(x) = 2^{-n} \) over an n-dimensional ball, for \( n = 2, 3, 4, 5 \) and 6.

<table>
<thead>
<tr>
<th>Dimension(n)</th>
<th>Exact solution</th>
<th>Results using proposed method</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td>Computed Value</td>
</tr>
<tr>
<td>2</td>
<td>0.785398163397448</td>
<td>0.785398163397452</td>
</tr>
<tr>
<td>3</td>
<td>0.523598775598299</td>
<td>0.523598775598319</td>
</tr>
<tr>
<td>4</td>
<td>0.308425137534042</td>
<td>0.308425137533993</td>
</tr>
<tr>
<td>5</td>
<td>0.164493406684823</td>
<td>0.164493416750893</td>
</tr>
<tr>
<td>6</td>
<td>0.080745512188281</td>
<td>0.080026617550037</td>
</tr>
</tbody>
</table>
5.6 Numerical integration formula over an irregular n-dimensional domain

In this section, a numerical integration formula is derived over an n-dimensional irregular domain. Let \( D \) be an n-dimensional closed region with boundary in polar coordinates, \( r = u(\varphi_1, \varphi_2, \ldots, \varphi_{n-1}) \).

To evaluate,

\[
I = \int_D f(x_1, x_2, \ldots, x_n) \, dx_n dx_{n-1} \ldots dx_1
\]

(5.8)

the domain \( D \) is transformed to an n-dimensional cube using the transformation,

\[
\begin{align*}
x_1 &= r \cos \varphi_1 \\
x_2 &= r \sin \varphi_1 \cos \varphi_2 \\
x_3 &= r \sin \varphi_1 \sin \varphi_2 \cos \varphi_3 \\
\cdots \\
x_{n-1} &= r \sin \varphi_1 \sin \varphi_2 \ldots \sin \varphi_{n-2} \cos \varphi_{n-1} \\
x_n &= r \sin \varphi_1 \sin \varphi_2 \ldots \sin \varphi_{n-2} \sin \varphi_{n-1}.
\end{align*}
\]

The Jacobian of this transformation is,

\[
|J_1| = r^{n-1} \sin^{n-2} \varphi_1 \sin^{n-3} \varphi_2 \ldots \sin \varphi_{n-2}.
\]

After the transformation, the integral in Eq. (5.8) will be

\[
I = \int_{0}^{\frac{\pi}{2n}} \int_{0}^{\pi} \ldots \int_{0}^{\pi} \int_{0}^{\frac{\pi}{2n-1}} f(\bar{x}(r, \varphi_1, \varphi_2, \ldots, \varphi_{n-1})) |J_1| \, dr \, d\varphi_1 \ldots d\varphi_{n-2} \, d\varphi_{n-1}
\]

(5.9)

The domain of integration of the integral in Eq. (5.9) is transformed to a zero-one n-cube

\[
C^* = \{(\xi_1, \xi_2, \ldots, \xi_n) \mid 0 \leq \xi_i \leq 1, i = 1, 2, \ldots, n\},
\]
using the transformation,

\[ \varphi_{n-1} = 2\pi \xi_n \]

\[ \varphi_{n-2} = \pi \xi_{n-1} \]

...\[ \varphi_2 = \pi \xi_3 \]

\[ \varphi_1 = \pi \xi_2 \]

\[ r = u(\pi \xi_2, \pi \xi_3, \ldots, \pi \xi_{n-1}, 2\pi \xi_n) \xi_1. \]

The Jacobian of this transformation is \(|J_2| = 2\pi^{n-1} u(\pi \xi_2, \pi \xi_3, \ldots, \pi \xi_{n-1}, 2\pi \xi_n)\) and the integral (5.9) will now be,

\[ I = \int_0^1 \int_0^1 \ldots \int_0^1 f(\bar{x}(u\xi_1, \pi \xi_2, \pi \xi_3, \ldots, \pi \xi_{n-1}, 2\pi \xi_n)) |J_1| \, d\xi_1 \ldots d\xi_2 \, d\xi_1. \]

Taking \(N_1, N_2, \ldots, N_n\) quadrature points along the \(\xi_1, \xi_2, \ldots, \xi_n\) directions respectively, the integral would be,

\[ I \approx \sum_{i_1=1}^{N_1} \sum_{i_2=1}^{N_2} \ldots \sum_{i_n=1}^{N_n} w_1^{i_1} w_2^{i_2} \ldots w_n^{i_n} f(\bar{x}(u\xi_1^{i_1}, \pi \xi_2^{i_2}, \pi \xi_3^{i_3}, \ldots, \pi \xi_{n-1}^{i_{n-1}}, 2\pi \xi_n^{i_n})) |J_1| |J_2| \]

where \(\bar{x} = (x_1, x_2, \ldots, x_n)\)

\[ \therefore I \approx \sum_{m=1}^{N_1N_2\ldots N_n} c_m f(x_{1m}, x_{2m}, \ldots, x_{nm}) \]

(5.10)

where,

\[ c_m = 2 \left[ u(\pi \xi_2^{i_2}, \pi \xi_3^{i_3}, \ldots, \pi \xi_{n-1}^{i_{n-1}}, 2\pi \xi_n^{i_n}) \right] \left( \pi \xi_1^{i_1} \right)^{n-1} \sin^{n-2}(\pi \xi_2^{i_2}) \sin^{n-3}(\pi \xi_3^{i_3}) \ldots \sin(\pi \xi_{n-1}^{i_{n-1}}) w_1^{i_1} w_2^{i_2} \ldots w_n^{i_n}; \]

\[ x_{1m} = u(\pi \xi_2^{i_2}, \pi \xi_3^{i_3}, \ldots, \pi \xi_{n-1}^{i_{n-1}}, 2\pi \xi_n^{i_n}) \xi_1^{i_1} \cos(\pi \xi_2^{i_2}); \]

\[ x_{2m} = u(\pi \xi_2^{i_2}, \pi \xi_3^{i_3}, \ldots, \pi \xi_{n-1}^{i_{n-1}}, 2\pi \xi_n^{i_n}) \xi_1^{i_1} \sin(\pi \xi_2^{i_2}) \cos(\pi \xi_3^{i_3}); \]

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\[ x_{3m} = \left[u\left(\pi \xi_{2}^{l_{2}}, \pi \xi_{3}^{l_{3}}, \ldots, \pi \xi_{n-1}^{l_{n-1}}, 2\pi \xi_{n}^{l_{n}}\right)\right] \xi_{1}^{l_{1}} \sin(\pi \xi_{2}^{l_{2}}) \sin(\pi \xi_{3}^{l_{3}}) \cos(\pi \xi_{4}^{l_{4}}); \]
\[ \cdots \]
\[ x_{n-1m} = \left[u\left(\pi \xi_{2}^{l_{2}}, \pi \xi_{3}^{l_{3}}, \ldots, \pi \xi_{n-1}^{l_{n-1}}, 2\pi \xi_{n}^{l_{n}}\right)\right] \xi_{1}^{l_{1}} \sin(\pi \xi_{2}^{l_{2}}) \sin(\pi \xi_{3}^{l_{3}}) \cdots \sin(\pi \xi_{n-1}^{l_{n-1}}) \cos(2\pi \xi_{n}^{l_{n}}); \]
\[ x_{nm} = \left[u\left(\pi \xi_{2}^{l_{2}}, \pi \xi_{3}^{l_{3}}, \ldots, \pi \xi_{n-1}^{l_{n-1}}, 2\pi \xi_{n}^{l_{n}}\right)\right] \xi_{1}^{l_{1}} \sin(\pi \xi_{2}^{l_{2}}) \sin(\pi \xi_{3}^{l_{3}}) \cdots \sin(\pi \xi_{n-1}^{l_{n-1}}) \sin(2\pi \xi_{n}^{l_{n}}) \]

(5.10a)

The set of equations in Eq. (5.10a) provides the nodal points \((x_{1m}, x_{2m}, \ldots, x_{nm})\) (in \(D\)) and their corresponding weights \(c_{m}\) required for integration (using Eq. (5.10)) of any function \(f(x_{1}, x_{2}, \ldots, x_{n})\) over \(D\).

It can be noted that by taking \(r = u(\varphi_{1}, \varphi_{2}, \ldots, \varphi_{n-1}) = a\), the domain \(D\) would be an \(n\)-dimensional ball, \(\sum_{i=1}^{n} x_{i}^{2} \leq a^{2}\). Hence by substituting \(u(\varphi_{1}, \varphi_{2}, \ldots, \varphi_{n-1}) = a\) in Eq. (5.10), the integration formula over an \(n\)-ball can be obtained as in Eq. (5.7).

### 5.7 Conclusions

This chapter familiarizes a numerical method for constructing a nearly-optimal quadrature rule for integrating \(n\)-dimensional multiple integrals in general. The integration rule to evaluate integrals over an \(n\)-dimensional cube and an \(n\)-dimensional simplex is given as a special case of the general formula. Numerical results along with comparison from references are provided in the tables given in the chapter. An effective integration formula is derived over \(n\)-dimensional balls using a combination of polar and linear transformations. Another integration formula is presented to evaluate integrals over an \(n\)-dimensional irregular domain. Tabulated values in each section in the paper show that the integration rule proposed here gives a good accuracy. Any programming language or any mathematical software can be used to obtain the nodes and weights for the domain, using the derived formulae and these nodes and weights could be used to get the integral value of any function over that domain.