GENERALIZED GAUSSIAN QUADRATURE RULES OVER AN N-DIMENSIONAL BALL

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ABSTRACT

A nearly-optimal quadrature rule is developed to evaluate integrals over an n-dimensional ball, using an effective transformation which maps an n-dimensional ball to an n-dimensional cube and then again to a zero-one n-cube. The derivation of this formula over a 2-dimensional ball (circular disc), a 3-dimensional ball (sphere) and an n-dimensional ball is given along with numerical results for various types of integrals.

Keywords: Quadrature rules, transformation, Jacobian

1. INTRODUCTION

Integration of complicated functions over a circle or a sphere often arises in Computation a Chemistry (to evaluate surface integrals over unit sphere), while solving partial differential equations over circular boundaries (using finite element method or boundary element method), etc. Integrals which appear in such applications can barely be solved analytically, due to the nonlinearity of the boundary. Widespread research has taken place to derive numerical integration techniques over regions with linear boundaries [Bathe, 1996, Davis and Rabinowitz, 2007, Hughes, 1987, Sarada Jayan and Nagaraja, 2011, Krishnaraj, et al., 2012, Krishnaraj et al., 2016], integration over curved, circular(2-D) and spherical boundaries(3-D) is a field of ongoing research [Ahrens and Beylkin, 2009, Nagaraja and SaradaJayan, 2012, Navaneethasanthakumar, et al., 2012, SaradaJayan and Nagaraja, 2015]. In fact, to the authors' knowledge, quadrature/cubature rules over n dimensional regions are seldom found [Cools and Rabinowitz 1993, Cools, 1997, 2003, Sag and Szekeras, 1964]. In Sag and Szekeras [1964], the authors have demonstrated a numerical method to evaluate high dimensional integrals including integrals over an n-dimensional ball, using few transformation techniques.

In this paper also, we use some special transformations for deriving a quadrature rule to integrate functions over an n-dimensional ball. Anyhow, the results we got by our proposed method is giving much better accuracy than the one given in [Sag and Szekeras, 1964] for all dimensions (for different values of n). Also, these formulae are simple and very easy to apply. The paper is furnished in the following way. Section 2 is devoted for mathematical preliminaries required for the understanding of this paper. In section 3, using a combination of a polar and a linear transformation, we derive an effective quadrature rule to integrate a function over a circular disc $x^2 + y^2 \le a^2$. A modification of this rule, so to reduce the computational cost is also provided in this section with comparative results. Section 4 constitutes a similar derivation of a quadrature rule for a sphere $x^2 + y^2 + z^2 \le a^2$ and in section 5, this quadrature rule is extended to an ndimensional ball. The results of integration are tabulated in each section. Finally, in section 6, we present the conclusions.

2. Mathematical Preliminaries

2.1. Gaussian and Generalized Gaussian quadrature

An integral is typically approximated by a weighted sum of integrand evaluations in numerical integration.

$$I[f] = \int_{\Omega} f(\overline{x}) d\Omega \approx \sum_{i=1}^{M} w_i f(\overline{x}_i) = Q[f] \qquad (1)$$

The Gaussian quadrature formula is a numerical integration formula given by

$$\int_{a}^{b} q(x)\phi(x)dx \approx \sum_{i=1}^{N} w_{i}\phi(x_{i})$$
(2)

where $x_i \in [a, b]$ are referred to as the nodes and $w_i \in \mathbf{R}$ for i = 1, 2, ..., N, are the weights of the Gaussian quadrature formula. x_i and w_i for different Gaussian quadrature formulae like Gauss Legendre, Gauss Jacobi, Gauss Hermite etc. are available in literature.

The quadrature formula given in Eq. 2 is called a classical Gaussian quadrature rule if it integrates exactly all polynomials of order up to 2N-1, whereas Eq. 2 is said to be a generalized Gaussian quadrature rule with respect to a set of functions

 $\{\phi_1, \phi_2, ..., \phi_{2N}\}$ if it integrates exactly all the 2N functions in the set $\{\phi_1, \phi_2, ..., \phi_{2N}\}$. Table 1 in [8] gives the generalized Gaussian quadrature nodes and weights with respect to the set of function:

{1, lnx, x, xlnx, ..., x^{N-1} , $x^{N-1}lnx$ }.

We shall be using these nodes and weights in the product formula shown in section 3.

2.2. n-dimensional ball

An n-dimensional ball with origin as the center and radius *a* is given by

$$B_n = \left\{ (x_1, x_2, \dots, x_n) / \sum_{i=1}^n x_i^2 \le a^2 \right\}$$

where n represents the dimension of the region B_n . B_2 is a circular disc $x_1^2 + x_2^2 \le a^2$ and B_3 represents a sphere $x_1^2 + x_2^2 + x_3^2 \le a^2$.

2.3. n-dimensional cube

An n-dimensional cube is given by



Fig.1: Transformation of a $x^2+y^2\leq a^2$ in x-y plane to the rectan-gle $0\leq r\leq a$, $0\leq \theta \leq 2\pi$ in r- θ plane and then to a square $0\leq \xi\leq 1$, $0\leq \eta\leq 1$ in ξ - η plane

The derivation is as follows: The disc B_2 is transformed to a rectangle $R = \{(r, \theta)/0 \le r \le a, 0 \le \theta \le 2\pi\}$ in the $r - \theta$ plane using the polar transformation, $x = r \cos \theta$, $y = r \sin \theta$ The Jacobian of the transformation is

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$$D_{\rm rel}$$

|J| = r > 0in B_2 . Hence the integral in Eq. 3 becomes

$$I = \int_{-a}^{a} \int_{-\sqrt{a^2 - x^2}}^{\sqrt{a^2 - x^2}} f(x, y) \, dy \, dx$$
$$= \int_{0}^{a} \int_{0}^{2\pi} f(r \cos \theta, r \sin \theta) \, r \, d\theta \, dr \quad (4)$$

Next the domain of integration in (4), which is a rectangle is transformed to a zero-one square in the $\xi - \eta$ plane using the linear transformation, $r = a\xi, \theta = 2\pi\eta$, which has a Jacobian $|J| = 2\pi a > 0$

Hence, the integral I in Eq. (4) would be now $I = \int_0^1 \int_0^1 f(a\xi \cos(2\pi\eta), a\xi \sin(2\pi\eta)) a\xi 2\pi a \, d\eta \, d\xi$ Applying the quadrature formula for both the integrals, we get

$$I \approx \sum_{i=1}^{N} \sum_{j=1}^{N} w_{1_{i}} w_{2_{j}} 2\pi a^{2} \xi_{i}$$

$$f(a\xi_{i} \cos(2\pi\eta_{j}), a\xi_{i} \sin(2\pi\eta_{j}))$$

$$\approx \sum_{m=1}^{N^{2}} c_{m} f(x_{m}, y_{m}) \qquad (5)$$
where $x_{m} = a\xi_{i} \cos(2\pi\eta_{j})$,
 $y_{m} = a\xi_{i} \sin(2\pi\eta_{j}), c_{m} = w_{1_{j}} w_{2_{j}} 2\pi a^{2} \xi_{i} \qquad (6)$

 $C_n = \{ (x_1, x_2, \dots, x_n) \mid a_1 \le x_1 \le b_1, a_2 \le x_2 \\ \le b_2, \dots, a_n \le x_n \le b_n \}$

where n represents the dimension of the cube C_n . C_2 is a rectangle and C_3 represents a cuboid. An n-dimensional zero-one cube is given by $C_n^* = \{(x_1, x_2, ..., x_n) \mid 0 \le x_i \le 1, i = 1, 2, ..., n\}$

3. Numerical Integration over a 2-dimensional ball (Circular disc)

3.1. Derivation of an Integration method to integrate a function over a circular disc

In this section, we illustrate an effective integration method to integrate any arbitrary function over a circular disc, $B_2: x^2 + y^2 \le a^2$ using the concepts in transformation and generalized Gauss quadrature. Consider the integral:

Consider the integral:

$$I = \iint_{B_2} f(x, y) = \int_{-a}^{a} \int_{-\sqrt{a^2 - x^2}}^{\sqrt{a^2 - x^2}} f(x, y) \, dy \, dx \tag{3}$$

We initially transform the integration domain in the integral (3), B_2 , to a rectangle and then using a linear transformation again transform it to a zero-one square.

 (ξ_i, η_j) in Eqs. 6 are the node points in (0,1) and w_{1i}, w_{2j} are their corresponding weights in one dimension. Any quadrature points and their corres-

ponding weights can be applied in this formula, like the Gauss Legendre, Gauss Jacobi etc. We are using the generalized Gaussian quadrature nodes and weights given in [Ma et al., 1996] in our approach, as it is proved in [Ma et al., 1996, Nagaraja and SaradaJayan, 2012, SaradaJayan and Nagaraja, 2011] that these nodes and weights give better results compared to any other ones for one-dimensional integration as well as for integration over bounded two-dimensional regions.

After applying the generalized Gaussian quadrature points and their corresponding weights in Eq. 6, we get the nodal points (x_m, y_m) and the weights c_m , which are used in the integration formula (Eq. 5) for integrating a function f(x, y) over the circular disc B_2 . The node points (x_m, y_m) for the unit circle with N=10 (i.e 100 points) is plotted in Fig.2.



Fig.2: Distribution of the 100 node points for integration in the unit disc $x^2+y^2 \le 1$ using the formula in section 3.1.

The knowledge of this (x_m, y_m, c_m) is sufficient for the solver to integrate any function over the circular disc $x^2 + y^2 \le a^2$. We have tested a variety of functions using the method. Most of the functions are giving accurate integral values at least up to 10 significant digits. The results of integration of some functions over the unit circular disc $x^2 + y^2 \le 1$ for N=10 (100 points) 10.5 are tabulated in table 1.

Table 1:Integration results over the unit circular disc $x^2\!+\!y^2\!\leq\!1$ with errors

Integrand	Exact solution	Integral value using Eq.(5)	Absolut e Error
1	3.14159265358979	3.14159265358979	0
$\sqrt{x^2 + y^2}$	2.09439510239320	2.09439510239320	0
$\operatorname{Exp}(\sqrt{x^2 + y^2})$	5.28318530717959	6.28318530717966	7.02E-14
$\frac{2}{1+\sqrt{x^2+y^2}}$	3.85602625314476	3.85602625314438	3.80E-13
$ln(x^2+y^2+1)$	1.21357952701741	1.21357952710252	8.51E-11

3.2. Modified integration method to reduce the computational cost

The derivation of this method is same as the method in section 3 with respect to the transformations used. The only difference is that, while applying the quadrature rule in each direction, different number of node points (N₁, N₂) are taken in ξ and η directions, thus giving the integral rule as,

$$I = \int_{0}^{1} \int_{0}^{1} f(a\xi \cos(2\pi\eta), a\xi \sin(2\pi\eta))$$

$$a\xi 2\pi a \, d\eta \, d\xi$$

$$I \approx \sum_{i=1}^{N_{1}} \sum_{j=1}^{N_{2}} w_{1i} w_{2j} 2\pi a^{2} \xi_{i}$$

$$f(a\xi_{i} \cos(2\pi\eta_{j}), a\xi_{i} \sin(2\pi\eta_{j}))$$

$$\approx \sum_{m=1}^{N_{1}N_{2}} c_{m} f(x_{m}, y_{m}) \qquad (7)$$
where, $x_{m} = a\xi_{i} \cos(2\pi\eta_{j})$,
 $y_{m} = a\xi_{i} \sin(2\pi\eta_{j})$,
 $c_{m} = w_{1i} w_{2j} 2\pi a^{2} \xi_{i} \qquad (8)$

Eq. 8 gives the weights and nodes (c_m, x_m, y_m) for integrating any function over B_2 and Eq. 7 is used to evaluate the integral numerically.

The distribution of nodal points for integration (x_m, y_m) on the unit circular disc $x^2 + y^2 \le 1$, evaluated using Eq. 8 for N₁=5, N₂=20 (100 points), is shown in Fig.3.



Fig.3: Distribution of the 100 node points for integration in the unit disc $x^2+y^2 \le 1$ using the method in 3.2. (N₁=5, N₂=20)

In the figures, Fig. 2 and 3 we have 100 integration points. But the distribution of points is more uniform in Fig. 3 than in Fig. 2, due to which the integral value obtained using Eq. 7 is more accurate compared to the integral value obtained by Eq. 5. To demonstrate this, we show integration of five different type of integrand functions over the unit circular disc $x^2 + y^2 \le 1$. The error involved in evaluating these functions using both the methods along with the number of function evaluations required in each case is tabulated in Table 2.

While evaluating integral f_1 and f_2 , half the number of points are used by the modified method than the first method, even though the accuracy obtained in both the cases are the same. Whereas for f_2 , f_3 and f_4 we have used same number of points (m=400) to show that the modified method gives almost double accuracy than the first method.

When we take N₁ points along ξ direction and N₂ points along η direction, the distribution of points will be on N₁ concentric circles, each of which will have N₂ points on it. Hence depending on the radius of the circle *a*, we must decide how to choose N₁ and N₂.

In all the cases in Table 2, we have taken $N_1 < N_2$, since for a unit circle the radius (r = 1) is less than the angle, $\theta = 2\pi$.

4. Numerical Integration over a 3-dimensional ball (sphere)

Here we derive a numerical integration formula which can be used to integrate any function over a sphere $x^2 + y^2 + z^2 \le a^2$, I = $\int_{-a}^{a} \int_{-\sqrt{a^2-x^2}}^{\sqrt{a^2-x^2}} \int_{-\sqrt{a^2-x^2-y^2}}^{\sqrt{a^2-x^2-y^2}} f(x, y, z) dz dy dx$ (9) The domain of integration in Eq. 9 is transformed to a cuboid

$$0 < r < a, 0 < \varphi_1 < \pi, 0 < \varphi_2 < 2\pi$$

in the *r*- φ_1 - φ_2 spaceusing the transformation,
 $x = r \cos \varphi_1$,

$$y = r \sin \varphi_1 \cos \varphi_2,$$

$$z = r \sin \varphi_1 \sin \varphi_2$$

The Jacobian of transformation is

$$|J| = r^2 \sin \varphi_1 > 0$$

Hence, Eq. 9 now becomes

 $I = \int_{0}^{\infty} \int_{0}^{\pi} \int_{0}^{2\pi} r^2 \sin \varphi_1$

 $f(r \cos \varphi_1, r \sin \varphi_1 \cos \varphi_2, r \sin \varphi_1 \sin \varphi_2) d\varphi_2 d\varphi_1 dr(10)$ Next we transform the cuboid to a zero-one cube in the ξ - η - γ space using the linear transformation

 $r = a\xi, \varphi_1 = \pi\eta, \varphi_2 = 2\pi\gamma$ which gives the Jacobian as $|J| = 2\pi^2 a > 0$ $I \int_{0}^{1} \int_{0}^{1} \int_{0}^{1} 2\pi^2 a (a\xi)^2 \sin(\pi\eta) f(\bar{x}(\xi,\eta,\gamma)) d\gamma d\eta d\xi$

Applying the generalized Gaussian quadrature rule to this integral with different node points N_1 , N_2 and N_3 along each direction ξ , η and γ respectively, we approximate the integral I as

$$I \approx \sum_{i_{1}=1}^{N_{1}} \sum_{i_{2}=0}^{N_{2}} \sum_{i_{3}=1}^{N_{3}} 2\pi^{2} a^{3} (\xi_{i})^{2} \sin(\pi\eta_{j})$$

$$w_{1_{i}} w_{2_{j}} w_{3_{k}} f[a\xi_{i} \cos(\pi\eta_{j}),$$

$$a\xi_{i} \sin(\pi\eta_{j}) \cos(2\pi\gamma_{k}), a\xi_{i} \sin(\pi\eta_{j}) \sin(2\pi\gamma_{k})]$$

$$\therefore I \approx \sum_{m=1}^{N_{1}N_{2}N_{3}} c_{m} f(x_{m}, y_{m}, z_{m}) \qquad (11)$$
where $x_{m} = a\xi_{i} \cos(\pi\eta_{j}), y_{m} =$

$$a\xi_{i} \sin(\pi\eta_{j}) \cos(2\pi\gamma_{k}), z_{m} =$$

$$a\xi_{i} \sin(\pi\eta_{j}) \sin(2\pi\gamma_{k}), c_{m} = 2\pi^{2} a^{3} (\xi_{i})^{2} \sin(\pi\eta_{j}) w_{1_{i}} w_{2_{j}} w_{3_{k}} \qquad (12)$$

By taking the generalized Gaussian quadrature points in one dimension as ξ_i , η_j and γ_k and their corres-ponding weights as w_{1i} , w_{2j} and w_{3k} in Eqs. 12, we can evaluate the quadrature points (x_m, y_m, z_m) and the weight at these points c_m . Using these nodes and weights in Eq. 11, we can evaluate the integral of any function over the sphere, B_3 .

The distribution of nodal points (x_m, y_m, z_m) in a unit sphere, $x^2 + y^2 + z^2 \le 1$, is plotted in Fig.4 and results of integration of some functions over this unit sphere, using the proposed method is tabulated in Table 3.

5. Numerical Integration over n-dimensional ball

In this section, we extend our integration formula in 2-D and 3-D to n-D.

To integrate a function over an n-dimensional ball





$$B_n = \left\{ (x_1, x_2, \dots, x_n) / \sum_{i=1}^n x_i^2 \le a^2 \right\},\$$

we initially transform B_n to an n-dimensional cube

 $\begin{aligned} & \mathcal{C}_n = \{ (x_1, x_2, \dots, x_n) | 0 < r < a, 0 < \varphi_1 < \pi \\ & 0 < \varphi_2 < \pi, \dots, 0 < \varphi_{n-1} < \pi, 0 < \varphi_n < 2\pi \} \\ & \text{using the transformation, } x_1 = r \cos\varphi_1 \end{aligned}$

 $x_2 = r \sin \varphi_1 \cos \varphi_2, x_3 = r \sin \varphi_1 \sin \varphi_2 \cos \varphi_3$

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

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

The Jacobian of this transformation is

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

Hence, the integral over B_n would be

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

=
$$\int_{r=0}^{a} \int_{\varphi_1=0}^{\pi} \int_{\varphi_2=0}^{\pi} \dots \int_{\varphi_{n-2}=0}^{\pi} \int_{\varphi_{n-1}=0}^{2\pi} F d\varphi_{n-1} \dots d\varphi_2 d\varphi_1 dr$$

where, $F = f(\overline{x}(r, \varphi_1, \varphi_2, ..., \varphi_{n-1}))|J_1|$

Next, we apply a linear transformation

$$r = a\xi_1, \varphi_1 = \pi\xi_2, \varphi_2 = \pi\xi_3, ...,$$
$$\varphi_{n-2} = \pi\xi_{n-1}, \varphi_{n-1} = 2\pi\xi_n$$

to transform C_n to a zero-one n-cube,

 $\Omega = \{ (\xi_1, \xi_2, \dots, \xi_n) \mid 0 \le \xi_i \le 1, i = 1, 2, \dots, n \}.$ The Jacobian of this transformation is:

 $|J_2| = 2\pi^{n-1}a$. Now, the integral will be

$$I = \int_{\xi_1=0}^{1} \int_{\xi_2=0}^{1} \dots \int_{\xi_n=0}^{1} G d\xi_n \dots d\xi_2 d\xi_1$$

$$G = f(\overline{x}(a\xi_1, \pi\xi_2, \pi\xi_3, \dots, \pi\xi_{n-1}, 2\pi\xi_n))|J_1||J_2|$$

Taking N₁,N₂,..., N_n quadrature points along the $\xi_1, \xi_2, ..., \xi_n$ directions respectively, we get the integral as,

$$I \approx \sum_{i_1=1}^{N_1} \sum_{i_2=1}^{N_2} \dots \sum_{i_n=1}^{N_n} w_1^{i_1} w_2^{i_2} \dots w_n^{i_n}$$
$$f\left(\overline{x} \left(a\xi_1^{i_1}, \pi\xi_2^{i_2}, \pi\xi_3^{i_3}, \dots, \pi\xi_{n-1}^{i_{n-1}}, 2\pi\xi_n^{i_n}\right)\right) |J_1| |J_2|$$
where $\overline{x} = (x_1, x_2, \dots, x_n)$

$$\therefore I \approx \sum_{m=1}^{N_1 N_2 \dots N_n} c_m f(x_{1_m}, x_{2_m}, \dots, x_{n_m})$$
(12)

where,

The above set of equations gives the weights and nodes required for integration (using Eq. 12) of any function $f(x_1, x_2, ..., x_n)$ over an ndimensional ball. Table 4 gives results for the constant test function $f(x) = 2^{-n}$ for dimensions from 2 to 5 [Krishnaraj et al., 2016] over a unit n-sphere.

7. Conclusions

In this paper, we introduce a general numerical method for constructing nearly-optimal quadrature rules over an n-dimensional ball. The strength and efficiency of the formula is due to the transformation used in its derivation. Due to this transformation, the distribution of the nodal points is in a circular fashion like its boundary and this distribution leads to good numerical results over 2-dimensional ball(disc), 3-dimensional ball and n-dimensional ball. Any programming language or any mathematical software can be used to obtain the nodes, weights and the integral value of a function over an n-dimensional ball. Tabulated values in the paper show that the integration rule proposed here gives a very good accuracy for almost all functions including transcendental functions. Applications of the present method in solving boundary value problems are underway and the results will be reported in the future.

Table 2: Comparison of errors and number of function evaluations while finding the integrals using the methods in section3 and section $4f_1 = x + y$; $f_2 = sin(x + y)$; $f_3 = x^4 + y^3$; $f_4 = \frac{x^4 + y^3}{1 + x^2}$; $f_5 = -2x + 8y + 10x^2 - 12xy + 10y^2 - 12x^3 - 60xy^2 - 12y^3 + 36x^3y + 36xy^3$

	Exact solution	Method in section 3.1		Method in section 3.2	
Integrand		Absolute Error	Number of function evaluations	Absolute Error	Number of function evaluations
f_1	0	1.37E-15	20×20=400	2.80E-15	5×10=50
f_2	0	1.48E-9	20×20=400	2.09E-15	10×40=400
f_3	0.392699081698	5.79E-11	20×20=400	0	10×40=400
f_4	0.246386078944	8.12E-06	20×20=400	6.96E-10	10×40=400
f_5	15.70796326794	4.71E-11	20×20=400	4.74E-11	10×20=200

Integrand	Exact solution	Absolute Error	Number of function evaluations
$\frac{1}{2^3}$	0.5235987755982	0.3E-14	$10 \times 20 \times 20 = 4000$
$\sqrt{y^2 + z^2} exp(x/3)$	2.490326881282	5.9E-14	$10 \times 20 \times 20 = 4000$
$x\sqrt{y^2+z^2}$	0	1.6E-15	$10 \times 20 \times 20 = 4000$
$\sqrt{x^2 + y^2 + z^2}$	3.141592653589	1.3E-13	$10 \times 20 \times 20 = 4000$
$(y^2 + z^2)Cos(x)$	1.559110909311	3.1E-13	$10 \times 20 \times 20 = 4000$

Table 4:Results of integration of $f(x)=2^{-n}$ over n-sphere

Dimension(n)	Exact solution	Results using proposed method		
		Computed Value	Absolute Error	
2	0.7853981633974	0.7853981633974	4.1E-15	

3	0.5235987755983	0.5235987755983	1.9E-14
4	0.3084251375340	0.3084251375339	4.9E-14
5	0.1644934066848	0.1644934167508	1.0E-08

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