EFFECTIVE NUMERICAL INTEGRATION OVER N-DIMENSIONAL SIMPLEXES

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Abstract: This paper gives a numerical integration rule for integrating functions over an n-simplex. The rule is derived using a simple transformation of the given n-simplex to a zero-one n-cube. The proposed method is proved to be near-optimal for integration of an arbitrary function over n-simplexes. The performance of the method is illustrated for different type of integrands over different two, three, four and five simplexes.

Keywords: Numerical integration, Gaussian quadrature, n-simplex, linear transformation, Jacobian

Introduction

Evaluation of multiple integrals numerically is a challenging work in numerical analysis. At the same time such integrals appear in many fields, such as finite element methods (to calculate the stiffness matrix), in fluid mechanics, 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.

Most of the multiple integration formulae are derived by solving many systems of non-linear equations which is a very tedious procedure. Due to this difficulty, derivation of cubature rules becomes a challenge, even though these rules are effective to some extent. For this reason the formulation of quadrature rules over multidimensional regions remains an open area of research as demonstrated by many authors. The integration rule proposed in this paper doesn't require solving non-linear systems of equations, as we are deriving a product formula using the one-dimensional quadrature points given in Ma *et.al.*[1996].

In Ma *et.al.*[1996], the authors have given the generalized Gaussian quadrature rules over different functions for one-dimensional integration and proved that their results are better compared to all other quadrature rules. In Sarada and Nagaraja [2011,2012], the authors have used these generalized Gaussian quadrature rules to derive a quadrature rule over any bounded two dimensional regions. In Sarada and Nagaraja [2014], a generalized Gaussian quadrature rule over n-dimensional cubes is derived. In this paper a numerical integration formula is derived to integrate functions over n-dimensional simplexes and the generalized Gaussian quadrature rules are used for numerical evaluation.

The remainder of this paper is organized as follows: Section 2 presents the mathematical preliminaries required for understanding the derivation. Section 3 explains the derivation of the method and section 5 elucidates the numerical results. Finally, in section 6 we give the conclusions.

Mathematical Preliminaries

Numerical Integration

In numerical integration an integral is typically approximated by a weighted sum of integrand evaluations.

$$\text{I[f]} = \int_{\Omega} f(\overline{\boldsymbol{x}}) d\Omega = \sum_{i=1}^{N} w_i f(\overline{\boldsymbol{x}_i}) = \text{Q[f]} \ \text{ with } \overline{\boldsymbol{x}_i} \epsilon\ \Omega \tag{1}$$

If the dimension of the integration region d=1 the approximation in (1) is called a *quadrature formula*. If d ≥2 the approximation in (1) is called a *cubature formula*. The term *integration rule* is also used.

Generalized Gaussian quadrature

The Gaussian quadrature is a numerical integration formula given by

$$\int_a^b q(x)\phi(x)dx = \sum_{i=1}^{N} w_i \phi(x_i) \tag{2}$$

where $x_i \, \epsilon \, [a, b] \; and \; w_i \, \epsilon \, \boldsymbol{R}$, for all $i = 1, 2, \dots, N$. The points x_i and the coefficients w_i are referred to as the nodes and weights of the quadrature formula. The quadrature formula given in eq.(1) is called a classical Gaussian quadrature rule if it integrates exactly all polynomials of order upto 2N-1, whereas eq. (2) is said to be a generalized Gaussian quadrature rule with respect to a set of functions $\{\phi_1, \phi_2, \dots, \phi_{2N}\}$ if it integrates exactly all the 2N functions in the set $\{\phi_1, \phi_2, \dots, \phi_{2N}\}$.

The generalized Gaussian quadrature with respect to the set of functions $\{1, lnx, x, xlnx, \dots, x^{N-1}, x^{N-1}lnx\}$ for N = 5, 10, 15, 20, 40 are given in the table 1 of [8]. We shall be using these nodes and weights in the product formula shown in the next section.

n-Simplex

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

$$X_n = \left\{ (x_1, x_2, \dots, x_n) / \sum_{i=1}^{n} x_i \le a \, , x_i > 0 \right\}$$

Here n represents the dimension of the region X_n.

A 2-simplex is the triangle with endpoints (0,0), (a,0) and (0,a) whereas a 3-simplex is a tetrahedron with corners at (0,0,0), (a,0,0), (0,a,0) and (0,0,a).

Derivation of the numerical integration rule over n-simplex

Consider the integral,

$$I[f] = \int_{X_n} f(\overline{\boldsymbol{x}}) \boldsymbol{d} X_n \tag{3}$$

of a function $f(\overline{\boldsymbol{x}})$ over the n-simplex,

$$X_n = \left\{ (x_1, x_2, \dots, x_n) / \sum_{i=1}^{n} x_i \le a \, , x_i > 0 \right\}$$

To evaluate the integral in Eq.(3) numerically, we derive a quadrature formula by transforming X_n to a zero-one n-cube in $\xi_1 - \xi_2 - \dots \xi_n$,

$$C_n = \{(\xi_1, \xi_2, \dots, \xi_n) \mid 0 \le \xi_i \le 1, i = 1,2, \dots, n\}$$

using the transformation

$$x_1 = a\xi_1$$

$$x_2 = a(1 - \xi_1)\xi_2$$

$$x_3 = a(1 - \xi_1)\,(1 - \xi_2)\,\xi_3$$

$$\dots$$

$$x_n = a(1-\xi_1)\,(1-\xi_2)\dots\,(1-\xi_{n-1})\,\xi_n$$

The Jacobian of this transformation is

$|\,J\,| = a^n(1-\xi_1)^{n-1}\,(1-\xi_2)^{n-2}\dots\,(1-\xi_{n-2})^2\,(1-\xi_{n-1})$

Hence, the integral in Eq.(3) will now be

$$\begin{aligned} I[f] &= \int_{X_n} f(\overline{\boldsymbol{x}})\boldsymbol{d}X_n \\ &= \int_0^a \int_0^{a-x_1} \int_0^{a-x_1-x_2} \dots \int_0^{a-x_1-x_2-\dots-x_{n-1}} f(x_1, x_2, \dots, x_n)\;\, dx_n \dots dx_2 dx_1 \\ &= \int_0^1 \int_0^1 \dots \int_0^1 f(\overline{\boldsymbol{x}}(\,\bar{\xi}\,))\,|\,J\,|\;\, d\xi_n \dots d\xi_2 d\xi_1 \end{aligned}$$

After applying the generalized Gaussian quadrature rule to each directions, we get

$$I \approx \sum_{i_1=1}^{N}\sum_{i_2=1}^{N}\dots\sum_{i_n=1}^{N} w_1^{i_1} w_2^{i_2}\dots w_n^{i_n}\, f\big(\overline{\boldsymbol{x}}(\xi_1^{i_1}, \xi_2^{i_2}, \dots, \xi_n^{i_n})\big)\,|\,J\,|$$

where $\overline{\boldsymbol{x}} = (x_1, x_2, \dots, x_n)$

$$\therefore I \approx \sum_{m=1}^{N^n} c_m f(x_{1_m}, x_{2_m}, \dots, x_{n_m}) \tag{4}$$

where $c_m = w_1^{i_1} w_2^{i_2}\dots w_n^{i_n}\,|\,J\,|$

i.e. $c_m = a^n\big(1-\xi_1^{i_1}\big)^{n-1}(1-\xi_2^{i_2})^{n-2}\dots(1-\xi_{n-2}^{i_{n-2}})^2(1-\xi_{n-1}^{i_{n-1}})\, w_1^{i_1} w_2^{i_2}\dots w_n^{i_n}$ (5)

and $x_{j_m} = a\big(1-\xi_1^{i_1}\big)\big(1-\xi_2^{i_2}\big)\dots(1-\xi_{j-1}^{i_{j-1}})\,\xi_j^{i_j}$ for $j = 1, 2, \dots, n$ (6)

$\xi_1^{i_1}, \xi_2^{i_2}, \dots, \xi_n^{i_n}$ in Eqs.(5 & 6) are the node points in (0,1) and $w_1^{i_1}, w_2^{i_2}, \dots, w_n^{i_n}$ are their corresponding weights in one dimension. Any quadrature points and their corresponding 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], Sarada and Nagaraja [2011,2012, 2014] that these nodes and weights give better results compared to any other ones for integration over any bounded regions.

After applying the generalized Gaussian quadrature points and their corresponding weights in Eq.(5&6), we get the weights c_m and the nodal points $(x_{1m,}\, x_{2m}, \dots, x_{nm})$, which are used in the integration formula (Eq.(4)) for integrating a function $f(x, y)$ over the n-simplex X_n.

Numerical Results

In this section, we write the formula for integration over the 2-simplex(triangle), 3-simplex(tetrahedron), 4-simplex and 5-simplex along with numerical results.

Integration over a 2-simplex

When n=2, the simplex is a triangle in the first quadrant with endpoints (0,0),(1,0) and (0,1), the quadrature rule as derived in section 3 will be,

$$\int_{X_2} f(\overline{\boldsymbol{x}})\boldsymbol{d}X_2 = \int_0^a \int_0^{a-x_1} f(x_1, x_2)dx_2x_1 \approx \sum_{m=1}^{N^2} c_m f(x_{1_m}, x_{2_m})$$

where, $c_m = a^2(1 - \xi_1^{i_1})\, w_1^{i_1} w_2^{i_2}$

$$x_{1_m} = a\xi_1^{i_1}$$

$$x_{2_m} = a\left(1 - \xi_1^{i_1}\right)\xi_2^{i_2}$$

Integration over a 3-simplex

The 3-simplex is a tetrahedron in the first octant bounded by the XY plane, YZ plane, XZ plane and the plane $+y + z = a$. By giving n=3, in Eqs.(4), (5) and (6), we get

$$\int_{X_3} f(\overline{\boldsymbol{x}})\boldsymbol{d}X_3 = \int_0^a \int_0^{a-x_1} \int_0^{a-x_1-x_2} f(x_1, x_2, x_3)dx_3dx_2x_1 \approx \sum_{m=1}^{N^3} c_m f(x_{1_m}, x_{2_m}, x_{3_m})$$

where, $c_m = a^3(1 - \xi_1^{i_1})^2\ (1 - \xi_2^{i_2})\, w_1^{i_1} w_2^{i_2} w_3^{i_3}$

$$x_{1_m} = a\xi_1^{i_1}$$

$$x_{2_m} = a\left(1 - \xi_1^{i_1}\right)\xi_2^{i_2}$$

$$x_{3_m} = a\left(1 - \xi_1^{i_1}\right)(1 - \xi_2^{i_2})\ \xi_3^{i_3}$$

Integration over a 4-simplex

To integrate a function over the 4-simplex, the formula to be used is

$$\int_{X_4} f(\overline{\boldsymbol{x}})\boldsymbol{d}X_4 = \int_0^a \int_0^{a-x_1} \int_0^{a-x_1-x_2} \int_0^{a-x_1-x_2-x_3} f(x_1, x_2, x_3, x_4)dx_4dx_3dx_2x_1$$

$$\approx \sum_{m=1}^{N^4} c_m f(x_{1_m}, x_{2_m}, x_{3_m}, x_{4_m})$$

where, $c_m = a^4(1 - \xi_1^{i_1})^3\ (1 - \xi_2^{i_2})^2\ \ (1 - \xi_3^{i_3})\, w_1^{i_1} w_2^{i_2} w_3^{i_3} w_4^{i_4}$

$$x_{1_m} = a\xi_1^{i_1}$$

$$x_{2_m} = a\left(1 - \xi_1^{i_1}\right)\xi_2^{i_2}$$

$$x_{3_m} = a\left(1 - \xi_1^{i_1}\right)(1 - \xi_2^{i_2})\ \xi_3^{i_3}$$

$$x_{4_m} = a\left(1 - \xi_1^{i_1}\right)(1 - \xi_2^{i_2})\ (1 - \xi_3^{i_3})\ \xi_4^{i_4}$$

Integration over a 5-simplex

Substituting n=5 in the derived formula in section 3, we get the quadrature formula for integrating a function on a 5-simplex as,

$$\int_{X_5} f(\overline{\boldsymbol{x}})\boldsymbol{d}X_5 = \int_0^a \int_0^{a-x_1} \int_0^{a-x_1-x_2} \int_0^{a-x_1-x_2-x_3} \int_0^{a-x_1-x_2-x_3} f(x_1, x_2, x_3, x_4, x_5)dx_5dx_4dx_3dx_2x_1$$

$$\approx \sum_{m=1}^{N^3} c_m f(x_{1_m}, x_{2_m}, x_{3_m}, x_{4_m}, x_{5_m})$$

where, $c_m = a^5(1-\xi_1^{i_1})^4\,(1-\xi_2^{i_2})^3\,(1-\xi_3^{i_3})^2\,(1-\xi_4^{i_4})\,w_1^{i_1}w_2^{i_2}w_3^{i_3}w_4^{i_4}w_5^{i_5}$

$$x_{1_m} = a\xi_1^{i_1}$$

$$x_{2_m} = a\left(1-\xi_1^{i_1}\right)\xi_2^{i_2}$$

$$x_{3_m} = a\left(1-\xi_1^{i_1}\right)(1-\xi_2^{i_2})\,\xi_3^{i_3}$$

$$x_{4_m} = a\left(1-\xi_1^{i_1}\right)(1-\xi_2^{i_2})\,(1-\xi_3^{i_3})\,\xi_4^{i_4}$$

$$x_{5_m} = a\left(1-\xi_1^{i_1}\right)(1-\xi_2^{i_2})\,(1-\xi_3^{i_3})\left(1-\xi_4^{i_4}\right)\xi_5^{i_5}$$

Numerical Results

In this section, we provide the numerical results of integration using the proposed method for various functions over different dimensional simplex.

In the first table, we consider the constant function $f(x,y)=1$ as the integrand. The value of the integral over the n-simplex is $\frac{1}{n!}$.

Table 1:Integration of $f(\overline{x}) = 1$

Dimension	Exact integral value	Computed value	Absolute Error
2	0.5	0.500000000000001	9.9E-16
3	0.166666666666667	0.166666666666640	2.7E-14
4	0.0416666666666667	0.0416666666666516	1.5E-14
5	0.00833333333333333	0.00833333333333050	2.8E-15

In the second table we take the integrand as $f(\overline{\boldsymbol{x}}) = \sqrt{\sum_{i=1}^{n} x_i}$

Table 2: Integration of $f(\overline{x}) = \sqrt{\sum_{i=1}^{n} x_i}$

Dimension	Exact integral value	Computed value	Absolute Error
2	0.4	0.399999999999480	5.2E-13
3	0.142857142857143	0.142857142857151	8.0E-15
4	0.0370370370370370	0.0370370370370237	1.3E-14
5	0.00757575757575758	0.00757575757575657	1.0E-15

In the last table we take the integrand as $f(\overline{\boldsymbol{x}}) = \frac{1}{\sqrt{\sum_{i=1}^{n} x_i}}$

Table 3: Integration of $f(\overline{x}) = 1/\sqrt{\sum_{i=1}^{n} x_i}$

Dimension	Exact integral value	Computed value	Absolute Error
2	0.666666666666666	0.666666667673585	1.0E-09
3	0.2	0.200000000004725	4.7E-12
4	0.0476190476190476	0.0476190476190462	1.4E-15
5	0.00925925925925926	0.00925925925929113	3.1E-14

Conclusions

The proposed integration formula is very simple at the same time very effective. The knowledge of the boundaries of the simplex and the generalized Gaussian quadrature rules is sufficient to apply these quadrature rules. Most of the results obtained here are exact up to 10 decimal places and the proposed method can be used to integrate a wide class of functions including functions with end-point singularities.

Further developments of the present method and their applications in Science and Engineering fields are underway and the results will be reported in the near future.

Acknowledgement

The continuous research support and encouragement of the management of Amrita Vishwa Vidyapeetham is gratefully acknowledged.

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