Symmetric Gauss Legendre Quadrature Rules for Numerical Integration over an Arbitrary Linear Tetrahedra in Euclidean Three-Dimensional Space

K. V. Nagaraja a, H. T. Rathod b

a Department of Mathematics, Amrita School of Engineering, # 26&27 Kasavanahalli, Carmelram post, Bangalore - 560035, India
nagarajaitec123@yahoo.com

b Department of Mathematics, Bangalore University, Bangalore - 560035, India

Abstract

In this paper it is proposed to compute the volume integral of certain functions whose antiderivatives with respect to one of the variates (say either x or y or z) is available. Then by use of the well known Gauss Divergence theorem, it can be shown that the volume integral of such a function is expressible as sum of four integrals over the unit triangle. The present method can also evaluate the triple integrals of trivariate polynomials over an arbitrary tetrahedron as a special case. It is also demonstrated that certain integrals which are nonpolynomial functions of trivariates x, y, z can be computed by the proposed method. Then we have applied the symmetric Gauss Legendre quadrature rules to evaluate the typical integrals governed by the proposed method.

Mathematics Subject Classification: 65D32

Keywords: Numerical integration, quadrature rules, tetrahedron
1. Introduction

Volume, center of mass, moment of inertia and other geometric properties of rigid homogeneous solids frequently arise in a large number of engineering applications, in CAD/CAE/CAM applications in geometric modelling as well as in robotics. Integration formulas for multiple integrals have always been of great interest in computer applications, a good overview of available methods for evaluating volume integrals is given by Lee and Requicha [14]. Timmer and Stern [4] discussed a theoretical approach to the evaluation of volume integrals by transforming the volume integral to a surface integral over the boundary of the integration domain. Lien and Kajiya [13] presented an outline of a closed form formula for volume integration by decomposing the solid into a set of solid tetrahedra. Cattani and paoluzzi [1, 2] gave a symbolic solution to both the surface and volume integration of polynomials by using a triangulation of the solid boundary. In a recent paper, Bernardini [3] has presented explicit formulas and algorithms for computing integrals of polynomials over n-dimensional polyhedra by using the decomposition representation and the boundary representation of the polyhedron. Rathod and Govind Rao [5] derived explicit integration formulas for computing volume integrals of trivariate polynomials over an arbitrary tetrahedron in Euclidean three-dimensional space. They proposed two different approaches; the first method evaluates this volume integral by mapping the tetrahedron into orthogonal unit tetrahedron and the second method computes the same integral as a sum of four integrals over the unit triangle. The present work enhances the second method by considering the evaluation of some functions by use of the well known Gauss Divergence theorem.

2. Problem statement for present work

Most computational studies of triple integrals deal with problems in which the domain of integration is very simple, like a cube or a sphere, but the integrand is complicated. However, in real applications, we confront the inverse problem: the integrating function \( f(x,y,z) \) is usually simple; but the domain is very complicated. Hence in this paper and in other previous works [3, 11, 13] an attempt is made to obtain practical formulas for the exact evaluation of integrals.

\[
\iiint_V f(x,y,z) \, dV
\]

Where \( P \) is a three-polyhedron in \( \mathbb{R}^3 \) and \( dV \) is the differential volume. The integrating-function is a trivariate monomial.

\[
f(x,y,z) = x^\alpha y^\beta z^\gamma,
\]

where \( \alpha, \beta, \gamma \) are non negative integers

or
Symmetric Gauss Legendre quadrature rules

\[ f(x, y, z) = \frac{\partial F}{\partial x}, \text{ or } f(x, y, z) = \frac{\partial F}{\partial y}, \text{ or } f(x, y, z) = \frac{\partial F}{\partial z} \]

However the paper is focused on the calculation of the following integral:

\[ \iiint_V f(x, y, z) \, dV \]

Where \( f(x, y, z) = \frac{\partial F}{\partial x}, \text{ or } f(x, y, z) = \frac{\partial F}{\partial y}, \text{ or } f(x, y, z) = \frac{\partial F}{\partial z} \), for some suitable function \( F \) and \( V \) is an arbitrary tetrahedron with four vertices \((x_i, y_i, z_i)\), \((i=1,2,3,4)\). Two different approaches are possible. The first approach is direct and it transforms an arbitrary tetrahedron into an orthogonal tetrahedron by means of a mapping. The second approach is based on the fact that certain triple integrals can be reduced to surface integrals by use of the well known Gauss’s divergence theorem. This paper is concerned with the second approach.

3. Volume integration over an arbitrary tetrahedron

In this section, we first obtain the volume integral of a scalar function \( f(p) = f(x, y, z) \) \((\alpha, \beta, \gamma \text{ are positive integers})\) over an arbitrary tetrahedron by transforming it to an orthogonal unit tetrahedron. That is we are actually interested in evaluating

\[ \iiint_V f(x, y, z) \, dV \] (1)

where \( V \) is an arbitrary tetrahedron in the \(x, y, z\) Cartesian coordinate system.

We have, over the unit orthogonal tetrahedron \( \overline{V} = \{(0,0,0),(1,0,0),(0,1,0),(0,1,0)\} \) in the \(\xi, \eta, \zeta\) Cartesian coordinate system. The volume (natural) coordinates are related to Cartesian coordinates by the well-known relations [5]

\[
x = L_1x_1 + L_2x_2 + L_3x_3 + L_4x_4 \\
y = L_1y_1 + L_2y_2 + L_3y_3 + L_4y_4 \\
z = L_1z_1 + L_2z_2 + L_3z_3 + L_4z_4
\]

and \(L_1 + L_2 + L_3 + L_4 = 1\)

where \((x_i, y_i, z_i)\) refer to the Cartesian coordinates of vertex \(i\) of the tetrahedron.

Letting \(L_1 = \xi, L_2 = \eta, L_3 = \zeta\), we can rewrite the relations (2) as:

\[
x(\xi, \eta, \zeta) = x_4 + \xi x_{14} + \eta x_{24} + \gamma x_{34} \\
y(\xi, \eta, \zeta) = y_4 + \xi y_{14} + \eta y_{24} + \gamma y_{34} \\
z(\xi, \eta, \zeta) = z_4 + \xi z_{14} + \eta z_{24} + \gamma z_{34}
\]

with \(x_{ij} = x_i - x_j, y_{ij} = y_i - y_j, z_{ij} = z_i - z_j\).
If we consider the mapping (see fig.1) between the three-dimensional space \((X, Y, Z)\) and the three-dimensional space \((\xi, \eta, \zeta)\) by the parametric eqn (3), we have for the volume element
\[
dx dy dz = \left| \det J \right| d\xi d\eta d\zeta
\] (4)

where
\[
\det J = \begin{vmatrix}
(x_1 - x_4) & (x_2 - x_4) & (x_3 - x_4) \\
(y_1 - y_4) & (y_2 - y_4) & (y_3 - y_4) \\
(z_1 - z_4) & (z_2 - z_4) & (z_3 - z_4)
\end{vmatrix}
\]
\[|\det J| = 6 \times \text{volume of tetrahedron} \quad (5)
\]

So, if we change the coordinates according to eqn (3) and express consistently the volume element, we obtain
\[
\int \int \int V = \left| \det J \right| \iiint f(x(\xi, \eta, \zeta), y(\xi, \eta, \zeta), z(\xi, \eta, \zeta)) d\xi d\eta d\zeta.
\] (6)

where \(V\) is the unit orthogonal tetrahedron \(\{(0,0,0),(1,0,0),(0,1,0),(0,0,1)\}\).

Fig.1. Three-dimensional mapping of an arbitrary tetrahedron in \((X,Y,Z)\) space into an unit orthogonal tetrahedron in \((\xi, \eta, \zeta)\) space.

4. Surface integration over an arbitrary tetrahedron

**Theorem:** Let \(V\) be a three-dimensional linear tetrahedron bounded by a tetrahedral surface \(S\). Then the structure product over a linear three-tetrahedron (linear arbitrary tetrahedron in three-dimensional space) is given by the equation:
Symmetric Gauss Legendre quadrature rules

\[ III_v = \iiint_{\mathcal{V}} f(x, y, z) \, dx \, dy \, dz = \frac{\text{det} J}{\text{det} \tau} \iiint_{\mathcal{V}} \{A(u, v) - B(u, v) - C(u, v) - D(u, v)\} \, du \, dv, \]

(7)

where \( \tau \) is the unit triangle \( \{(0,0),(1,0),(0,1)\} \) in the uv-plane and \( A(u,v),B(u,v),C(u,v) \) and \( D(u,v) \) are explained in the body of the following proof of this theorem.

5. Application example

We consider some typical integrals with known exact values.

5.1 Evaluate

\[ I_1 = \int_0^1 \int_0^1 \int_0^1 \sqrt{\xi + \eta + \zeta} \, d\eta \, d\xi \, d\zeta = \int_0^1 \int_0^1 \frac{2}{3} \left[ 1 - (\xi + \eta)^3 \right] \, d\eta \, d\xi = 0.142857142857 \]

\[ I_2 = \int_0^1 \int_0^1 \int_0^1 \frac{d\xi \, d\eta \, d\zeta}{\sqrt{\xi + \eta + \zeta}} = \int_0^1 \int_0^1 2 \left[ 1 - \sqrt{\xi + \eta} \right] \, d\eta \, d\xi = 0.200000000000 \]

\[ I_3 = \int_0^1 \int_0^1 \int_0^1 \sin(\xi + 2\eta + 4\zeta) \, d\zeta \, d\eta \, d\xi \]

\[ = \int_0^1 \int_0^1 \frac{1}{4} [\cos(\xi + 2\eta) - \cos(4 - 3\xi - 2\eta)] \, d\eta \, d\xi = 0.13190232688 \]

\[ I_4 = \int_0^1 \int_0^1 \int_0^1 (1 + \xi + \eta + \zeta)^{-2} \, d\zeta \, d\eta \, d\xi \]

\[ = \int_0^1 \int_0^1 \left[ \frac{1}{3} - \frac{1}{24} \right] \, d\eta \, d\xi = 0.0208333333333333 \]

5.2 Evaluate

\[ I_{a,\beta} = \iiint_{\mathcal{V}} \frac{x^\alpha y^\beta}{\sqrt{x+y+z}} \, dx \, dy \, dz = \int_0^1 \int_0^1 \int_0^1 \left[ 10(8 - 3x + 2y)^\alpha (7 - 2x + 3y)^\beta \sqrt{(23 - 13x - 3y)} 
+ 20(10 - 2y)^\alpha (5 + 5x + 2y)^\beta \sqrt{(15 + 5x + 8y)} 
+ 20(10 - 5x - 2y)^\alpha (5 + 2y)^\beta \sqrt{(15 - 5x + 8y)} 
- 50(10 - 5x)^\alpha (5 + 5y)^\beta \sqrt{(15 - 5x + 5y)} \right] \, dx \, dy \]

(8)
6. Integration of double integrals over a triangular surface

In a recent work Rathod et al [9, 10, 11], the procedure to evaluate the double integrals over a triangular surface was discussed in great detail. We can now evaluate the triple integrals \( I_1, I_2, I_3, I_4, I_5 \) and \( I_{a,\beta} \), we find excellent convergence to the exact value in each case. The results are summarized in Tables I-II.

**Table I:** Numerical results of double integration using symmetric Gauss Legendre quadrature rules (\( n=2,3,4,\ldots,10 \))

<table>
<thead>
<tr>
<th>n</th>
<th>( I_1 )</th>
<th>( I_2 )</th>
<th>( I_3 )</th>
<th>( I_4 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>0.142 360 381</td>
<td>0.202 452 031</td>
<td>0.128 735 364</td>
<td>0.021 952 283</td>
</tr>
<tr>
<td>3</td>
<td>0.142 830 669</td>
<td>0.200 375 176</td>
<td>0.131 958 161</td>
<td>0.020 910 819</td>
</tr>
<tr>
<td>4</td>
<td>0.142 853 394</td>
<td>0.200 099 231</td>
<td>0.131 901 781</td>
<td>0.020 837 464</td>
</tr>
<tr>
<td>5</td>
<td>0.142 856 304</td>
<td>0.200 035 102</td>
<td>0.131 902 330</td>
<td>0.020 833 525</td>
</tr>
<tr>
<td>6</td>
<td>0.142 856 895</td>
<td>0.200 014 921</td>
<td>0.131 902 327</td>
<td>0.020 833 342</td>
</tr>
<tr>
<td>7</td>
<td>0.142 857 055</td>
<td>0.200 007 205</td>
<td>0.131 902 327</td>
<td>0.020 833 334</td>
</tr>
<tr>
<td>8</td>
<td>0.142 857 107</td>
<td>0.200 004 125</td>
<td>0.131 902 327</td>
<td>0.020 833 333</td>
</tr>
<tr>
<td>9</td>
<td>0.142 857 127</td>
<td>0.200 002 178</td>
<td>0.131 902 327</td>
<td>0.020 833 333</td>
</tr>
<tr>
<td>10</td>
<td>0.142 857 135</td>
<td>0.200 001 315</td>
<td>0.131 902 327</td>
<td>0.020 833 333</td>
</tr>
</tbody>
</table>

**Exact** 0.142 857 142 0.200 000 000 0.131 902 327 0.020 833 333

**Table II:** Numerical results of double integration using symmetric Gauss Legendre quadrature rules (\( n=2,3,4,\ldots,10 \))

\[
I_{a,\beta} = \iiint_{V} \frac{x^{\alpha}y^{\beta}}{\sqrt{x+y+z}} \, dx \, dy \, dz
\]

<table>
<thead>
<tr>
<th>n</th>
<th>( I_{2,1} )</th>
<th>( I_{2,2} )</th>
<th>( I_{4,4} )</th>
</tr>
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<tbody>
<tr>
<td>2</td>
<td>3796.025407</td>
<td>26476.103434</td>
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<tr>
<td>3</td>
<td>3784.408139</td>
<td>26253.172039</td>
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<td>4</td>
<td>3784.400698</td>
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<td>3784.400650</td>
<td>26253.291320</td>
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</table>
7. Conclusions

This paper proposes to compute the volume integral of certain functions whose antiderivatives with respect to one of the variates (say either x or y or z) is available. Then by use of the well known Gauss Divergence theorem, it can be shown that the volume integral of such a function is expressible as sum of four integrals over the unit triangle. The present method can also evaluate the triple integrals of trivariate polynomials over an arbitrary tetrahedron as a special case. It is also demonstrated that certain integrals which are nonpolynomial functions of trivariates x, y, z can be computed by the proposed method. We have applied symmetric Gauss Legendre Quadrature rules to evaluate the typical integrals governed by the proposed method. The results obtained are in excellent agreement with the exact value.

References


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