Analytical Formulae for Two of A. H. Stroud’s Quadrature Rules

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September 28, 2009

Abstract

Analytical formulae for the points and weights of two fifth-order quadrature rules for $C_3$, the 3-cube, are given. The rules, originally formulated by A. H. Stroud in 1967, are discussed in greater detail in terms of both the setup of the basic equations and the method of obtaining their solutions analytically. The primary purpose of this paper is to better document what we feel is a particularly practical quadrature rule (e.g. in finite element calculations) and one for which we felt comprehensive information was scarce.

Keywords: quadrature, Stroud, fifth-order rule, 3-cube

1 Introduction

In 1967, A. H. Stroud published an article [8] on fifth-degree integration formulas for several symmetric, $n$-dimensional regions. In the first sentence of Section 2 of that article, Stroud mentions that “Unless stated otherwise we assume that $n \geq 4$.” He goes on to give a general description of what is now a well-known method for determining non-product quadrature rules for several standard regions including the $n$-cube, $n$-sphere, and the entire $n$-space.

This description is followed by a number of tabulated quadrature rules for specific $n$ having about six digits of precision. A particularly interesting rule (herein referred to as “Stroud’s first rule”) is given for the 3-cube, “$C_3$”.
In the last sentence of the paper, Stroud states: “Previously no such 13 point formula was known for $C_3$.” A second rule (herein referred to as “Stroud’s second rule”) for the 3-cube, having some points outside the region, is given as well.

Unfortunately, the generic equations for the $n$-cube given by Stroud in [8] do not apply to the $n = 3$ case. This fact makes it impossible to reproduce Stroud’s tabulated results (in order to e.g. compute the points and weights to a higher precision) without investing some amount of time redoing the algebra oneself for the $n = 3$ case. In Stroud’s famous 1971 compendium on quadrature rules [9], the first rule for the 3-cube is given in additional detail: fifteen decimal digits of precision (suitable for double-precision calculations) are given for the points and weights, and an eighth-order polynomial is given for determining two of the rule parameters, but no additional guidance is given in this short table entry. Stroud’s second rule for the 3-cube is also not given in detail in [9].

In this paper we provide additional details on Stroud’s first and second rules for the 3-cube. In particular, we give analytical formulae for the points and weights, which, to our knowledge, have not been previously published. Although we came across a number of potential references for these rules [1, 2, 3, 4, 5, 7], none were found that contained exactly the information given here. The purpose of this paper is therefore to provide an accessible reference for what we feel is an especially practical rule. For example, the analytical formulae presented here are now being used in the general purpose finite element library, LibMesh [6]. The reasons for preferring an analytical solution over tabulated numerical values are obvious, chief among them being adequate precision in any computing environment, even those not yet in existence.

2 Basic Equations for Stroud’s Fifth-Order Rules for the 3-cube

Stroud’s technique for obtaining fifth-order quadrature rules for symmetric regions $R$ is summarized as follows: choose $N$ points $\nu_i$ and weights $A_i$ such that the approximation

$$\sum_{i=1}^{N} A_i f(\nu_i) \approx \int_{R} f dx$$

(1)
is exact for all monomial functions \( f := x_1^{\alpha_1}x_2^{\alpha_2}\cdots x_n^{\alpha_n} \) for which
\[
|\alpha| := \alpha_1 + \alpha_2 + \ldots + \alpha_n \leq 5 \quad (2)
\]
Due to the symmetry of the regions studied, Stroud additionally restricts the set of possible rules to only those which contain symmetric pairs of points ±\( \nu_i \) and their negatives, both having weight \( A_i \). (If \( \nu_i \) is the origin, then its negative is not included in the rule.) The rules are also restricted to have
\[
M = \frac{1}{2}(n^2 + n) + 1 \text{ distinct points. Such rules are then automatically exact for all monomials in which } |\alpha| \text{ is odd.}
\]
The condition that Eqn. (1) be exact for monomials with \( |\alpha| = 0, 2, 4 \) is then equivalent to the matrix equation
\[
X^TAX = C \quad (3)
\]
which is Stroud’s Eqn. (5), where \( A := \text{diag} (A_1, A_2, \ldots, A_M) \), \( X \) contains various (quadratic) products of the \( \nu_i \), and \( C \) contains corresponding exact monomial integrals for the given region. (The reader should refer to [8] for additional details.) Assuming \( C \) is non-singular, we can take inverses and thus Eqn. (3) is equivalent to
\[
XC^{-1}X^T = A^{-1} \quad (4)
\]
which is Stroud’s Eqn. (7). Finally, Stroud chooses the \( M \) points and weights in a special way by taking (for the particular case \( n = 3, M = 7 \))
\[
\nu_1 = (\eta, \eta, \eta) \quad \text{weight } A
\]
\[
\nu_2 = (\lambda, \xi, \xi) \quad \nu_3 = (\xi, \lambda, \xi) \quad \nu_4 = (\xi, \xi, \lambda) \quad \text{weight } B
\]
\[
\nu_5 = (\mu, \mu, \gamma) \quad \nu_6 = (\mu, \gamma, \mu) \quad \nu_7 = (\gamma, \mu, \mu) \quad \text{weight } C
\]
With this special choice of points, and taking \( \eta := 0 \), Eqn. (4) has the left-hand side
\[
XC^{-1}X^T = \begin{bmatrix}
19 & M_1^T(\lambda, \xi) & M_1^T(\gamma, \mu) \\
M_1(\lambda, \xi) & M_2(\lambda, \xi) & M_3 \\
M_1(\gamma, \mu) & M_3 & M_2(\gamma, \mu)
\end{bmatrix} \quad (5)
\]
and the right-hand side

\[ A^{-1} = 32 \text{diag} \left( A^{-1}, B^{-1}, B^{-1}, B^{-1}, C^{-1}, C^{-1}, C^{-1} \right) \]  

(6)

We have added extra horizontal and vertical lines to the matrix given in Eqn. (5) to emphasize the symmetric sub-structure present in the governing equations. In Eqns. (5) and (6) we have also introduced the following submatrices:

\[ \mathbf{M}_1(x, y) := \begin{bmatrix} m_1 \\ m_1 \\ m_1 \end{bmatrix}, \quad m_1(x, y) := 19 - 15x^2 - 30y^2 \]  

(7)

\[ \mathbf{M}_2(x, y) := \begin{bmatrix} m_2 & m_3 & m_3 \\ m_3 & m_2 & m_3 \\ m_3 & m_3 & m_2 \end{bmatrix}, \quad m_2(x, y) := 45x^4 - 30x^2 - 60y^2 + 126y^2 + 72x^2y^2 + 19 \]  

(8)

\[ m_3(x, y) := 45y^4 - 30x^2 - 60y^2 + 126x^2y^2 + 72xy^3 + 19 \]  

(9)

\[ \mathbf{M}_3 := \begin{bmatrix} m_4 & m_4 & m_5 \\ m_4 & m_5 & m_4 \\ m_5 & m_4 & m_4 \end{bmatrix}, \quad m_4 := 45\xi^2\mu^2 - 30\xi^2 + 45\mu^2\lambda^2 - 15\lambda^2 + 45\gamma^2\xi^2 + 36\lambda\xi\mu^2 \\
+ 36\xi^2\mu\gamma + 36\lambda\xi\mu\gamma - 30\mu^2 - 15\gamma^2 + 19 \]  

(10)

\[ m_5 := 126\xi^2\mu^2 - 30\xi^2 + 45\gamma^2\lambda^2 - 15\lambda^2 + 72\lambda\xi\mu\gamma \\
- 30\mu^2 - 15\gamma^2 + 19 \]  

(11)

The special form assumed for the quadrature points and weights has reduced the size of the original system of equations quite drastically, from \( 7^2 = 49 \) equations to fewer than 10.
3 Analytical Solution of the Equations

The equations defined by $M_1$ and $M_2$ may be used to determine all possible solutions for the triplets $(\lambda, \xi, B)$ and $(\gamma, \mu, C)$ independently and simultaneously. The following procedure is used: we rearrange Eqn. (7) to solve for $y$ (resp. $x$) and insert it into the $m_3$ equation, (9). Since the equation for $m_3$ has odd powers of both $x$ and $y$, we obtain two possible forms of the $m_3$ equation: one for the positive square root of $x$ (resp. $y$) and one for the negative square root. Setting the product of the positive- and negative-root versions of Eqn. (9) equal to zero leads to an eighth-order polynomial equation in $x$ (resp. $y$) which is equivalent to a quartic polynomial equation in $x^2$ (resp. $y^2$). We can solve this quartic equation for $x^2$ (resp. $y^2$) analytically, and, finally, the resulting $(x^2, y^2)$ pairs may be substituted into the $m_2$ equation, (8) to solve for the weights.

The eighth-order polynomial in $x$ (quartic in $x^2$) arising from the previously-described procedure is given by

$$1330425x^8 - 3108780x^6 + 2339622x^4 - \frac{2828796}{5} x^2 + 361 = 0 \quad (12)$$

while the eighth-order equation for $y$ is

$$53217y^8 - \frac{363204}{5} y^6 + \frac{833454}{25} y^4 - \frac{30324}{5} y^2 + 361 = 0 \quad (13)$$

We can use any suitable CAS to solve Eqn. (12) and obtain the four solutions of $x^2$ (recall that our generic $x$ variable corresponds to either $\lambda$ or $\gamma$) analytically. The result is

$$x^2 = \{x_{1,2}^2, x_{3,4}^2\}$$

$$= \left\{ \frac{1919 + 148\sqrt{19} \pm 4t_-}{3285}, \frac{1919 - 148\sqrt{19} \pm 4t_+}{3285} \right\} \quad (14)$$

where the short-hand notation

$$t_\pm := \sqrt{71440 \pm 6802\sqrt{19}}$$

is used, and will also be used throughout this paper. In Eqn. (14) and those which follow, for any quantity with an $i, j$ subscript and an ambiguous “±”
sign, the \(i\) subscript always refers to the top sign throughout the equation, while the \(j\) subscript refers to the bottom sign.

In a similar manner, we obtain the following analytical solutions for \(y^2\) (recall that our generic \(y\) variable corresponds to either \(\xi\) or \(\mu\)) by solving Eqn. (13)

\[
y^2 = \begin{cases} y_{1,2}^2, & y_{3,4}^2 \\
\frac{1121 - 74\sqrt{19} \mp 2t_-}{3285}, & \frac{1121 + 74\sqrt{19} \mp 2t_+}{3285}
\end{cases}
\] (16)

(Note: we have ordered the \(x_i^2\) and \(y_i^2\) solutions such that pairs \((x_i, y_i)\) satisfy the \(m_1\) equation (7).) We can now substitute the \((x_i, y_i)\) pairs given above into the generic \(m_2\) equation (repeated here)

\[
45x^4 - 30x^2 - 60y^2 + 126y^4 + 72x^2y^2 + 19 = 32w^{-1}
\] (17)

to solve for the generic weights \(w\). The weights \(w_i\) (which we have already scaled by \(\frac{1}{2}\), since each weight solved for in Eqn. (17) is actually twice the true value) correspond to the \(B\) and \(C\) parameters in the original equations, and are given by

\[
w = \begin{cases} w_{1,2}, & w_{3,4} \\
\frac{133225}{260072 + 1520\sqrt{19} \pm (133 + 37\sqrt{19}) t_-}, & \frac{133225}{260072 - 1520\sqrt{19} \pm (133 - 37\sqrt{19}) t_+}
\end{cases}
\] (18)

Upon simplification, the \(m_5\) equation, (11) yields

\[
126\xi^2\mu^2 + 45\gamma^2\lambda^2 + 72\lambda\xi\mu\gamma + 19 = 0
\] (19)

This implies that exactly one of the four parameters \(\lambda, \xi, \mu, \gamma\) must be negative. (Note: Conversely, three of the four parameters could instead be negative, but since the rule always includes a point and its negative, this is equivalent to one of the four parameters being negative.) This means that, when taking square roots of the \(x^2\) and \(y^2\) values obtained previously, exactly one negative root must be selected. In both of his rules, Stroud [8] has
selected $\xi$ as the negative root, and we shall follow the same convention here. Using the rest of Stroud’s tabulated results as a guide, we have compiled Table 1, which gives the corresponding analytically-obtained $x_i$, $y_i$, and $w_i$ values. It may of course be verified that these analytical values also satisfy Eqns. (10) and (11).

Table 1: The middle column gives numerical approximations to the analytical results obtained in this section, for reference. In the right-hand column, we give the corresponding parameter originally obtained by Stroud [8]. The 1 and 2 subscripts in the third column correspond to the first (with all points inside the region) and second (with some points outside the region) rules reported by Stroud.

| $x_1$ | 1.0146309695 | $\gamma_2$ |
|-------|---------------|-------------|
| $x_2$ | 0.7291297984 | $\lambda_2$ |
| $x_3$ | 0.8803044067 | $\lambda_1$ |
| $x_4$ | 0.0252937117 | $\gamma_1$ |
| $y_1$ | 0.3443767286 | $\mu_2$ |
| $y_2$ | 0.6062327951 | $-\xi_2$ |
| $y_3$ | 0.4958481715 | $-\xi_1$ |
| $y_4$ | 0.7956214222 | $\mu_1$ |
| $w_1$ | 0.4075948702 | $C_2$ |
| $w_2$ | 0.6450367090 | $B_2$ |
| $w_3$ | 0.5449873514 | $B_1$ |
| $w_4$ | 0.5076442277 | $C_1$ |

4 Summary

To summarize the analytical results reported, we give both numerical approximations and analytical forms for the various parameters in this section. In Tables 2 and 3 the numerical and analytical values, respectively, for Stroud’s first quadrature rule are given. The numerical approximations are given to 32
digits of accuracy for convenience and because in the case of the second rule, such highly-accurate values have not been previously published. Stroud’s second fifth-order rule (which is less useful for finite element calculations due to the fact that some of the points lie outside the region of integration) is likewise summarized in Tables 4 and 5.

Table 2: Values for Stroud’s first fifth order quadrature rule for the 3-cube, originally reported in [8], to 32 decimal digits.

|    | 0.00000000000000000000000000000000E+00 |
|----|-----------------------------------|
| η  | 8.80304406699309780477378182098603E−01 |
| λ  | −4.9584817142571152814212423642879E−01 |
| ξ  | 7.95621422164095415429824825675787E−01 |
| μ  | 2.52937117448425813473892559293236E−02 |
| γ  | 1.68421052631578947368421052631579E+00 |
| A  | 5.44987351277576716846907821808944E−01 |
| C  | 5.07644227669791704205723757138424E−01 |
Table 3: Analytical representations for Stroud’s first fifth order quadrature rule for the 3-cube, originally reported in [8]. The results correspond to the numerical approximations given in Table 2. When taking the square root, the positive root is always assumed unless specified otherwise.

|   |   |   |
|---|---|---|
| $\eta$ | 0 | $\sqrt{1919 - 148\sqrt{19} + 4t_+}$ |
| $\lambda$ | $\sqrt{\frac{1121 + 74\sqrt{19} - 2t_+}{3285}}$ | $\sqrt{\frac{1121 + 74\sqrt{19} + 2t_+}{3285}}$ |
| $\xi$ | $\sqrt{\frac{1919 - 148\sqrt{19} - 4t_+}{3285}}$ | $\sqrt{\frac{1919 - 148\sqrt{19} - 4t_+}{3285}}$ |
| $\mu$ | $\sqrt{\frac{1919 - 148\sqrt{19} + 4t_+}{3285}}$ | $\sqrt{\frac{1919 - 148\sqrt{19} + 4t_+}{3285}}$ |

$A = \frac{32}{19}$

$B = \frac{133225}{260072 - 1520\sqrt{19} + (133 - 37\sqrt{19})t_+}$

$C = \frac{133225}{260072 - 1520\sqrt{19} - (133 - 37\sqrt{19})t_+}$

$t_\pm := \sqrt{71440 \pm 6802\sqrt{19}}$
Table 4: More accurate values for Stroud’s second fifth order quadrature rule for the 3-cube, originally reported in [8], to 32 decimal digits.

| Symbol | Value                                      |
|--------|--------------------------------------------|
| $\eta$ | 0.00000000000000000000000000E+00           |
| $\lambda$ | 7.29129798350178619517304350180274E−01     |
| $\xi$  | −6.06232795147414690867819787871004E−01    |
| $\mu$  | 3.44376728634554308789703229927940E−01      |
| $\gamma$ | 1.01463096947441524044348381753366E+00     |
| $A$    | 1.68421052631578947368421052631579E+00     |
| $B$    | 6.45036708927015064146303620658267E−01     |
| $C$    | 4.07594870020353356906327958289101E−01     |
Table 5: Analytical representations for Stroud’s second fifth-order quadrature rule for the 3-cube, originally reported in [8]. The results correspond to the numerical approximations given in Table 4. When taking the square root, the positive root is always assumed unless specified otherwise.

| Symbol | Expression |
|--------|------------|
| η      | 0          |
| λ      | $\sqrt{\frac{1919 + 148\sqrt{19} - 4t_-}{3285}}$ |
| ξ      | $-\sqrt{\frac{1121 - 74\sqrt{19} + 2t_-}{3285}}$ |
| μ      | $\sqrt{\frac{1121 - 74\sqrt{19} - 2t_-}{3285}}$ |
| γ      | $\sqrt{\frac{1919 + 148\sqrt{19} + 4t_-}{3285}}$ |

| A      | $\frac{32}{19}$ |
|--------|-----------------|
| B      | $\frac{133225}{260072 + 1520\sqrt{19} - (133 + 37\sqrt{19}) t_-}$ |
| C      | $\frac{133225}{260072 + 1520\sqrt{19} + (133 + 37\sqrt{19}) t_-}$ |

$t_\pm := \sqrt{\frac{71440 \pm 6802\sqrt{19}}{11}}$
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