Approximate Integration Formulas of Degree 3 for Simplexes

By A. H. Stroud

1. Introduction. Here we consider approximate integration formulas of the form

\[ \int_{S_n} \cdots \int f(x_1, \cdots, x_n) \, dx_1 \cdots dx_n \simeq \sum_{i=1}^{N} A_i f(p_i) \]

where \( S_n \) is an \( n \)-dimensional simplex (a triangle for \( n = 2 \); a tetrahedron for \( n = 3 \)). The \( A_i \) are constants and the \( p_i = (p_{i1}, p_{i2}, \cdots, p_{in}) \) are points in the space. The formulas we consider all have degree 3, that is they are exact whenever \( f \) is a polynomial, in the \( n \) variables, of degree \( \leq 3 \).

We show how to obtain such formulas in which all the \( A_i \) are equal and which contain \( N = n(n + 1) \) points. This can be done for all \( n \geq 2 \). For \( 2 \leq n \leq 8 \) such formulas exist with all the points interior to \( S_n \). For \( n \geq 9 \), however, the formulas have the undesirable feature that all the points are exterior to \( S_n \).

Other formulas of degree 3 with unequal coefficients are known for \( S_n \). Hammer and Stroud [1] give a formula using \( n + 2 \) points and Stroud [3] gives a formula with \( 2n + 3 \) points. By the method described in [4] formulas of degree 3 can be constructed using \( 2^n \) points. Since the only previously known formulas, with all positive coefficients, of degree 3 for \( S_n \) were the \( 2^n \) point formulas, the ones given here become the formulas with the fewest points with this property (for \( n \geq 5 \)). (The \( (n + 2) \)-point formula has one negative coefficient for \( n \geq 2 \); the \( (2n + 3) \)-point formula has one negative coefficient for \( n \geq 4 \). Formulas of degree 3 are known for the \( n \)-dimensional cube and sphere which have \( 2^n \) points with equal coefficients [2].)

To develop the formulas below we use the special simplex \( S_n \) with vertices

\[
\begin{align*}
(0, 0, 0, & \cdots, 0) \\
(1, 0, 0, & \cdots, 0) \\
(0, 1, 0, & \cdots, 0) \\
(0, 0, 0, & \cdots, 1).
\end{align*}
\]

For this simplex the monomial integrals are

\[
\int_{S_n} \cdots \int x_1^{a_1} \cdots x_n^{a_n} \, dx = \frac{a_1! \cdots a_n!}{(n + a_1 + \cdots + a_n)!}.
\]

2. The Triangle. Before discussing higher values of \( n \), \( n \geq 3 \), we first discuss the somewhat special case \( n = 2 \).

We wish to construct an approximate integration formula of degree 3 for \( S_2 \) with 6 points in which the coefficients \( A_i \) are equal:

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\[ A_1 = A_2 = \cdots = A_6 = A. \]

We will seek such a formula using the following points

\[(v_1, v_2), \quad (v_1, v_3), \quad (v_2, v_3), \]
\[(v_2, v_1), \quad (v_3, v_1), \quad (v_3, v_2), \]

where

\[ v_1 + v_2 + v_3 = 1, \quad 0 \leq v_i \leq 1, \quad i = 1, 2, 3. \]

It should be noted that this set of points maps onto itself under any linear transformation of \( S_2 \) onto itself.

If these points are to form the desired integration formula the following equations must be satisfied:

\[(1) \quad 6A = \frac{1}{2} = \int_{S_2} dx, \]
\[(2) \quad 2A[v_1 + v_2 + v_3] = \frac{1}{6} = \int_{S_2} x_i dx, \]
\[(3) \quad 2A[v_1^2 + v_2^2 + v_3^2] = \frac{2}{24} = \int_{S_2} x_i^2 dx, \]
\[(4) \quad 2A[v_1 v_2 + v_1 v_3 + v_2 v_3] = \frac{1}{24} = \int_{S_2} x_1 x_2 dx, \]
\[(5) \quad 2A[v_1^3 + v_2^3 + v_3^3] = \frac{6}{120} = \int_{S_2} x_i^3 dx, \]
\[(6) \quad A[v_1 v_2^2 + v_1 v_3^2 + v_2 v_3^2 + v_1 v_3^2 + v_2 v_3^2 + v_1 v_2] = \frac{2}{120} = \int_{S_2} x_i^2 x_j dx. \]

Here \( i, j = 1, 2 \) and \( i \neq j \). We must then have

\[ A = \frac{1}{2}, \]
\[ v_1 + v_2 + v_3 = 1, \]
\[ v_1 v_2 + v_1 v_3 + v_2 v_3 = \frac{1}{4}, \]
\[ v_1 v_2 v_3 = \frac{1}{8}. \]

This last equation follows from

\[ (\sum v_i)^3 - 3 \sum v_i^2 v_j - \sum v_i^3 = 1 - 3(\frac{1}{8}) - \frac{1}{8} = \frac{1}{8} = 6v_1 v_2 v_3. \]

It is not difficult to show that if equations (7), (8) and (9) are satisfied then (3), (5) and (6) are also satisfied. For example, to verify (6):

\[ \sum v_i \sum v_i v_j - 3v_1 v_2 v_3 = \frac{1}{4} - \frac{1}{8} = \frac{1}{8} = \sum v_i^2 v_j. \]

This shows that \( v_1, v_2, v_3 \) must be the zeros of

\[ P_3(x) = x^3 - x^2 + \frac{1}{4}x - \frac{1}{8}. \]

These zeros are irrational; their approximate values will be given in the next section.
3. Higher $n$. We now seek an approximate integration formula for $S_n$, $n \geq 3$, with equal coefficients by selecting a point

$$\nu = (\nu_1, \nu_2, \cdots, \nu_n)$$

in the simplex and taking, together with this point, the set $F$ of all points $\nu$ maps into under the symmetric group $G_n$ of all linear transformations of $S_n$ onto itself. Since $G_n$ contains $(n + 1)!$ transformations the set $F$ contains $(n + 1)!$ points (including $\nu$). This is true if all the coordinates $\nu_1, \nu_2, \cdots, \nu_n$ are distinct; if $k$ of the $\nu_i$ are equal then $F$ contains $(n + 1)!/k!$ points.

At first we assume that all the $\nu_i$, $i = 1, 2, \cdots, n$, are distinct, but later we will choose some of them to be equal.

Another way to describe the set of points $F$ is to take real numbers $\nu_1, \nu_2, \cdots, \nu_{n+1}$ for which

$$\nu_1 + \nu_2 + \cdots + \nu_{n+1} = 1$$

and take as the points in $F$ points

$$(\nu_1, \nu_2, \cdots, \nu_{n-2}, \nu_{n-1}, \nu_n),$$

$$(\nu_1, \nu_2, \cdots, \nu_{n-2}, \nu_{n-1}, \nu_{n+1}),$$

$$(\nu_1, \nu_2, \cdots, \nu_{n-2}, \nu_n, \nu_{n+1}),$$

$$(\nu_1, \nu_2, \cdots, \nu_{n-1}, \nu_n, \nu_{n+1}),$$

$$(\nu_2, \nu_3, \cdots, \nu_{n-1}, \nu_n, \nu_{n+1}),$$

$$(\nu_1, \nu_2, \cdots, \nu_{n-2}, \nu_{n-1}, \nu_n),$$

together with all points which can be obtained from any one of these by all possible permutations of its coordinates. That is each of the $n + 1$ points give rise to $n!$ points for a total of $(n + 1)!$.

If the points in $F$ are to be an integration formula of degree 3 for $S_n$ in which the coefficients are all equal, then the following seven equations must be satisfied:

\begin{align*}
(10) & \quad (n + 1)! A = \frac{1}{n!} = \int_{S_n} dx, \\
(11) & \quad n! A[\nu_1 + \nu_2 + \cdots + \nu_{n+1}] = \frac{1}{(n + 1)!} = \int_{S_n} x_i dx, \\
(12) & \quad n! A[\nu_1^2 + \nu_2^2 + \cdots + \nu_{n+1}^2] = \frac{2}{(n + 2)!} = \int_{S_n} x_i^2 dx, \\
(13) & \quad 2(n - 1)! A[\nu_1 \nu_2 + \nu_1 \nu_3 + \cdots + \nu_n \nu_{n+1}] = \frac{1}{(n + 2)!} = \int_{S_n} x_i x_j dx, \\
(14) & \quad n! A[\nu_1^3 + \nu_2^3 + \cdots + \nu_{n+1}^3] = \frac{6}{(n + 3)!} = \int_{S_n} x_i^3 dx, \\
& \quad (n - 1)! A[\nu_1 \nu_2 + \nu_1 \nu_3 + \nu_2 \nu_3 + \cdots + \nu_n \nu_{n+1} + \nu_n^2 \nu_{n+1}] = \frac{2}{(n + 3)!} = \int_{S_n} x_i^2 x_j dx.
\end{align*}
\[6(n - 2)! \ A[v_1 v_2 v_3 + v_1 v_2 v_4 + \cdots + v_{n-1} v_n v_{n+1}] \]

(16)

\[= \frac{1}{(n + 3)!} = \int_{S_n} x_1 x_2 x_n \, dx.\]

Then \( A = 1/[n!(n + 1)!] \) and to solve the remainder of the equations for the \( v_i \) we seek these to satisfy (11), (13) and (16), that is

\[v_1 + v_2 + \cdots + v_{n+1} = 1,\]

\[v_1 v_2 + v_1 v_3 + \cdots + v_n v_{n+1} = \frac{n}{2(n + 2)},\]

\[v_1 v_2 v_3 + \cdots + v_{n-1} v_n v_{n+1} = \frac{n(n - 1)}{6(n + 2)(n + 3)}.\]

If these equations are satisfied then, as for \( n = 2 \), it is easy to verify that (12), (14) and (15) are also satisfied.

This shows that the \( v_i, i = 1, \ldots, n + 1 \), must be the zeros of a polynomial

\[P_{n+1}(x) = x^{n+1} - x^n + \frac{n}{2(n + 2)} x^{n-1} - \frac{n(n - 1)}{6(n + 2)(n + 3)} x^{n-2} + k_{n-2} x^{n-3} + \cdots + k_1 x + k_0.\]

We now seek a polynomial of this type with all real zeros with the property that \( n - 1 \) of the zeros are equal. If \( P_{n+1}(x) \) is to have a zero \( v_1 \) of multiplicity \( n - 1 \) then \( v_1 \) must also be a zero of

\[P^{(n-2)}_{n+1}(x) = (n + 1)x^3 - 3x^2 + \frac{3}{n + 2} x - \frac{1}{(n + 2)(n + 3)}\]

and then

\[P_{n+1}(x) = (x - v_1)^{n-1}(x^2 - bx + c),\]

\[b = 1 - (n - 1)v_1,\]

\[c = \frac{n}{2(n + 2)} - (n - 1)v_1 + \frac{n(n - 1)}{2} v_1^2.\]

Let \( v_n, v_{n+1} \) denote the zeros of \( x^2 - bx + c \). We can now construct formulas for various values of \( n \). In principle for each \( n \) there should be 3 such formulas, one corresponding to each zero of (17). Since we will not admit points with complex coordinates this will be true only if \( v_1 \) and the corresponding \( v_n, v_{n+1} \) are real.

In Table 1 we tabulate these real solutions for certain \( n \). Equation (17) always has 3 real zeros, but the largest of these always gives complex values for \( v_n, v_{n+1} \).

For \( n \geq 9 \) the smallest zero of (17) also gives complex \( v_n, v_{n+1} \). For \( 3 \leq n \leq 8 \) there are 2 real solutions and for \( 5 \leq n \leq 8 \) one of these gives a formula for \( S_n \) with all points exterior to \( S_n \) (since \( v_n \) is negative). For \( n \geq 9 \) the single solution also is exterior to \( S_n \).

We will not carry out proofs, for all large \( n \), of these statements about the behavior of the three possible solutions. We have verified, by computation, that they
Table 1
Coordinates of Points in Approximate Integration Formulas

<table>
<thead>
<tr>
<th>n</th>
<th>(v_1)</th>
<th>(v_n)</th>
<th>(v_{n+1})</th>
</tr>
</thead>
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<tr>
<td>2</td>
<td>0.1090390091</td>
<td>0.231933368</td>
<td>0.659027624</td>
</tr>
<tr>
<td>3</td>
<td>0.09484726491</td>
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<td>0.5690284733</td>
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<tr>
<td>4</td>
<td>0.1881284504</td>
<td>0.05236466588</td>
<td>0.5713784333</td>
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<td>5</td>
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<td>0.2460180205</td>
<td>0.5015684822</td>
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<tr>
<td>6</td>
<td>0.1582718214</td>
<td>0.01736377592</td>
<td>0.5078207600</td>
</tr>
<tr>
<td>7</td>
<td>0.07573830688</td>
<td>0.2489442226</td>
<td>0.4481025499</td>
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<tr>
<td>8</td>
<td>0.1366074267</td>
<td>0.250852934</td>
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<td>9</td>
<td>0.06760619726</td>
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<td>10</td>
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<td>500</td>
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<tr>
<td>1000</td>
<td>0.04478490125</td>
<td>-0.06983053166</td>
<td>0.2189172279</td>
</tr>
</tbody>
</table>

are true for \(n \leq 1000\). Proofs could be given based on estimates for the zeros of (17). For example, the middle zero of (17) lies in the interval \((n + 3)^{-1} < x < (n + 2)^{-1}\) and in this interval \(c < 0\) (for large \(n\)) which means \(b^2 - 4c > 0\) and \(v_n < 0\).

The values for \(n = 2\) are those found in the previous section. However, if \(n = 2\) is substituted in (17) and in the expressions for \(b\) and \(c\) we arrive at the same results.

4. Relationship to Orthogonal Polynomials. We will show that the \(n(n + 1)\) points in any one of the formulas described above can be considered as the complete solution of a certain system of \(n\) polynomial equations which have a certain orthogonality property.

First consider the case \(n = 2\). The 6 points in the constructed formula are the solution of the simultaneous equations

\[ P_1(x_1) = (x_1 - v_1)(x_1 - v_2)(x_1 - v_3) = 0, \]
\[ P_2(x_1, x_2) = x_1^2 + x_2^2 + x_1x_2 - x_1 - x_2 + \frac{1}{4} = 0. \]

(The easiest way to show that this is true is to assume a \(P_2\) with this property can be found of the form

\[ P_2(x_1, x_2) = a(x_1^2 + x_2^2) + bx_1x_2 + c(x_1 + x_2) + \frac{1}{4}. \]

Then we must have

\[ P_2(v_1, v_2) = P_2(v_1, v_3) = P_2(v_2, v_3) = 0. \]
and using equations (7), (8), (9) it can be shown that $P_2$ has coefficients $a = b = -c = 1$.) Since the points in the formula are zeros of both $P_1$ and $P_2$ it is immediately obvious that these polynomials satisfy the orthogonality conditions

$$\int_{s_2} P_1(x_1) \, dx = 0,$$

$$\int_{s_2} P_2(x_1, x_2) Q(x_1, x_2) \, dx = 0$$

where $Q$ is any polynomial of degree zero or one.

In a similar way we can show that for $n = 3$ the points in each of the two distinct formulas are the solution of a system of the form

$$P_1(x_1) = 0,$$

$$P_2(x_1, x_2) = 0,$$

$$P_3(x_1, x_2, x_3) = 0$$

where $P_1$, $P_2$ have degree 3 and $P_3$ has degree 2. To do this we take polynomials of the form

$$P_1(x_1) = (x_1 - v_1)(x_1 - v_2)(x_1 - v_3),$$

$$P_2(x_1, x_2) = (x_2 - v_1)[a_2(x_1^2 + x_2^2) + b_2x_1x_2 + c_2(x_1 + x_2) + 1],$$

$$P_3(x_1, x_2, x_3) = a_3(x_1^2 + x_2^2 + x_3^2) + b_3(x_1x_2 + x_1x_3 + x_2x_3) + c_3(x_1 + x_2 + x_3) + 1$$

and calculate the unknown coefficients in $P_2$ and $P_3$ by the requirements

$$P_2(v_1, v_2) = P_2(v_1, v_3) = P_2(v_2, v_3) = 0,$$

$$P_3(v_1, v_2, v_3) = P_3(v_1, v_2, v_4) = P_3(v_1, v_3, v_4) = 0.$$

A proof that the 12 points in the integration formula satisfy the resulting system of equations, and that there are no other solutions, can be made by simply enumerating all possible solutions. As before, it is obvious that $P_1$ and $P_2$ are orthogonal to any polynomial of degree zero and that $P_3$ is orthogonal to any polynomial of degree zero or one.

The generalization to arbitrary $n$ is now almost obvious. The $n(n + 1)$ points in the constructed formula are the solution of a system

$$P_1(x_1) = 0,$$

$$P_2(x_1, x_2) = 0,$$

$$\hdots$$

$$P_{n-1}(x_1, \cdots, x_{n-1}) = 0,$$

$$P_n(x_1, x_2, \cdots, x_n) = 0,$$

where $P_1$, $\cdots$, $P_{n-1}$ have degree 3 and $P_n$ has degree 2. These polynomials are constructed as follows:
\[ P_1(x_1) = (x_1 - v_1)(x_1 - v_n)(x_1 - v_{n+1}), \]

\[ P_k(x_1, \ldots, x_k) = (x_k - v_1) \left[ a_k \sum_{i=1}^{k} x_i^2 + b_k \sum_{i,j=1}^{k} x_i x_j + c_k \sum_{i=1}^{k} x_i + 1 \right], \quad k = 2, 3, \ldots, n - 1, \]

\[ P_n(x_1, \ldots, x_n) = a_n \sum_{i=1}^{n} x_i^2 + b_n \sum_{i,j=1}^{n} x_i x_j + c_n \sum_{i=1}^{n} x_i + 1 \]

where the unknown coefficients \( a_k, b_k, c_k, k = 2, \ldots, n \) are found by the requirements that

\[ P_k(v_1, \ldots, v_n) = P_k(v_1, \ldots, v_1, v_{n+1}) = P_k(v_1, \ldots, v_n, v_{n+1}) = 0, \quad k = 2, 3, \ldots, n. \]

The proof can be made by induction on \( n \). Assuming that the form of the solution is correct for order \( n - 1 \), then all possible solutions of the \( n \)th order system can also be enumerated (which we will not do) and thus it can be shown that the result is also true for order \( n \). \( P_1, \ldots, P_{n-1} \) are orthogonal to any polynomial of degree zero and \( P_n \) is orthogonal to any polynomial of degree zero or one.

5. Concluding Remarks. As a simple example of the application of these integration formulas let us evaluate numerically the integral

\[ \int_{\mathbb{S}_3} (1 + x_1 + x_2 + x_3)^{-4} \, dx = \frac{1}{16} \approx 0.0208333333. \]

Here \( n = 3 \) and in addition to the two 12-point formulas given in Table 1 above we also use for comparison the formulas of degree 3 given in [1], [3] and [4] mentioned in the introduction. The results are summarized below:

<table>
<thead>
<tr>
<th>Approximation to (18)</th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>First formula of Table 1.</td>
<td>0.0206178943</td>
</tr>
<tr>
<td>Second formula of Table 1.</td>
<td>0.0206308008</td>
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<tr>
<td>Formula of [1], 5 points.</td>
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<td>Formula of [3], 8 points.</td>
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<td>Formula of [4], 8 points.</td>
<td>0.0206454784</td>
</tr>
</tbody>
</table>

It should be noted that the third degree formula of [3] involves, in principle, \( 2n + 3 = 9 \) points for \( n = 3 \). For \( n = 3 \), however, one of the coefficients reduces to zero so, in effect, there are only 8 points.

In a certain sense the \( n(n+1) \)-point formulas developed here are a generalization of the classical Gaussian 2-point formula of degree 3 for a one-dimensional interval. The most obvious similarity between these formulas is that in each case the formula has all equal coefficients and in each case the formula is mapped onto itself under all linear transformations of the region onto itself. The \( n(n+1) \)-point formulas, however, do not have the property of having a minimal number of points as is true of the Gaussian formula.

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