Approximate Integration Formulas of Degree 3 for Simplexes

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

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

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 $\leqq 3$.

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 $n \geqq 2$. For $2 \leqq n \leqq 8$ such formulas exist with all the points interior to S_n. For $n \geqq 9$, 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 $n \geqq 5$). (The $(n + 2)$-point formula has one negative coefficient for $n \geqq 2$; the $(2n + 3)$-point formula has one negative coefficient for $n \geqq 4$. Formulas of degree 3 are known for the n-dimensional cube and sphere which have $2n$ points with equal coefficients [2].)

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

$$\begin{array}{c} (0, 0, 0, \cdots, 0) \\ (1, 0, 0, \cdots, 0) \\ (0, 1, 0, \cdots, 0) \\ \cdots\cdots\cdots\cdots \\ (0, 0, 0, \cdots, 1). \end{array}$$

For this simplex the monomial integrals are

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

2. The Triangle. Before discussing higher values of n, $n \geqq 3$, 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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$$A_1 = A_2 = \cdots = A_6 \equiv A.$$

We will seek such a formula using the following points

$$(\nu_1, \nu_2), \quad (\nu_1, \nu_3), \quad (\nu_2, \nu_3),$$
$$(\nu_2, \nu_1), \quad (\nu_3, \nu_1), \quad (\nu_3, \nu_2),$$

where

$$\nu_1 + \nu_2 + \nu_3 = 1, \qquad 0 \leqq \nu_i \leqq 1, \qquad i = 1, 2, 3.$$

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:

$$(1) \qquad 6A = \frac{1}{2} = \int_{S_2} dx,$$

$$(2) \qquad 2A[\nu_1 + \nu_2 + \nu_3] = \frac{1}{6} = \int_{S_2} x_i \, dx,$$

$$(3) \qquad 2A[\nu_1^2 + \nu_2^2 + \nu_3^2] = \frac{2}{24} = \int_{S_2} x_i^2 \, dx,$$

$$(4) \qquad 2A[\nu_1 \nu_2 + \nu_1 \nu_3 + \nu_2 \nu_3] = \frac{1}{24} = \int_{S_2} x_1 x_2 \, dx,$$

$$(5) \qquad 2A[\nu_1^3 + \nu_2^3 + \nu_3^3] = \frac{6}{120} = \int_{S_2} x_i^3 \, dx,$$

$$(6) \qquad A[\nu_1^2\nu_2 + \nu_1 \nu_2^2 + \nu_1^2\nu_3 + \nu_1 \nu_3^2 + \nu_2^2\nu_3 + \nu_2 \nu_3^2] = \frac{2}{120} = \int_{S_2} x_i^2 x_j \, dx.$$

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

$$A = \tfrac{1}{12},$$

$$(7) \qquad \nu_1 + \nu_2 + \nu_3 = 1,$$

$$(8) \qquad \nu_1\nu_2 + \nu_1\nu_3 + \nu_2\nu_3 = \tfrac{1}{4},$$

$$(9) \qquad \nu_1\nu_2\nu_3 = \tfrac{1}{60}.$$

This last equation follows from

$$\left(\sum \nu_i\right)^3 - 3 \sum \nu_i^2 \nu_j - \sum \nu_i^3 = 1 - 3(\tfrac{2}{10}) - \tfrac{3}{10} = \tfrac{1}{10} = 6\nu_1\nu_2\nu_3 .$$

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):

$$\sum \nu_i \sum \nu_i\nu_j - 3\nu_1\nu_2\nu_3 = \tfrac{1}{4} - \tfrac{3}{60} = \tfrac{1}{5} = \sum \nu_i^2 \nu_j .$$

This shows that ν_1, ν_2, ν_3 must be the zeros of

$$P_3(x) \equiv x^3 - x^2 + \tfrac{1}{4}x - \tfrac{1}{60}.$$

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, $n \geqq 3$, 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 ν 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 ν). This is true if all the coordinates $\nu_1, \nu_2, \cdots, \nu_n$ are distinct; if k of the ν_i are equal then F contains $(n+1)!/k!$ points.

At first we assume that all the ν_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

$$\begin{array}{l} (\nu_1, \nu_2, \cdots, \nu_{n-2}, \nu_{n-1}, \nu_n), \\ (\nu_1, \nu_2, \cdots, \nu_{n-2}, \nu_{n-1}, \nu_{n+1}), \\ (\nu_1, \nu_2, \cdots, \nu_{n-2}, \nu_n, \nu_{n+1}), \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ (\nu_1, \nu_3, \cdots, \nu_{n-1}, \nu_n, \nu_{n+1}), \\ (\nu_2, \nu_3, \cdots, \nu_{n-1}, \nu_n, \nu_{n+1}), \end{array}$$

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:

$$(n+1)!\,A = \frac{1}{n!} = \int_{S_n} dx, \tag{10}$$

$$n!\,A[\nu_1 + \nu_2 + \cdots + \nu_{n+1}] = \frac{1}{(n+1)!} = \int_{S_n} x_i\,dx, \tag{11}$$

$$n!\,A[\nu_1^2 + \nu_2^2 + \cdots + \nu_{n+1}^2] = \frac{2}{(n+2)!} = \int_{S_n} x_i^2\,dx, \tag{12}$$

$$2(n-1)!\,A[\nu_1\nu_2 + \nu_1\nu_3 + \cdots + \nu_n\nu_{n+1}] = \frac{1}{(n+2)!} = \int_{S_n} x_i x_j\,dx, \tag{13}$$

$$n!\,A[\nu_1^3 + \nu_2^3 + \cdots + \nu_{n+1}^3] = \frac{6}{(n+3)!} = \int_{S_n} x_i^3\,dx, \tag{14}$$

$$\begin{aligned} (n-1)!\,A[\nu_1^2\nu_2 + \nu_1\nu_2^2 + \nu_1^2\nu_3 + \cdots + \nu_n^2\nu_{n+1} + \nu_n\nu_{n+1}^2] \\ = \frac{2}{(n+3)!} = \int_{S_n} x_i^2 x_j\,dx \end{aligned} \tag{15}$$

$$6(n-2)!\,A[\nu_1\nu_2\nu_3+\nu_1\nu_2\nu_4+\cdots+\nu_{n-1}\nu_n\nu_{n+1}] = \frac{1}{(n+3)!} = \int_{S_n} x_i\,x_j\,x_k\,dx. \tag{16}$$

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

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

$$\nu_1\nu_2+\nu_1\nu_3+\cdots+\nu_n\nu_{n+1} = \frac{n}{2(n+2)},$$

$$\nu_1\nu_2\nu_3+\cdots+\nu_{n-1}\nu_n\nu_{n+1} = \frac{n(n-1)}{6(n+2)(n+3)}.$$

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 ν_i, $i = 1, \cdots, n+1$, must be the zeros of a polynomial

$$P_{n+1}(x) \equiv x^{n+1} - x^n + \frac{n}{2(n+2)}x^{n-1} - \frac{n(n-1)}{6(n+2)(n+3)}x^{n-2} + k_{n-3}x^{n-3} + \cdots + k_1x + k_0.$$

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 ν_1 of multiplicity $n-1$ then ν_1 must also be a zero of

$$P_{n+1}^{(n-2)}(x) = (n+1)x^3 - 3x^2 + \frac{3}{n+2}x - \frac{1}{(n+2)(n+3)} \tag{17}$$

and then

$$P_{n+1}(x) = (x-\nu_1)^{n-1}(x^2-bx+c),$$

$$b = 1-(n-1)\nu_1,$$

$$c = \frac{n}{2(n+2)} - (n-1)\nu_1 + \frac{n(n-1)}{2}\nu_1^2.$$

Let ν_n, ν_{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 ν_1 and the corresponding ν_n, ν_{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 ν_n, ν_{n+1}. For $n \geqq 9$ the smallest zero of (17) also gives complex ν_n, ν_{n+1}. For $3 \leqq n \leqq 8$ there are 2 real solutions and for $5 \leqq n \leqq 8$ one of these gives a formula for S_n with all points exterior to S_n (since ν_n is negative). For $n \geqq 9$ 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

n	ν_1	ν_n	ν_{n+1}
2	0.1090390091	0.2319333686	0.6590276224
3	0.09484726491	0.2412769968	0.5690284733
	0.1881284504	0.05236466588	0.5713784333
4	0.08413783241	0.2460180205	0.5015684822
	0.1582718214	0.01736377592	0.5078207600
5	0.07573830688	0.2489442226	0.4481025499
	0.1366074267	−0.005814213043	0.4593845062
6	0.06895619726	0.2515528295	0.4036661842
	0.1201666155	−0.02192591378	0.4210928365
7	0.06335425440	0.2550852934	0.3647891803
	0.1072617271	−0.03352878861	0.3899584259
8	0.05864185796	0.2618241841	0.3276828101
	0.09686195317	−0.04210939636	0.3640757242
9	0.08830191983	−0.04858472329	0.3421693647
10	0.08113284981	−0.05354757701	0.3233519287
20	0.04478490125	−0.06983035166	0.2189172279
50	0.01910896646	−0.06445758604	0.1281182294
100	0.009772078935	−0.05308566241	0.08564984787

are true for $n \leqq 1000$. 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 $\nu_n < 0$.

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

$$P_1(x_1) \equiv (x_1 - \nu_1)(x_1 - \nu_2)(x_1 - \nu_3) = 0,$$

$$P_2(x_1, x_2) \equiv x_1^2 + x_2^2 + x_1x_2 - x_1 - x_2 + \tfrac{1}{4} = 0.$$

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

$$P_2(x_1, x_2) = a(x_1^2 + x_2^2) + bx_1x_2 + c(x_1 + x_2) + \tfrac{1}{4}.$$

Then we must have

$$P_2(\nu_1, \nu_2) = P_2(\nu_1, \nu_3) = P_2(\nu_2, \nu_3) = 0$$

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

$$P_1(x_1) = (x_1 - \nu_1)(x_1 - \nu_3)(x_1 - \nu_4),$$
$$P_2(x_1, x_2) = (x_2 - \nu_1)[a_2(x_1^2 + x_2^2) + b_2x_1x_2 + c_2(x_1 + x_2) + 1],$$
$$P_3(x_1, x_2, x_3) = a_3(x_1^2 + x_2^2 + x_3^2) + b_3(x_1x_2 + x_1x_3 + x_2x_3) + c_3(x_1 + x_2 + x_3) + 1$$

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

$$P_2(\nu_1, \nu_3) = P_2(\nu_1, \nu_4) = P_2(\nu_3, \nu_4) = 0,$$
$$P_3(\nu_1, \nu_1, \nu_3) = P_3(\nu_1, \nu_1, \nu_4) = P_3(\nu_1, \nu_3, \nu_4) = 0.$$

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

$$P_1(x_1) = 0,$$
$$P_2(x_1, x_2) = 0,$$
$$\cdots\cdots\cdots\cdots\cdots\cdots$$
$$P_{n-1}(x_1, \cdots, x_{n-1}) = 0,$$
$$P_n(x_1, x_2, \cdots, x_n) = 0,$$

where $P_1, \cdots, P_{n-1}$ have degree 3 and P_n has degree 2. These polynomials are constructed as follows:

$$P_1(x_1) = (x_1 - \nu_1)(x_1 - \nu_n)(x_1 - \nu_{n+1}),$$

$$P_k(x_1, \cdots, x_k) = (x_k - \nu_1)\left[a_k \sum_{i=1}^{k} x_i^2 + b_k \sum_{i,j=1}^{k} x_i x_j + c_k \sum_{i=1}^{k} x_i + 1\right], \quad k = 2, 3, \cdots, n-1,$$

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

where the unknown coefficients a_k, b_k, c_k, $k = 2, \cdots, n$ are found by the requirements that

$$P_k(\nu_1, \cdots, \nu_n) = P_k(\nu_1, \cdots, \nu_1, \nu_{n+1}) = P_k(\nu_1, \cdots, \nu_1, \nu_n, \nu_{n+1}) = 0, \quad k = 2, 3, \cdots, n.$$

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 nth 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. $P_1, \cdots, P_{n-1}$ 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

$$\int_{S_3} (1 + x_1 + x_2 + x_3)^{-4}\, dx = \tfrac{1}{48} \simeq 0.0208333333. \tag{18}$$

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:

	Approximation to (18)
First formula of Table 1.	0.0206178943
Second formula of Table 1.	0.0206308008
Formula of [1], 5 points.	0.0205151884
Formula of [3], 8 points.	0.0218716667
Formula of [4], 8 points.	0.0206454784

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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