Numerical Integration Formulas of Degree 3 for Product Regions and Cones

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1. Introduction. Here we discuss approximate integration formulas of degree 3; that is, formulas which are exact for polynomials of degree ≤ 3 , of the form

$$\int_R f(x_1, \dots, x_n) dx_n \cdots dx_1 \simeq \sum b_i f(v_{i1}, \dots, v_{in})$$

for certain regions R in n -dimensional, real, Euclidean space E_n .

If R is the Cartesian product of an r -dimensional and an s -dimensional region, $R = R_r \times R_s$, $r + s = n$, and if formulas of degree k involving p and q points are known for R_r and R_s , then Hammer and Wymore [4] have shown that a formula of degree k may be obtained for R which involves pq points. Similarly, if R is a cone (or pyramid) with $(n - 1)$ -dimensional base B , and if a formula of degree k involving p points is known for B , and further, if a formula of degree k of the form

$$\int_0^1 x^{n-1} g(x) dx \simeq \sum a_i g(v_i)$$

is known involving q points, then Hammer, Marlowe and Stroud [2] have shown that a formula of degree k can be obtained for R which involves pq points.

For $k = 3$ we will show that these results can be improved as follows. If $R = R_r \times R_s$ and formulas of degree 3 involving p and q points are known for R_r and R_s , then a formula of degree 3 can be found for R involving $p + q + 1$ points (and in some cases this may be reduced to $p + q$ or $p + q - 1$ points). If R is a cone and a formula of degree 3 involving p points is known for its base B , then a formula of degree 3 involving $p + 3$ points (in some cases $p + 2$ or $p + 1$ points) can be found for R , whereas the method of [2] would involve $2p$ points. We also give a $p + 2$ point formula of degree 3 for certain double cones, where p is the number of points in a formula for the base, and a $2n + 3$ point formula of degree 3 for an n -dimensional simplex.

2. Formulas for Product Regions. For convenience let us assume that the centroid of R_r is at the origin of coordinates in the subspace E_r of E_n for which $x_{r+1} = \dots = x_n = 0$, and also that the centroid of R_s is at the origin in the subspace E_s for which $x_1 = \dots = x_r = 0$. Then the centroid of R is at the origin in E_n . Also, for convenience in notation, we will write

$$R_r(x_1^{\alpha_1} \cdots x_r^{\alpha_r}) \equiv \int_{R_r} x_1^{\alpha_1} \cdots x_r^{\alpha_r} dx_r \cdots dx_1$$

with similar notations for R_s and R . Then, for example, $R_r(1)$ is the r -dimensional content or volume of R_r and $R(1) = R_r(1)R_s(1)$ is the n -dimensional volume of R .

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Suppose an approximate integration formula of degree 3 for R_r is given by:

$$(1) \quad \nu_i = (\nu_{i1}, \dots, \nu_{ir}) \quad a_i, \quad i = 1, 2, \dots, p.$$

Also suppose that a formula of degree 3 for R_s is given by:

$$(2) \quad \nu_{p+j} = (\nu_{p+j,r+1}, \dots, \nu_{p+j,n}) \quad a_{p+j}, \quad j = 1, 2, \dots, q.$$

At first it is assumed no ν_i coincides with the origin in E_r and no ν_{p+j} coincides with the origin in E_s . An integration formula for degree 3 for R is given by:

$$(3) \quad \begin{aligned} \nu_0 &= (0, \dots, 0, 0, \dots, 0) & b_0 &= -R(1) \\ \nu_i &= (\nu_{i1}, \dots, \nu_{ir}, 0, \dots, 0) & b_i &= a_i R_s(1), \\ & & i &= 1, 2, \dots, p \\ \nu_{p+j} &= (0, \dots, 0, \nu_{p+j,r+1}, \dots, \nu_{p+j,n}) & b_{p+j} &= a_{p+j} R_r(1), \\ & & j &= 1, 2, \dots, q. \end{aligned}$$

To prove this statement, it suffices to prove that the formula is exact for the following ten types of monomials: 1, $x_{r_1}, x_{s_1}, x_{r_1}x_{r_2}, x_{r_1}x_{s_1}, x_{s_1}x_{s_2}, x_{r_1}x_{r_2}x_{r_3}, x_{r_1}x_{r_2}x_{s_1}, x_{r_1}x_{s_1}x_{s_2}, x_{s_1}x_{s_2}x_{s_3}$ where $r_1, r_2, r_3 = 1, 2, \dots, r$ and $s_1, s_2, s_3 = r+1, r+2, \dots, n$:

The monomial 1. Since $a_1 + \dots + a_p = R_r(1)$ and $a_{p+1} + \dots + a_{p+q} = R_s(1)$ we have

$$\begin{aligned} -R(1) + [a_1 + \dots + a_p]R_s(1) + [a_{p+1} + \dots + a_{p+q}]R_r(1) \\ = -R(1) + 2R_r(1)R_s(1) = R(1). \end{aligned}$$

The type $x_{r_1}x_{r_2}x_{r_3}$. The formula gives for the integral of $x_{r_1}x_{r_2}x_{r_3}$ over R

$$[a_1\nu_{1r_1}\nu_{1r_2}\nu_{1r_3} + \dots + a_p\nu_{pr_1}\nu_{pr_2}\nu_{pr_3}]R_s(1) = R_r(x_{r_1}x_{r_2}x_{r_3})R_s(1).$$

Thus the formula is exact because

$$R(x_{r_1}x_{r_2}x_{r_3}) = R_r(x_{r_1}x_{r_2}x_{r_3})R_s(1).$$

The proofs for types $x_{r_1}, x_{s_1}, x_{r_1}x_{r_2}, x_{s_1}x_{s_2}, x_{s_1}x_{s_2}x_{s_3}$ are similar.

The type $x_{r_1}x_{r_2}x_{s_1}$. By the formula the integral of $x_{r_1}x_{r_2}x_{s_1}$ over R is zero since each term of the sum is zero. However

$$R(x_{r_1}x_{r_2}x_{s_1}) = R_r(x_{r_1}x_{r_2})R_s(x_{s_1}) = 0$$

because $R_s(x_{s_1}) = 0$. The proofs for the types $x_{r_1}x_{s_1}$ and $x_{r_1}x_{s_1}x_{s_2}$ are similar.

If the formulas for R_r and R_s already include the origin, then the formula for R will involve either $p+q$ or $p+q-1$ points according as the origin is included in one or both of these formulas. In the former case, if ν_{p+1} in (2) is the origin, then $b_0 = -[a_{p+2} + \dots + a_{p+q}]R_r(1)$. In the latter case, if both ν_1 in (1) and ν_{p+1} in (2) are the origin, then

$$b_0 = R(1) - [a_2 + \dots + a_p]R_s(1) - [a_{p+2} + \dots + a_{p+q}]R_r(1).$$

Depending on the particular structure of the formulas (1) and (2) it may be possible in special cases to eliminate the origin in the formula (3) for R . Suppose in the formula (2) for R_s , ν_{p+1} is the origin and a_{p+1} is positive. Also suppose R_r is centrally symmetric. Then, as shown in [6], we may obtain $2r$ point formulas for

R_r with $-v_{r+i} = v_i$, $a_{r+i} = a_i$, $i = 1, 2, \dots, r$. In addition to the assumptions already made about R_r , we may also assume $R_r(x_1^2) = \dots = R_r(x_r^2)$ and $R_r(x_i x_j) = 0$, for $i \neq j$; then in order that (1) be a formula of degree 3 it is necessary and sufficient that $v_1, \dots, v_r$ be orthogonal vectors with $a_i = \frac{R_r(x_1^2)}{2|v_i|^2}$ where $|v_i|$ is the distance of v_i from the origin. Since in the formula for $R_r \times R_s$ it is no longer necessary that $b_1 + \dots + b_{2r} = R(1)$, a formula of degree 3 for $R_r \times R_s$ is given by the $2r + q - 1$ points:

$$\begin{aligned}
 -v_{r+i} &= v_i = (v_{i1}, \dots, v_{ir}, 0, \dots, 0) & b_{r+i} &= b_i, \\
 & & i &= 1, 2, \dots, r \\
 v_{2r+j} &= (0, \dots, 0, v_{2r+j, r+1}, \dots, v_{2r+j, n}) & b_{2r+j} &= a_{2r+j} R_r(1), \\
 & & j &= 2, \dots, q
 \end{aligned}$$

where the only conditions that the b_i and v_i , $i = 1, 2, \dots, r$, must satisfy are $2(b_1 + \dots + b_r) = a_{2r+1} R_r(1)$ and $v_1, \dots, v_r$ are any set of orthogonal vectors for which $|v_i|^2 = \frac{R_r(x_1^2)}{2b_i}$; the b_i must all be positive.

Of course if both R_r and R_s are centrally symmetric then $R_r \times R_s$ is also centrally symmetric and the results of [6] may be applied directly to obtain $2n$ point formulas. Some of the resulting formulas may also be obtained from the separate formulas for R_r and R_s by a method somewhat similar to that described in the preceding paragraph.

As an example of a specific formula we give a formula for the region $C_r \times S_{n-r}$, $1 \leq r \leq n - 2$, where C_r is the r -cube with vertices $(\pm 1, \pm 1, \dots, \pm 1)$ and S_{n-r} is the $(n - r)$ -simplex with vertices $(-1, -1, \dots, -1)$, $(1, 0, \dots, 0)$, $(0, 1, \dots, 0)$, $\dots$, $(0, 0, \dots, 1)$. For $r = 1$, $C_1 \times S_{n-1}$ can be considered as a prism (or in the terminology of Sommerville [5], p. 113, a prism of the first species) with base S_{n-1} ; for general r , $C_r \times S_{n-r}$ is a prism of species r . Since C_r is centrally symmetric the remarks made above apply. A formula of degree 3 is known for S_{n-r} using $n - r + 2$ points, [3], one of which is the origin, but the origin is taken with a negative weight so that it is necessary to use $n + r + 2$ points in the formula for $C_r \times S_{n-r}$. A particular formula is:

$$\begin{aligned}
 v_0 &= (0, 0, \dots, 0, 0, 0, \dots, 0) & b_0 &= \\
 & & &= 2^r S_{n-r}(1) \left[1 - \frac{r}{3} - \frac{(n-r+3)^2}{4(n-r+2)} \right] \\
 -v_{r+1} &= v_1 = (1, 0, \dots, 0, 0, 0, \dots, 0) & b_{r+1} &= b_1 = \dots = \\
 -v_{r+2} &= v_2 = (0, 1, \dots, 0, 0, 0, \dots, 0) & &= b_{2r} = b_r = \frac{2^{r-1}}{3} S_{n-r}(1) \\
 & \dots & & \\
 -v_{2r} &= v_r = (0, 0, \dots, 1, 0, 0, \dots, 0) \\
 v_{2r+1} &= \left(0, 0, \dots, 0, \frac{-2}{n-r+3}, \right.
 \end{aligned}$$

$$\begin{aligned} & \left(\frac{-2}{n-r+3}, \dots, \frac{-2}{n-r+3} \right) \quad b_{2r+1} = \dots = b_{n+r+1} = \\ \nu_{2r+2} &= \left(0, 0, \dots, 0, \frac{2}{n-r+3}, 0, \dots, 0 \right) = \frac{(n-r+3)^2 2^r S_{n-r}(1)}{4(n-r+1)(n-r+2)} \\ & \dots \\ \nu_{n+r+1} &= \left(0, 0, \dots, 0, 0, 0, \dots, \frac{2}{n-r+3} \right) \end{aligned}$$

3. Formulas for Cones. Suppose the centroid of the $(n-1)$ -dimensional base B is at the origin in the subspace E_{n-1} of E_n for which $x_1 = 0$ and that the vertex of R is at $(1, 0, \dots, 0)$ in E_n . Suppose further a formula of degree 3 for B is given by

$$(4) \quad \nu_i = (\nu_{i2}, \nu_{i3}, \dots, \nu_{in}) \quad a_i, \quad i = 1, 2, \dots, p.$$

We assume at first that no ν_i coincides with the origin in E_{n-1} . An integration formula of degree 3 for R can be found of the form

$$(5) \quad \begin{aligned} \nu_i &= (\eta, \gamma\nu_{i2}, \gamma\nu_{i3}, \dots, \gamma\nu_{in}) & b_i &= \alpha a_i, \quad i = 1, 2, \dots, p \\ \nu_{p+j} &= (\xi_j, 0, 0, \dots, 0) & b_j &, \quad j = 1, 2, 3. \end{aligned}$$

To prove this we must first calculate the monomial integrals over R in terms of those over B . These are

$$\begin{aligned} \int_R x_1^\beta x_2^{\beta_2} \dots x_n^{\beta_n} dx_n \dots dx_1 \\ = \int_0^1 (1-x_1)^{n+\beta_2+\dots+\beta_n-1} x_1^\beta dx_1 \int_B x_2^{\beta_2} \dots x_n^{\beta_n} dx_n \dots dx_2. \end{aligned}$$

The equations which must be satisfied by (5) if it is to integrate each monomial are given below (where the monomial from which the equation arises is indicated at the left):

$$[x_1^\beta] \quad b_1 \xi_1^\beta + b_2 \xi_2^\beta + b_3 \xi_3^\beta + \alpha \eta^\beta [a_1 + \dots + a_p] = \frac{\beta!(n-1)!}{(n+\beta)!} B(1),$$

$$\beta = 0, 1, 2, 3.$$

$$[x_1^\beta x_i] \quad \alpha \gamma \eta^\beta [a_1 \nu_{1i} + \dots + a_p \nu_{pi}] = \frac{\beta! n!}{(n+\beta+1)!} B(x_i),$$

$$\beta = 0, 1, 2$$

$$[x_1^\beta x_i x_j] \quad \alpha \gamma^2 \eta^\beta [a_1 \nu_{1i} \nu_{1j} + \dots + a_p \nu_{pi} \nu_{pj}] = \frac{\beta!(n+1)!}{(n+\beta+2)!} B(x_i x_j),$$

$$\beta = 0, 1$$

$$[x_i x_j x_k] \quad \alpha \gamma^3 [a_1 \nu_{1i} \nu_{1j} \nu_{1k} + \dots + a_p \nu_{pi} \nu_{pj} \nu_{pk}] = \frac{1}{n+3} B(x_i x_j x_k)$$

where $i, j, k = 2, 3, \dots, n$. Because we have assumed $B(x_i) = 0$, the three equations $[x_1^\beta x_i]$ are of the form $0 = 0$. From the equations $[x_i x_j]$ and $[x_i x_j x_k]$ it imme-

diately results that $\eta = 1/(n+3)$. From equations $[x, x_j]$ and $[x, x_j, x_k]$ it follows that

$$\alpha = \frac{(n+3)^2}{(n+2)^3}, \quad \gamma = \frac{n+2}{n+3}.$$

Since $a_1 + \dots + a_p = B(1)$ the equations that remain become

$$[x_1^\beta] \quad b_1 \xi_1^\beta + b_2 \xi_2^\beta + b_3 \xi_3^\beta + \frac{(n+3)^2}{(n+2)^3} \frac{1}{(n+3)^\beta} B(1) = \frac{\beta!(n-1)!}{(n+\beta)!} B(1),$$

$$\beta = 0, 1, 2, 3.$$

In these equations we cannot take, say, $b_3 = 0$, which would in effect reduce by one the number of points in the formula, because the resulting equations do not have a real solution. It might be expected, however, that there would be many solutions with all $b_i \neq 0$. Here we give just one of the simplest solutions. If we choose

$$b_3 = -\frac{(n+3)^2}{(n+2)^3} B(1), \quad \xi_3 = \frac{1}{n+3}$$

then the other values are

$$b_1 = b_1' B(1) = \frac{2(n+1) - (n-1) \sqrt{2(n+1)(n+2)}}{4n(n+1)^2} B(1)$$

$$\xi_1 = \frac{2(n+2) + \sqrt{2(n+1)(n+2)}}{(n+2)(n+3)}$$

$$b_2 = b_2' B(1) = \frac{2(n+1) + (n-1) \sqrt{2(n+1)(n+2)}}{4n(n+1)^2} B(1)$$

$$\xi_2 = \frac{2(n+2) - \sqrt{2(n+1)(n+2)}}{(n+2)(n+3)}.$$

These values of b_1' , b_2' , ξ_1 , ξ_2 have been given in connection with numerical integration with respect to a weight function x^{n-1} by Fishman [1] for $n = 1(1)6$ to 12D and in [2] for $n = 2(1)4$ to 18S. These authors have used n where we use $n-1$ and for $m=2$, $j=1, 2$, their $1-x_j$ is our ξ_j , their b_j is our b_j' . It is proved in [2] that the $2p$ points

$$(\xi_j, (1-\xi_j)\nu_{i2}, (1-\xi_j)\nu_{i3}, \dots, (1-\xi_j)\nu_{in}) \quad b_j' a_i$$

$i = 1, 2, \dots, p$, $j = 1, 2$, are an integration formula of degree 3 for R .

If one of the ν_i in (4), say ν_1 , is the origin in E_{n-1} then it may be possible to determine b_1 , b_2 , ξ_1 , ξ_2 with $b_3 = 0$ to give a formula which involves only $p+1$ points $\nu_2, \dots, \nu_{p+2}$. The formula using $n+2$ points when R is an n -simplex, [3], can be derived in this manner; the formula for B , which is an $(n-1)$ -simplex, involves $n+1$ points of which one is the origin in E_{n-1} . In any event, if ν_1 is the origin, we may derive a formula of degree 3 for R involving $p+2$ points $\nu_2, \dots, \nu_{p+3}$ where

$$b_3 = -\frac{(n+3)^2}{(n+2)^3} [a_2 + \dots + a_p]$$

and the other values as before. Usually there will be other $p+2$ point formulas as well.

Now we briefly discuss formulas for regions which are double cones; that is, regions which are the union of two cones with vertices $(1, 0, \dots, 0)$ and $(-1, 0, \dots, 0)$ and with a common base B of the type we have just considered. By a combination of the methods of this section and the preceding it is easy to see that from a formula (4) for B we may obtain the following formula involving $p + 2$ points for the double cone R :

$$\begin{aligned} \nu_i &= (0, \gamma\nu_2, \gamma\nu_3, \dots, \gamma\nu_n) & b_i &= \frac{2(n+3)^2}{(n+2)^3} a_i, & i &= 1, 2, \dots, p \\ -\nu_{p+2} &= \nu_{p+1} = (\xi, 0, 0, \dots, 0) & b_{p+2} &= b_{p+1} = \frac{3n+8}{n(n+2)^3} B(1) \end{aligned}$$

where

$$\gamma = \frac{n+2}{n+3} \quad \text{and} \quad \xi = \sqrt{\frac{2n^2 + 8n + 8}{3n^2 + 11n + 8}}.$$

Since $\xi < 1$ for all n , the points ν_{p+1} and ν_{p+2} are always interior to R . In this formula the origin is not required if it does not occur in (4) and b_{p+1} and ξ are uniquely determined. If the origin does occur in (4), then in some cases it can be eliminated in the formula for R ; if ν_1 is the origin, then b_{p+1} , ξ , and b_1 will not be uniquely determined and we may take ξ arbitrary, which will then determine

$$\begin{aligned} b_{p+1} &= \frac{2}{\xi n(n+1)(n+2)} B(1) \\ b_1 &= \frac{2}{n} B(1) - 2b_{p+1} - \frac{2(n+3)^2}{(n+2)^3} [a_2 + \dots + a_p]. \end{aligned}$$

Since b_{p+1} is required to be positive, we could, providing

$$[a_2 + \dots + a_p] < \frac{(n+2)^3}{n(n+3)^2} B(1),$$

or, in other words, providing

$$a_1 > -\frac{(3n+8)}{n(n+3)^2} B(1),$$

choose $b_1 = 0$. In this case the formula for R would involve only the $p + 1$ points $\nu_2, \dots, \nu_{p+2}$ and b_{p+1} and ξ would again be uniquely determined. In this paragraph R has been a double cone of the first species with base B ; this method may be repeated to give a formula for a double cone of species r . If we take a double cone of species r with base S_{n-r} , $1 \leq r \leq n-2$, then this region has a formula of degree 3 which involves $n + r + 2$ points.

4. A Special Formula for Simplexes. We digress here from the methods of the previous sections to give a special formula of degree 3 for a simplex S_n in E_n . The formula involves $2n + 3$ points, $n \geq 2$, all but one of which are on the surface of S_n ; the formula involves the $n + 1$ vertices, the $n + 1$ centroids of the $(n - 1)$ -dimensional faces, and the centroid of S_n .

To develop the formula it is most convenient to take S_n to have vertices $(0, 0, \dots, 0), (1, 0, \dots, 0), \dots, (0, 0, \dots, 1)$. Then the monomial integrals over S_n are

$$\int_{S_n} x_i^{\alpha_i} x_j^{\alpha_j} x_k^{\alpha_k} dx_n \cdots dx_1 = \frac{\alpha_i! \alpha_j! \alpha_k!}{(n + \alpha_i + \alpha_j + \alpha_k)!}.$$

The formula is then:

$$\begin{aligned} \nu_0 &= \left(\frac{1}{n+1}, \frac{1}{n+1}, \dots, \frac{1}{n+1} \right) & b_0 &= -\frac{(n+1)^2(n-3)}{(n+2)(n+3)} S_n(1) \\ \nu_1 &= (0, 0, \dots, 0) & b_1 &= \dots = b_{n+1} = \\ \nu_2 &= (1, 0, \dots, 0) & &= \frac{3}{(n+1)(n+2)(n+3)} S_n(1) \\ &\dots & & \\ \nu_{n+1} &= (0, 0, \dots, 1) & & \\ \nu_{n+2} &= \left(\frac{1}{n}, \frac{1}{n}, \dots, \frac{1}{n} \right) & b_{n+2} &= \dots = b_{2n+2} = \\ \nu_{n+3} &= \left(0, \frac{1}{n}, \dots, \frac{1}{n} \right) & &= \frac{n^3}{(n+1)(n+2)(n+3)} S_n(1) \\ &\dots & & \\ \nu_{2n+2} &= \left(\frac{1}{n}, \frac{1}{n}, \dots, 0 \right) \end{aligned}$$

where $S_n(1) = 1/(n!)$ is the volume of S_n . Because of the symmetries of this particular simplex, the proof that this is a formula of degree 3 can be established by verifying that it is exact for the 7 monomials: $1, x_1, x_1^2, x_1x_2, x_1^3, x_1^2x_2, x_1x_2x_3$. For $n = 1$ this formula gives us Simpson's formula, since for S_1 , a line segment, the vertices coincide with the $(n-1)$ -faces; the weight for each end point of S_1 is $b_1 + b_4 = b_2 + b_3$. For $n = 3$, $b_0 = 0$, and in this one case the centroid does not occur in the formula; for $n > 3$, b_0 is negative.

This formula will be useful when it is desired to integrate over a region by subdividing the region into simplexes and then applying a formula of degree 3 to each simplex. For a large number of subdivisions the total number of points used in applying this formula to each simplex will be less than the total number of points used if the $n+2$ point formula is applied to each simplex. For example, for $n = 3$ suppose we desire to integrate over an icosahedron (which has 20 triangular faces) by subdividing it into 20 tetrahedra (each tetrahedron having as vertices the vertices of a face plus the center of the icosahedron). Repeated use of the formula given here would involve a total of 63 points whereas use of the 5-point formula for each tetrahedron would involve 100 points.

5. Concluding Remarks. From the formulas we have discussed, formulas may be obtained for regions which are linear transforms of the particular regions we have considered. While these results add greatly to our knowledge of formulas of degree 3

nothing is yet known concerning such formulas for regions which are less regular than those considered here.

It seems certain, although no proof is known, that the $n + 2$ point formula of degree 3 for S_n and the $2n$ point formulas of degree 3 for C_n involve the minimal number of points for this degree. If this is true, then it is also likely that the $n + r + 2$ point formulas for both $C_r \times S_{n-r}$ and the double cone of species r with base S_{n-r} are also minimal. For fixed r these latter regions are the duals of each other (see [5], p. 56) and thus have the same symmetries. This seems to indicate that the minimal point formulas of degree 3 for a region are related to the group of symmetries of the region.

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