

Rotation Invariant Cubature Formulas over the n -Dimensional Unit Cube

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Rotation Invariant Cubature Formulas over the n -Dimensional Unit Cube

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Abstract

We consider cubature formulas to approximate multivariate integrals that remain unchanged under the orientation preserving transformation of a cube. The use of invariant theory (Molien series, Reynold operator) for the construction of such cubature formula is investigated. Some new cubature formulas for the unit cube that are obtained using this approach, are presented.

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1 Introduction

An integral I is a positive linear continuous functional

$$I[f] := \int_{\Omega} w(\mathbf{x})f(\mathbf{x})d\mathbf{x} \quad (1)$$

where the region $\Omega \subset \mathbb{R}^n$ and the weight function $w(\mathbf{x}) \geq 0$, for all $\mathbf{x} \in \Omega$. It is often desirable to approximate I by a weighted sum of functionals that are easier to evaluate, e.g., point evaluations, such that

$$I[f] \approx Q_m[f] := \sum_{i=1}^m w_i f(\mathbf{x}_i), \quad (2)$$

where $w_i \in \mathbb{R} \setminus \{0\}$, $\mathbf{x}_i \in \mathbb{R}^n$, and $m \in \mathbb{N}$. Here \mathbb{N} denotes the set of positive integers. For multivariate integrals such an approximation is called a cubature formula.

We will only consider cubature formulas that are exact for a vector space of algebraic polynomials. Let \mathcal{P}^n denote the vector space of all polynomials in n variables and let \mathcal{P}_d^n denote the subspace of polynomials of degree at most d .

Q_m is said to be of degree d if $I[p] = Q_m[p]$ whenever $p \in \mathcal{P}_d^n$ and $I[q] \neq Q_m[q]$ for at least one $q \in \mathcal{P}_{d+1}^n$.

The theory we use to exploit symmetry is called *invariant theory*. For some general facts about invariant theory, we refer to [11,12]. Overviews concerning its use to construct cubature formulas are presented in [16,19,4].

Let G be a finite group of linear transformations and let $|G|$ denote the order of the group. If a linear transformation acts on a vector space \mathbb{R}^n for which an orthonormal basis is fixed, then the linear transformation can be represented by a matrix. We will denote by g both the transformation and the matrix that represents it. A set $\Omega \subset \mathbb{R}^n$ is said to be invariant with respect to a group G if Ω is left unchanged by each transformation of the group, that is, $g(\Omega) = \Omega$, for all $g \in G$. A function f is said to be invariant with respect to the group G if it is left unchanged by each transformation of the group, that is, $f(g(\mathbf{x})) = f(\mathbf{x})$ for all $g \in G$. An integral is invariant with respect to G if both its region and weight function are invariant with respect to G . The G -orbit of a point $y \in \mathbb{R}^n$ is the set $\{g(y) : g \in G\}$. A cubature formula Q_m is said to be G -invariant if the region Ω and the weight function $w(\mathbf{x})$ are G -invariant, if the set of points is a union of G -orbits and all points of one and the same orbit have the same weight. A G -invariant cubature formula can be written as

$$Q[f] := \sum_{j=1}^K w_j Q_G(\mathbf{x}_j)[f], \quad (3)$$

where K is the number of distinct G -orbits and the functional $Q_G(\mathbf{x}_j)$ maps a function f to the average of its values in the points of the G -orbit of \mathbf{x}_j .

The space of all G -invariant polynomials in n -variables is

$$\mathcal{P}^n(G) := \{p \in \mathcal{P}^n : p \circ g = p \text{ for every } g \in G\}. \quad (4)$$

The subspace of $\mathcal{P}^n(G)$ of all G -invariant polynomials of degree at most d is denoted by $\mathcal{P}_d^n(G)$. The usefulness of all this is highlighted by the following theorem, usually called Sobolev's theorem.

Theorem 1 *Let the cubature formula Q be G -invariant. The cubature formula has degree d if it is exact for all invariant polynomials of degree at most d and if it is not exact for at least one polynomial of degree $d + 1$.*

Proof: See, e.g., [4]. \square

This theorem teaches us that the points and weights of a G -invariant cubature

formula (3) are a solution of the system of nonlinear equations

$$\sum_{j=1}^K w_j Q_G(\mathbf{x}_j)[f_i] = I[f_i] \quad , \quad i = 1, \dots, \dim \mathcal{P}_d^n(G), \quad (5)$$

where $\{f_i | i = 1, \dots, \dim \mathcal{P}_d^n(G)\}$ is a basis for $\mathcal{P}_d^n(G)$.

For all $i \geq 0$ the homogeneous G -invariant polynomials of degree i form a finite dimensional vector space over \mathbb{R} . The dimension c_i of these spaces can be obtained using Molien's formula.

Theorem 2 (*Molien's formula*) *Let $c_i := \dim \mathcal{P}_i^n(G) - \dim \mathcal{P}_{i-1}^n(G)$ and let $\lambda_1(g), \dots, \lambda_n(g)$ be the eigenvalues of $g \in G$. Then*

$$\sum_{i=0}^{\infty} c_i t^i = \frac{1}{|G|} \sum_{g \in G} \frac{1}{(1 - \lambda_1(g)t) \cdots (1 - \lambda_n(g)t)} \quad (6)$$

Proof: See, e.g., [18]. \square

For $p \in \mathcal{P}_d^n$ the Reynold operator “ $*$ ” is defined through

$$p_* := \sum_{g \in G} \frac{p \circ g}{|G|}. \quad (7)$$

This operator can be used to describe all elements of $\mathcal{P}^n(G)$.

Theorem 3 *Using the Reynold operator (7) the space $\mathcal{P}_d^n(G)$ of all G -invariant polynomials of degree at most d can be obtained as*

$$\mathcal{P}_d^n(G) = \{p_* : p \in \mathcal{P}_d^n\}. \quad (8)$$

Proof: See [14]. \square

In this paper we will be concerned with so-called fully symmetric integrals. For such integrals, the region Ω and the weight function $w(\mathbf{x})$ are invariant with respect to the symmetry group of a cube. The unit cube $\Omega = [-1, 1]^n$ and the unit ball $\Omega = \{\mathbf{x} \mid \|\mathbf{x}\|_2 \leq 1\}$ with constant weight function $w(\mathbf{x}) = 1$ are examples. This symmetry will be exploited to construct cubature formulas. The results are directly applicable to other regions and weight functions with the same symmetry.

Definition 1 *A symmetry g of a set $\Omega \subset \mathbb{R}^n$ is an orthogonal transformation of G which leaves Ω unchanged, i.e., $g(\Omega) = \Omega$.*

Let G_n be the group of symmetries of the n -cube with vertices $(\pm 1, \pm 1, \dots, \pm 1)$. This group consists of the $2^n n!$ linear transformations

$$(x_1, x_2, \dots, x_n) \mapsto (\pm x_{p(1)}, \pm x_{p(2)}, \dots, \pm x_{p(n)}),$$

the \pm signs being chosen independently and $(p(1), \dots, p(n))$ an arbitrary permutation of $(1, 2, \dots, n)$.

The integrals we consider in this paper are invariant with respect to a subgroup of the symmetry group of the cube: the orientation preserving transformations. In Section 2 we will describe this subgroup and collect known results relevant to our work. In Section 3 we will derive the general form of the nonlinear equations that determine cubature formulas and give some rules to obtain cubature formulas with a reasonable small number of points. In Section 4 we report on the new cubature formulas for the cube that we obtained. Although the number of new cubature formulas incorporated in this paper is limited, they convince us that this approach deserves more attention. This approach becomes useful for high degrees but obviously one then has to face large systems of nonlinear equations.

2 Orientation preserving transformations

For the classical space of polynomials one can choose between several bases depending on the application one has in mind. Sometimes a basis formed by monomials is used, some other times a basis of orthogonal polynomials is used. For invariant polynomials a very convenient basis is the so-called good integrity basis.

Definition 2 *Let $\phi_1, \phi_2, \dots, \phi_l$ be invariant polynomials of G . $\phi_1, \phi_2, \dots, \phi_l$ form an integrity basis for the invariant polynomials of G if every invariant polynomial of G is a polynomial in $\phi_1, \phi_2, \dots, \phi_l$. Each polynomial ϕ_j ($1 \leq j \leq l$) is called a basic invariant polynomial of G .*

Definition 3 *Polynomials $\phi_1(\mathbf{x}), \phi_2(\mathbf{x}), \dots, \phi_l(\mathbf{x})$ are called algebraically dependent if there is a polynomial $f(\mathbf{x})$ in l variables with not all coefficients equal to zero, such that $f(\phi_1(\mathbf{x}), \phi_2(\mathbf{x}), \dots, \phi_l(\mathbf{x})) = 0$. Otherwise the polynomials $\phi_1(\mathbf{x}), \phi_2(\mathbf{x}), \dots, \phi_l(\mathbf{x})$ are algebraically independent.*

The ring of all polynomials in the variables x_1, x_2, \dots, x_n over \mathbb{R} is denoted by $\mathbb{R}[x_1, x_2, \dots, x_n]$.

Definition 4 *A good integrity basis for $\mathcal{P}^n(G)$ consists of homogeneous invariant polynomials $\phi_1(\mathbf{x}), \dots, \phi_l(\mathbf{x})$ ($l \geq n$) with respect to G where $\phi_1(\mathbf{x}),$*

$\dots, \phi_n(\mathbf{x})$ are algebraically independent and

$$\begin{aligned} \mathcal{P}^n(G) &= \mathbb{R}[\phi_1(\mathbf{x}), \dots, \phi_n(\mathbf{x})] \quad \text{if } l = n, \\ &= \mathbb{R}[\phi_1(\mathbf{x}), \dots, \phi_n(\mathbf{x})] \oplus \phi_{n+1}(\mathbf{x}) \mathbb{R}[\phi_1(\mathbf{x}), \dots, \phi_n(\mathbf{x})] \\ &\quad \oplus \dots \oplus \phi_l(\mathbf{x}) \mathbb{R}[\phi_1(\mathbf{x}), \dots, \phi_n(\mathbf{x})] \quad \text{if } l > n. \end{aligned}$$

We will now describe the group of orientation preserving transformations. Let $W \subseteq \mathbb{R}^n$ be a subspace of dimension m and let $W^\perp \subseteq \mathbb{R}^n$ be the orthogonal complement of a subspace W . Hence $\mathbb{R}^n = W \oplus W^\perp$.

Definition 5 *The reflection s with respect to W^\perp is the linear transformation on \mathbb{R}^n which maps each $\mathbf{x} \in W$ to $-\mathbf{x}$ and leaves W^\perp pointwise invariant.*

Definition 6 *An orthogonal transformation g of G is orientation preserving if $\det(g) = +1$. An orthogonal transformation g of G is orientation reversing if $\det(g) = -1$.*

A reflection s with respect to W^\perp is said to be of type m if $\dim W = m$. A reflection of type 1 is an orientation reversing transformation with one eigenvalue equal to -1 and $(n - 1)$ eigenvalues equal to $+1$. Let \mathbf{a} be the eigenvector of length 1 corresponding to the eigenvalue -1 . The vectors \mathbf{a} and $-\mathbf{a}$ are called the roots of the reflection s with respect to W^\perp .

In the following, we mean by a reflection a reflection of type 1.

Definition 7 *G is a finite reflection group acting on \mathbb{R}^n if G is a finite group generated by reflections on \mathbb{R}^n .*

Theorem 4 *Let G be a finite reflection group acting on the n -dimensional space \mathbb{R}^n . Let $\phi_1, \phi_2, \dots, \phi_n$ be homogeneous polynomials forming an integrity basis for the invariant polynomials of G . Let $\nu_1, \nu_2, \dots, \nu_n$ be the respective degrees of $\phi_1, \phi_2, \dots, \phi_n$. Then*

$$\prod_{j=1}^n \nu_j = |G| \quad , \quad \sum_{j=1}^n (\nu_j - 1) = r,$$

where r is the number of reflections in G .

Proof: See [12]. \square

Theorem 5 *Let G be a reflection group of a regular polytope and let G^{op} be the subgroup of the orientation preserving transformations. A good integrity basis for $\mathcal{P}^n(G^{op})$, the invariant polynomials of the group G^{op} , can be written as follows:*

$$\mathcal{P}^n(G^{op}) = \mathbb{R}[\phi_1, \phi_2, \dots, \phi_n] \oplus \phi_{n+1} \mathbb{R}[\phi_1, \phi_2, \dots, \phi_n].$$

The polynomials $\phi_1, \phi_2, \dots, \phi_n$ are the basic invariant polynomials of G and

$$\phi_{n+1}(x) = \prod_{j=1}^r (\mathbf{a}_j \cdot \mathbf{x}).$$

\mathbf{a}_j is one of the two roots of the reflection $s_j \in G$, $j = 1, 2, \dots, r$.

Proof: See [2]. \square

From the above two theorems, we obtain that the degree of ϕ_{n+1} is

$$\deg(\phi_{n+1}) = r = \sum_{j=1}^n (\nu_j - 1). \quad (9)$$

Let G_n^{op} be the set of all orientation preserving transformations of G_n , the symmetry group of the n -cube, and G_n^{or} the set of all orientation reversing transformations of G_n . We know that G_n^{op} is a subgroup of G_n with order equal to the order of G_n^{or} and so $|G_n^{op}| = n!2^{n-1}$.

The basic invariant polynomials ϕ_i 's of G_n are known [7]:

$$\begin{aligned} \phi_1 &:= \sum_{j=1}^n x_j^2 & \deg(\phi_1) &= 2 \\ \phi_2 &:= \sum_{k<l} x_k^2 x_l^2 & \deg(\phi_2) &= 4 \\ \dots & & \deg(\phi_i) &= 2i \\ \phi_n &:= \prod_{j=1}^n x_j^2 & \deg(\phi_n) &= 2n \end{aligned} \quad (10)$$

Therefore for the group G_n^{op} we get $r = n^2$. The following polynomial can be added to (10) to obtain a good integrity basis for G_n^{op} (see [2]):

$$\phi_{n+1} := \prod_{j=1}^n x_j \prod_{1 \leq j < l \leq n} (x_l^2 - x_j^2).$$

A basis for $\mathcal{P}_d^n(G_n^{op})$ is thus given by

$$\{\phi_1^{i_1} \cdots \phi_n^{i_n} \cdot \phi_{n+1}^{i_{n+1}} \mid i_j \in \mathbb{N} \cup \{0\}, i_{n+1} \in \{0, 1\}, \sum_{j=1}^n 2ji_j + n^2 i_{n+1} \leq d\}.$$

The right hand side of the expression in Theorem 2 can be simplified in this case.

Corollary 1 For G_n , the symmetry group of the n -cube ($n \geq 2$), the right

hand side of (6) is equal to

$$\frac{1}{\prod_{i=1}^n (1 - t^{2i})}.$$

For G_n^{op} , the group of orientation preserving transformations of the symmetry group of the n -cube ($n \geq 2$), the right hand side of (6) is equal to

$$\frac{1 + t^{n^2}}{\prod_{i=1}^n (1 - t^{2i})}. \quad (11)$$

The dimensions of the G_n^{op} -invariant spaces of homogeneous polynomials follow directly from the series expansion of (11). It is very interesting to note that the additional basic invariant polynomial ϕ_{n+1} has a very large degree. Consequently, for $d < n^2$ we have $\mathcal{P}_d^n(G_n) = \mathcal{P}_d^n(G_n^{op})$. So, for a moderate degree of precision the number of equations in (5) is the same for the groups G_n and G_n^{op} .

Because we will use this in the following sections, we give here the series expansions for $n = 3$:

$$\begin{aligned} \frac{1}{(1-t^2)(1-t^4)(1-t^6)} &= 1 + t^2 + 2t^4 + 3t^6 + 4t^8 + 5t^{10} + 7t^{12} + 8t^{14} \\ &\quad + 10t^{16} + 12t^{18} + \mathcal{O}(t^{20}), \end{aligned}$$

$$\begin{aligned} \frac{1+t^9}{(1-t^2)(1-t^4)(1-t^6)} &= 1 + t^2 + 2t^4 + 3t^6 + 4t^8 + t^9 + 5t^{10} + t^{11} + 7t^{12} \\ &\quad + 2t^{13} + 8t^{14} + 3t^{15} + 10t^{16} + 4t^{17} + 12t^{18} \\ &\quad + 5t^{19} + \mathcal{O}(t^{20}). \end{aligned}$$

Definition 8 For a given dimension n and $j \in \{0, 1, \dots, n\}$ we set

$$\begin{aligned} T_j^n := \{ &(k_{j1}, k_{j2}, \dots, k_{jn}) \mid \sum_{i=1}^n k_{ji} = j, k_{j1} \geq k_{j2} \geq \dots \geq k_{jn} \text{ and} \\ &k_{ji} \in \mathbb{N} \cup \{0\}\}. \end{aligned}$$

The elements of T_j^n , denoted by $T_{j,i}^n$ for $i = 1, \dots, |T_j^n|$, can be ordered as follows:

$$\begin{aligned} T_{j,1}^n &:= (j, 0, \dots, 0) < T_{j,2}^n := (j-1, 1, 0, \dots, 0) < T_{j,3}^n := (j-2, 2, 0, \dots, 0) \\ &< T_{j,4}^n := (j-2, 1, 1, 0, \dots, 0) < \dots < T_{j,|T_j^n|}^n := (1, 1, \dots, 1, 0, \dots, 0), \end{aligned}$$

where the first j coordinates of $T_{j,|T_j^n|}^n$ are equal to 1. For example, when n and j are both equal to 4, $T_{4,1}^4 = (4, 0, 0, 0) < T_{4,2}^4 = (3, 1, 0, 0) < T_{4,3}^4 = (2, 2, 0, 0) < T_{4,4}^4 = (2, 1, 1, 0) < T_{4,5}^4 = (1, 1, 1, 1)$.

The maximum number of points in a G_n^{op} -orbit is equal to $n!2^{n-1} = |G_n^{op}|$, which is equal to $|G_n^{op}|$. However, for special choices some of these points may coincide, so that the orbit in fact has less points. We will consider several types of G_n^{op} -orbits corresponding to the elements of T_j^n , $j = 0, 1, \dots, n$.

Definition 9 With $(k_{j_1}, k_{j_2}, \dots, k_{j_n}) \in T_j^n$ we associate a type of generator of the form

$$\underbrace{(x_1, \dots, x_1)}_{k_{j_1} \text{ times}}, \underbrace{(x_2, \dots, x_2)}_{k_{j_2} \text{ times}}, \dots, \underbrace{(x_n, \dots, x_n)}_{k_{j_n} \text{ times}}, \underbrace{(0, \dots, 0)}_{n-j \text{ times}}. \quad (12)$$

If $k_{j_m}, \dots, k_{j_n} = 0$ then x_m, \dots, x_n do not appear in the generator.

Let ψ_n be the number of types of G_n^{op} -orbits induced this way, then

$$\psi_n = \sum_{j=0}^n |T_j^n|. \quad (13)$$

For example, we consider the following 7 G_3^{op} -orbits (only one representative of each orbit is given):

$T_{j,i}^3$	\mapsto generator	number of elements in an orbit
$T_{0,1}^3 = (0, 0, 0)$	$\mapsto (0, 0, 0)$	1
$T_{1,1}^3 = (1, 0, 0)$	$\mapsto (x_1, 0, 0)$	6
$T_{2,1}^3 = (2, 0, 0)$	$\mapsto (x_1, x_1, 0)$	12
$T_{2,2}^3 = (1, 1, 0)$	$\mapsto (x_1, x_2, 0)$	24
$T_{3,1}^3 = (3, 0, 0)$	$\mapsto (x_1, x_1, x_1)$	8
$T_{3,2}^3 = (2, 1, 0)$	$\mapsto (x_1, x_1, x_2)$	24
$T_{3,3}^3 = (1, 1, 1)$	$\mapsto (x_1, x_2, x_3)$	24

With $G_n^{op}(k_{j_1}, k_{j_2}, \dots, k_{j_n})$ we denote a minimal subset of G_n^{op} that, when applied to a generator that corresponds to $(k_{j_1}, k_{j_2}, \dots, k_{j_n})$, generates all points of its orbit. The number of distinct points in an orbit then follows directly:

$$|G_n^{op}(k_{j1}, k_{j2}, \dots, k_{jn})| = 2^j \times \binom{n}{n-j} \times \prod_{u=1}^n \binom{\sum_{i=u}^n k_{ji}}{k_{ju}}$$

if $(k_{j1}, \dots, k_{jn}) \neq (1, \dots, 1)$

and $|G_n^{op}(1, 1, \dots, 1)| = 2^{n-1} n!$ otherwise.

It is interesting to note that all G_n^{op} -orbits are G_n -orbits *except* the orbit of type $(1, 1, \dots, 1)$. Each orbit introduces a number of unknowns in the nonlinear equations (5): the weight and the coordinate of a generator. The number of unknowns introduced by an orbit of type $T_{j,p}^n$ is

$$[T_{j,p}^n] := 1 + |\{k_{ji} | k_{ji} \neq 0, k_{ji} \text{ is a component of } T_{j,p}^n \text{ and } i = 1, 2, \dots, n\}|,$$

where $p = 1, 2, \dots, |T_j^n|$.

Let $t_{j,p}$ be the number of orbits associated to $T_{j,p}^n$. The total number of unknowns in the system of nonlinear equations (5) is then

$$s := \sum_{j=0}^n \sum_{p=1}^{|T_j^n|} t_{j,p} [T_{j,p}^n]. \quad (14)$$

3 Study of the system of nonlinear equations

In the previous section we observed that as long as $d < n^2$, we have $\mathcal{P}_d^n(G_n) = \mathcal{P}_d^n(G_n^{op})$. We also observed that all G_n^{op} -orbits are G_n -orbits *except* the orbit of type $(1, 1, \dots, 1)$. Consequently for moderate degrees of precision $d < n^2$ and as long as no orbits of type $(1, 1, \dots, 1)$ are used, the system of nonlinear equations that defines a G_n^{op} -invariant cubature formula is identical to the system of equations that defines a G_n -invariant (a so-called fully symmetric) cubature formula. The possible choices of orbits and the construction of such cubature formulas have been already investigated a lot, see for example [17,15,13,8–10,3,20]. For consistency conditions we refer to [15,13] and for a survey of known cubature formulas we refer to [6,5].

Rabinowitz and Richter [17] introduced the notion of consistency conditions. A consistency condition is an inequality for the $t_{j,p}$ that must be satisfied in order to obtain a system of nonlinear equations where the number of unknowns is greater than or equal to the number of equations in each subsystem. If one recognises the subsystems, the consistency conditions can immediately be derived from what we know about the good integrity basis, see [4, §10.2]. We will now derive *some* of these conditions *to illustrate* this approach and to point the reader's attention to some pitfalls.

3.1 Consistency conditions

Demanding that the number of unknowns exceeds the number of equations gives a first consistency condition:

$$\text{CC1 : } \sum_{j=0}^n \sum_{p=1}^{|T_j^n|} [T_{j,p}^n] t_{j,p} \geq \dim P_d^n(G_n^{op}). \quad (15)$$

This condition is in some way too pessimistic whenever $t_{n,|T_n^n|} = 0$. Indeed, $P_d^n(G_n^{op})$ contains odd polynomials whenever $d \geq n^2$. Such polynomials are dealt with automatically whenever $t_{n,|T_n^n|} = 0$, because then the cubature formula will be fully symmetric and odd polynomials are integrated to zero. Consequently, in the above consistency condition, as well as in all that we will show below, one has to subtract the number of odd invariant polynomials from the right hand side of the consistency condition whenever $t_{n,|T_n^n|} = 0$. Actually in that case, the consistency conditions reduce to the well known conditions for fully symmetric cubature formulas. We will therefore always assume in what follows that $t_{n,|T_n^n|} \neq 0$.

To integrate the polynomials

$$\phi_1^{i_1} \cdots \phi_n^{i_n} \cdot \phi_{n+1}, \quad i_j \in \mathbb{N} \cup \{0\} \text{ and } \sum_{j=1}^n 2ji_j \leq d - n^2,$$

one needs orbits with all components distinct and different from zero, i.e., orbits of type $(1,1, \dots, 1)$. So, we obtain a second consistency condition:

$$\text{CC2 : } [T_{n,|T_n^n|}^n] t_{n,|T_n^n|} = (n+1)t_{n,|T_n^n|} \geq \dim P_{d-n^2}^n(G_n). \quad (16)$$

Orbits with generators with a zero component do not help to integrate the polynomials

$$\phi_1^{i_1} \cdots \phi_n^{i_n} \cdot \phi_{n+1}^{i_{n+1}} \quad (17)$$

with $i_n \geq 1$ or $i_{n+1} = 1$. From an observation of this kind follows a consistency condition. In this case, both the left and right hand side will include those of (16). The additional polynomials in (17) are

$$\phi_n \phi_1^{i_1} \cdots \phi_n^{i_n}, \quad i_j \in \mathbb{N} \cup \{0\} \text{ and } \sum_{j=1}^n 2ji_j \leq d - 2n.$$

This gives us a third consistency condition:

$$\text{CC3 : } \sum_{p=1}^{|T_n^n|} [T_{n,p}^n] t_{n,p} \geq \dim P_{d-2n}^n(G_n) + \dim P_{d-n^2}^n(G_n) \quad (18)$$

Now we investigate the influence of orbits with generators with at least two zero components. The additional polynomials that vanish are

$$\phi_{n-1}\phi_1^{i_1}\cdots\phi_{n-1}^{i_{n-1}}, \quad i_j \in \mathbb{N} \cup \{0\} \text{ and } \sum_{j=1}^{n-1} 2ji_j \leq d - 2(n-1).$$

This gives us a fourth consistency condition:

$$\begin{aligned} \text{CC4 : } \sum_{j=n-1}^n \sum_{p=1}^{|T_j^n|} [T_{j,p}^n] t_{j,p} &\geq \dim P_{d-2n}^n(G_n) + \dim P_{d-n^2}^n(G_n) \\ &+ \dim P_{d-2(n-1)}^{n-1}(G_{n-1}) \end{aligned} \quad (19)$$

Similarly one can obtain consistency conditions by investigating the influence of orbits with at least three, four, \dots , n zeros. The last consistency condition of this set is

$$\begin{aligned} \text{CC}(n+2) : \sum_{j=1}^n \sum_{p=1}^{|T_j^n|} [T_{j,p}^n] t_{j,p} &\geq \dim P_{d-2n}^n(G_n) + \dim P_{d-n^2}^n(G_n) \\ &+ \sum_{k=1}^{n-1} \dim P_{d-2k}^k(G_k). \end{aligned} \quad (20)$$

At this point, it will be clear that one can obtain the consistency conditions this way.

One also has to be careful to investigate all special cases. That was the major contribution of [13].

In addition to the conditions obtained above, there are many others. Consider for example the invariant polynomial

$$\varphi := (n-1)\phi_1^2 - 2n\phi_2 = \sum_{k < j} (x_j^2 - x_k^2)^2.$$

This fourth degree polynomial, and all its multiples, vanish in the points of orbits of type $(n, 0, \dots, 0)$, i.e., those with a generator with identical components.

Orbits with generators with at least one zero component or with identical components do not help to integrate the polynomials

$$\begin{aligned} \varphi\phi_n\phi_1^{i_1}\cdots\phi_n^{i_n}\phi_{n+1}^{i_{n+1}} &\text{ with } i_j \in \mathbb{N} \cup \{0\}, i_{n+1} \in \{0, 1\} \\ \text{and } \sum_{j=1}^n 2ji_j + n^2i_{n+1} &\leq d - (2n+4). \end{aligned}$$

These polynomials can be split into two disjoint sets:

$$\varphi\phi_n\phi_1^{i_1}\cdots\phi_n^{i_n}, \quad i_j \in \mathbb{N} \cup \{0\} \text{ and } \sum_{j=1}^n 2ji_j \leq d - (2n + 4)$$

and

$$\varphi\phi_n\phi_{n+1}\phi_1^{i_1}\cdots\phi_n^{i_n}, \quad i_j \in \mathbb{N} \cup \{0\} \text{ and } \sum_{j=1}^n 2ji_j \leq d - (2n + 4) - n^2.$$

From this we obtain the consistency condition

$$\text{CC}(n + 3) : \sum_{p=2}^{|T_n^n|} [T_{n,p}^n] t_{n,p} \geq \dim P_{d-(2n+4)}^n(G_n) + \dim P_{d-n^2-(2n+4)}^n(G_n). \quad (21)$$

More conditions can be obtained by extending this.

For example, for $n = 3$ and $t_{3,3} \neq 0$ we obtain

	left hand side	$d = 8$	$d = 9$
CC0	$t_{0,1} \leq$	1	1
CC1	$t_{0,1} + 2t_{1,1} + 2t_{2,1} + 3t_{2,2} + 2t_{3,1} + 3t_{3,2} + 4t_{3,3} \geq$	11	12
CC2	$4t_{3,3} \geq$	0	1
CC3	$2t_{3,1} + 3t_{3,2} + 4t_{3,3} \geq$	2	3
CC4	$2t_{2,1} + 3t_{2,2} + 2t_{3,1} + 3t_{3,2} + 4t_{3,3} \geq$	6	7
CC5	$2t_{1,1} + 2t_{2,1} + 3t_{2,2} + 2t_{3,1} + 3t_{3,2} + 4t_{3,3} \geq$	10	11
CC6	$3t_{3,2} + 4t_{3,3} \geq$	0	0

The number of points will be

$$N = t_{0,1} + 6t_{1,1} + 8t_{3,1} + 12t_{2,1} + 24(t_{2,2} + t_{3,2} + t_{3,3}). \quad (22)$$

Consistency conditions are used in the following way. One starts with the following integer linear programming problem: search the integer solutions of the consistency conditions that minimize (22). For each of these solutions one tries to find a real solution of the nonlinear equations (5). If such a solution is not found or the solution has points outside the region Ω (this seems to happen in most cases), then one searches integer solutions of the consistency conditions with more points than the minimum. For low dimensions, a small program with ψ_n nested loops that simply tries $t_{i,j} = 0, 1, \dots$ suffices.

3.2 An equivalent system of equations

In the articles that deal with the construction of fully symmetric formulas by directly solving a system of nonlinear equations, one seldom uses the equations (5) with the basic invariant polynomials (10). Instead one tries to solve the equations

$$\sum_{j=1}^K w_j f_i(\mathbf{x}_j) = I[f_i]$$

where

$$f_i \in \{x_1^{i_1} \cdots x_n^{i_n} \mid i_j \text{ even integers, } \sum_{j=1}^n i_j \leq d \text{ and } i_1 \geq i_2 \geq \cdots \geq i_n\}.$$

In this subsection we will show that the two approaches are equivalent thanks to the Reynold operator. This motivates the following definitions.

For non-negative integers j we define the following sets of n -tuples:

$$E_j^n := \{(k_{j1}, k_{j2}, \dots, k_{jn}) \mid j = \sum_{i=1}^n k_{ji}, k_{ji} \text{ even integers and } k_{j1} \geq k_{j2} \geq \cdots \geq k_{jn}\}.$$

$$O_j^n := \{(k_{j1}, k_{j2}, \dots, k_{jn}) \mid j = \sum_{i=1}^n k_{ji}, k_{ji} \text{ odd integers and } k_{j1} > k_{j2} > \cdots > k_{jn}\}$$

Observe that $O_j^n = \emptyset$ for $j < n^2$.

Theorem 6 *Let*

$$M_j^n := \{x^{k_{j1}} x^{k_{j2}} \cdots x^{k_{jn}} \mid (k_{j1}, k_{j2}, \dots, k_{jn}) \in V_j^n\} \quad (23)$$

where

$$V_j^n := \begin{cases} O_j^n & \text{if } n \text{ and } j \text{ are odd} \\ E_j^n & \text{if } n \text{ is odd and } j \text{ is even} \\ E_j^n \cup O_j^n & \text{if } n \text{ and } j \text{ are even} \\ \emptyset & \text{if } n \text{ is even and } j \text{ is odd} \end{cases}$$

Then a set of c_j linearly independent homogeneous G_n^{op} -invariant polynomials of degree j is obtained by applying the Reynold operator to each monomial of the set M_j^n .

Proof: Let us analyze the G_n^{op} -orbit of a point $\mathbf{x} = (x_1, x_2, \dots, x_n)$ of type $(1, 1, \dots, 1)$. This orbit will always contain $n!$ points of the form $(\alpha_1 x_{p(1)}, \alpha_2 x_{p(2)}, \dots, \alpha_n x_{p(n)})$ where $(p(1), \dots, p(n))$ is a permutation of $(1, 2, \dots, n)$ and $\alpha_i = 1$ or -1 , $i = 1, 2, \dots, n$. The α_i must be chosen such that the transformation that maps (x_1, x_2, \dots, x_n) onto $(\alpha_1 x_{p(1)}, \dots, \alpha_n x_{p(n)})$ is orientation preserving. These points can be obtained by rotating \mathbf{x} successively over an angle $\pi/2$ in some of the planes formed by two coordinate axes: each such rotation corresponds to a transposition of 2 coordinates with a change of signs. The set of all these points is denoted by $G_n^{op(\pi/2)}(\mathbf{x})$.

If the permutation is odd (i.e., if the determinant of the permutation matrix $= -1$) then $\alpha_1 \alpha_2 \cdots \alpha_n = -1$ is necessary in order to turn the transformation into an orientation preserving one. Otherwise $\alpha_1 \alpha_2 \cdots \alpha_n = 1$. Because the number of odd permutations is equal to the number of even permutations, one has

$$\left| \{ \mathbf{y} \in G_n^{op(\pi/2)}(\mathbf{x}) : \prod_{i=1}^n \alpha_i = 1 \} \right| = \left| \{ \mathbf{y} \in G_n^{op(\pi/2)}(\mathbf{x}) : \prod_{i=1}^n \alpha_i = -1 \} \right|. \quad (24)$$

Consider one of the points $\tilde{\mathbf{x}} = (\alpha_1 x_{p(1)}, \alpha_2 x_{p(2)}, \dots, \alpha_n x_{p(n)})$ with $\alpha_1 \alpha_2 \cdots \alpha_n = -1$. By rotating $\tilde{\mathbf{x}}$ over an angle π in the planes formed by every combination of two coordinate axes, we obtain distinct points of the form $(\beta_1 x_{p(1)}, \beta_2 x_{p(2)}, \dots, \beta_n x_{p(n)})$, with $\beta_i = 1$ or -1 , $i = 1, 2, \dots, n$ and $\beta_1 \beta_2 \cdots \beta_n = -1$. We denote the set of all these points, including $\tilde{\mathbf{x}}$, by $G_n^{op(\pi)}(\tilde{\mathbf{x}})$. The order of this set

$$\left| G_n^{op(\pi)}(\tilde{\mathbf{x}}) \right| = 2^{n-1}.$$

Indeed, one can choose the sign of $n - 1$ coordinates. The sign of the n th coordinate follows from the constraint $\alpha_1 \alpha_2 \cdots \alpha_n = \beta_1 \beta_2 \cdots \beta_n = -1$.

Similarly, we can obtain a set $G_n^{op(\pi)}(\tilde{\mathbf{x}})$ if the point $\tilde{\mathbf{x}} = (\alpha_1 x_{p(1)}, \alpha_2 x_{p(2)}, \dots, \alpha_n x_{p(n)})$ satisfies $\alpha_1 \alpha_2 \cdots \alpha_n = 1$.

Because a G_n^{op} -orbit of a point of type $(1, 1, \dots, 1)$ consists of $n!2^{n-1}$ points, each point can be obtained by a combination of two of the transformations described above, i.e., the G_n^{op} -orbit of \mathbf{x} is

$$\{ \mathbf{y} \in G_n^{op(\pi)}(\tilde{\mathbf{x}}) : \tilde{\mathbf{x}} \in G_n^{op(\pi/2)}(\mathbf{x}) \}.$$

We can use this to see the effect of applying the Reynold operator (7) to a monomial.

Let p be a monomial having at least one even exponent (including 0) and at the same time at least one odd exponent. From the construction of $G_n^{op(\pi)}(\tilde{\mathbf{x}})$

follows that

$$\sum_{\mathbf{y} \in G_n^{op(\pi)}(\tilde{\mathbf{x}})} p(\mathbf{y}) \equiv 0$$

and consequently $p_* \equiv 0$

Let p be a monomial having only odd exponents, but not all distinct. Then the terms in

$$\sum_{g \in G_n^{op}} p(g(\mathbf{x}))$$

will cancel pairwise because of (24).

We thus obtain that all monomials (disregarding the order of exponents) not having elements of the sets O_j^n or E_j^n as exponents are converted into zero by applying the Reynold operator to them. Furthermore it can be seen that all invariant polynomials obtained by applying the Reynold operator to all monomials that correspond to $E_j^n \cup O_j^n$ are linearly independent. \square

For example, consider the case $n = 3$ and $d = 9$. The set $G_3^{op(\pi/2)}(\mathbf{x})$ has 3! elements:

$$G_3^{op(\pi/2)}(\mathbf{x}) = \{\mathbf{x}_1 = (x_1, x_2, x_3), \mathbf{x}_2 = (x_2, -x_1, x_3), \mathbf{x}_3 = (x_3, -x_1, -x_2), \\ \mathbf{x}_4 = (x_3, -x_2, x_1), \mathbf{x}_5 = (-x_2, -x_3, x_1), \mathbf{x}_6 = (x_1, -x_3, x_2)\}$$

There are other possibilities, depending on the selected rotations. This will however only influence the signs. Once this set is fixed, for each of its points \mathbf{x}_i we can compute $G_3^{op(\pi)}(\mathbf{x}_i)$. E.g.,

$$G_3^{op(\pi)}(x_1, -x_3, x_2) = \{(x_1, -x_3, x_2), (-x_1, x_3, x_2), (x_1, x_3, -x_2), (-x_1, -x_3, -x_2)\}.$$

For the monomials p having both at least one even exponent (including 0) and at the same time at least one odd exponent, $x, xy, x^3, x^2y, x^3y, x^5, x^4y, x^3y^2, x^2y^2z, \dots$,

$$\sum_{\mathbf{y} \in G_3^{op(\pi)}(\mathbf{x}_i)} p(\mathbf{y}) \equiv 0.$$

Next consider the monomial $p = x^5yz$. Then

$$\sum_{\mathbf{y} \in G_3^{op(\pi)}(\mathbf{x}_1)} p(\mathbf{y}) + \sum_{\mathbf{y} \in G_3^{op(\pi)}(\mathbf{x}_6)} p(\mathbf{y}) \equiv 0, \\ \sum_{\mathbf{y} \in G_3^{op(\pi)}(\mathbf{x}_2)} p(\mathbf{y}) + \sum_{\mathbf{y} \in G_3^{op(\pi)}(\mathbf{x}_5)} p(\mathbf{y}) \equiv 0$$

and

$$\sum_{\mathbf{y} \in G_3^{op(\pi)}(\mathbf{x}_3)} p(\mathbf{y}) + \sum_{\mathbf{y} \in G_3^{op(\pi)}(\mathbf{x}_4)} p(\mathbf{y}) \equiv 0.$$

Similarly, the monomials $xyz, x^3yz, x^3y^3z, x^7yz, x^3y^3z^3$ vanish.

Obviously, all monomials having elements of the set $E_0^3 \cup E_2^3 \cup E_4^3 \cup E_6^3 \cup E_8^3 \cup O_9^3$ as exponents don't vanish and by applying the Reynold operator to them all linearly independent polynomials are obtained for $n = 3$ and $d = 9$. If we take, e.g., $E_4^3 = \{(4, 0, 0), (2, 2, 0)\}$ then we obtain the invariant polynomials

$$(x^4)_* = \frac{1}{3}(x^4 + y^4 + z^4) \quad \text{and} \quad (x^2y^2)_* = \frac{1}{3}(x^2y^2 + y^2z^2 + x^2z^2).$$

These can be written in term of the basic invariant polynomials:

$$(x^4)_* = \frac{1}{3}(\phi_1^2 - 2\phi_2) \quad \text{and} \quad (x^2y^2)_* = \frac{1}{3}\phi_2.$$

The monomials in M_j^n are called the *monomial generators*. A side-effect of the previous proof is the following.

Corollary 2 *For non-negative integer j and dimension $n \geq 2$, the dimension c_j of the space of homogeneous G_n^{op} -invariant polynomials of degree j are*

- (1) for odd n
 - (a) for odd j
 - (i) $c_j = 0$ for $j < n^2$;
 - (ii) $c_j =$ the number of all elements of the set O_j^n ;
 - (b) for even j ,
 - (i) $c_j =$ the number of all elements of the set E_j^n ;
- (2) for even n
 - (a) for odd j , $c_j = 0$;
 - (b) for even j ,
 - (i) $c_j =$ the number of all elements of the set E_j^n for $j < n^2$;
 - (ii) $c_j =$ the number of all elements of the set $E_j^n \cup O_j^n$ for $j \geq n^2$.

4 Results

In this section we present some results for the unit cube with constant weight function obtained using the approach described in the previous sections to illustrate its power and problems. We aim to obtain cubature formulas with a number of points lower than in results that were known before. In our search

we will restrict ourselves to cubature formulas that are *not* fully symmetric and thus assume that $t_{3,3} \geq 1$. We will see however that sometimes the structure of the solution will be changed. E.g., an orbit generated by (x_1, x_2, x_3) introduces 4 unknowns in the system of equations but it might happen that a solution is obtained with $x_2 = x_3$. And so it is still possible to obtain a fully symmetric formula.

In this paper we will also restrict ourselves to cubature formulas with no free parameters, in other words, we only consider the case where consistency condition CC1 is an equality.

All results were verified in extended precision, using Bailey's Fortran 90 multiprecision modules [1], and the results are believed to be correctly rounded up to the last digit shown.

The first interesting case under these assumptions is degree 8 in three dimensions.

4.1 Degree 8

G_n^{op} -invariant cubature formulas of degree 8 are determined by 11 equations (5).

The previously known cubature formula with lowest number of points has 47 points with structure $(1, 1, 0, 0, 2, 0, 1)$ and was obtained in [14]. It has all points inside the region of integration. For better accessibility we repeat this recomputed formula in Table 1.

We obtained a formula having 45 points, with structure $(1, 2, 0, 0, 1, 0, 1)$. It has however some points outside the region of integration. This formula is given in Table 2. As far as we know this formula is new and has the lowest known number of points, see [6,5].

4.2 Degree 10

G_n^{op} -invariant cubature formulas of degree 10 are determined by 17 equations (5).

In [14] a cubature formula of degree 10 having 77 points with structure $(1, 2, 0, 0, 2, 0, 2)$ is presented. Observe that this structure introduces 17 unknowns (14). We could not improve this result.

4.3 Degree 11

G_n^{op} -invariant cubature formulas of degree 11 are determined by 18 equations (5).

The three previously known cubature formulas with lowest number of points have 89 points [9,10,14]. These are all fully symmetric.

We obtained a formula with 84 points with structure $(0, 2, 2, 0, 3, 0, 1)$ with one generator far outside the region of integration, see Table 3. This result is however remarkable because it shows that the structure can be changed into a fully symmetric formula. This one has structure $(0, 2, 2, 0, 3, 1, 0)$, so a generator of the form (x_1, x_2, x_3) , which introduced 4 unknowns in the system of 18 equations, lead to a solution with $x_2 = x_3$.

4.4 Degree 12

G_n^{op} -invariant cubature formulas of degree 12 are determined by 25 equations (5).

In [14] cubature formulas of degree 12 with 137 and 127 points were presented as a solution of the system of equations with structure $(1, 2, 1, 1, 2, 1, 2)$ and $(1, 3, 1, 1, 3, 1, 1)$. Both structures introduce 25 unknowns. We could not improve these results.

In retrospect, the obtained results in [14] are fully symmetric and consequently have an odd degree of precision. So although they are presented as cubature formulas of degree 12, they really have degree 13! If one directly searches for fully symmetric cubature formulas of degree 13 with the structure of this result, then the formula with 127 is a solution of a system of 23 equations with 24 unknowns, i.e., a system with one free parameter.

4.5 Degree 13

G_n^{op} -invariant cubature formulas of degree 13 are determined by 27 equations (5).

As far as we know only one formula of degree 13 has been published and this uses 151 points, some of which are outside the region of integration [9]. In addition, there are the formulas with 137 and 127 points published in [14] as having degree 12. These have also some points outside the region of integration.

For better accessibility we repeat the recomputed cubature formula with 127 points in Table 4.

We obtained formulas with 149, 145 and 143 points. One of the cubature formulas with 143 points, with structure (1, 3, 1, 1, 2, 1, 2), has all points inside the region of integration. This formula is given in Table 5. Observe that the actual result is also a fully symmetric formula with structure (1, 3, 1, 1, 2, 3, 0).

Table 1: Cubature formula of degree 8 with 47 points.

weight	generator point		
0.4519037148751997	0.0	0.0	0.0
0.2993791773523389	0.7824607964359516	0.0	0.0
0.3008761593712400	0.4880946697063665	0.4880946697063665	0.4880946697063665
0.04948432558770381	0.8622189276614812	0.8622189276614812	0.8622189276614812
0.1228723892224673	0.2811139094083419	0.9441965782920082	0.6975748337072370

Table 2: Cubature formula of degree 8 with 45 points.

weight	generator point		
-2.463199622285841	0.0	0.0	0.0
0.9133715960969999	0.4382032850415545	0.0	0.0
0.1139966594179854	0.9773391544061192	0.0	0.0
1.236499932378910 10^{-3}	1.224744871391589	1.224744871391589	1.224744871391589
0.1787124204057041	0.8848065928534505	0.3861200022666244	0.7246871699123335

Table 3: Cubature formula of degree 11 with 84 points.

weight	generator point		
$1.899392614715866 \cdot 10^{-12}$	8.910406659693070	0.0	0.0
0.1509766120915464	0.9253947441376310	0.0	0.0
0.2543904602021154	0.5787192007068168	0.5787192007068168	0.0
0.04773107751169104	0.9260902491961117	0.9260902491961117	0.0
0.09468587065692231	0.2050794278938527	0.2050794278938527	0.2050794278938527
0.03469495002113647	0.8795398628617438	0.8795398628617438	0.8795398628617438
-0.1421221169310977	0.7060290954549611	0.7060290954549611	0.7060290954549611
0.1487755102040816	0.8819171036881969	0.5773502691896258	0.5773502691896258

Table 4: Cubature formula of degree 13 with 127 points.

weight	generator point		
-0.07392803169551410	0.0	0.0	0.0
0.01047790153440169	1.511521614586340	0.0	0.0
-9.844095092340856 10^{-3}	1.518036150896988	0.0	0.0
0.2566798947018500	0.4789453644853970	0.0	0.0
5.698078501485224 10^{-3}	1.010788881812447	1.010788881812447	0.0
0.1210486991503321	0.8759698649844666	0.4687839764804761	0.0
8.524241405662044 10^{-3}	0.9312968210145930	0.9312968210145930	0.9312968210145930
0.02774661970591842	0.8008618355165513	0.8008618355165513	0.8008618355165513
0.1896430443832050	0.5012617586565738	0.5012617586565738	0.5012617586565738
0.05956382874226242	0.8504419008369039	0.8504419008369039	0.3858343598195990
0.01331904039306980	1.029692626670945	0.64276930417252580	0.64276930417252580

Table 5: Cubature formula of degree 13 with 143 points.

weight	generator point		
-1.437929681007702	0.0	0.0	0.0
0.2751638314548124	0.4271982785522924	0.0	0.0
0.05969737985407605	0.9759258101988700	0.0	0.0
0.1957779899572527	4.597174699741714 10^{-8}	0.0	0.0
-0.06349777333388220	0.9758804588167024	0.9758804588167024	0.0
0.06641612493626893	0.8905259344452349	0.6348385168267266	0.0
5.588460949347480 10^{-3}	0.9514802502494549	0.9514802502494549	0.9514802502494549
0.06190603644353458	0.7865944923816076	0.7865944923816076	0.7865944923816076
0.1277083009214507	0.3767337028665920	0.3767337028665920	0.7370109241895892
0.02489821355566059	0.6067691727170686	0.6067691727170686	0.9839971199914726
0.05081535118138582	0.9645114312097896	0.9645114312097896	0.1790934033355623

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