Acta Numerica (1997), *pp.* 1–54

Constructing cubature formulae: the science behind the art

Ronald Cools
Katholieke Universiteit Leuven
Dept. of Computer Science
Celestijnenlaan 200A
B-3001 Heverlee, Belgium
E-mail: Ronald.Cools@cs.kuleuven.ac.be

In this paper we present a general, theoretical foundation for the construction of cubature formulae to approximate multivariate integrals. The focus is on cubature formulae that are exact for certain vector spaces of polynomials. Our main quality criteria are the algebraic and trigonometric degrees. The constructions using ideal theory and invariant theory are outlined. The known lower bounds for the number of points are surveyed and characterizations of minimal cubature formulae are given. We include references to all known minimal cubature formulae. Finally, some methods to construct cubature formulae illustrate the previously introduced concepts and theorems.

CONTENTS

1. What to expect

This is a paper for patient readers. The reader has to digest several pages before being enlightened on the direction taken by this paper. Following a short section with historical notes, Section 3 describes the problem this paper concentrates upon, approximating multivariate integrals, and presents my favourite quality criteria. Section 4 sketches several ways to construct such approximations, one of which is this paper's real subject. After introducing concrete integrals and a tool to deal with symmetries in Section 5, we are ready for the real work.

In Section 6, interpolatory cubature formulae are characterized and the connection with orthogonal polynomials and ideal theory is in the spotlight. Sections 7 and 8 are devoted to the determination of lower bounds and the characterization of minimal cubature formulae. Finally, Sections 9 and 10 concentrate on the art of constructing cubature formulae.

Readers familiar with the construction of quadrature formulae may find it helpful to spell out the meaning in one dimension of the definitions and theorems given for arbitrary dimensions.

2. On the origin of cubature formulae

2.1. The prehistory

According to the Oxford English Dictionary, cubature is the determination of the cubic contents of a solid, that is, the computation of a volume. We are interested in the construction of cubature formulae, that is, formulae to estimate volumes. The problem of measuring areas and volumes has always been present in everyday life. The ancient Babylonians and Egyptians already had precise and correct rules for finding the areas of triangles, trapezoids and circles (for the Babylonians π equalled 3, for the Egyptians 235/81) and the volumes of parallelepipeds, pyramids and cylinders. They thought of these figures in concrete terms, mainly as storage containers for grain. They discovered these rules empirically.

The first abstract proofs of rules for finding some areas and volumes are said to have been developed by Eudoxus of Cnidus in about 367 BC. About a century later, his method was further developed by Archimedes. In the middle of the 16th century Archimedes' work became available in Greek and Latin and in the 17th century his method became known as the method of exhaustion. It culminated in the 19th century in the isolation of the concept of Riemann integration, defined by approximating Riemann sums.

In southern Germany, due to increased commerce, measuring the contents of wine barrels became important in the 15th century, and therefore approximations were introduced. In 1613, Johannes Kepler witnessed a salesman using *one* gauging-rod to measure the contents of *all* Austrian wine barrels *without* further calculations. This was the motivation for what became his book *Nova Stereometria Doliorum Vinariorum*[1] (Kepler 1615). It turned out that for the type of barrels used in Austria, the approximation used by the salesman was quite good. At the end of the book Kepler wrote that his book was longer than he had expected and people could just as well continue to use the approximation. In his final sentence he philosophizes on the eternal compromise between approximations and exact calculations:

Et cum pocula mille mensi erimus,
Conturbabimus illa, ne sciamus.[2]

The start of the modern study of volume computation is usually linked with Kepler.

The word 'cubature' appeared in the written English language around the same time. The oldest known reference, according to the Oxford English Dictionary, is a letter from Collins in 1679 containing the sentence: 'In order to the quadrature of these figures and the cubature of their solids.' From 1877 we cite Williamson: 'The cube ... is ... the measure of all solids, as the square is the measure of all areas. Hence the finding the volume of a solid is called its cubature.'

The formulation of the problem of measuring in terms of integrals and functions is much more recent. The first cubature formula in the form we are now familiar with was constructed by Maxwell (1877). And that is when our story starts. For us, a cubature formula is a weighted sum of function evaluations used to approximate a multivariate integral. (The function is not necessarily the integrand, nor is the same function used for each evaluation.) The prehistory of our field of interest thus ends in 1877. In the following section we briefly sketch different approaches and specify the approach we follow in the rest of this paper.

2.2. In search of a pedigree

There are several criteria to specify and classify cubature formulae based on their behaviour for specific classes of functions. A classical way to present a survey is to sketch the pedigree of different approaches.

The oldest criterion is the *algebraic degree* of a cubature formula, used by James Clerk Maxwell in 1877[3]. This criterion is obviously inherited from the work on quadrature formulae. We have no idea what a cubature formula of algebraic degree d will give us when applied to a function that is not a polynomial of degree smaller than or equal to d.

[1] *Solid Geometry of Wine Barrels*
[2] After measuring a thousand cups, we will be so confused that we lose our head.
[3] When we write that something happened in a particular year, we in fact refer to the year the results were published.

The second oldest approach to approximate multivariate integrals does not have this problem. One evaluates the integrand function in a number of randomly selected points and uses the average function value. This is the classical *Monte Carlo method.* The idea came to Stanislaw Ulam, Nick Metropolis and John von Neumann while working on the Manhattan Project in 1945. From the Strong Law of Large Numbers it follows that the expected value this method delivers is the integral. If one restricts the integrands to the class of square integrable functions, the Central Limit Theorem gives rise to a probabilistic error bound known as the '$N^{1/2}$ law': for a fixed level of confidence, the error bound varies inversely as $N^{1/2}$.

Because truly random samples are not available and the error estimate of the Monte Carlo method is only probabilistic, researchers in the early 1950s became interested in *quasi-Monte Carlo methods.* The method received its name from R. D. Richtmyer (1952). In these methods one uses, as in the classical Monte Carlo method, an equal-weights cubature formula but chooses the points to be 'better than random'. One obtains rigorous error bounds that behave better than the $N^{1/2}$ law. The first quasi-Monte Carlo methods were based on low discrepancy sequences. Another type of quasi-Monte Carlo method is the *method of good lattice points* introduced by Nikolai M. Korobov (1959). The more general notion of a lattice rule was introduced by Konstantin K. Frolov (1977) and rediscovered by Ian H. Sloan and Philip Kachoyan (1987).

It should be noted that Frolov did not see his rules as quasi-Monte Carlo methods. He constructed cubature formulae that are exact for a set of trigonometric polynomials, that is, his criterion is the *trigonometric degree.* It is strange that his paper is not cited in the Russian literature on cubature formulae of trigonometric degree. We will see that there are many similarities between the construction of cubature formulae of algebraic degree and the construction of formulae of trigonometric degree. In addition, Frolov made the link with lattice rules. Hence the pedigree approach breaks down here and we will use another thread for this story.

We will focus on cubature formulae that are exact for a certain class of functions: polynomials, both algebraic and trigonometric. Cubature formulae of algebraic degree and lattice rules fit in this single framework.

Cubature formulae of algebraic degree play an important role for low dimensions and are essential building blocks for adaptive routines to compute integrals. Practical experience with lattice rules is still limited. Most people expect them to be important for high dimensions. However, there already exist two-dimensional applications that benefit from their properties.

3. Problem setting and criteria

An integral I is a linear continuous functional

$$I[f] := \int_{\Omega} w(\mathbf{x}) f(\mathbf{x}) \, \mathrm{d}\mathbf{x} \tag{3.1}$$

where the region $\Omega \subset \mathbb{R}^n$. We use $\mathbf{x}$ as a shorthand for the variables $x_1, x_2, \ldots, x_n$. We will always assume that $w(\mathbf{x}) \geq 0$, for all $\mathbf{x} \in \Omega$, that is, I is a positive functional.

It is often desirable to approximate I by a weighted sum of (easier) functionals such that

$$I[f] \simeq Q[f] = \sum_{j=1}^{N} w_j L_j[f] \tag{3.2}$$

where $w_j \in \mathbb{R}$. We will only consider approximations that are exact for a given vector space of functions and we start with a very general result on the existence of such approximations, due to Sobolev (1962); see also Mysovskikh (1981).

We will need the following lemma.

Lemma 3.1 The system of linear equations

$$A\mathbf{x} = \mathbf{b} \quad \text{with} \quad A \in \mathbb{C}^{\mu \times \nu}, \quad \mathbf{b} \in \mathbb{C}^{\mu}, \quad \mathbf{x} \in \mathbb{C}^{\nu}$$

has a solution if and only if $\sum_{j=1}^{\mu} b_j \mathbf{y}_j = 0$ for all solutions $\mathbf{y}$ of $A^{\star}\mathbf{y} = 0$ ($A^{\star} = \bar{A}^T$; $\bar{y}$ is the complex conjugate of y).

Proof. Let L be the vector space generated by the columns $a^{(1)}, \ldots, a^{(\nu)}$ of A, and $L^{\perp} \subset \mathbb{C}^n$ the orthogonal complement of L. Thus $\mathbf{y} \in L^{\perp}$ if and only if $\mathbf{y}$ is orthogonal to all columns of A. Hence $L^{\perp}$ is the subspace of all solutions of $A^{\star}\mathbf{y} = 0$.

$A\mathbf{x} = \mathbf{b}$ has a solution if and only if $\mathbf{b} \in L$. But $\mathbf{b} \in L$ if and only if $\mathbf{b}$ is orthogonal to $\mathbf{y}$ and $A^{\star}\mathbf{y} = 0$. $\square$

Let F be a vector space of functions defined on $\Omega \subset \mathbb{R}^n$ and $F_1 \subset F$ a subspace. Let I be a linear, continuous functional defined on F, that is approximated by a linear combination of other functionals (3.2) with constant coefficients. Let

$$F_0 = \{f \in F_1 : L_j[f] = 0, j = 1, \ldots, N\} \subset F_1.$$

Theorem 3.1 A necessary and sufficient condition for the existence of an approximation (3.2) that is exact for all $f \in F_1$ is

$$f \in F_0 \Rightarrow I[f] = 0. \tag{3.3}$$

Proof. It is trivial that the condition is necessary. It remains to be proven that it is sufficient.

Let f_i, $i = 1, \ldots, \mu$ be a basis of F_1. Then the approximation (3.2) is exact for all $f \in F_1$ if and only if it is exact for f_i, $i = 1, \ldots, \mu$:

$$\sum_{j=1}^{N} w_j L_j[f_i] = I[f_i]. \tag{3.4}$$

(3.4) is a system of linear equations for the weights w_j, $j = 1, \ldots, N$.
Let $(a_1, \ldots a_\mu)^T$ be the solution of the adjoint homogeneous system:

$$\sum_{j=1}^{\mu} a_j L_i[f_j] = 0, \quad i = 1, \ldots, N. \tag{3.5}$$

The lemma implies that (3.4) has a solution if and only if $\sum_{j=1}^{\mu} a_j I[f_j] = 0$ which is equivalent to

$$I\left[\sum_{j=1}^{\mu} a_j f_j\right] = 0. \tag{3.6}$$

But (3.5) is equivalent to

$$L_i\left[\sum_{j=1}^{\mu} a_j f_j\right] = 0, \quad i = 1, \ldots, N,$$

which means that $f = \sum_{j=1}^{\mu} a_j f_j \in F_0$. Hence the necessary and sufficient condition (3.6) for the solvability of (3.4) can be written as $I[f] = 0$. From the solvability of (3.4) follows the sufficientness of (3.3). □

We will only consider functionals L_j that are point evaluations. Most often $L_j[f] = f(\mathbf{y}^{(j)})$ for a $\mathbf{y}^{(j)} \in \mathbb{R}^n$ but occasionally one encounters approximations that use partial derivatives of f, that is,

$$L_j[f] = \frac{\partial^{j_1+\cdots+j_n} f}{\partial x_1^{j_1} \ldots x_n^{j_n}}(\mathbf{y}^{(j)}).$$

Unless stated otherwise, we shall concentrate on approximations that use function values only. If $n = 1$, then Q is called a *quadrature formula.* If $n \geq 2$, then Q is called a *cubature formula.* If partial derivatives are used, Q is called a *generalized cubature formula.* So, for our purposes, a cubature formula Q has the form

$$I[f] \approx Q[f] := \sum_{j=1}^{N} w_j f(\mathbf{y}^{(j)}). \tag{3.7}$$

The choice of the points $\mathbf{y}^{(j)}$ and weights w_j is independent of the function f. They are chosen so that the formula gives a good approximation for some class of functions.

According to Rabinowitz and Richter (1969), a *good quadrature or cubature formula* has all points $\mathbf{y}^{(j)}$ inside the region Ω and all weights w_j positive. Positive weights imply that Q is also a positive functional. As Maxwell (1877) noted when he obtained a cubature formula for the cube with 27 points, some outside the cube, it might be difficult to apply a cubature formula when points are outside the region Ω:

This, of course, renders the method useless in determining the integral from the *measured values* of the quantity u, as when we wish to determine the weight of a brick from the specific gravities of samples taken from 27 selected places in the brick, for we are directed by the method to take some of the samples from places outside the brick.

In the remainder of the paper, we will only consider cubature formulae that are exact for algebraic or trigonometric polynomials.

Let $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_n) \in \mathbb{Z}^n$ and $|\alpha| = \sum_{j=1}^n |\alpha_j|$. An (algebraic) monomial in the variables $x_1, x_2, \ldots, x_n$ is a function of the form $\prod_{j=1}^n x_j^{\alpha_j}$, also denoted by $\mathbf{x}^\alpha$, for $\alpha \in \mathbb{N}^n$. A trigonometric monomial is a function of the form

$$\prod_{j=1}^{n} e^{2\pi\, \mathrm{i}\alpha_j x_j}, \quad \text{where} \quad \mathrm{i}^2 = -1,$$

also denoted by $e^{2\pi\,\mathrm{i}\alpha\mathbf{x}}$. An algebraic, respectively trigonometric, polynomial in n variables is a finite linear combination of monomials, that is,

$$p(\mathbf{x}) = \sum_{\alpha_1,\ldots,\alpha_n=0}^{\infty} a_\alpha \mathbf{x}^\alpha, \qquad \text{respectively} \quad t(\mathbf{x}) = \sum_{\alpha_1,\ldots,\alpha_n=-\infty}^{\infty} a_\alpha e^{2\pi\,\mathrm{i}\alpha\mathbf{x}}.$$

For trigonometric polynomials, some authors add the restriction that a_α and $a_{-\alpha}$ are complex conjugates. One can of course also use sine and cosine functions to describe real trigonometric polynomials. This restriction is unnecessary here.

The *degree* of a multivariate algebraic or trigonometric polynomial v is defined as

$$\deg(v) = \begin{cases} \max\{|\alpha| : a_\alpha \neq 0\} & \text{if } v \neq 0, \\ -\infty & \text{if } v = 0. \end{cases}$$

The vector space of all algebraic polynomials in n variables of degree at most d is denoted by $\mathcal{P}_d^n$. The vector space of all trigonometric polynomials in n variables of degree at most d is denoted by $\mathcal{T}_d^n$. The dimensions of these vector spaces are:

$$\begin{aligned} \dim \mathcal{P}_d^n &= \binom{n+d}{d} \quad \text{and} \\ \dim \mathcal{T}_d^n &= \sum_{i=0}^{n} \binom{n}{i}\binom{d}{i} 2^i. \end{aligned}$$

We can now formulate the criterion we will most often use.

Definition 3.1 A cubature formula Q for an integral I has algebraic, respectively trigonometric, degree d if it is exact for all polynomials of algebraic, respectively trigonometric, degree at most d and it is not exact for at least one polynomial of degree $d+1$.

Cubature formulae of algebraic degree are available for a large variety of regions and weight functions. For a survey, we refer to Stroud (1971) and Cools and Rabinowitz (1993). Cubature formulae of trigonometric degree are only published for $\Omega = [0,1]^n$ and $w(\mathbf{x}) \equiv 1$, and in this paper we will only consider this region. For a survey, we refer to Cools and Sloan (1996).

The *overall degree* of a multivariate polynomial v is defined as

$$\overline{\deg}(v) = \begin{cases} \max\{\max\{|\alpha_j| : j = 1, \ldots, n\} : a_\alpha \neq 0\} & \text{if } v \neq 0, \\ -\infty & \text{if } v = 0. \end{cases}$$

The vector space of all algebraic polynomials in n variables of overall degree at most d is denoted by $\overline{\mathcal{P}}_d^n$. The vector space of all trigonometric polynomials in n variables of overall degree at most d is denoted by $\overline{\mathcal{T}}_d^n$. The dimension of these vector spaces are:

$$\dim \overline{\mathcal{P}}_d^n = (d+1)^n \quad \text{and} \quad \dim \overline{\mathcal{T}}_d^n = (2d+1)^n.$$

We can now define another criterion for cubature formulae.

Definition 3.2 A cubature formula Q for an integral I has algebraic, respectively trigonometric, overall degree d if it is exact for all algebraic, respectively trigonometric polynomials of overall degree at most d, and it is not exact for at least one polynomial of overall degree $d+1$.

A notable example of cubature formulae with overall algebraic degree d is the family of Gauss-product rules, obtained from quadrature formulae of degree d.

Most known cubature formulae for integrals of periodic functions on the unit cube $[0,1)^n$ are so-called *lattice rules* and for them a criterion used much more often than the trigonometric degree is the *Zaremba index*. The Zaremba index is related to the dominant terms in the error of the lattice rule for a worst possible function in a particular class of functions.

Definition 3.3 A *multiple integration lattice* L in $\mathbb{R}^n$ is a subset of $\mathbb{R}^n$ which is discrete and closed under addition and subtraction and which contains $\mathbb{Z}^n$ as a subset. A *lattice rule* is a cubature formula for approximating integrals over $[0,1)^n$ where the N points are the points of a multiple integration lattice L that lie in $[0,1)^n$ and the weights are all equal to $1/N$.

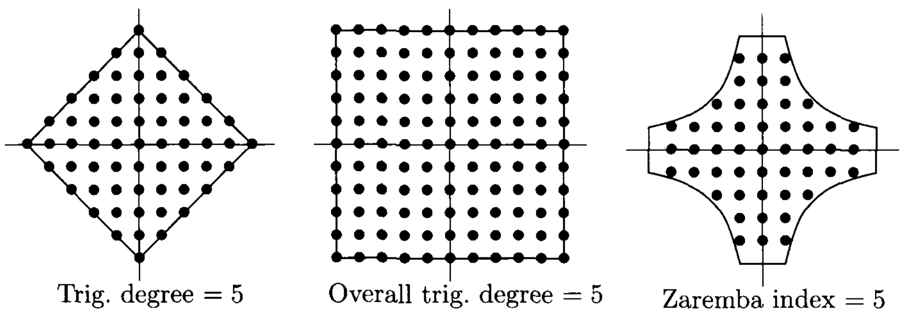

Fig. 1. Monomials for which a two-dimensional cubature formula is exact

Definition 3.4 A cubature formula Q for an integral I has Zaremba index d if it is exact for all trigonometric monomials $e^{2\pi\,\mathrm{i}\alpha\mathbf{x}}$ with

$$\prod_{i=1}^{n} r_i < d \quad \text{with} \quad r_i := \begin{cases} 1 & \text{if} \quad \alpha_i = 0, \\ |\alpha_i| & \text{if} \quad \alpha_i \neq 0, \end{cases}$$

and it is not exact for at least one monomial with $d = \prod_{i=1}^{n} r_i$.

Why is the algebraic degree of a cubature formula a measure of its quality? The main argument is that a well-behaved function is expected to be well approximated by a polynomial (for instance a Taylor series) and consequently its integral is expected to be well approximated by a cubature formula of a suffienciently high algebraic degree. Another argument, which applies only to some regions, is that the rate of convergence of a compound cubature formula as the mesh size shrinks is directly related to the algebraic degree of the basic cubature formula. This follows from the asymptotic error expansion for compound cubature formulae, which we will encounter in Section 4.

Why is the trigonometric degree, as well as other criteria based on trigonometric polynomials, a measure of the quality of a cubature formula? The main argument is that a well-behaved function is expected to be well approximated by a trigonometric polynomial (for instance its Fourier series) and consequently its integral is expected to be well approximated by a cubature formula of a sufficiently high trigonometric degree.

One uses other criteria, such as the overall algebraic or trigonometric degree or the Zaremba index, if one has reasons to believe that the corresponding set of monomials is more relevant. This is obviously connected to one's favourite way to study the error of a cubature formula when applied to a function for which it does not give the exact value of the integral.

We will use the symbol $\mathcal{V}_d^n$ to refer to one of the vector spaces $\mathcal{P}_d^n$, $\overline{\mathcal{P}}_d^n$, $\mathcal{T}_d^n$ or $\overline{\mathcal{T}}_d^n$. The results we present in this paper are also valid for other vector spaces, but one has to be cautious. A property that is needed to generalize several proofs is that the convex hull of the powers of α of the monomials in $\mathcal{V}_n^d$ contains only these monomials. In Figure 1 we illustrate this for the trigonometric degree, overall trigonometric degree and Zaremba index. It is obvious that the Zaremba index no longer has a role to play in this paper. The role of this criterion is important in the context of quasi-Monte Carlo methods. For readers who want to know more about this, we recommend Niederreiter (1992) and Sloan and Joe (1994).

4. Different ways to construct cubature formulae

In Section 2.2 we mentioned that there is more than one way to obtain a cubature formula. Much depends on the quality criterion used. As stated earlier, in this paper we restrict our attention to cubature formulae that are designed to be exact for a vector space of algebraic or trigonometric polynomials. Even then there are several ways to reach this goal and in this section we will briefly outline some of these. The examples in this section will only be two-dimensional but the ideas behind them are perfectly general.

4.1. Repeated quadrature

No doubt the field of quadrature is more threaded and explored than its multivariate counterpart. It is hence not surprising that even today many people use the product of two quadrature formulae to integrate over a square. Let

$$\int_0^1 g(x)\,\mathrm{d}x \simeq \sum_{j=1}^{N} w_j g(x^{(j)}) \tag{4.1}$$

be a quadrature formula of degree d_x, then

$$\int_0^1 \int_0^1 f(x,y)\,\mathrm{d}x\,\mathrm{d}y \simeq \sum_{i=1}^{N}\sum_{j=1}^{N} w_i w_j f(x^{(i)}, x^{(j)}). \tag{4.2}$$

If the quadrature formula (4.1) has algebraic degree d, then the cubature formula (4.2) has overall algebraic degree d.

One can use different quadrature formulae for each of the one-dimensional integrals. Even the one-dimensional integrals may have different limits or weight functions. If the quadrature formula in x has degree d_x with N_x points and the formula in y has degree d_y with N_y points, the resulting cubature formula will be exact for a space of polynomial 'between' $\bar{\mathcal{P}}_d^n$ and $\bar{\mathcal{P}}_D^n$ with $d := \min\{d_x, d_y\}$ and $D := \max\{d_x, d_y\}$, and has $N = N_x N_y$ points.

4.2. Change of variables

If one encounters a new problem, it is tempting to transform it into a problem for which a solution is familiar. For instance, an integral over a circle or triangle can be transformed into an integral over a square:

$$\begin{aligned}\int_0^1 \int_0^x f(x,y)\,\mathrm{d}y\,\mathrm{d}x &= \int_0^1 x \int_0^1 f(x,xt)\,\mathrm{d}t\,\mathrm{d}x, \\ \int_{-1}^1 \int_{-\sqrt{1-x^2}}^{\sqrt{1-x^2}} f(x,y)\,\mathrm{d}y\,\mathrm{d}x &= \int_0^1 \int_0^{2\pi} r f(r\cos\theta, r\sin\theta)\,\mathrm{d}\theta\,\mathrm{d}r.\end{aligned}$$

One can then use repeated quadrature, preferably using quadrature formulae that take the Jacobian of the transformation into account. For the above examples a possible choice is a combination of a Gauss–Legendre and an appropriate Gauss–Jacobi quadrature formula. This results in a so-called Conical Product rule for the triangle and a Spherical Product rule for the circle (Stroud 1971).

Transformations can have surprising advantages and disadvantages. For example, the above transformation of a triangle into a square, mentioned by Stroud (1971), but now usually referred to as the Duffy transformation (Duffy 1982), removes some types of singularity from the integrand (Lyness 1992, Lyness and Cools 1994), but the resulting cubature formula lacks symmetry. In fact there are three distinct Conical Products rules for each degree, depending on which vertex of the triangle is the preferred one.

4.3. Compound rules and copy rules

It can happen that the given integration region has an unusual shape for which no cubature formula is available, but that it can be subdivided into standard regions for which cubature formulae are available. The sum of all cubature formulae on all subregions is a so-called *compound rule.* If a cubature formula on a standard region does not give a result that is accurate enough, because it is applied to a function for which it was not designed to give the exact result, one can also subdivide and apply a properly scaled version of the given cubature formula on each subregion. And so on until one obtains the desired accuracy.

If the given region can be subdivided in congruent regions, a special kind of compound rule, the *copy rule*, becomes interesting. If, for example, the integration region is a square, one can divide this into m^2 identical squares, each of side $1/m$th the original side, and apply a properly scaled version of the given cubature formula to each. This approach looks expensive, especially if the dimension goes up, but is appealing because an error expansion is readily available.

So far, we have considered cubature formulae that are exact for a certain vector space. Almost all users will apply them to functions for which they do not give the exact result. So, we have arrived at a point where we need to say something about the error, that is, $Q[f] - I[f]$.

For regular $f(x, y) \in C^p$, $p \in \mathbb{N}$, the almost self-evident extension of the one-dimensional Euler–Maclaurin expansion may be expressed as

$$Q^{(m)}[f] - I[f] = \sum_{i=1}^{p-1} \frac{B_i(Q, f)}{m^i} + \mathcal{O}(m^{-p}), \tag{4.3}$$

where $Q^{(m)}$ is the m^2-copy of Q and the coefficients B_i depend on the cubature formula Q, the integral I and the integrand f.

Once it is known that an error expansion such as (4.3) exists, Richardson extrapolation (Richardson 1927) can be used to speed up convergence (by eliminating terms of the error expansion). In order to apply extrapolation one need not know all details: the value of the B_i need not be known.

The m-copy rules for cubes and simplices have received considerable attention, because for some classes of non-regular functions, error expansions are also available and Richardson extrapolation can be used to speed up convergence. It is beyond the scope of this text to pursue this further. The situation seems to be that for many algebraic or logarithmic singularities that occur at a vertex or along a side, an appropriate expansion exists. For a brief survey of what is available for a triangle we refer to Lyness and Cools (1994). Readers who want to know more about this topic will find it in Lyness and McHugh (1970), Lyness and Puri (1973), Lyness (1976), de Doncker (1979), Lyness and Monegato (1980), Lyness and de Doncker-Kapenga (1987), Lyness and de Doncker (1993), Verlinden and Haegemans (1993).

4.4. Direct construction of cubature formulae

In the previous subsections we described indirect approaches to constructing cubature formulae. These are not the main subject of the article. We are especially interested in the direct approach.

Suppose one wants a cubature formula that is exact for all functions of a vector space of functions. Because an integral and a cubature formula are linear operators, it is sufficient and necessary that the cubature formula is exact for all functions of a basis of the vector space. Hence, if one desires a cubature formula that is exact for a vector space $\mathcal{V}_d^n$ and if the functions f_i form a basis for $\mathcal{V}_d^n$, then it is necessary and sufficient that

$$Q[f_i] = I[f_i], \quad i = 1, \ldots, \dim \mathcal{V}_d^n. \tag{4.4}$$

If the f_i are monomials, then the right-hand sides of (4.4), the so-called *moments*, are known in closed form or can be evaluated. When the left-hand sides of (4.4) are replaced by the weighted sum of function values (3.7) and the number of points N is fixed, then one obtains a system of nonlinear equations in the unknown points $\mathbf{y}^{(j)}$ and weights w_j:

$$\sum_{j=1}^{N} w_j f_i(\mathbf{y}^{(j)}) = I[f_i], \quad i = 1, \ldots, \dim \mathcal{V}_d^n. \tag{4.5}$$

We are interested in cubature formulae with a 'low' number of points. In Section 7.1 we will search for a lower bound for the number of points depending on $\mathcal{V}_d^n$.

At this point we want to mention that one can distinguish between two approaches to construct cubature formulae the direct way:

- one may proceed directly to solve the system of nonlinear equations, or
- one can search for polynomials that vanish at the points of the formula.

The foundation for successful application of the first approach is laid in Section 5. The building blocks for the second approach are presented in Section 6. The second approach has been very successful in (one-dimensional) quadrature. Most published cubature formulae were, however, obtained using the first approach.

5. On regions and symmetry

We will always try to be as general as possible but we will soon discover that, for instance, lower bounds for the number of points depend on the specific region Ω and weight function $w(\mathbf{x})$. In this section we will define some standard regions and describe their most important property, namely symmetry.

5.1. Standard regions

In this paper we will encounter the following regions and weight functions for the algebraic-degree case:

C_n: the n-dimensional cube

$$\Omega := \{(x_1, \ldots, x_n) : -1 \leq x_i \leq 1, i = 1, \ldots, n\}$$

with weight function $w(\mathbf{x}) := 1$,

C_2^α: the square

$$\Omega := \{(x_1, x_2) : -1 \leq x_i \leq 1, i = 1, 2\}$$

with weight function

$$w(x_1, x_2) := (1 - x_1^2)^\alpha (1 - x_2^2)^\alpha, \quad \alpha > -1,$$

S_n: the n-dimensional ball

$$\Omega := \left\{ (x_1, \ldots, x_n) : \sum_{j=1}^{n} x_i^2 \leq 1 \right\}$$

with weight function $w(\mathbf{x}) := 1$,

U_n: the n-dimensional sphere, that is, the surface of the ball

$$\Omega := \left\{ (x_1, \ldots, x_n) : \sum_{j=1}^{n} x_i^2 = 1 \right\}$$

with weight function $w(\mathbf{x}) := 1$,

T_n: the n-dimensional simplex

$$\Omega := \left\{ (x_1, \ldots, x_n) : \sum_{j=1}^{n} x_i \leq 1 \text{ and } x_i \geq 0, i = 1, \ldots, n \right\}$$

with weight function $w(\mathbf{x}) := 1$,

$E_n^{r^2}$: the entire n-dimensional space $\Omega := \mathbb{R}^n$ with weight function

$$w(\mathbf{x}) := e^{-r^2} \quad \text{with} \quad r^2 := \sum_{j=1}^{n} x_j^2,$$

E_n^r: the entire n-dimensional space $\Omega := \mathbb{R}^n$ with weight function

$$w(\mathbf{x}) := e^{-r}.$$

The trigonometric-degree case deals usually with the following region:

C_n^*: the n-dimensional cube

$$\Omega := \{(x_1, \ldots, x_n) : 0 \leq x_i < 1, i = 1, \ldots, n\}$$

with weight function $w(\mathbf{x}) := 1$.

We will use the above notation to refer to both the region and weight function and to the integral over this region with this weight function.

5.2. Symmetry groups

The symmetry of an integral is described by its symmetry group. Let G be any group of orthogonal transformations that have a fixed point at the origin, and let $|G|$ denote the order of the group.

Definition 5.1 A set $\Omega \subset \mathbb{R}^n$ is said to be invariant with respect to (w.r.t.) 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 w.r.t. G

if it is left unchanged by each transformation of the group, that is, $f(\mathbf{x}) = f(g(\mathbf{x}))$ for all $g \in G$. An integral is invariant w.r.t. G if both its region and weight function are invariant w.r.t. G.

Note that S_n, U_n, $E_n^{r^2}$ and E_n^r are invariant w.r.t. each group of orthogonal transformations.

Definition 5.2 The *G-orbit* of a point $\mathbf{y} \in \mathbb{R}^n$ is the set $\{g(\mathbf{y}) : g \in G\}$.

A G-orbit of a given point is obviously an invariant set w.r.t. G. Observe that the number of points in an orbit depends on the given point.

Example 5.1 Let $n = 2$, $\Omega = \{(x, y) : -1 \le x, y \le 1\}$ and G the group of linear transformations for which Ω is G-invariant. The group can be represented by the following set of matrices:

$$\left\{ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}, \right.$$

$$\left. \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \right\}.$$

The orbit of an arbitrary point (a, b) is

$$\{(a, b), (b, -a), (-a, -b), (-b, a), (a, -b), (b, a), (-a, b), (-b, -a)\}.$$

Orbits can have less than 8 points:

- the orbit of (a, a), $a \neq 0$, is $\{(a, a), (-a, a), (a, -a), (-a, -a)\}$
- the orbit of $(a, 0)$, $a \neq 0$, is $\{(a, 0), (-a, 0), (0, a), (0, -a)\}$
- the orbit of $(0, 0)$ is $\{(0, 0)\}$.

The most important symmetries for our purposes are *central symmetry* and *shift symmetry.*

Definition 5.3 A set, integral or, respectively, cubature formula is called *centrally symmetric* if it remains unchanged under reflection through the origin, that is, it is invariant w.r.t. the group of transformations

$$G_{cs} := \{\mathbf{x} \mapsto \mathbf{x}, \mathbf{x} \mapsto -\mathbf{x}\}.$$

Given $\mathbf{a} \in \mathbb{R}^n$, let $\{\mathbf{a}\} \in [0, 1)^n$ denote the vector each of whose components is the fractional part of the corresponding component of $\mathbf{a}$.

Definition 5.4 A set, integral or cubature formula is called *shift symmetric* if it is invariant w.r.t. the group of transformations

$$G_{ss} := \left\{ \mathbf{x} \rightarrow \mathbf{x}, \mathbf{x} \rightarrow \left\{ \mathbf{x} + \left(\tfrac{1}{2}, \ldots, \tfrac{1}{2} \right) \right\} \right\}.$$

Shift symmetry is for the trigonometric-degree case what central symmetry is for the algebraic case. C_n is centrally symmetric and $C_n^\star$ is shift symmetric.

The other important groups are the symmetry groups of regular polytopes and their subgroups. The most common are:

$A_n, n \geq 2$	:	symmetry group of a regular simplex
$B_n, n \geq 2$	:	symmetry group of a cube
$H_2^m, n = 2$	:	dihedral group, that is, symmetry group of regular m-gon
$I_3, n = 3$	:	symmetry group of a regular icosahedron.

(The origin is the barycentre of the regular polytopes.)

In addition, the associated group $A_n^\star$ is obtained from A_n by adding the reflection through the origin as generator to the group.

Regions and cubature formulae are often called *fully symmetric* when they are B_n-invariant, that is, when they are invariant w.r.t. the following group of transformations:

$$\begin{aligned} G_{B_n} \;:=\; & G_{FS} := \{(x_1, \ldots, x_n) \mapsto (s_1 x_{p_1}, \ldots, s_n x_{p_n}) : \\ & s_i \in \{-1, +1\}, i \in \{1, \ldots, n\}, \{p_1, \ldots, p_n\} = \{1, \ldots, n\}\}. \end{aligned}$$

Example 5.1 dealt with this group. Observe that fully symmetric regions are also centrally symmetric.

Regions and cubature formulae are often called *symmetric* when they are invariant w.r.t. the following subgroup of G_{FS}:

$$G_S := \{(x_1, \ldots, x_n) \mapsto (s_1 x_1, \ldots, s_n x_n) : s_i \in \{-1, +1\}, i \in \{1, \ldots, n\}\}.$$

Definition 5.5 A cubature formula is said to be invariant w.r.t. a group G if the region Ω and the weight function $w(\mathbf{x})$ are G-invariant and if the set of points is a union of G-orbits. All points of one and the same orbit have the same weight.

A G-invariant cubature formula can be written as

$$Q[f] := \sum_{j=1}^{K} w_j Q_G(\mathbf{y}^{(j)})[f], \tag{5.1}$$

where the functional $Q_G(\mathbf{y}^{(j)})$ is the average of the function values of f in the points of the G-orbit of $\mathbf{y}^{(j)}$. $Q_G(\mathbf{y})$ is called a *basic G cubature rule operator.*

5.3. Usefulness for cubature formula construction

The usefulness of symmetry groups in the context of constructing cubature formulae is highlighted by the following result, due to Sobolev (1962). Let F be a vector space of functions defined on $\Omega \subset \mathbb{R}^n$ that is G-invariant, so that $g(f) \in F$ for all $f \in F$ and $g \in G$.

The G-invariant functions of F

$$F(G) := \{f \in F : g(f) = f \text{ for all } g \in G\}.$$

form a subspace

Theorem 5.1 Let G be a finite group of linear transformations acting on F. Then, every G-invariant linear functional on F is determined by its restriction to $F(G)$.

Proof. For every $h \in G$ we have

$$h\left(\sum_{g\in G} g(f)\right) = \sum_{g\in G} h(g(f)) = \sum_{hg\in G} h(g(f)) = \sum_{g\in G} g(f),$$

hence $\sum_{g\in G} g(f) \in F(G)$.

Let I be a G-invariant linear functional on F, so that $I[g(f)] = I[f]$ for all $f \in F$ and $g \in G$. Hence we have

$$I[f] = \frac{1}{|G|}\sum_{g\in G} I[g(f)] = I\left[\frac{1}{|G|}\sum_{g\in G} g(f)\right].$$

This proves the theorem, since we showed that for each $f \in F$, a function in $F(G)$ exists such that the functional gives the same result for both. □

The usual formulation of this theorem is an obvious corollary and is generally known as Sobolev's theorem.

Corollary 5.1 (Sobolev's theorem) 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 $d + 1$.

The exploitation of the symmetry of the region by imposing a structure to the cubature formula has a simplifying effect. If one wants a G-invariant cubature formula (5.1), the necessary and sufficient conditions (4.4) can be replaced by the reduced system of nonlinear equations

$$Q[\phi_i] = I[\phi_i], \quad i = 1, \dots \dim \mathcal{V}_d^n(G), \tag{5.2}$$

where the ϕ_i form a basis for $\mathcal{V}_d^n(G)$. The larger the symmetry group G, the lower the dimension of the space of all G-invariant functions and, consequently, the easier it will be to determine a cubature formula.

Example 5.2 If $p(\mathbf{x})$ is an algebraic monomial, deg(p) is odd, and Q is a centrally symmetric cubature formula, then $I[f] = Q[f] = 0$. If $t(\mathbf{x})$ is a trigonometric monomial, deg(t) is odd and Q is a shift symmetric cubature formula, then $I[f] = Q[f] = 0$. So the symmetry of the cubature formula suffices to integrate odd-degree monomials exactly. This is in agreement with Sobolev's theorem because all invariant polynomials for both groups have even degree, and thus odd-degree monomials need not be taken into account.

5.4. Invariant theory

We will now mention some results from invariant theory, a tool for working with vector spaces of invariant polynomials. This will help us to set up the system of nonlinear equations (5.2).

Definition 5.6 The G-invariant polynomials $\phi_1, \dots, \phi_l$ form an *integrity basis* for the invariant polynomials of G if and only if every invariant polynomial of G is a polynomial in $\phi_1, \dots, \phi_l$. Each polynomial ϕ_i is called a *basic invariant polynomial* of G.

Because the degree of a polynomial is left unchanged by a linear transformation of the variables, one can restrict the search of basic invariant polynomials to homogeneous polynomials. If the number of basic invariant polynomials $l > n$, then there exist polynomials equations, called *syzygies*, relating $\phi_1, \dots, \phi_l$. Syzygies come into play when calculating the dimension of a vector space of invariant polynomials.

Some properties are summarized by the following theorems.

Theorem 5.2 There always exists a finite integrity basis for the invariant polynomials of a finite group G.

Theorem 5.3 Let G be a finite group acting on the n-dimensional vector space $\mathbb{R}^n$. G is a finite reflection group if and only if the invariant polynomials of G have an integrity basis consisting of n homogeneous polynomials which are algebraically independent.

Example 5.3 For the symmetry group of a regular m-gon, H_2^m, it is very convenient to use basic invariant polynomials in the variables x and y, or in polar coordinates r and θ:

$$\begin{aligned} \sigma_2 &:= r^2 = x^2 + y^2, \\ \sigma_m &:= r^m \cos(m\theta) = \sum_{i=0}^{\lfloor \frac{m}{2} \rfloor} (-1)^i \binom{m}{2i} x^{m-2i} y^{2i}. \end{aligned}$$

In H_2^m one can distinguish two types of element: there are orientation-reversing transformations (reflections) and orientation-preserving transformations (rotations). The rotations of H_2^m form a subgroup R_2^m of order m. R_2^m is not a reflection group and thus an integrity basis consists of more than two polynomials. In addition to σ_2 and σ_m one can use as basic invariant polynomial

$$\sigma'_m := r^m \sin(m\theta).$$

The syzygy relating σ_2, σ_m and σ'_m is

$$\sigma_2^m - \sigma_m^2 - \sigma_m'^2 = 0.$$

For proofs of the theorems, basic invariant polynomials and other information we refer to Fisher (1967) and Flatto (1978).

6. Characterization of cubature formulae

6.1. Interpolatory cubature formulae

Because we are interested in cubature formulae with a 'low' number of points, we can restrict our attention to interpolatory cubature formulae. Indeed, when a non-interpolatory cubature formula is given, by applying Steinitz's *Austauschsatz* (Davis 1967) an interpolatory cubature formula that uses a subset of the given points can be constructed.

Definition 6.1 If the weights of a cubature formula of degree d are uniquely determined by the points, the cubature formula is called an *interpolatory cubature formula.*

A cubature formula that is exact for all elements of $\mathcal{V}_d^n$ is determined by a system of nonlinear equations (4.4) or (5.2):

$$Q[f_i] = I[f_i], \quad i = 1, \ldots, \dim \mathcal{V}_d^n, \tag{6.1}$$

where the f_i form a basis for $\mathcal{V}_d^n$. If the points of a cubature formula are given, then (6.1) is a system of $\dim \mathcal{V}_d^n$ linear equations in the N unknown weights. Hence an interpolatory cubature formula has $N \leq \dim \mathcal{V}_d^n$ and there exist N linearly independent polynomials $U_1, \ldots, U_N \in \mathcal{V}_d^n$ such that

$$\det \begin{pmatrix} U_1(\mathbf{y}^{(1)}) & \ldots & U_N(\mathbf{y}^{(1)}) \\ \vdots & & \vdots \\ U_1(\mathbf{y}^{(N)}) & \ldots & U_N(\mathbf{y}^{(N)}) \end{pmatrix} \neq 0.$$

These polynomials generate a maximal, not uniquely determined, vector space of polynomials that do not vanish at all given points.

One can always find $t := \dim \mathcal{V}_d^n - N$ polynomials $p_1, \ldots, p_t$ such that the polynomials

$$U_1, \ldots, U_N, p_1, \ldots, p_t$$

form a basis for $\mathcal{V}_d^n$. Then one can solve

$$\begin{pmatrix} U_1(\mathbf{y}^{(1)}) & \ldots & U_N(\mathbf{y}^{(1)}) \\ \vdots & & \vdots \\ U_1(\mathbf{y}^{(N)}) & \ldots & U_N(\mathbf{y}^{(N)}) \end{pmatrix} \begin{pmatrix} a_{i1} \\ \vdots \\ a_{iN} \end{pmatrix} = \begin{pmatrix} p_i(\mathbf{y}^{(1)}) \\ \vdots \\ p_i(\mathbf{y}^{(N)}) \end{pmatrix}, \quad i = 1, \ldots, t,$$

and so obtain $t = \dim \mathcal{V}_d^n - N$ linearly independent polynomials

$$R_i = p_i - \sum_{j=1}^{N} a_{ij} U_j, \quad i = 1, \ldots, t \tag{6.2}$$

that vanish at the given points of the cubature formula. We can replace the polynomials p_i in the basis of $\mathcal{V}_d^n$ by the polynomials R_i.

With every cubature formula of degree d one can associate a basis of $\mathcal{V}_d^n$ that consists of $\dim \mathcal{V}_d^n - N$ polynomials R_i that vanish at all the points of the cubature formula and N polynomials U_i that do not vanish at all points. A cubature formula is thus fully characterized by the polynomials R_i. The polynomials U_i give rise to a linear system that determines the weights.

These characterizing polynomials provide the links between cubature formulae on one hand, and orthogonal polynomials and ideal theory on the other hand.

6.2. Orthogonal polynomials

Because each R_i (6.2) vanishes at all points of the cubature formula,

$$Q[R_i P] = 0, \quad \text{for all } P \in \mathcal{V}^n.$$

Because the cubature formula has degree d,

$$I[R_i P] = Q[R_i P] = 0 \quad \text{whenever} \quad R_i P \in \mathcal{V}_d^n.$$

And that brings us to orthogonality.

Definition 6.2 A polynomial $f \in \mathcal{V}^n$ is called d-orthogonal (w.r.t. a given integral I), if $I[fg] = 0$ whenever $fg \in \mathcal{V}_d^n$.

Definition 6.3 A polynomial $f \in \mathcal{V}^n$ is called orthogonal (w.r.t. a given integral I), if $I[fg] = 0$ whenever $\deg(g) < \deg(f)$.

The polynomials R_i that characterize a cubature formula of degree d are d-orthogonal.

In contrast with the one-dimensional case, in the n-dimensional case more than one orthogonal polynomial of a given degree d exists. Sequences of orthogonal polynomials can be constructed with $\dim \mathcal{V}_d^{n-1}$ linearly independent polynomials of degree d and many such sequences exist.

The trigonometric case

For the integral with region $C_n^\star$,

$$I[f] = \int_{[0,1)^n} f(\mathbf{x})\, \mathrm{d}\mathbf{x},$$

any trigonometric monomial is orthogonal to every trigonometric monomial of a lower degree. Hence, these are the obvious choice when $w(\mathbf{x}) \equiv 1$.

We have only found other weight functions in theoretical results where orthogonal polynomials are only used implicitly.

The algebraic case
It is a generalization of a result of Jackson (1936) that there exist $\dim \mathcal{P}_d^{n-1}$ unique orthogonal polynomials of degree d of the form

$$P^{\alpha_1,\alpha_2,\ldots,\alpha_n}(x_1,x_2,\ldots,x_n) = x_1^{\alpha_1}x_2^{\alpha_2}\ldots x_n^{\alpha_n} + Q \tag{6.3}$$

with $\sum_{i=1}^n \alpha_i = d$ and $Q \in \mathcal{P}_{d-1}^n$. The polynomials of the form (6.3) are called *basic orthogonal polynomials.*

For so-called *product regions*, that is, when the region of integration is a product of intervals and the weight function is a product of univariate functions, so that

$$I[f] = \int_{a_1}^{b_1} w_1(x_1)\ldots\int_{a_n}^{b_n} w_n(x_n)f(\mathbf{x})\,\mathrm{d}x_n\ldots\,\mathrm{d}x_1,$$

the basic invariant polynomials are products of monic univariate orthogonal polynomials. For example, in C_2, we have $P^{k,l}(x,y) = P_k(x)P_l(y)$, where $P_i(x)$ is the monic Legendre polynomial of degree i in x. The regions C_n and $E_n^{r^2}$ are product regions and their basic invariant polynomials are the product of monic Legendre and Hermite polynomials, respectively.

As the explicit expressions for the basic orthogonal polynomials for S_n and T_n are not well known, we list them here.

S_n: Let $\alpha \in \mathbb{N}^n$ and $\beta \le \alpha/2$ (that is, $0 \le \beta_i \le \alpha_i/2$ for $i = 1,\ldots,n$). Then,

$$P^\alpha(\mathbf{x}) = \sum_{\beta\le\alpha/2}(-1)^{|\beta|}\frac{\Gamma(|\alpha|-|\beta|+n/2)}{\Gamma(|\alpha|+n/2)2^{2|\beta|}}\left(\prod_{j=1}^n\frac{\alpha_j!}{(\alpha_j-2\beta_j)!\beta_j!}\right)\mathbf{x}^{\alpha-2\beta}.$$

See Appell and Kampé de Fériet (1926).

T_n: Let $\alpha \in \mathbb{N}^n$ and $\beta \le \alpha$ (that is, $0 \le \beta_i \le \alpha_i$ for $i = 1,\ldots,n$). Then,

$$P^\alpha(\mathbf{x}) = \sum_{\beta\le\alpha}(-1)^{|\alpha|+|\beta|}\frac{(|\alpha|+|\beta|+n-1)!}{(2|\alpha|+n-1)!}\left(\prod_{i=1}^n\binom{\alpha_i}{\beta_i}\frac{\alpha_i!}{\beta_i!}\right)\mathbf{x}^\beta.$$

See Appell and Kampé de Fériet (1926) for $n=2$ and Grundmann and Möller (1978) for $n \in \mathbb{N}$.

E_n^r: An explicit expression for the basic invariant polynomials has not yet been shown.

The basic orthogonal polynomials reflect the symmetry of the integral. If the integral is centrally symmetric then the basic orthogonal polynomials of even (odd) degree consist of even (odd) degree monomials only. If the integral is fully symmetric then the basic orthogonal polynomial $P^\alpha(\mathbf{x})$ with all α_i even (odd) consists only of monomials with even (odd) powers of x_i, for all $i \in \{1, \ldots, n\}$. Furthermore, $P^{p(\alpha)}(\mathbf{x}) = P^\alpha(p(\mathbf{x}))$ where p performs a permutation on the components of its vector argument.

The structure of basic invariant polynomials motivates the following.

Definition 6.4 A set of polynomials S is called *fundamental of degree d* whenever $\dim \mathcal{V}_d^{n-1} (= \dim \mathcal{V}_d^n - \dim V_{d-1}^n)$ linearly independent polynomials of the form $x_1^{\alpha_1} \ldots x_n^{\alpha_n} + Q_\alpha$, $Q_\alpha \in \mathcal{V}_{d-1}^n$, $|\alpha| = d$, belong to span S.

6.3. Polynomial ideals

The polynomials U_i and R_i are not uniquely determined. The direct sum of the vector spaces generated by these polynomials is

$$\text{span}\{U_i\} \oplus \text{span}\{R_i\} = \mathcal{V}_d^n.$$

span$\{R_i\}$ is more than simply a vector space. Indeed, if one multiplies a polynomial that vanishes at all points of the cubature formula by an arbitrary polynomial, the product also vanishes at all points. And that brings us to ideals.

Definition 6.5 A *polynomial ideal* $\mathfrak{A}$ is a subset of the ring of polynomials in n variables $\mathcal{V}^n$ such that if $f_1, f_2 \in \mathfrak{A}$ and $g_1, g_2 \in \mathcal{V}^n$, then $f_1g_1 + f_2g_2 \in \mathfrak{A}$.

The genesis of ideal theory is described in Edwards (1980). In this section we describe the part of ideal theory needed in this paper.

Definition 6.6 If $\mathfrak{A}$ is a polynomial ideal, then the set of polynomials $\{f_1, \ldots, f_s\} \subset \mathfrak{A}$ form a basis for $\mathfrak{A}$ if each $f \in \mathfrak{A}$ can be written in the form

$$f = \sum_{j=1}^{s} g_j f_j \quad \text{where} \quad g_j \in \mathcal{V}^n.$$

The ideal generated by $\{f_1, \ldots, f_s\}$ is

$$(f_1, \ldots, f_s) := \left\{ f = \sum_{j=1}^{s} g_j f_j : g_j \in \mathcal{V}^n \right\}.$$

The polynomials R_i that characterize a cubature formula generate an ideal, denoted by $(R_1, \ldots, R_t)$.

Theorem 6.1 For any polynomial ideal there exists a finite basis.

Proof. See Hilbert (1890). □

There are several types of bases for ideals. For our purposes, H-bases and G-bases are important. H-bases are important as a theoretical tool. Their power will be shown by the short proof of Theorem 6.7. G-bases are important because algorithms exist to construct them and to derive properties of the ideal. It is thus very convenient for us that with some restrictions a G-basis is also an H-basis (Buchberger 1985, Möller and Mora 1986, Sturmfels 1996).

Definition 6.7 Let $\mathfrak{A}$ be a polynomial ideal. The set $\{f_1, \ldots, f_s\} \subset \mathfrak{A}$ is an H-basis for $\mathfrak{A}$ if for all $f \in \mathfrak{A}$ there exist polynomials $g_1, \ldots, g_s$ such that

$$f = \sum_{j=1}^{s} g_j f_j \quad \text{and} \quad \deg(g_j f_j) \leq \deg(f), \quad j = 1, \ldots, s.$$

Theorem 6.2 For any polynomial ideal an H-basis exists.

Proof. See Möller (1973). □

Other names for an H-basis are canonical basis and Macaulay basis.

Before defining G-bases, also called Gröbner-bases, we have to introduce some notation. Let the set of monomials $M = \{\mathbf{x}^\alpha : \alpha \in \mathbb{N}^n\}$ be ordered by $<$ such that, for any $f, f_1, f_2 \in M$, $1 \leq f$ and $f_1 \leq f_2$ imply $ff_1 \leq ff_2$. Let $f = \sum_{i=1}^{m} c_i f_i$ with $f_i \in M$ and $c_i \in \mathbb{R}_0$. Then the *headterm* of $f = \text{Hterm}(f) := f_m$, and the *maximal part* of $f = M(f) := c_m f_m$. For $f, g \in \mathcal{P}^n \backslash \{0\}$ let

$$H(f, g) := \text{lcm}\{\text{Hterm}(f), \text{Hterm}(g)\}. \tag{6.4}$$

Let $F \subset \mathcal{P}^n \backslash \{0\}$ be a finite set. We write $f \longrightarrow_F g$ if $f, g \in \mathcal{P}^n$ and there exist $h \in \mathcal{P}^n$, $f_i \in F$ such that $f = g + hf_i$, $\text{Hterm}(g) < \text{Hterm}(f)$ or $g = 0$. The map $\underset{F}{\longrightarrow}$ is called a reduction modulo F. By $\underset{F}{\longrightarrow}^{+}$ we denote the reflexive transitive closure of $\underset{F}{\longrightarrow}$.

Definition 6.8 A set $F := \{f_1, \ldots, f_l\}$ is a Gröbner basis (G-basis) for the ideal $\mathfrak{A}$ generated by F if

$$f \in \mathfrak{A} \text{ implies } f \underset{F}{\longrightarrow}^{+} 0.$$

Theorem 6.3 Let $F := \{f_1, \ldots, f_s\} \subset \mathcal{P}^n \backslash \{0\}$ and let $\mathfrak{A}$ be the ideal generated by F. Then the following conditions are equivalent.

- F is a Gröbner basis of $\mathfrak{A}$.
- For all (i, j) with $1 \leq i < j \leq s$,

$$SP(f_i, f_j) = \frac{H(f_i, f_j)}{M(f_i)} f_i - \frac{H(f_i, f_j)}{M(f_j)} f_j \underset{F}{\longrightarrow}^{+} 0.$$

Proof. See Möller and Mora (1986). □

Theorem 6.3 provides an algorithmic way to verify if a given set is a G-basis. Practical implementations incorporate several shortcuts. For example, according to Gebauer and Möller (1988), a pair (f_i, f_j) is superfluous if $H(f_l, f_j)$ divides properly $H(f_i, f_j)$ and $l < j$.

Theorem 6.4 If $<$ is compatible with the partial ordering by degrees, that is, $\deg(f) < \deg(g)$ implies $\mathrm{Hterm}(f) < \mathrm{Hterm}(g)$, then a G-basis with respect to $<$ is also an H-basis.

Proof. See Möller and Mora (1986). □

Definition 6.9. (Nullstellengebilde) The *zero set* of an ideal $\mathfrak{A}$ is

$$\mathsf{NG}(\mathfrak{A}) := \{\mathbf{y} \in \mathbb{C}^n : f(\mathbf{y}) = 0 \quad \text{for all } f \in \mathfrak{A}\}$$

If $\mathsf{NG}(\mathfrak{A})$ is a finite set of points, then the ideal is called *zero-dimensional*, and obviously any basis for $\mathfrak{A}$ consists of at least n polynomials.

An important function of a polynomial ideal is the Hilbert function (Hilbert 1890). It is useful to count the number of elements of $\mathsf{NG}(\mathfrak{A})$.

Definition 6.10 The *Hilbert function* $\mathcal{H}$ is defined as

$$\mathcal{H}(k;\mathfrak{A}) := \begin{cases} \dim \mathcal{P}_k^n - \dim(\mathfrak{A} \cap \mathcal{P}_k^n), & k \in \mathbb{N}, \\ 0, & -k \in \mathbb{N}_0. \end{cases}$$

Theorem 6.5 If $\mathcal{H}(k;\mathfrak{A}) = \mathcal{H}(K;\mathfrak{A})$ for all $k \geq K$ holds for a sufficiently large K, then the polynomials in $\mathfrak{A}$ have exactly $\mathcal{H}(K;\mathfrak{A})$ (complex) common zeros if these are counted with multiplicities.

Proof. See Gröbner (1949). □

Definition 6.11 An ideal $\mathfrak{A}$ is a real ideal if all polynomials vanishing at $\mathsf{NG}(\mathfrak{A}) \cap \mathbb{R}^n$ belong to $\mathfrak{A}$, that is,

$$f \in \mathfrak{A} \quad \text{if and only if} \quad f(\mathbf{y}) = 0, \quad \text{for all } \mathbf{y} \in \mathsf{NG}(\mathfrak{A}) \cap \mathbb{R}^n.$$

Note that the theorems given in this subsection are proven only for algebraic polynomials in the literature. We do not see any problem in their application to ideals of invariant algebraic polynomials or trigonometric polynomials.

Within the ideal theoretical framework we can rephrase Theorem 3.1.

Theorem 6.6 Let I be an integral over an n-dimensional region. Let $\{\mathbf{y}^{(1)}, \ldots, \mathbf{y}^{(N)}\} \subset \mathbb{C}^n$ and $\mathfrak{A} := \{f \in \mathcal{V}^n : f(\mathbf{y}^{(i)}) = 0, i = 1, \ldots, N\}$. Then the following statements are equivalent.

- $f \in \mathfrak{A} \cap \mathcal{V}_d^n$ implies $I[f] = 0$.
- There exists a cubature formula Q (3.7) such that $I[f] = Q[f]$, for all $f \in \mathcal{V}_d^n$, with at most $\mathcal{H}(d;\mathfrak{A})$ (complex) weights different from zero.

Proof. This theorem is proven by Möller (1973) for the case $\mathcal{V}_d^n = P_d^n$. □

The role of H-bases is illustrated by the following theorem by Möller (1973).

Theorem 6.7 If $\{f_1, \ldots, f_s\}$ is an H-basis of a polynomial ideal $\mathfrak{A}$ and if the set of common zeros of $f_1, \ldots, f_s$ is finite and nonempty, then the following statements are equivalent.

- There is a cubature formula of degree d for the integral I which has as points the common zeros of $f_1, \ldots, f_s$. (These zeros may be multiple, leading to the use of function derivatives in the cubature formula.)
- f_i is d-orthogonal for $I, i = 1, 2, \ldots, s$.

Proof.

'$\Rightarrow$': Let $gf_i \in \mathcal{P}_d^n$. Then $I[gf_i] = \sum_{j=1}^N w_j g(\mathbf{y}^{(j)}) f_i(\mathbf{y}^{(j)}) = 0$, since $f_i \in \mathfrak{A}$.
'$\Leftarrow$': Let $f \in \mathfrak{A} \cup \mathcal{P}_d^n$. Then, with g_i as given in the definition of H-basis, $I[f] = I[\sum_{i=1}^s g_i f_i] = 0$.

□

Schmid managed to give a characterization of cubature formulae with real points and positive weights using real ideals.

Theorem 6.8 Let $\{R_1, \ldots, R_t\} \subset \mathcal{P}_{d+1}^n$ be a set of linearly independent d-orthogonal polynomials that is fundamental of degree $d+1$. Let $\mathfrak{A} := (R_1, \ldots, R_t)$ and $V :=$ span$\{R_1, \ldots, R_t\}$. Let $N + t = \dim \mathcal{P}_{d+1}^n$ and U an arbitrary but fixed vector space such that $\mathcal{P}_{d+1}^n = V \oplus U$. Then the following statements are equivalent.

- There exists an interpolatory cubature formula of degree d
$$Q[f] := \sum_{j=1}^N w_j f(\mathbf{y}^{(j)}), \quad \mathbf{y}^{(j)} \in \mathbb{R}^n, \quad w_j > 0$$
with $\{\mathbf{y}^{(1)}, \ldots, \mathbf{y}^{(N)}\} \subset \mathsf{NG}(\mathfrak{A})$.
- $\mathfrak{A}$ and U are characterized by:
  (i) $\mathfrak{A} \cap U = \{0\}$
  (ii) $I[f^2 - R^+] > 0$ for all $f \in U$, where $R^+ \in \mathfrak{A}$ is chosen such that $f^2 - R^+ \in \mathcal{P}_d^n$.
- $\mathfrak{A}$ is a real ideal and $|\mathsf{NG}(\mathfrak{A}) \cap \mathbb{R}^n| = N$. The points of the cubature formula are the elements of $\mathsf{NG}(\mathfrak{A}) \cap \mathbb{R}^n$.

Proof. See Schmid (1980*a*). □

This characterization was used to develop the T-method for constructing cubature formulae; see Section 9.2.

6.4. *Tchakaloff's upper bound*

To conclude this section we will prove an upper bound for the number of points in an interpolatory cubature formula using the concepts from ideal theory just introduced. We mentioned this result at the beginning of this section.

Corollary 6.1 If an interpolatory cubature formula of degree d for an integral over an n-dimensional region has N points, then $N \leq \dim \mathcal{V}_d^n$.

Proof. Suppose a given cubature formula of degree d has M points. Let $\mathfrak{A}$ be the ideal of all polynomials that vanish at these points. According to Theorem 6.6, there exists a cubature formula with $N \leq \mathcal{H}(d; \mathfrak{A}) \leq M$ of these points, and from the definition of the Hilbert function, it follows immediately that $N \leq \mathcal{H}(d; \mathfrak{A}) \leq \dim \mathcal{V}_d^n$. A basis of any complement of $\mathfrak{A} \cap \mathcal{V}_d^n$ in $\mathcal{V}_d^n$ can be used to construct a set of linear equations to determine the weights. □

The above corollary is an elementary version of Tchakaloff's theorem.

Theorem 6.9 (Tchakaloff's theorem) Let I be an integral over an n-dimensional region Ω with a weight function that is nonnegative in Ω and for which the integrals of all monomials exist. Then a cubature formula of degree d with $N \leq \dim \mathcal{V}_d^n$ points exists with all points inside Ω and all weights positive.

Proof. This theorem was proven by Tchakaloff (1957) for bounded regions and by Mysovskikh (1975) for unbounded regions for $\mathcal{V}_d^n = \mathcal{P}_d^n$. □

We will now prove, along the lines of Mysovskikh (1981), that this is the smallest general upper bound. We will construct an n-dimensional region for which a cubature formula of degree d with fewer points than $\dim \mathcal{V}_d^n$ does not exist.

Let $\mu := \dim \mathcal{V}_d^n$ and choose distinct points $\mathbf{a}^{(1)}, \ldots, \mathbf{a}^{(\mu)} \in \mathbb{R}^n$ that do not lie on a curve of order d. Let C_i be a cube with centre $\mathbf{a}^{(i)}$ and side ρ, such that the μ cubes do not intersect. We will now show that, for sufficiently small ρ, no cubature formula of degree d exists for $\Omega = C_1 \cup \ldots \cup C_\mu$ and $w(\mathbf{x}) \equiv 1$ with all points inside Ω and all weights positive.

Assume that such a cubature formula exists and let C_1 be the subregion containing no point of the cubature formula. Let $p(\mathbf{x}) \in \mathcal{V}_d^n$ satisfy

$$p(\mathbf{a}^{(1)}) = 1, \quad p(\mathbf{a}^{(i)}) = 0 \quad \text{for} \quad i = 2, \ldots, \mu,$$

and σ a number such that

$$0 < \sigma < \frac{1}{2\mu}. \tag{6.5}$$

Take ρ small enough such that $p(\mathbf{x}) \geq 1-\sigma$, for $\mathbf{x} \in C_1$, and $|p(\mathbf{x})| \leq \sigma$, for $\mathbf{x} \in \cup_{i=2}^{\mu} C_i$. Then

$$\begin{aligned} \left|\int_\Omega p(\mathbf{x})\,\mathrm{d}\mathbf{x}\right| &= \left|\int_{C_1} p(\mathbf{x})\,\mathrm{d}\mathbf{x} + \sum_{i=2}^{\mu} \int_{C_i} p(\mathbf{x})\,\mathrm{d}\mathbf{x}\right| \\ &\geq \left|\int_{C_1} p(\mathbf{x})\,\mathrm{d}\mathbf{x}\right| - \sum_{i=2}^{\mu} \left|\int_{C_i} p(\mathbf{x})\,\mathrm{d}\mathbf{x}\right| \\ &\geq (1-\sigma)\rho^n - (\mu-1)\sigma\rho^n \\ &= \rho^n(1-\mu\sigma). \end{aligned}$$

On the other hand,

$$\sum_{j=1}^{\mu} w_j p(\mathbf{y}^{(j)}) \leq \sigma \sum_{j=1}^{\mu} w_j = \sigma\mu\rho^n.$$

From the exactness of the cubature formula it follows that

$$(1-\mu\sigma)\rho^n \leq \sigma\mu\rho^n \quad \text{if and only if} \quad 1 \leq 2\mu\sigma,$$

which contradicts (6.5).

7. In search of minimal formulae

7.1. A general lower bound

We consider cubature formulae of the form

$$Q[f] = \sum_{j=1}^{N} w_j f(\mathbf{y}^{(j)}), \quad w_j \in \mathbb{R}, \tag{7.1}$$

for the approximation of the integral (3.1). In this section we identify the polynomials which are identical on the integration region Ω, and we restrict our attention to cubature formulae with all points inside Ω. This identification leaves the polynomial space unchanged if and only if Ω contains inner points.

Example 7.1 Consider the surface of the unit ball: $\Omega = \{\mathbf{x} : \sum_{i=1}^{n} x_i^2 = 1\}$. Then the polynomials $(\sum_{i=1}^{n} x_i^2)^p$, $p \in \mathbb{N}$, are all identified with the constant polynomial 1. So,

$$\dim \mathcal{P}_d^n|_\Omega = \binom{n+d}{n} - \binom{n+d-2}{n}.$$

Theorem 3.1 can be used to derive a very general lower bound. Good lower bounds are important because any method to construct cubature formulae (implicitly or explicitly) depends on a bound or estimate of the number of points. If a lower bound is known, then a method to construct cubature formulae attaining this bound is usually known.

Theorem 7.1 If the cubature formula (7.1) is exact for all polynomials of $\mathcal{V}^n_{2k}$, then the number of points $N \geq \dim \mathcal{V}^n_{k|\Omega}$.

Proof. Let $F = \mathcal{V}^n|_\Omega$, $F_1 = \mathcal{V}^n_k|_\Omega$ and

$$F_0 = \{f \in F_1 : f(\mathbf{y}^{(j)}) = 0, j = 1, \ldots, N\}.$$

If $f \in F_0$, then $\deg(f) \leq k$ and $f(\mathbf{y}^{(j)}) = 0$, $j = 1, \ldots, N$. Because f^2 is of degree at most $2k$, the cubature formula is exact and $I[f^2] = 0$. Hence, on Ω, $f \equiv 0$. So far, we have proved that

$$f \in F_0 \quad \text{implies} \quad f \equiv 0.$$

Let Q be a linear functional defined on $\mathcal{V}^n_k|_\Omega$. Then

$$f \in F_0 \Rightarrow f \equiv 0 \Rightarrow Q[f] = 0.$$

From Theorem 3.1 it follows that weights w_j can be found such that

$$Q[f] = \sum_{j=1}^{N} w_j f(\mathbf{y}^{(j)}), \quad \text{for all } f \in \mathcal{V}^n_k.$$

So, the vector space spanned by the functionals $L_j[f] = f(\mathbf{y}^{(j)})$ is equal to the space of all linear functionals defined on $\mathcal{V}^n_k|_\Omega$. Its dimension is also $\dim \mathcal{V}^n_k|_\Omega$. Hence $N \geq \dim \mathcal{V}^n_k|_\Omega$. $\square$

For regions with interior points and algebraic degree, Theorem 7.1 is given by Radon (1948) for $n = 2$, and for general n by Stroud (1960). It should be noted that the well-known proof of the Radon–Stroud lower bound does not assume all points are inside the region. This restriction plays a role if one includes regions such as the surface of the n-ball, without interior points. For the surface of the n-ball, this result was given by Mysovskikh (1977). Table 1 lists all known formulae that attain the lower bound, for the regions we mentioned in Section 5.

For trigonometric degree, this theorem was probably first mentioned by Mysovskikh (1988). Table 2 lists all known formulae that attain the lower bound. Cools and Reztsov (1997) proved it for other spaces of trigonometric polynomials.

For regions with interior points and product algebraic degree, this theorem was presented by Gout and Guessab (1986). The bound is attained by Gauss product formulae. For other spaces of algebraic polynomials it was presented by Guessab (1986). The general formulation we gave is from Möller (1979) with a proof due to Mysovskikh (1981).

Because $\dim \overline{\mathcal{P}}^n_d = (\dim \overline{\mathcal{P}}^1_d)^n$ and $\dim \overline{\mathcal{T}}^n_d = (\dim \overline{\mathcal{T}}^1_d)^n$, this bound is attained for the overall degree case by the product rules based on minimal quadrature rules. Hence in the rest of this paper, not much attention is paid to this case. As Tables 1 and 2 illustrate, the ordinary degree case is totally

Table 1. *Minimal formulae of algebraic degree*

n	d	N	regions	references
n	2	$n+1$	C_n, S_n, T_n, U_n	see Stroud (1971), Mysovskikh (1981)
2	d	$d+1$	U_n	see Stroud (1971)
	$2k$	$\frac{k^2+3k+2}{2}$	$C_2^{0.5}$	Morrow and Patterson (1978)
	4	6	$C_2, S_2, T_2, E_2^{r^2}$	see Stroud (1971), Cools and Rabinowitz (1993)
	6	10	C_2	Schmid (1983)
			T_2	Rasputin (1983*a*)
			S_2	Rasputin (1986), Wissman and Becker (1986)
	8	15	C_2	Morrow and Patterson (1978)
			T_2	Cools and Haegemans (1987*c*)
3	4	10	C_3	Weiß (1991)

Table 2. *Minimal formulae of trigonometric degree for* C_n^*

n	d	N	references
n	2	$2n+1$	Noskov (1988*b*)
2	$2k$	$2k^2+2k+1$	Noskov (1988*b*)

different: odd degree formulae do not appear in these tables (except for U_2) and the known even degree formulae are rare.

The following theorem teaches us something about the weights. It generalizes a theorem from Mysovskikh (1981).

Theorem 7.2 If the cubature formula (7.1) is exact for all polynomials of degree $d > 0$ and has only real points and weights, then it has at least $\dim \mathcal{V}_k^n$ positive weights, $k = \lfloor \frac{d}{2} \rfloor$.

Proof. According to Theorem 7.1, $N \geq \dim \mathcal{V}_k^n = \kappa$. Because $d > 0$, the cubature formula is exact for $f \equiv 1$, that is, $\sum_{j=1}^N w_j = I[1] > 0$. Hence there must be positive weights. If $d = 1$, then $\kappa = 1$ and the theorem holds.

We now consider $d \geq 2$ and assume the theorem does not hold. Let the number of positive weights $\nu < \kappa$ and order the points of the cubature formula such that these positive weights correspond to $\mathbf{y}^{(1)}, \ldots, \mathbf{y}^{(\nu)}$. Then one can find a polynomial $p \in \mathcal{V}_k^n$ such that $p(\mathbf{y}^{(j)}) = 0$, $j = 1, \ldots, \nu$.

The cubature formula is exact for p^2, hence

$$I[p^2] = \sum_{j=\nu+1}^{N} w_j p^2(\mathbf{y}^{(j)}).$$

Because $I[p^2] > 0$, $p^2(\mathbf{y}^{(j)}) \geq 0$ and $w_j < 0$ we obtain a contradiction, hence our assumption was wrong. $\square$

Corollary 7.1 If a cubature formula attains the lower bound of Theorem 7.1, then all its weights are positive.

Theorem 7.1 gives the same lower bound for cubature formulae of degree $2k$ and $2k+1$.

7.2. The characterization of minimal formulae and the reproducing kernel

For even degrees, I am unaware of any greater lower bound than that given in Theorem 7.1. The fact that not many formulae that attain this bound exist for the ordinary algebraic or trigonometric degree case has to do with the practical problems one encounters while attempting to construct these formulae. In this section, the reproducing kernel approach to construct cubature formulae is explained.

The concept of 'reproducing kernel' was first used for the construction of cubature formulae of algebraic degree by Mysovskikh (1968). For the trigonometric degree case it was first used by Mysovskikh (1990).

Choose the polynomials $\phi_1(\mathbf{x}), \phi_2(\mathbf{x}), \ldots \in \mathcal{V}^n$ such that $\phi_i(\mathbf{x})$ is orthogonal to $\phi_i(\mathbf{x})$, for all $j < i$, and $I[\phi_i\bar{\phi}_i] = 1$. This means that $\{\phi_i(\mathbf{x})\}_{i=1}^{\infty}$ is an orthonormal basis of $\mathcal{V}^n$. For a given $k \in \mathbb{N}$ we set $\kappa := \dim \mathcal{V}_k^n$ and

$$K(\mathbf{x}, \mathbf{y}) := \sum_{i=1}^{\kappa} \bar{\phi}_i(\mathbf{x})\phi_i(\mathbf{y}).$$

$K(\mathbf{x}, \mathbf{y})$ is a reproducing kernel in the space $\mathcal{V}_k^n$: if $f \in \mathcal{V}_k^n$, then f coincides with its expansion in ϕ_i, so that for $a \in \mathbb{C}^n$ fixed,

$$f(\mathbf{a}) = I[f(\mathbf{x})K(\mathbf{x}, \mathbf{a})] = \sum_{i=1}^{\kappa} I[f(\mathbf{x})\bar{\phi}_i(\mathbf{x})]\phi_i(\mathbf{a}).$$

The reproducing kernel $K(\mathbf{x}, \mathbf{y})$ plays an important role in connection with Theorem 7.1, as the next theorem illustrates.

Theorem 7.3 A necessary and sufficient condition for the points $\mathbf{y}^{(j)}$, $j = 1, \ldots, N = \dim \mathcal{V}_k^n$, to be the points of a cubature formula that is exact for $\mathcal{V}_{2k}^n$ is that

$$K(\mathbf{y}^{(r)}, \mathbf{y}^{(s)}) = b_r \delta_{rs}, \qquad (7.2)$$

with $b_r \neq 0$ and δ_{rs} the Kronecker symbol.

Proof. To prove the necessity, assume a cubature formula (7.1) exists that is exact on $\mathcal{V}^n_{2k}$. Hence, it is exact for

$$\phi_l(\mathbf{x})\phi_m(\mathbf{x}), \quad l, m = 1, \ldots, N,$$

and due to the orthonormality of the ϕ_i, we obtain

$$\sum_{j=1}^{N} w_j \bar{\phi}_l(\mathbf{y}^{(j)})\phi_m(\mathbf{y}^{(j)}) = \delta_{lm}. \tag{7.3}$$

Let $W := \mathrm{diag}(w_1, \ldots, w_N)$, E the unit matrix, and let A be

$$A = \begin{pmatrix} \phi_1(\mathbf{y}^{(1)}) & \ldots & \phi_1(\mathbf{y}^{(N)}) \\ \vdots & & \vdots \\ \phi_N(\mathbf{y}^{(1)}) & \ldots & \phi_N(\mathbf{y}^{(N)}) \end{pmatrix}.$$

Then (7.3) can be written as

$$AWA^\star = E,$$

where $A^\star$ denotes the Hermitian conjugate of A. A is non-singular, for otherwise there is an element of $\mathcal{V}^n_k$ that vanishes at all points of the cubature formula, which is impossible.

W is also non-singular, so we obtain

$$W = A^{-1}(A^\star)^{-1}$$

or

$$A^\star A = W^{-1}.$$

We deduce (7.2) with

$$b_r = 1/w_r = \sum_{i=1}^{N} |\phi_1(\mathbf{y}^{(r)})|^2 > 0.$$

(Remember Corollary 7.1!)

Sufficiency remains to be proven. Conditions (7.2) can be written as

$$A^\star A = B,$$

where $B := \mathrm{diag}(b_1, \ldots, b_N)$ is non-singular. This is equivalent to

$$AB^{-1}A^\star = E,$$

which in turn is equivalent to saying that the cubature formula with points $\mathbf{y}^{(j)}$, $j = 1, \ldots, N$, and weights $w_j = 1/b_j$ is exact for

$$\phi_l(\mathbf{x})\phi_m(\mathbf{x}), \quad l, m = 1, \ldots, N,$$

and thus for all elements of $\mathcal{V}^n_{2k}$. (The final step of this proof motivated the warning at the end of Section 3.) $\square$

For the algebraic-degree case, the reproducing kernel approach has not been very successful in constructing minimal cubature formulae. It can, however, also be used to construct non-minimal formulae; see Möller (1973) and Mysovskikh (1980). Möller (1973) also gave a modified reproducing kernel method to construct centrally symmetric cubature formulae of odd algebraic degree. This modification is based on the same idea we use in the following section to derive a lower bound for such formulae. Cools and Sloan (1996) used a similar modified method to construct minimal shift symmetric cubature formulae of odd trigonometric degree. In this case an infinite number of minimal cubature formulae for each odd degree was obtained in the two-dimensional case.

The reproducing kernel approach has also led to interesting results on the weights of cubature formulae (Cools and Haegemans 1988*c*, Cools 1989, Beckers and Cools 1993). Such results have also led to the following theorem.

Theorem 7.4 A cubature formula of degree $d = 2k$ with $N = \dim \mathcal{P}_d^n$ points does not exist for U_n if $n > 2$ and $k > 2$.

Proof. See Taylor (1995). □

For other characterizations of cubature formulae attaining the bound of Theorem 7.1, see, for instance, Morrow and Patterson (1978), Schmid (1978), and Schmid (1995).

7.3. The general lower bound for some invariant formulae

Although Theorem 7.1 has already shown many of its faces in the literature, it has not yet unveiled all. We will now show what it can teach us about centrally symmetric cubature formulae. In combination with Theorem 5.1, Theorem 7.1 gives a lower bound for the number of G-orbits in a G-invariant cubature formula. This can be translated into a lower bound for the number of points by multiplying it with the highest possible cardinality of a G-orbit, but one expects this will not usually give strict bounds. There is, however, an interesting exception ...

Consider centrally symmetric cubature formulae of algebraic degree $2k+1$ with k even. According to Theorem 7.1, the number of orbits of this cubature formula, K, satisfies

$$K \geq \dim \mathcal{P}_k^n(G_{cs}) = \sum_{i=0}^{k/2} \binom{n-1+2i}{n-1}.$$

A G_{cs}-orbit has one or two points and there can be only one orbit with one point. Hence the above bound for K implies a bound for the number of points:

$$N \geq 2 \dim \mathcal{P}_k^n(G_{cs}) - 1. \tag{7.4}$$

For example, for $n = 2$, we obtain

$$N \geq 2\sum_{i=0}^{k/2}(2i+1) - 1 = \frac{k^2}{2} + 2k + 1 = \binom{k+2}{2} + \frac{k}{2}.$$

For C_2, for instance, this bound is now known to be sharp for degrees 1,5 and 9. Consider shift symmetric cubature formulae of trigonometric degree $2k+1$. A G_{ss}-orbit always has two points. Using the same arguments as in the previous paragraph, we obtain the lower bound

$$N \geq 2 \dim \mathcal{T}_k^n(G_{ss}).$$

for the number of points.

These results, which are derived under the restriction of central symmetry and shift symmetry, will appear again in Section 8.3.

The following questions have probably already occurred in the reader's mind while reading this section.

- Under what conditions is the lower bound of Theorem 7.1 sharp?
- What is the minimum number of points for a cubature formula for a given region?
- Is the symmetry of the region somehow reflected in the structure of minimal formulae?

These questions have kept researchers busy for approximately 50 years now, and are still only partially answered. We return to them in the next section.

8. In search of better bounds for odd degree formulae

8.1. The need for a better bound

In Section 7.1 we obtained a lower bound for the number of points N of a cubature formula that is exact on a vector space of functions $\mathcal{V}_d^n$. This bound, presented in Theorem 7.1, depends only on $\mathcal{V}_d^n$, restricted to Ω. In this section we will see that this bound is in general too low for odd degrees d. Higher lower bounds have to take into account more information on the region Ω and weight function $w(\mathbf{x})$.

Suppose we have a cubature formula of algebraic degree $d = 2k+1$ that attains the lower bound of Theorem 7.1, and let $\mathfrak{A}$ be the corresponding ideal. Then

$$\mathcal{H}(k; \mathfrak{A}) = \dim \mathcal{P}_k^n = N = \mathcal{H}(d; \mathfrak{A}).$$

Hence the ideal contains $\dim \mathcal{P}_{k+1}^n - \dim \mathcal{P}_k^n$ linearly independent polynomials of degree $k+1$. These polynomials must be d-orthogonal and thus, because of their degree, simply orthogonal. So we have in fact proved the following theorem.

Theorem 8.1 A necessary condition for the existence of a cubature formula of algebraic degree $2k+1$ with $N = \dim \mathcal{P}_k^n$ points is that the basic orthogonal polynomials of degree $k+1$ have N common zeros.

The condition of Theorem 8.1 does not hold for standard regions such as C_n, T_n, S_n, $E_n^{r^2}$ and E_n^r. Radon (1948) discovered that no cubature formula of degree 5 with 6 points exists for C_2, T_2, and S_2.

8.2. The quest for exceptional regions

Fritsch (1970) searched for an n-dimensional region for which a formula of degree 3 with $n+1$ points exists. He defined a region $S_n(d)$ as follows. Let S_n be the n-simplex with vertices $v_0, v_1, \ldots, v_n$ and centroid c. Let F_k be the face of S_n that does not contain the vertex v_k and let c_k be the centroid of F_k. Let $d > 0$ and define the points $u_k(d)$ by

$$u_k(d) = dc_k + (1-d)c \ , \ k = 0, 1, \ldots, n.$$

Let $S_{nk}(d)$ be the simplex with base F_k and vertex $u_k(d)$. Define

$$S_n(d) = \begin{cases} S_n \cup (\bigcup_{k=0}^n S_{nk}(d)) \ , & d \geq 1, \\ S_n - (\bigcup_{k=0}^n S_{nk}(d)) \ , & 0 < d < 1. \end{cases}$$

Fritsch constructed a cubature formula of degree 3 with $n+2$ points depending on n and d for the region $S_n(d)$. He proved that there exists a $d_n > 1$, a zero of a known polynomial, such that his formula has a zero weight, and thus uses only $n+1$ points. For two dimensions he found two such regions, as shown in Figure 2. He also proved that there exists one $d_n^\star$ for which a formula of the form he looked for does not exist. For two and three dimensions the region $S_n(d_n^\star)$ is centrally symmetric (that is, the region and weight function remain invariant after reflection through the centre) and we will see later that the minimal number of points in a formula of degree 3 for such a region requires $2n$ points.

Mysovskikh and Černicina (1971) constructed a region $\Omega = \Omega_1 \cup \Omega_2$ with

$$\begin{aligned} \Omega_1 &= \{(x,y) : -\tau \leq x \leq \tau \ , \ 0 \leq y \leq e^{-|x|}\}, \\ \Omega_2 &= \{(x,y) : -\sigma \leq x \leq \sigma \ , \ -\epsilon \leq y \leq 0\}, \end{aligned}$$

$$\tau = 3 \ , \ \epsilon \simeq 0.048 \ , \ \sigma \simeq 1.266,$$

for which there exists a cubature formula of degree 5 with 6 points.

Recently, Schmid and Xu (1994) found a two-dimensional region for which formulae with $\dim \mathcal{P}_k^2$ points exist for each degree $2k+1$.

Theorem 8.2 Let $W(u,v) := w(x)w(y)$ with $w(t) := (1-t)^\alpha(1+t)^\beta$ and let

$$\Omega := \{(u,v) : (x,y) \in [-1,1]^2 \ , \ x < y \ , \ u = x+y \ , \ v = xy\}.$$

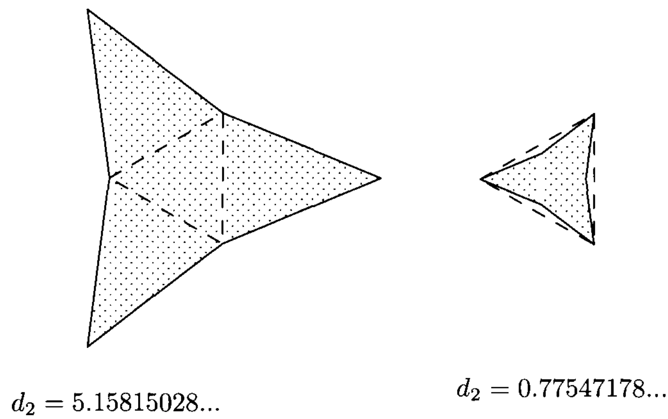

Fig. 2. Regions $S_2(d_2)$ for which a formula of degree 3 with 3 points exists

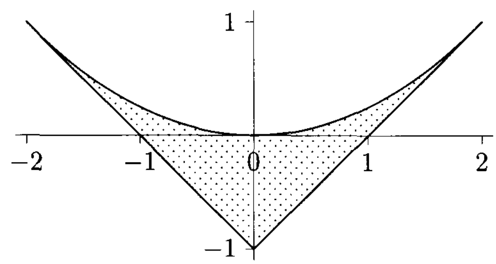

Fig. 3. Region for which a formula of degree $2k+1$ attains the bound of Theorem 7.1

Then there exists an infinite number of minimal cubature formulae of degree $2k$ and one (uniquely determined) minimal formula of degree $2k+1$ (both with $\dim \mathcal{P}_k^2$ points) for the following two classes of integrals,

$$\int_\Omega f(u,v)W(u,v)(u^2-4v)^\gamma \,du\,dv \quad \text{with} \quad \alpha,\beta > -1,\ \gamma = \pm\tfrac{1}{2}.$$

Proof. See Schmid and Xu (1994). □

Figure 3 displays Ω. Berens, Schmid and Xu (1995) obtained a similar result for arbitrary dimensions.

8.3. Improved bounds for centrally symmetric formulae

In Example 5.2 and at the end of Section 5 we encountered the pleasant effect of central symmetry on cubature formulae of algebraic degree. Mysovskikh (1966) showed that for centrally symmetric n-dimensional regions, the minimal number of points in a cubature formula of algebraic degree 3 is $2n$. The construction of such formulae is summarized by Stroud (1971). Möller (1973) generalized this improved lower bound for all odd degrees.

Theorem 8.3 Let R_{2k} denote the vector space of even polynomials of $\mathcal{P}^n_{2k+1}|_\Omega$ and R_{2k+1} denote the vector space of odd polynomials of $\mathcal{P}^n_{2k+1}|_\Omega$, $k \in \mathbb{N}_0$. If the algebraic degree of the cubature formula (7.1) for a centrally symmetric integral is $d = 2k+1$, then

$$\begin{array}{ll} N \geq 2\dim R_k - 1, & \text{if } k \text{ even and } 0 \text{ is a point,} \\ N \geq 2\dim R_k, & \text{otherwise.} \end{array}$$

A cubature formula that attains this bound is centrally symmetric and has all weights positive.

Proof. See Möller (1973) for the case where Ω has interior points and Möller (1979) for the general case. □

A similar result holds for cubature formulae of trigonometric degree.

Theorem 8.4 Let $R_k \subset \mathcal{T}^n_k$ denote the vector space of polynomials whose degree has the same parity as k. If the trigonometric degree of the cubature formula (7.1) for an integral over $C^\star_n$ is $d = 2k+1$, then

$$N \geq 2\dim R_k.$$

Proof. See Mysovskikh (1988). □

A nice result about the weights was obtained using the reproducing kernel.

Theorem 8.5 A cubature formula that attains the bound of Theorem 8.4 has all weights equal to $1/N$.

Proof. See Beckers and Cools (1993). □

To illustrate my belief in the similarities between the algebraic degree case and the trigonometric degree case, as well as the similarities between central-symmetry and shift symmetry, I dare to pose the following conjecture.

Conjecture 8.1 Any cubature formula attaining the bound of Theorem 8.4 is shift symmetric.

How good are the lower bounds of Theorems 8.3 and 8.4? For two dimensions it is now known that these bounds are the best possible if further information on the integral is not available.

For the regions $C_2^{0.5}$ and $C_2^{-0.5}$, cubature formulae attaining the lower bound of Theorem 8.3 exist for arbitrary odd degree (Cools and Schmid 1989). In Table 3, we list the known minimal formulae for standard regions. For some regions, for instance S_2 and $E_2^{r^2}$, it has been proved that the bound of Theorem 8.3 cannot be attained for degrees $4k+1$, $k > 1$. For C_2, it is known that a cubature formula of degree 13 with 31 points cannot exist. For these regions at least one additional point is required (Verlinden and Cools 1992, Cools and Schmid 1993).

Table 3. *Minimal formulae of odd algebraic degree*

n	d	N	references C_n	S_n	$E_n^{r^2}$	E_n^r
2	3	4	[1]	[1]		
	5	7	[1]	[1]		
	7	12	[1]*	[1]	[1]	[1,4]
	9	17(18)	[3]	[2]	[4]	
	11	24	[5]			
3	3	6	[1]			
	5	13	[1]*	[1]	[1]	[1]

[1] = Stroud (1971), [2] = Piessens and Haegemans (1975), [3] = Möller (1976),
[4] = Haegemans and Piessens (1977), [5] = Cools and Haegemans (1988*a*),
* = Many known formulae; see also Cools and Rabinowitz (1993).

Table 4. *Minimal formulae of odd trigonometric degree for* $C_n^\star$

n	d	N	references
n	1	2	Mysovskikh (1988)
	3	$4n$	Noskov (1988*a*)
2	d	$\frac{(d+1)^2}{2}$	Beckers and Cools (1993)
			Cools and Sloan (1996)
3	5	38	Frolov (1977)

For $C_2^\star$, cubature formulae attaining the lower bound of Theorem 8.4 exist for arbitrary odd degree (Cools and Sloan 1996). In Table 4, we list the known minimal formulae for $C_n^\star$.

8.4. An improved general bound for odd degrees

We will now present a lower bound especially derived for odd algebraic degrees, $d = 2k+1$, without any assumptions on the symmetry of the region. Let

$$O_{k+1} := \{f \in \mathcal{P}_{k+1}^n : g \in \mathcal{P}_k^n \Rightarrow I[fg] = 0\},$$

Table 5. *Minimal formulae of odd algebraic degree for T_n*

n	d	N	references
2	3	4	Stroud (1971), Hillion (1977)
	5	7	Stroud (1971)
	7	12	Gatermann (1988), Becker (1987)
n	3	$n+2$	Stroud (1971)
4	3	6	Stroud (1971), Grundmann and Möller (1978), de Doncker (1979)

and define for arbitrary $l \in \{2, \ldots, n\}$

$$\begin{aligned} \gamma_l &:= \dim \left\{ (f_1, \ldots, f_l) \in O_{k+1}^l \,\middle|\, \sum_{i=1}^{l} x_i f_i \in \mathcal{P}_{k+1}^n \right\}, \\ &- \dim \left\{ (f_1, \ldots, f_l) \in O_{k+1}^l \,\middle|\, \sum_{i=1}^{l} x_i f_i \in O_{k+1} \right\}. \end{aligned}$$

Theorem 8.6 If a cubature formula has algebraic degree $2k+1$, then $N \geq \dim \mathcal{P}_k^n + \frac{\gamma_l}{l}$.

Proof. See Möller (1976) ($l = 2$, Ω with interior points), and Möller (1979). □

For two dimensions, the bounds of Theorems 8.3 and 8.6 coincide for centrally symmetric integrals:

$$N \geq \frac{(k+1)(k+2)}{2} + \left\lfloor \frac{k+1}{2} \right\rfloor. \tag{8.1}$$

For more than two dimensions, Theorem 8.3 gives a higher lower bound than Theorem 8.6 for centrally symmetric integrals. Theorem 8.6 was applied by Möller to the triangle T_2. He obtained (8.1) for $0 \leq k \leq 5$. Rasputin (1983*b*) generalized this to all k. Berens and Schmid (1992) proved that the same lower bound is obtained for some non-constant weight functions. In addition, Möller (1976) obtained the following results for T_n: for $k = 1$, $\gamma_2 = 2$ and for $k = 2$, $\gamma_2 = 2n - 2$. In Table 5 the known minimal formulae for this region are listed.

8.5. The quality of lower bounds

In this section we have presented the best known lower bounds for the number of points in cubature formulae of odd degree. We gave examples showing that these bounds can be attained for some regions. If one looks at Tables 3, 4 and 5, the results for standard regions look meagre: minimal formulae, that is, formulae attaining a known lower bound, are known only for low dimensions and low degrees. It is likely, but not certain, that these bounds are too low for standard regions and for higher degrees or dimensions. This uncertainty is one of the main problems in the construction of cubature formulae and the construction methods based on characterizing polynomials suffer from it, as we shall see in the following section.

9. Constructing cubature formulae using ideal theory

9.1. A bird's-eye view

Orthogonal polynomials were already being used by Appell (1890) and Radon (1948) to construct cubature formulae of algebraic degree for two-dimensional integrals. Radon tried without success to construct cubature formulae of degree 5 with 6 points. He constructed formulae of degree 5 with 7 points using the common zeros of three orthogonal polynomials. His work marked a starting point of a theory. During the 1960s, Stroud and Mysovskikh studied the relation between orthogonal polynomials and cubature formulae for n-dimensional integrals. In the mid-1970s, many new, mainly symmetric, cubature formulae were obtained using the common zeros of three orthogonal polynomials in two and three variables; see, for instance, Piessens and Haegemans (1975), Haegemans and Piessens (1976), Haegemans and Piessens (1977), Haegemans (1982). The theoretical results were put in the framework of ideal theory by Möller (1973). Methods to construct cubature formulae based on these and other theoretical achievements were derived by Morrow and Patterson (1978), Schmid (1980*b*) and Cools and Haegemans (1987*b*), amongst others.

We mentioned that one can also work with ideals of invariant polynomials. Gatermann (1992) combined ideal theory with the theory of linear representations of finite groups.

We will now present two successful methods to construct cubature formulae of algebraic degree. In order not to over-complicate everything, we restrict this to two dimensions.

9.2. The T-method

A starting point in Theorem 6.8 is that the ideal $\mathfrak{A}$ is fundamental of degree $d+1$. In general, $\mathfrak{A}$ will be fundamental of degree $l, l+1, \ldots$ where $\lfloor d/2 \rfloor + 1 \leq l \leq d+1$. Let m be such that $\mathfrak{A}$ is fundamental of degree m, but is not fundamental of degree $m-1$. One can try to determine a set of polynomials of degree m that form a basis of an ideal satisfying the conditions of Theorem 6.8. This idea was first suggested by Morrow and Patterson (1978) and Schmid (1978) for two-dimensional regions. It was further developed by Schmid (1980*a*); see also Schmid (1980*b*) and Schmid (1995).

Consider the case where the ideal $\mathfrak{A}$ associated with a cubature formula of degree $2k-1$ is fundamental of degree $k+1$. Let $R_0, \ldots, R_{k+1}$ be linearly independent polynomials of degree $k+1$ in two variables, x and y. These polynomials are orthogonal to all polynomials of degree $k-2$ if they vanish at the points of a cubature formula of degree $2k-1$. Thus the R_is can be written as

$$R_i = P^{k+1-i,i} + \sum_{j=0}^{k} \beta_{ij} P^{k-j,j} + \sum_{j=0}^{k-1} \gamma_{ij} P^{k-1-j,j}, \quad i = 0, \ldots, k+1,$$

where the $P^{a,b}$ are the basic orthogonal polynomials (6.3). The β_{ij} and γ_{ij} are parameters which have to be determined such that the R_is belong to an ideal $\mathfrak{A}$ satisfying the conditions of Theorem 6.8. When the integral is centrally symmetric, the basic orthogonal polynomials have a special form and the β_{ij} vanish.

The construction is based on the following observations.

- Let $Q_i := yR_i - xR_{i+1}$, $i = 0, \ldots, k$. Then Q_i is a polynomial of degree k and Q_i has to be orthogonal.
- The polynomials $xQ_i, yQ_i, i = 0, \ldots, k$, are of degree $k+1$ and they belong to $\mathfrak{A}$. Thus $xQ_i, yQ_i \in \text{span}\{R_0, \ldots, R_{k+1}\}$.

Both conditions lead to necessary conditions: linear and quadratic equations in the γ_{ij}s. Starting from the explicit expressions for the basic orthogonal polynomials, a computer algebra system can be programmed to derive these equations. The linear equations can then be used to reduce the number of unknowns in the system of quadratic equations. In the resulting system the number of equations and unknowns is usually different. More recently, Schmid (1995) worked this out in detail using matrix equations.

The inequality in Theorem 6.8 translates into inequalities for the γ_{ij}. These inequalities together with the linear and quadratic equations give necessary and sufficient conditions for the γ_{ij}s so that all conditions of Theorem 6.8 are satisfied. Schmid (1983) used this method to construct cubature formulae of degree ≤ 9 for C_2^{α}. Cools and Schmid (1989) used it to construct formulae of arbitrary odd degree for $C_2^{-0.5}$ and $C_2^{0.5}$.

We will now prove, using G-bases, that the above method works. A similar proof for the n-dimensional case is given by Möller (1987).

Theorem 9.1 Let

$$\begin{aligned} R_i &= P^{k+1-i,i} + \textstyle\sum_{j=0}^{k-1} \gamma_{ij} P^{k-1-j,j}, & j &= 0, \ldots, k+1, \\ Q_i &= yR_i - xR_{i+1}, & i &= 0, \ldots, k. \end{aligned} \tag{9.1}$$

If the polynomials Q_i are $(2k-1)$-orthogonal and if all polynomials xQ_i, yQ_i are elements of $\text{span}\{R_0, \ldots, R_{k+1}\}$, then $F := \{R_0, \ldots, R_{k+1}, Q_0, \ldots, Q_k\}$ is a G-basis.

Proof. We use the term ordering $1 < y < x < y^2 < xy < x^2 < \ldots$, apply Theorem 6.3 and distinguish three cases.

Case 1: (R_i, R_j), $i, j = 0, \ldots, k+1$.
$H(R_l, R_j) = x^{k+1-l}y^j$. This is a divisor of $H(R_i, R_j) = x^{k+1-i}y^j$ for $i < j$, if $i < l$. Hence the pair (R_i, R_j) is superfluous if there exists a l such that $i < l < j$. Therefore we only have to check pairs (R_i, R_{i+1}). But

$$\begin{aligned} SP(R_i, R_{i+1}) &= \frac{H(R_i, R_{i+1})}{M(R_i)} R_i - \frac{H(R_i, R_{i+1})}{M(R_{i+1})} R_{i+1} \\ &= \frac{x^{k+1-i}y^{i+1}}{x^{k+1-i}y^i} R_i - \frac{x^{k+1-i}y^{i+1}}{x^{k-i}y^{i+1}} R_{i+1} \\ &= yR_i - xR_{i+1} \\ &= Q_i, \end{aligned}$$

and thus $SP(R_i, R_{i+1}) \xrightarrow[F]{}^{+} 0$.

Case 2: (Q_i, Q_j), $i, j = 0, \ldots, k$.
If $\mathrm{Hterm}(Q_i) = \mathrm{Hterm}(Q_j)$ then $SP(Q_i, Q_j) \in \mathrm{span}\{Q_i\}$ and thus $SP(Q_i, Q_j) \xrightarrow[F]{}^{+} 0$.
If $\mathrm{Hterm}(Q_i) \neq \mathrm{Hterm}(Q_j)$ then there exist $u, v \in \{x, y\}$ for which $SP(Q_i, Q_j) = SP(uQ_i, vQ_j)$.
Because $xQ_i, yQ_i \in \mathrm{span}\{R_0, \ldots R_{k+1}\}$ this reduces to Case 1.

Case 3: (R_i, Q_j), $i = 0, \ldots, k+1$, $j = 0, \ldots, k$.
One can always find a $u \in \{x, y\}$ such that $SP(R_i, Q_j) = SP(R_i, uQ_j)$. Since x, Q_i, yQ_i are in $\mathrm{span}\{R_0, \ldots, R_{k+1}\}$, this reduces to Case 1.

□

Theorem 9.2 Let F be as defined in Theorem 9.1. If the common zeros of the polynomials in F are real and simple, then there exists a cubature formula of degree $2k-1$ with the elements of $\mathsf{NG}(F)$ as points. The number of points $N \leq \frac{k(k+3)}{2}$.

Proof. The ordering used in the proof of Theorem 9.1 is compatible with the partial ordering by degree. According to Theorem 6.4, F is thus an H-basis. Theorem 6.7 then guarantees the existence of the cubature formula.

An upper bound for the number of points in the cubature formula is given by the Hilbert function. Because F is fundamental of degree $k+1$,

$$\begin{aligned} \mathcal{H}(2k-1, F) &= \mathcal{H}(k, F) \\ &= \dim \mathcal{P}_k^2 - \dim(\mathcal{P}_k^2 \cap F) \\ &= \dim \mathcal{P}_{k-1}^2 + \operatorname{codim}(F \cap \mathcal{P}_k^2). \end{aligned}$$

There will be at least one polynomial Q_i, hence $\operatorname{codim}(F \cap \mathcal{P}_k^2) \leq k$. Thus $N \leq \frac{k(k+1)}{2} + k$. □

The upper bound of Theorem 9.2 is very weak. A tighter result is known.

Theorem 9.3 If the ideal of all polynomials that vanish at the N points of a cubature formula of degree $2k-1$ contains a fundamental set of degree $k+1$, then

$$\frac{k(k+1)}{2} + \left\lfloor \frac{k}{2} \right\rfloor \leq N \leq \frac{k(k+1)}{2} + \left\lfloor \frac{k}{2} \right\rfloor + 1.$$

Proof. See Cools (1989) or Schmid (1995). □

This clearly shows that the success of this method strongly depends on the quality of the lower bound (8.1) for the particular integral for which a cubature formula is wanted.

If the lower bound (8.1) underestimates the real minimal number of points by more than one, then the method is useless. At the moment it looks as if this is the case for $d \geq 15$ for the regions C_2, S_2 $E_2^{r^2}$ and E_2^r. The known exceptions are $C_2^{0.5}$ and $C_2^{-0.5}$.

9.3. The S-method

The S-method was suggested by Cools and Haegemans (1987*b*) in an attempt to find a method that is less dependent on the lower bound (8.1) than the T-method. If the T-method is used to construct symmetric cubature formulae for a two-dimensional symmetric integral, then $\gamma_{ij} = 0$ if $i+j$ is odd, in the polynomials R_i (9.1). The polynomials R_i can be divided into two sets: $A := \{R_i : i \text{ is even}\}$ and $B := \{R_i : i \text{ is odd}\}$. Instead of demanding that $(A \cup B) \subset \mathfrak{A}$, as in the T-method, we demand that $A \subset \mathfrak{A}$ or $B \subset \mathfrak{A}$. We assign $C := A$ and $q := 0$ if we want to investigate the case $A \subset \mathfrak{A}$. We assign $C := B$ and $q := 1$ if we want to investigate the case $B \subset \mathfrak{A}$. The S-method is based on the following observations.

- Let $S_i := y^2 R_i - x^2 R_{i+2}$, $i = q, q+2, \ldots, k-1$. Then S_i is a polynomial of degree $k+1$ and S_i must be orthogonal to all polynomials of degree $k-2$.
- Because S_i has degree $k+1$, $S_i \in \operatorname{span}(C)$.

Both conditions lead to necessary conditions for γ_{ij}: linear and quadratic equations in the γ_{ij}s. In Cools and Haegemans (1988*b*), necessary and sufficient conditions are given for this method, with proofs along the lines of the proof of Theorem 9.1.

The S-method has been used to construct cubature formulae of degree 13 with 36, 35 and 34 points for C_2, S_2, $E_2^{r^2}$, and of degree 17 with 57 points for C_2.

9.4. Evaluation

Orthogonal polynomials and ideal theory are powerful tools for theoretical investigations of cubature formulae. The most complex concepts of ideal theory have only been used to develop construction methods and to prove theorems about cubature formulae. The reader has probably noticed that we do not need the most sophisticated part of ideal theory to construct formulae: operations on vector spaces of polynomials suffice. This is one of the beautiful aspects of ideal theory. The construction methods described require the solution of systems of linear and quadratic equations. These systems are in general smaller than the systems that determine the formulae. One problem for these methods is that they stand or fall with the quality of the lower bounds given in Sections 7 and 8.

10. Constructing cubature formulae using invariant theory

10.1. A bird's-eye view

In this section we will describe how one tries to construct cubature formulae by solving the associated system of nonlinear equations (4.4). Sobolev's theorem plays a very important role: it is essential to limit the size of the nonlinear system by imposing structure on the cubature formulae. It suggests that we look for invariant cubature formulae, that is, solutions of the equations

$$Q[\phi_i] = I[\phi_i], \quad i = 1, \ldots, \dim \mathcal{P}_d^n(G), \tag{10.1}$$

where the ϕ_i form a basis for the space of G-invariant polynomials $\mathcal{P}_d^n(G)$.

The idea of demanding that a cubature formula has the same symmetries as the given integral is as old as the construction of cubature formulae itself. Indeed, when Maxwell (1877) constructed cubature formulae for the square and the cube, he considered only cubature formulae that are invariant with respect to the groups of symmetries of these regions, that is, G_{FS}.

There is no reason why a cubature formula should have the same structure as the integral. (What should a formula for a circle look like?) Cubature formulae that are invariant with respect to a subgroup of the symmetry group of the integral were already obtained by Radon (1948). His formula for C_2 is symmetric, that is, G_s-invariant, and his formula for S_2 has the origin and the vertices of a regular hexagon as points, that is, H_2^6-invariant.

Russian researchers, aware of Sobolev's result, applied the tools of invariant theory to construct cubature formulae invariant with respect to the symmetry groups of regular polytopes A_n, B_n and I_3 and the extension group $A_n^\star$. Notable results are those of Lebedev (1976) for U_n (see also Lebedev and Skorokhodov (1992) and Lebedev (1995)) and Konjaev (1977) for S_3, $E_2^{r^2}$ and E_2^r.

Table 6. *Different types of H_2^4-orbit*

type	generator	number of unknowns	number of points in an orbit	unknowns
0	(0,0)	1	1	weight
1	(a,0)	2	4	a, weight
2	(a,a)	2	4	a, weight
3	(a,b)	3	8	a, b, weight

Western researchers also considered subgroups without using the general theory. They realized that imposing too much structure on a formula prohibits attaining the minimal number of points. For instance, a fully symmetric formula for C_2 of degree 9 requires 20 points, a symmetric formula 18, but a rotational invariant (R_4) cubature formula requires 17, and this is minimal. Humans seem to have a preference for certain symmetries. Symmetry with respect to the axes (G_s) is studied regularly but symmetry with respect to the diagonals has been used only recently. The symmetry groups are nevertheless isomorphic. Rotational symmetries turned up unexpectedly in Möller (1976) and were later used to construct some other minimal formulae (Cools and Haegemans 1988*a*).

We will now present the consistency conditions approach to constructing fully symmetric cubature formulae. For simplicity, we again restrict ourselves to two dimensions.

10.2. Consistency conditions and fully symmetric regions

In this section, fully symmetric cubature formulae for two-dimensional integrals will be considered. The symmetry group is the dihedral group $H_2^4 = B_2 = G_{FS}$. In Example 5.1 it was shown that not all orbits have the same number of points. Each orbit in an invariant cubature formula introduces a number of unknowns in the nonlinear equations (5.2) and gives a number of points in the cubature formula (5.1). The role of the different types of orbit is described in Table 6.

Let K_i be the number of orbits of type i in an invariant cubature formula. One does not expect a solution of a system of nonlinear equations if there are more equations than unknowns. The previous sentence is the foundation upon which all work in this area is based. It sounds very reasonable but it also incorporates the weakness of this approach.

Rabinowitz and Richter (1969) introduced the notion of *consistency conditions*. A consistency condition is an inequality for the K_i 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. Cubature formulae that do not satisfy the consistency conditions are called 'fortuitous' and are thought to be rare.

We encountered basic invariant polynomials for H_2^4 in Example 5.3:

$$\sigma_2 := x^2 + y^2 \quad \text{and} \quad \sigma_4 := x^4 - 6x^2y^2 + y^4.$$

For this particular group it is more common to use $\phi_1 := x^2 + y^2$ and $\phi_2 := x^2y^2$ as basic invariant polynomials.

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

$$K_0 + 2K_1 + 2K_2 + 3K_3 \geq \dim \mathcal{P}_d^2(G_{FS}). \tag{10.2}$$

For $d = 2k+1$, $\dim \mathcal{P}_d^2(G_{FS}) = 1 + k + \lfloor \frac{k^2}{4} \rfloor$.

A cubature formula that is exact for ϕ_2 cannot use orbits of types 0 and 1 only, because such orbits have a zero contribution in a G_{FS}-invariant cubature formula. Thus, to integrate the polynomials

$$\phi_2(\phi_1^i \phi_2^j) \quad \text{for all } i, j : 0 \leq 2i + 4j \leq d - 4,$$

orbits of types 2 and 3 are needed. So we obtain the second consistency condition:

$$2K_2 + 3K_3 \geq \dim \mathcal{P}_{d-4}^2(G_{FS}). \tag{10.3}$$

A cubature formula that is exact for $(x-y)^2(x+y)^2 = \phi_1^2 - 4\phi_2$ cannot use orbits of types 0 and 2 only, for the same reasons as in the previous case. Analogously, the third consistency condition is obtained:

$$2K_1 + 3K_3 \geq \dim \mathcal{P}_{d-4}^2(G_{FS}). \tag{10.4}$$

A cubature formula that is exact for $x^2y^2(x-y)^2(x+y)^2 = \phi_1^2\phi_2 - 4\phi_2^2$ must use orbits of type 3 because all other orbits have a zero contribution. Thus, to integrate the polynomials

$$(\phi_1^2\phi_2 - 4\phi_2^2)(\phi_1^i \phi_2^j) \quad \text{for all } i, j : 0 \leq 2i + 4j \leq d - 8,$$

orbits of type 3 are needed. From this follows the fourth consistency condition:

$$3K_3 \geq \dim \mathcal{P}_{d-8}^2(G_{FS}). \tag{10.5}$$

The final consistency condition is that there can be only one orbit of type 0:

$$K_0 \leq 1. \tag{10.6}$$

The above consistency conditions were first derived by Mantel and Rabinowitz (1977).

If the structure of a cubature formula with $N = K_0 + 4K_1 + 4K_2 + 8K_3$ points satisfies the consistency conditions (10.2), (10.3), (10.4), (10.5) and

(10.6), the system of nonlinear equations (10.1), as well as each subsystem, has a number of unknowns that exceeds the number of equations and that looks promising to those interested in a solution of such a system. However, appearances can be deceptive.

The construction of a cubature formula with the lowest possible number of points requires two steps.

(1) Solve the integer programming problem:

$$\text{minimize } N(K_i : i = 0, 1, \ldots),$$

where the integers K_i satisfy the consistency conditions.

(2) Solve the system of polynomial equations (10.1). If no solution of the polynomial equations is found, then another (non-optimal) solution of the consistency conditions must be tried.

Example 10.1 For a fully symmetric formula of degree 7, the consistency conditions become

$$\begin{aligned} K_0 + 2K_1 + 2K_2 + 3K_3 &\geq 6, \\ 2K_2 + 3K_3 &\geq 2, \\ 2K_1 + 3K_3 &\geq 2, \\ 3K_3 &\geq 0, \\ K_0 &\leq 1. \end{aligned}$$

Optimal solutions are $[K_0, K_1, K_2, K_3] = [0, 1, 2, 0]$, and $[0, 2, 1, 0]$. (Optimal solutions are not necessarily unique!) This second structure corresponds to a cubature formula of the form

$$\begin{aligned} Q[f] = \; & w_1(f(x_1, 0) + f(-x_1, 0) + f(0, x_1) + f(0, -x_1)) \\ & + w_2(f(x_2, 0) + f(-x_2, 0) + f(0, x_2) + f(0, -x_2)) \\ & + w_3(f(x_3, x_3) + f(-x_3, x_3) + f(x_3, -x_3) + f(-x_3, -x_3)). \end{aligned}$$

The system of nonlinear equations (5.2) for this case is

$$\left\{ \begin{array}{lll} 4w_3\phi_2(x_3, x_3) & = 4w_3x_3^4 & = I[\phi_2], \\ 4w_3\phi_1(x_3, x_3)\phi_2(x_3, x_3) & = 8w_3x_3^6 & = I[\phi_1\phi_2] \end{array} \right.$$

$$\left\{ \begin{array}{ll} 4w_1 + 4w_2 & = I[0] - 4w_3, \\ 4w_1\phi_1(x_1, 0) + 4w_2\phi_1(x_2, 0) & = I[\phi_1] - 4w_3\phi_1(x_3, x_3), \\ 4w_1\phi_1^2(x_1, 0) + 4w_2\phi_1^2(x_2, 0) & = I[\phi_1^2] - 4w_3\phi_1^2(x_3, x_3), \\ 4w_1\phi_1^3(x_1, 0) + 4w_2\phi_1^3(x_2, 0) & = I[\phi_1^3] - 4w_3\phi_1^3(x_3, x_3). \end{array} \right.$$

From the first two equations one determines w_3 and x_3. Then w_1, x_1, w_2, and x_2 follow from the remaining four equations. Both systems have the familiar form of systems that determine a Gauss quadrature problem.

10.3. How to exploit symmetries

Invariant theory is very useful for constructing a system of nonlinear equations that determines a cubature formula with a particular structure. One advantage of imposing a structure is that the number of nonlinear equations is reduced. For instance, a cubature formula of degree 7 for a two-dimensional region is a solution of a system of $\dim \mathcal{P}_7^2 = 36$ equations. A fully symmetric formula of the same degree is determined by 6 equations.

A second advantage is that one can often find a basis for the invariant polynomials such that the equations are easy to solve. Typically, the system of nonlinear equations is split into several smaller subsystems which can be solved sequentially.

A third advantage is that, if the basis is chosen carefully, then each of these subsystems of nonlinear equations can be solved easily, because they have the same form as the systems that determine a quadrature formula.

The success of this approach depends on the selection of a proper basis for the invariant polynomials, and that is definitely more of an art than a science. This is clearly illustrated in Example 10.1. Other nice examples are given by Cools and Haegemans (1987*a*) and Beckers and Haegemans (1991).

10.4. Some critical notes

Consistency conditions can be derived for every structure and dimension. They can help to set up a system of nonlinear equations where in each subsystem the number of unknowns is larger than or equal to the number of equations. See, for example, Lyness and Jespersen (1975), Mantel and Rabinowitz (1977), Keast and Lyness (1979), Cools (1992), and Maeztu and Sainz de la Maza (1995).

In general, the system of nonlinear equations is still too large to be solved completely with currently available tools. One usually has to use an iterative zero finder and must provide very good starting values.

It must be emphasized that consistency conditions are neither sufficient nor necessary conditions. Even if a system of equations has more unknowns than equations, it might not have a real solution. Furthermore, fortuitous cubature formulae are known, for instance the minimal formulae for $C_2^{0.5}$ and $C_2^{-0.5}$.

The success of this approach depends on the quality of the lower bound for the number of points provided by the integer programming problem. For higher degrees and dimensions, many solutions of the consistency conditions exist for which no solutions of the nonlinear equations are known.

Most researchers have studied consistency conditions without worrying about the associated cubature formula. It is often easier to derive these conditions and, at the same time, obtain a system with a special structure that makes it easier to solve it, using the tools from invariant theory. See, for example, Beckers and Haegemans (1991).

Although the foundations of consistency conditions are built on quicksand, it must be said that most known cubature formulae of algebraic degree are obtained this way. In fact, for higher dimensions and higher degrees, only this approach has so far delivered cubature formulae.

11. A never-ending story

Let those patient readers who have borne with me thus far now join with me in looking back. We started from a solid, general theoretical foundation. Almost immediately we restricted our attention to the most common vector spaces, hence limiting consideration to cubature formulae of algebraic and trigonometric degree. We paid attention to lower bounds for the number of points and saw that they can easily be attained in the overall algebraic or trigonometric degree case. Following that, we searched for better bounds that, at least in the two-dimensional case, are attained for the trigonometric degree case. The rest of our time we spent on the most difficult and interesting algebraic degree case and ended with two approaches to constructing such formulae.

From the above, it is clear that solving systems of polynomial equations is very near to our heart. We therefore welcome the survey of Li (1997) in this volume.

Our list of references may seem long, yet it is incomplete. And there is much more to say: see also Engels (1980) and Davis and Rabinowitz (1984), and, if you can wait, Davis, Rabinowitz and Cools (199x). Let me whet your appetite.

A cubature formula is meant to be used to approximate integrals. Users want to have an indication of the accuracy of the approximation. A classical way to obtain an error estimate is to compare several approximations of different degrees of precision. Sequences of embedded cubature formulae help to reduce the burden. Indeed, these have already been investigated. As Cools (1992) incorporates a survey of some of the obtained results, I resist the temptation to elaborate on this subject.

Acknowledgements
The author gratefully acknowledges helpful comments by Professors Ann Haegemans, Dirk Laurie, Philip Rabinowitz and Hans Joachim Schmid on an earlier version of this paper. To the author alone belongs the responsibility for the selection of the material included.

REFERENCES

P. Appell (1890), 'Sur une classe de polynômes à deux variables et le calcul approché des intégrales double', *Ann. Fac. Sci. Univ. Toulouse* **4**, H1–H20.

P. Appell and J. Kampé de Fériet (1926), *Fonctions Hypergéométriques et Hypersphériques - Polynomes d'Hermite*, Gauthier-Villars, Paris.

T. Becker (1987), Konstruktion von interpolatorischen Kubaturformeln mit Anwendungen in der Finit-Element-Methode, PhD thesis, Technische Hochschule Darmstadt.

M. Beckers and R. Cools (1993), A relation between cubature formulae of trigonometric degree and lattice rules, in *Numerical Integration IV* (H. Brass and G. Hämmerlin, eds), Birkhäuser, Basel, pp. 13–24.

M. Beckers and A. Haegemans (1991), 'The construction of three-dimensional invariant cubature formulae', *J. Comput. Appl. Math.* **35**, 109–118.

H. Berens and H. J. Schmid (1992), On the number of nodes of odd degree cubature formulae for integrals with Jacobi weights on a simplex, in *Numerical Integration - Recent Developments, Software and Applications* (T. Espelid and A. Genz, eds), Vol. 357 of *NATO ASI Series C: Math. and Phys. Sciences*, Kluwer, Dordrecht, pp. 37–44.

H. Berens, H. J. Schmid and Y. Xu (1995), 'Multivariate Gaussian cubature formulae', *Arch. Math.* **64**, 26–32.

B. Buchberger (1985), Gröbner bases: An algorithmic method in polynomial ideal theory, in *Progress, Directions and Open Problems in Multidimensional Systems Theory* (N. Bose, ed.), Reidel, Dordrecht, pp. 184–232.

R. Cools (1989), The construction of cubature formulae using invariant theory and ideal theory, PhD thesis, Katholieke Universiteit Leuven.

R. Cools (1992), A survey of methods for constructing cubature formulae, in *Numerical Integration - Recent Developments, Software and Applications* (T. Espelid and A. Genz, eds), Vol. 357 of *NATO ASI Series C: Math. and Phys. Sciences*, Kluwer, Dordrecht, pp. 1–24.

R. Cools and A. Haegemans (1987*a*), 'Automatic computation of knots and weights of cubature formulae for circular symmetric planar regions', *J. Comput. Appl. Math.* **20**, 153–158.

R. Cools and A. Haegemans (1987*b*), 'Construction of fully symmetric cubature formulae of degree $4k-3$ for fully symmetric planar regions', *J. Comput. Appl. Math.* **17**, 173–180.

R. Cools and A. Haegemans (1987*c*), Construction of minimal cubature formulae for the square and the triangle using invariant theory, Report TW 96, Dept. of Computer Science, Katholieke Universiteit Leuven.

R. Cools and A. Haegemans (1988*a*), 'Another step forward in searching for cubature formulae with a minimal number of knots for the square', *Computing* **40**, 139–146.

R. Cools and A. Haegemans (1988*b*), Construction of symmetric cubature formulae with the number of knots (almost) equal to Möller's lower bound, in *Numerical Integration III* (H. Brass and G. Hämmerlin, eds), Birkhäuser, Basel, pp. 25–36.

R. Cools and A. Haegemans (1988c), 'Why do so many cubature formulae have so many positive weights?', *BIT* **28**, 792–802.

R. Cools and P. Rabinowitz (1993), 'Monomial cubature rules since 'Stroud': A compilation', *J. Comput. Appl. Math.* **48**, 309–326.

R. Cools and A. Reztsov (1997), 'Different quality indexes for lattice rules', *J. Complexity*. To appear.

R. Cools and H. J. Schmid (1989), 'Minimal cubature formulae of degree $2k-1$ for two classical functionals', *Computing* **43**, 141–157.

R. Cools and H. J. Schmid (1993), A new lower bound for the number of nodes in cubature formulae of degree $4n+1$ for some circularly symmetric integrals, in *Numerical Integration IV* (H. Brass and G. Hämmerlin, eds), Birkhäuser, Basel, pp. 57–66.

R. Cools and I. H. Sloan (1996), 'Minimal cubature formulae of trigonometric degree', *Math. Comp.* **65**, 1583–1600.

P. J. Davis (1967), 'A construction of nonnegative approximate quadratures', *Math. Comp.* **21**, 578–582.

P. J. Davis and P. Rabinowitz (1984), *Methods of Numerical Integration*, Academic, London.

P. J. Davis, P. Rabinowitz and R. Cools (199x), *Methods of Numerical Integration.* Work in progress.

E. de Doncker (1979), 'New Euler–Maclaurin expansions and their application to quadrature over the s-dimensional simplex', *Math. Comp.* **33**, 1003–1018.

M. G. Duffy (1982), 'Quadrature over a pyramid or cube of integrands with a singularity at a vertex', *SIAM J. Numer. Anal.* **19**, 1260–1262.

H. M. Edwards (1980), 'The genesis of ideal theory', *Arch. Hist. Exact Sci.* **23**, 321–378.

H. Engels (1980), *Numerical Quadrature and Cubature*, Academic, London.

C. S. Fisher (1967), 'The death of a mathematical theory: a study in the sociology of knowledge', *Arch. Hist. Exact Sci.* **3**, 136–159.

L. Flatto (1978), 'Invariants of finite reflection groups', *Enseign. Math.* **24**, 237–292.

F. N. Fritsch (1970), 'On the existence of regions with minimal third degree integration formulas', *Math. Comp.* **24**, 855–861.

K. K. Frolov (1977), 'On the connection between quadrature formulas and sublattices of the lattice of integral vectors', *Soviet Math. Dokl.* **18**, 37–41.

K. Gatermann (1988), 'The construction of symmetric cubature formulas for the square and the triangle', *Computing* **40**, 229–240.

K. Gatermann (1992), Linear representations of finite groups and the ideal theoretical construction of G-invariant cubature formulas, in *Numerical Integration – Recent Developments, Software and Applications* (T. Espelid and A. Genz, eds), Vol. 357 of *NATO ASI Series C: Math. and Phys. Sciences*, Kluwer, Dordrecht, pp. 25–35.

R. Gebauer and H. M. Möller (1988), 'On an installation of Buchberger's algorithm', *J. Symb. Computation* **6**, 275–286.

J. L. Gout and A. Guessab (1986), 'Sur les formules de quadrature numérique à nombre minimal de noeuds d'intégration', *Numer. Math.* **49**, 439–455.

W. Gröbner (1949), *Moderne Algebraische Geometrie*, Springer, Wien.

A. Grundmann and H. M. Möller (1978), 'Invariant integration formulas for the n-simplex by combinatorial methods', *SIAM J. Numer. Anal.* **15**, 282–290.

A. Guessab (1986), 'Cubature formulae which are exact on spaces P, intermediate between P_k and Q_k', *Numer. Math.* **49**, 561–576.

A. Haegemans (1982), Construction of known and new cubature formulas of degree five for three-dimensional symmetric regions, using orthogonal polynomials, in *Numerical Integration*, Birkhäuser, Basel, pp. 119–127.

A. Haegemans and R. Piessens (1976), 'Construction of cubature formulas of degree eleven for symmetric planar regions, using orthogonal polynomials', *Numer. Math.* **25**, 139–148.

A. Haegemans and R. Piessens (1977), 'Construction of cubature formulas of degree seven and nine symmetric planar regions, using orthogonal polynomials', *SIAM J. Numer. Anal.* **14**, 492–508.

D. Hilbert (1890), 'Über die Theorie der algebraischen Formen', *Math. Ann.* **36**, 473–534.

P. Hillion (1977), 'Numerical integration on a triangle', *Internat. J. Numer. Methods Engrg.* **11**, 797–815.

D. Jackson (1936), 'Formal properties of orthogonal polynomials in two variables', *Duke Math. J.* **2**, 423–434.

P. Keast and J. N. Lyness (1979), 'On the structure of fully symmetric multidimensional quadrature rules', *SIAM. J. Numer. Anal.* **16**, 11–29.

J. Kepler (1615), *Nova stereometria doliorum vinariorum, in primis Austriaci, figuræ omnium aptissimæ*, Authore Ioanne Kepplero, imp. Cæs. Matthiæ I. ejusq; fidd. Ordd. Austriæ supra Anasum Mathematico, Lincii, Anno MDCXV.

S. I. Konjaev (1977), 'Ninth-order quadrature formulas invariant with respect to the icosahedral group', *Soviet Math. Dokl.* **18**, 497–501.

N. M. Korobov (1959), 'On approximate calculation of multiple integrals', *Dokl. Akad. Nauk SSSR* **124**, 1207–1210. Russian.

V. I. Lebedev (1976), 'Quadrature on a sphere', *USSR Comput. Math. and Math. Phys.* **16**, 10–24.

V. I. Lebedev (1995), 'A quadrature formula for the sphere of 59th algebraic order of accuracy', *Dokl. Math.* **50**, 283–286.

V. I. Lebedev and A. L. Skorokhodov (1992), 'Quadrature formulas of orders 41, 47, and 53 for the sphere', *Dokl. Math.* **45**, 587–592.

T. Y. Li (1997), Numerical solution of multivariate polynomial systems by homotopy continuation methods, in *Acta Numerica*, Vol. 6, Cambridge University Press, pp. 399–436.

J. N. Lyness (1976), 'An error functional expansion for N-dimensional quadrature with an integrand function singular at a point', *Math. Comp.* **30**, 1–23.

J. N. Lyness (1992), On handling singularities in finite elements, in *Numerical Integration – Recent Developments, Software and Applications* (T. Espelid and A. Genz, eds), Vol. 357 of *NATO ASI Series C: Math. and Phys. Sciences*, Kluwer, Dordrecht, pp. 219–233.

J. N. Lyness and R. Cools (1994), A survey of numerical cubature over triangles, in *Mathematics of Computation 1943–1993: A Half-Century of Computational Mathematics* (W. Gautschi, ed.), Vol. 48 of *Proceedings of Symposia in Applied Mathematics*, AMS, Providence, RI, pp. 127–150.

J. N. Lyness and E. de Doncker (1993), 'Quadrature error expansions, II. The full corner singularity', *Numer. Math.* **64**, 355–370.

J. N. Lyness and E. de Doncker-Kapenga (1987), 'On quadrature error expansions, part I', *J. Comput. Appl. Math.* **17**, 131–149.

J. N. Lyness and D. Jespersen (1975), 'Moderate degree symmetric quadrature rules for the triangle', *J. Inst. Math. Appl.* **15**, 19–32.

J. N. Lyness and B. J. J. McHugh (1970), 'On the remainder term in the N-dimensional Euler–Maclaurin expansion', *Numer. Math.* **15**, 333–344.

J. N. Lyness and G. Monegato (1980), 'Quadrature error functional expansion for the simplex when the integrand has singularities at vertices', *Math. Comp.* **34**, 213–225.

J. N. Lyness and K. K. Puri (1973), 'The Euler–Maclaurin expansion for the simplex', *Math. Comp.* **27**, 273–293.

J. I. Maeztu and E. Sainz de la Maza (1995), 'Consistent structures of invariant quadrature rules for the n-simplex', *Math. Comp.* **64**, 1171–1192.

F. Mantel and P. Rabinowitz (1977), 'The application of integer programming to the computation of fully symmetric integration formulas in two and three dimensions', *SIAM J. Numer. Anal.* **14**, 391–425.

J. C. Maxwell (1877), 'On approximate multiple integration between limits of summation', *Proc. Cambridge Philos. Soc.* **3**, 39–47.

H. M. Möller (1973), Polynomideale und Kubaturformeln, PhD thesis, Universität Dortmund.

H. M. Möller (1976), 'Kubaturformeln mit minimaler Knotenzahl', *Numer. Math.* **25**, 185–200.

H. M. Möller (1979), Lower bounds for the number of nodes in cubature formulae, in *Numerische Integration*, Vol. 45 of *ISNM*, Birkhäuser, Basel, pp. 221–230.

H. M. Möller (1987), On the construction of cubature formulae with few nodes using Gröbner bases, in *Numerical Integration* (P. Keast and G. Fairweather, eds), Reidel, Dordrecht, pp. 177–192.

H. M. Möller and F. Mora (1986), 'New constructive methods in classical ideal theory', *J. Algebra* **100**, 138–178.

C. R. Morrow and T. N. L. Patterson (1978), 'Construction of algebraic cubature rules using polynomial ideal theory', *SIAM J. Numer. Anal.* **15**, 953–976.

I. P. Mysovskikh (1966), 'A proof of minimality of the number of nodes of a cubature formula for a hypersphere', *Zh. Vychisl. Mat. Mat. Fiz.* **6**, 621–630. Russian. Published as I. P. Mysovskih 1966.

I. P. Mysovskikh (1968), 'On the construction of cubature formulas with fewest nodes', *Soviet Math. Dokl.* **9**, 277–280.

I. P. Mysovskikh (1975), 'On Chakalov's theorem', *USSR Comput. Math. and Math. Phys.* **15**, 221–227.

I. P. Mysovskikh (1977), 'On the evaluation of integrals over the surface of a sphere', *Soviet Math. Dokl.* **18**, 925–929. Published as I. P. Mysovskih 1977.

I. P. Mysovskikh (1980), The approximation of multiple integrals by using interpolatory cubature formulae, in *Quantitative Approximation* (R. D. Vore and K. Scherer, eds), Academic, New York, pp. 217–243.

I. P. Mysovskikh (1981), *Interpolatory Cubature Formulas*, Izdat. 'Nauka', Moscow-Leningrad. Russian. See I. P. Mysovskikh 1992.

I. P. Mysovskikh (1988), 'Cubature formulas that are exact for trigonometric polynomials', *Metody Vychisl.* **15**, 7–19. Russian.

I. P. Mysovskikh (1990), On the construction of cubature formulas that are exact for trigonometric polynomials, in *Numerical Analysis and Mathematical Modelling* (A. Wakulicz, ed.), Vol. 24 of *Banach Center Publications*, PWN – Polish Scientific Publishers, Warsaw, pp. 29–38. Russian.

I. P. Mysovskikh (1992), Interpolatorische Kubaturformeln, Bericht Nr. 74, Institut für Geometrie und Praktische Mathematik der RWTH Aachen. Translated from the Russian by I. Dietrich and H. Engels. Published as J. P. Mysovskih 1992.

I. P. Mysovskikh and V. Ja Černicina (1971), 'The answer to a question of Radon', *Soviet Math. Dokl.* **12**, 852–854. Published as I. P. Mysovskih and V. Ja Černicina 1971.

H. Niederreiter (1992), *Random Number Generation and Quasi-Monte Carlo Methods*, Vol. 63 of *CBMS-NSF regional conference series in applied mathematics*, SIAM, Philadelphia.

M. V. Noskov (1988*a*), 'Cubature formulae for the approximate integration of functions of three variables', *USSR Comput. Math. and Math. Phys.* **28**, 200–202.

M. V. Noskov (1988*b*), 'Formulas for the approximate integration of periodic functions', *Metody Vychisl.* **15**, 19–22. Russian.

R. Piessens and A. Haegemans (1975), 'Cubature formulas of degree nine for symmetric planar regions', *Math. Comp.* **29**, 810–815.

P. Rabinowitz and N. Richter (1969), 'Perfectly symmetric two-dimensional integration formulas with minimal number of points', *Math. Comp.* **23**, 765–799.

J. Radon (1948), 'Zur mechanischen Kubatur', *Monatsh. Math.* **52**, 286–300.

G. G. Rasputin (1983*a*), 'On the construction of cubature formulas containing prespecified knots', *Metody Vychisl.* **13**, 122–128. Russian.

G. G. Rasputin (1983*b*), 'On the question of numerical characteristics for orthogonal polynomials of two variables', *Metody Vychisl.* **13**, 145–154. Russian.

G. G. Rasputin (1986), 'Construction of cubature formulas containing preassigned nodes', *Soviet Math. (Iz. VUZ)* **30**, 58–67.

L. F. Richardson (1927), 'The deferred approach to the limit', *Philos. Trans. Royal Soc. London* **226**, 261–299.

R. D. Richtmyer (1952), The evaluation of definite integrals, and a quasi-Monte-Carlo method based on the properties of algebraic numbers, Report LA-1342, Los Alamos Scientific Laboratory.

H. J. Schmid (1978), 'On cubature formulae with a minimal number of knots', *Numer. Math.* **31**, 281–297.

H. J. Schmid (1980*a*), 'Interpolatorische Kubaturformeln und reelle Ideale', *Math. Z.* **170**, 267–282.

H. J. Schmid (1980*b*), Interpolatory cubature formulae and real ideals, in *Quantitative Approximation* (R. D. Vore and K. Scherer, eds), Academic, New York, pp. 245–254.

H. J. Schmid (1983), *Interpolatorische Kubaturformeln*, Vol. CCXX of *Dissertationes Math.*, Polish Scientific Publishers, Warsaw.

H. J. Schmid (1995), 'Two-dimensional minimal cubature formulas and matrix equations', *SIAM J. Matrix Anal.* **16**(3), 898–921.

H. J. Schmid and Y. Xu (1994), 'On bivariate Gaussian cubature formulae', *Proc. Amer. Math. Soc.* **122**, 833–842.

I. H. Sloan and S. Joe (1994), *Lattice Methods for Multiple Integration*, Oxford University Press.

I. H. Sloan and P. J. Kachoyan (1987), 'Lattice mathods for multiple integration: theory, error analysis and examples', *SIAM J. Numer. Anal.* **24**, 116–128.

S. L. Sobolev (1962), 'The formulas of mechanical cubature on the surface of a sphere', *Sibirsk. Mat. Ž.* **3**, 769–796. Russian.

A. H. Stroud (1960), 'Quadrature methods for functions of more than one variable', *New York Acad. Sci.* **86**, 776–791.

A. H. Stroud (1971), *Approximate calculation of multiple integrals*, Prentice-Hall, Englewood Cliffs, NJ.

B. Sturmfels (1996), *Gröbner Bases and Convex Polytopes*, Vol. 8 of *University Lecture Series*, AMS, Providence, RI.

M. Taylor (1995), 'Cubature for the sphere and the discrete spherical harmonic transform', *SIAM J. Numer. Anal.* **32**(2), 667–670.

V. Tchakaloff (1957), 'Formules de cubatures mécaniques à coefficients non négatifs', *Bull. des Sciences Math., 2^e^ série* **81**, 123–134.

P. Verlinden and R. Cools (1992), 'On cubature formulae of degree $4k+1$ attaining Möller's lower bound for integrals with circular symmetry', *Numer. Math.* **61**, 395–407.

P. Verlinden and A. Haegemans (1993), 'An error expansion for cubature with an integrand with homogeneous boundary singularities', *Numer. Math.* **65**, 383–406.

S. Weiß (1991), Über Kubaturformeln vom Grad $2k-2$, Master's thesis, Universität Erlangen.

J. W. Wissman and T. Becker (1986), 'Partially symmetric cubature formulas for even degrees of exactness', *SIAM J. Numer. Anal.* **23**, 676–685.