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Cubature formulae and orthogonal polynomials

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Abstract

The connection between orthogonal polynomials and cubature formulae for the approximation of multivariate integrals has been studied for about 100 yr. The article J. Radon published about 50 yr ago (J. Radon, *Zur mechanischen Kubatur*, *Monatsh. Math.* 52 (1948) 286–300) has been very influential. In this text we describe some of the results that were obtained during the search for answers to questions raised by his article. © 2001 Elsevier Science B.V. All rights reserved.

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1. Introduction

The connection between orthogonal polynomials and algebraic integration formulae in higher dimension was already studied about 100 yr ago (early papers are, e.g., [1,6]). The problem became widely noticed after the second edition of Krylov's book "On the approximate calculation of integrals" [43], published in 1967, wherein Mysovskikh introduced Radon's construction of a formula of degree 5 published in 1948 [72].

Though no final solution – similar to the one-dimensional case – has been found up to now, the work in this field has been tremendous. In the textbooks by Krylov [43], Stroud [90], Sobolev [84], Engels [20], Mysovskikh [66], Davis and Rabinowitz [17], Xu [94] and Sobolev and Vaskevich [85], and in the survey article of Cools [10], the growth of knowledge in the field is documented. In this text we will only try to describe some relevant results – following Radon's ideas – that have been found in the meantime.

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The one-dimensional algebraic case, i.e., interpolatory quadrature formulae and their relation to orthogonal polynomials, is well known. In dimension 2 and beyond, things look worse: there are more questions than answers. Nevertheless, some progress has been made. Though several essential problems – important in applications – are still open, e.g., how minimal formulae of an arbitrary degree of exactness look like for the integral over the square with constant weight function, several results of some generality have been found. They make transparent why answers to important questions must be quite complex. We leave aside many particular results, in spite of their importance for applications. For these we refer to the surveys in [90,14,11].

2. Basic concepts and notations

We would have liked to preserve the flair of the old papers; however, we finally decided to use modern notations in order to achieve an easy and consistent way of presenting the results.

We denote by \mathbb{N} the nonnegative integers. The monomials of degree m in n variables are written in the short notation

$$\mathbf{x}^{\mathbf{m}} = x_1^{m_1} x_2^{m_2} \cdots x_n^{m_n} \quad \text{with } |\mathbf{m}| = m,$$

where $\mathbf{x} = (x_1, x_2, \dots, x_n)$, $\mathbf{m} = (m_1, m_2, \dots, m_n) \in \mathbb{N}^n$, and

$$|\mathbf{m}| = \sum_{i=1}^n m_i \text{ is the length of the multi-index } \mathbf{m}.$$

A polynomial $f(\mathbf{x}) = f(x_1, x_2, \dots, x_n)$ of (total) degree m can be represented as

$$f(\mathbf{x}) = \sum_{s=0}^m \sum_{|\mathbf{k}|=s} c_{\mathbf{k}} \mathbf{x}^{\mathbf{k}}, \quad c_{\mathbf{k}} \in \mathbb{C},$$

and the summation in

$$g_s(\mathbf{x}) = \sum_{|\mathbf{k}|=s} c_{\mathbf{k}} \mathbf{x}^{\mathbf{k}}$$

is done over all multi-indices \mathbf{k} of length s . The polynomial g_s is called a *homogeneous component* of degree s . Hence f is an element of the ring of polynomials with complex coefficients, which will be denoted by $\mathbb{C}[\mathbf{x}] = \mathbb{C}[x_1, x_2, \dots, x_n]$. The degree of a polynomial f will be denoted by $\deg(f)$.

The number of linearly independent polynomials of degree $\leq m$ is

$$M(n, m) = \binom{m+n}{n},$$

the number of pairwise distinct monomials of degree m is $M(n-1, m)$. When the linearly independent monomials are needed as an ordered sequence, we will represent them by

$$\{\varphi_j(\mathbf{x})\}_{j=1}^{\infty},$$

where $j < k$ whenever $\deg(\varphi_j(\mathbf{x})) < \deg(\varphi_k(\mathbf{x}))$. Hence

$$\{\varphi_j(\mathbf{x})\}_{j=1}^{\mu}, \quad \mu = M(n, m),$$

contains all monomials of degree $\leq m$. Most of the results in the sequel will be stated in the ring of polynomials with real coefficients, $\mathbb{R}[x_1, x_2, \dots, x_n] = \mathbb{R}[\mathbf{x}]$, which will be denoted by \mathbb{P}^n . The

polynomials in \mathbb{P}^n of degree $\leq m$ will be denoted by \mathbb{P}_m^n . The elements of \mathbb{P}_m^n form a vector space over \mathbb{R} with dimension $\dim \mathbb{P}_m^n = M(n, m)$.

We consider integrals of the type

$$\mathcal{I}^n[f] = \int_{\Omega} f(\mathbf{x})\omega(\mathbf{x}) \, d\mathbf{x}, \quad f \in \mathcal{C}(\Omega), \tag{1}$$

where $\Omega \subseteq \mathbb{R}^n$ is a region with inner points and the real weight function ω is chosen such that the moments

$$\mathcal{I}^n[\mathbf{x}^m], \quad m \in \mathbb{N}^n,$$

exist. In many applications $\omega(\mathbf{x})$ is nonnegative. Hence \mathcal{I}^n is a positive linear functional. In most of the results presented, \mathcal{I}^n will be even strictly positive, i.e.,

$$\mathcal{I}^n[f] > 0 \text{ whenever } 0 \neq f \geq 0 \text{ on } \Omega,$$

so orthogonal polynomials with respect to \mathcal{I}^n are defined.

The type of integrals we consider includes integrals over the so-called *standard regions*, for which we follow Stroud’s notation [90].

C_n : the n -dimensional cube

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

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

S_n : the n -dimensional ball

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

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

T_n : the n -dimensional simplex

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

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

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

$$\omega(\mathbf{x}) = e^{-r^2}, \quad r^2 = \sum_{i=1}^n x_i^2,$$

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

$$\omega(\mathbf{x}) = e^{-r},$$

H_2 : the region bounded by the regular hexagon with vertices

$$(\pm 1, 0), (\pm \frac{1}{2}, \pm \frac{1}{2}\sqrt{3}) \text{ and weight function } \omega(\mathbf{x}) = 1.$$

A cubature formula for (1) is of the form

$$\mathcal{I}^n[f] = \mathcal{Q}[f] + R[f], \tag{2}$$

where

$$\mathcal{Q}[f] = \sum_{j=1}^N w_j f(\mathbf{x}^{(j)}) \tag{3}$$

is called a *cubature sum*. The $\mathbf{x}^{(j)}$'s are called *nodes*, the w_j 's *weights* or *coefficients*, and $R[f]$ is the error. The shorthand notation

$$\mathcal{I}^n[f] \cong \sum_{j=1}^N w_j f(\mathbf{x}^{(j)})$$

is often used.

A nonnegative integer d is called *degree of exactness* or *degree of precision* or simply *degree* of formula (2), if $R[f] = 0$ for all polynomials f with $\deg(f) \leq d$ and if a polynomial g with $\deg(g) = d + 1$ exists such that $R[g] \neq 0$.

Let $f \in \mathbb{C}[\mathbf{x}]$ be given and $\deg(f) = m$; the algebraic manifold of degree m generated by f will be denoted by

$$\mathcal{H}_m = \{\mathbf{x} \in \mathbb{C}^n : f(\mathbf{x}) = 0\}.$$

A cubature formula (2) with $N = M(n, m)$ which is exact for all polynomials of degree $\leq m$ is called *interpolatory* if the nodes do not lie on an algebraic manifold of degree m and the coefficients are uniquely determined by the nodes.

If $n = 1$, then $N = m + 1$ and the converse is true, too. If the degree of exactness of the quadrature formula is m , then it is interpolatory. For $n \geq 2$ this does not hold in general. The number of nodes might be lower than $M(n, m)$ since some of the coefficients may vanish.

Theorem 1. *Let (2) be given such that $R[f] = 0$ for all polynomials of degree $\leq m$ and $N \leq \mu = M(n, m)$. The formula is interpolatory if and only if*

$$\text{rank}([\varphi_1(\mathbf{x}^{(j)}), \varphi_2(\mathbf{x}^{(j)}), \dots, \varphi_\mu(\mathbf{x}^{(j)})]_{j=1}^N) = N.$$

We are specifying \mathcal{Q} by $\mathcal{Q}(n, m, N)$ if we refer to a cubature sum in n dimensions with a degree of exactness m and N nodes. We only consider interpolatory cubature formulae. A noninterpolatory formula can be transformed to an interpolatory formula by deleting nodes. In particular, minimal formulae (N is minimal for fixed m) are interpolatory.

A polynomial P with $\deg(P) = m$ is called *orthogonal* with respect to the underlying \mathcal{I}^n if $\mathcal{I}^n[PQ] = 0$ for all Q , $\deg(Q) \leq m - 1$. It is called *quasi-orthogonal* if $\mathcal{I}^n[PQ] = 0$ for all Q , $\deg(Q) \leq m - 2$.

A set of polynomials in $\mathbb{R}[x_1, \dots, x_n]$ is called a *fundamental system of degree m* whenever it consists of $M(n - 1, m)$ linearly independent polynomials of the form

$$\mathbf{x}^m + Q_m, \quad m \in \mathbb{N}^n, \quad \deg(Q_m) \leq |\mathbf{m}| - 1.$$

A set \mathcal{M} of polynomials is called a *fundamental set of degree m* if a fundamental system of degree m is contained in $\text{span}\{\mathcal{M}\}$.

In the two-dimensional case we drop the superscript n and use x and y as variables, i.e., \mathbb{P}, \mathbb{P}_m , and,

$$\mathcal{I}[f] = \int_{\Omega} f(x, y)\omega(x, y) dx dy, \quad f \in \mathcal{C}(\Omega), \quad \Omega \subseteq \mathbb{R}^2.$$

Whenever possible, one tries to find cubature sums (3) such that the following constraints are satisfied:

- (i) $w_j > 0$,
- (ii) $\mathbf{x}^{(j)} \in \Omega$,
- (iii) N is minimal for fixed degree m .

If $n = 1$, Gaussian quadrature formulae satisfy all constraints. These formulae are closely connected to orthogonal polynomials. The zeros of a quasi-orthogonal polynomial of degree k , $P_k^1 + \gamma P_{k-1}^1$ with free parameter γ , are the nodes of a minimal quadrature formula of degree $2k - 2$ with all weights positive. The parameter γ can be chosen such that all nodes are inside the domain of integration, and, if $\gamma = 0$ one obtains a uniquely determined formula of degree $2k - 1$ satisfying (i), (ii), (iii). Nonminimal interpolatory quadrature formulae have been characterised by Sottas and Wanner, Peherstorfer, and many others, most recently by Xu [86,68,69,96].

3. Radon’s formulae of degree 5

The paper by Johann Radon [72], which appeared in 1948, is not the oldest studying the application of orthogonal polynomials to cubature formulae (earlier papers are, e.g., [1] to which Radon refers, and [6]). However, Radon’s contribution became fundamental for all research in that field. Although the word “cubature” appeared in the written English language already in the 17th century, this paper is probably the first that used the term “Kubaturformel” (i.e., German for “cubature formula”) for a weighted sum of function values to approximate a multiple integral (in contrast to quadrature formula to approximate one-dimensional integrals). As an introduction to the survey which follows, we will briefly sketch its main ideas.

Radon discusses the construction of cubature formulae of degree 5 with 7 nodes for integrals over T_2, C_2, S_2 . We are sure Radon knew the estimate (22) and knew that this bound will not be attained for classical (standard) regions in the case of degree 5. In order to construct a cubature formula of degree m he counted the number of monomials of degree $\leq m$ and used this divided by 3 as number of necessary nodes. He was aware that for degrees 2, 3 and 4 this will not lead to a solution and thus degree 5 is the first nontrivial case he could consider.

Assuming a formula of degree 5 with 7 nodes for an integral \mathcal{I} , a geometric consideration leads to polynomials of degree 3 vanishing at the nodes. These polynomials have to be orthogonal with respect to \mathcal{I} to all polynomials of degree 2, and exactly three such polynomials, P_1, P_2, P_3 , can vanish at the nodes. In the next step further necessary conditions are derived for the P_i . They must satisfy

$$\sum_{i=1}^3 L_i P_i = 0 \tag{4}$$

for some linear polynomials $L_i \neq 0$. This can be reduced to

$$xK_1 + yK_2 = K_3, \tag{5}$$

where K_i are orthogonal polynomials of degree 3. Assuming the orthogonal basis of degree 3 in a form

$$P_i^3 = x^{3-i}y^i + Q_i, \quad Q_i \in \mathbb{P}_2, \quad i = 0, 1, 2, 3,$$

one obtains

$$K_1 = \alpha P_1^3 + \beta P_2^3 + \gamma P_3^3 \quad \text{and} \quad K_2 = -\alpha P_0^3 - \beta P_1^3 - \gamma P_2^3.$$

The parameters α, β, γ have to be chosen such that K_3 is also an orthogonal polynomial of degree 3. Thus, by setting

$$A = \mathcal{I}[P_0^3 P_2^3 - P_1^3 P_1^3], \quad B = \mathcal{I}[P_0^3 P_3^3 - P_1^3 P_2^3], \quad C = \mathcal{I}[P_1^3 P_3^3 - P_2^3 P_2^3], \tag{6}$$

one obtains the linear system

$$\begin{bmatrix} 0 & A & B \\ -A & 0 & C \\ -B & -C & 0 \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \\ \gamma \end{bmatrix} = 0. \tag{7}$$

Two cases may occur. The parameters α, β, γ can be determined up to a common factor, if

$$A^2 + B^2 + C^2 > 0, \tag{8}$$

otherwise they can be chosen arbitrarily. Radon did not further pursue the last case. He just remarked that he did not succeed in proving that this case never occurs.

In case (8) the polynomials K_1, K_2, K_3 can be computed. If they are linearly independent, the desired equation (4) is given by $xK_1 + yK_2 = K_3$. If these polynomials vanish at 7 pairwise distinct nodes, the degree of exactness follows from the orthogonality property of the K_i 's.

If the K_i are linearly dependent, it follows that

$$K_1 = yQ \quad \text{and} \quad K_2 = -xQ$$

for some $Q \in \mathbb{P}_2$. In this case it can be shown that there is a K_3 such that all K_i vanish at 7 pairwise distinct nodes. This construction again is based on geometric considerations and finally allows the conclusion that such K_3 's can be computed.

Radon's article continues with the construction of formulae of degree 5 with 7 nodes for integrals over the standard regions with constant weight function T_2, C_2 and S_2 . The amount of computational work – in a pre-computer time – is tremendous. The article finishes with an examination of the cubature error.

Though the results are limited to a special case, Radon's approach is the basis for fundamental questions that were studied in the years following the publication of his result:

- (i) Can this constructive method be generalised to a higher degree of exactness?
- (ii) Can this constructive method be generalised to more than two dimensions?
- (iii) Are there integrals for which the second case occurs, i.e., $A = B = C = 0$?
- (iv) Is 7 a lower bound for the number of nodes of cubature formulae of degree 5 if (8) holds?
- (v) Are there lower bounds of some generality for the number of nodes?
- (vi) What intrinsic tools were applied for the solution?

Fifty years after the publication of Radon’s paper, it is still not possible to answer these questions completely. We will outline what is known in the sequel.

4. Multivariate orthogonal polynomials

We assume that \mathcal{J}^n is strictly positive. Different methods of generating an orthogonal polynomial basis were discussed by Hirsch [34]. If the moments $\mathcal{J}^n[\mathbf{x}^m]$, $\mathbf{m} \in \mathbb{N}^n$, are known, one can either orthogonalise the monomial basis by the Gram–Schmidt procedure, or compute step by step fundamental systems of orthogonal polynomials of degree m .

A third way is to find a partial differential equation with boundary conditions the polynomial solutions of which lead to orthogonal systems. This permits finding formulae for the coefficients of the polynomials and deriving recursion formulae. However, one has to find out if there is an integral for which the polynomials form an orthogonal system.

4.1. Simple properties

The strictly positive integral (1) defines a scalar product in $\mathbb{C}[\mathbf{x}]$ by

$$(\phi, \psi) = \mathcal{J}^n[\phi, \bar{\psi}] = \int_{\Omega} \phi(\mathbf{x}) \overline{\psi(\mathbf{x})} \omega(\mathbf{x}) \, d\mathbf{x}, \quad \phi, \psi \in \mathbb{C}[\mathbf{x}]. \tag{9}$$

Consider the polynomial

$$P_{k+1}(\mathbf{x}) = g_{k+1}(\mathbf{x}) + \sum_{i=1}^{\kappa} a_i \varphi_i(\mathbf{x}), \quad \kappa = M(n, k), \tag{10}$$

where $g_{k+1}(\mathbf{x})$ is a given homogeneous component of degree $k + 1$ and the a_i ’s are unknown coefficients. Assuming (10) to be orthogonal to $\varphi_j(\mathbf{x})$, $j = 1, 2, \dots, \kappa$, with respect to (9), we obtain

$$\sum_{i=1}^{\kappa} a_i (\varphi_i, \varphi_j) = -(g_{k+1}(\mathbf{x}), \varphi_j), \quad j = 1, 2, \dots, \kappa. \tag{11}$$

The matrix of this system is the Gram matrix of the linearly independent polynomials $\varphi_1(\mathbf{x})$, $\varphi_2(\mathbf{x}), \dots, \varphi_{\kappa}(\mathbf{x})$. Hence, the a_i are uniquely determined. The polynomial (10) is uniquely determined by its homogeneous component of degree $k + 1$ and by orthogonality to all polynomials of degree $\leq k$.

We state some simple properties of orthogonal polynomials, which will be of use later.

Theorem 2. *The following properties hold for an orthogonal polynomial P_{k+1} .*

- (1) *If the homogeneous component of degree $k + 1$ has real coefficients, then all coefficients are real. This follows from (11).*
- (2) *A real polynomial P_{k+1} changes sign in Ω . In particular,*

$$\{\mathbf{x} \in \Omega: P_{k+1} > 0\} \quad \text{and} \quad \{\mathbf{x} \in \Omega: P_{k+1} < 0\}$$

are of positive measure, which follows from

$$\int_{\Omega} P_{k+1}(\mathbf{x}) \omega(\mathbf{x}) \, d\mathbf{x} = 0.$$

- (3) Whenever $P_{k+1} = UV$ with polynomials U and V of degree at least 1, then U is orthogonal with respect to Ω and the weight function $\omega(\mathbf{x})|V(\mathbf{x})|^2$. This implies Properties (1) and (2) for the factors as well.
- (4) If the coefficients belonging to the highest-degree terms in the homogeneous component of a factor are real, then the remaining coefficients are real, too.
- (5) A real factor U of an orthogonal polynomial changes sign in Ω . In particular,

$$\{\mathbf{x} \in \Omega: U > 0\} \quad \text{and} \quad \{\mathbf{x} \in \Omega: U < 0\}$$

are of positive measure. From this we obtain

- (6) An orthogonal polynomial has no real multiple factors.

We normalise the orthogonal polynomials of degree k to

$$P_k = \mathbf{x}^k + Q_k, \quad \mathbf{k} \in \mathbb{N}^n, \quad |\mathbf{k}| = k, \quad \deg(Q_k) \leq k - 1.$$

This fundamental system of degree k will be gathered in a polynomial vector of dimension $M(n-1, k)$ and be written as \mathbf{P}_k . We refer to the common zeros of all P_k as zeros of \mathbf{P}_k . The known explicit expressions for these normalised orthogonal polynomials are collected in [10].

4.2. Recursion formulae

For $n=2$ the following results were found. Jackson [37] discusses a three-term recursion formula for a given orthogonal system, Gröbner [27] generates orthogonal systems by solving a variational problem under constraints; Krall and Sheffer [42] study in a class of second-order differential equations special cases the polynomial solutions of which generate classical orthogonal systems. Since their approach is closely related to recursion formulae and leads to concrete results we will outline the main ideas.

Let

$$P_j^k = x^{k-j} y^j + Q_j, \quad Q_j \in \mathbb{P}_{k-1}, \quad j = 0, 1, \dots, k, \quad k \in \mathbb{N},$$

be a basis of \mathbb{P} . We can collect these fundamental systems of degree k in vectors

$$\mathbf{P}_k = (P_0^k, P_1^k, \dots, P_k^k)^T.$$

The basis \mathbf{P}_k , $k \in \mathbb{N}$, is said to be a *weak orthogonal system* if there exist matrices

$$C_k, \bar{C}_k \in \mathbb{R}^{k+1 \times k+1} \quad \text{and} \quad D_k, \bar{D}_k \in \mathbb{R}^{k+1 \times k},$$

such that

$$\begin{aligned} x\mathbf{P}_k &= L_{k+1}\mathbf{P}_{k+1} + C_k\mathbf{P}_k + D_k\mathbf{P}_{k-1}, \\ y\mathbf{P}_k &= F_{k+1}\mathbf{P}_{k+1} + \bar{C}_k\mathbf{P}_k + \bar{D}_k\mathbf{P}_{k-1}, \end{aligned} \tag{12}$$

with shift matrices L_{k+1} and F_{k+1} defined by $[E_k \ 0]$ and $[0 \ E_k]$, where E_k is the identity in $\mathbb{R}^{k+1 \times k+1}$ and $\mathbf{P}_{-1} = 0$.

A polynomial basis is said to be orthogonal with respect to a linear functional $\mathcal{L} : \mathbb{P} \rightarrow \mathbb{R}$, if, for each $k \in \mathbb{N}$, $\mathcal{L}[\mathbf{P}_k \mathbf{P}_l^T] = 0$, $l = 0, 1, \dots, k - 1$, and if $\text{rank}(\mathcal{L}[\mathbf{P}_k \mathbf{P}_k^T]) = k + 1$. Here, $\mathbf{P}_k \mathbf{P}_l^T$ is the tensor product of the vectors \mathbf{P}_k and \mathbf{P}_l , and $\mathcal{L}[\mathbf{P}_k \mathbf{P}_l^T]$ is the matrix whose elements are determined by the functional acting on the polynomial coefficients of the tensor product. The matrix $M_k = \mathcal{L}[\mathbf{P}_k \mathbf{P}_k^T]$ is

known as the k th moment matrix. The basis $\{\mathbf{P}_k\}_{k \in \mathbb{N}}$ is said to be a (*positive*) definite orthogonal system in case the matrices M_k , $k \in \mathbb{N}$, are (positive) definite.

A definite system $\{\mathbf{P}_k\}_{k \in \mathbb{N}}$ is a weak orthogonal system, i.e., it satisfies the recurrence relations (12). Conversely, it follows from work by Xu [93] that a weak orthogonal system is an orthogonal system with respect to some \mathcal{L} if and only if

$$\text{rank}(S_k) = k + 1 \quad \text{where } S_k = [D_k \quad \bar{D}_k] \in \mathbb{R}^{k+1 \times 2k}.$$

The associated moment problem consists in assigning a measure to the functional \mathcal{L} defined by a definite system. In particular, assigning a positive measure in case the system is positive definite (Favard’s theorem) is quite complicated. We refer to Fuglede [24] and Xu [95].

Krall and Sheffer [42] studied the orthogonal polynomial systems which are generated by the following second-order differential equation:

$$\mathcal{D}\omega = -\lambda_k \omega, \quad \lambda_k \in \mathbb{R}, \quad k \in \mathbb{N}, \tag{13}$$

where

$$\begin{aligned} \mathcal{D}\omega = & (ax^2 + d_1x + e_1y + f_1) \frac{\partial^2 \omega}{\partial x^2} + (2axy + d_2x + e_2y + f_2) \frac{\partial^2 \omega}{\partial x \partial y} \\ & + (ay^2 + d_3x + e_3y + f_3) \frac{\partial^2 \omega}{\partial y^2} + (gx + h_1) \frac{\partial \omega}{\partial x} + (gy + h_2) \frac{\partial \omega}{\partial y} \end{aligned}$$

for some real constants $a \neq 0, g, d_i, e_i, f_i, h_i$, and for

$$\lambda_k = -k((k - 1)a + g), \quad g + ka \neq 0, \quad k \in \mathbb{N}.$$

They determined all weak orthogonal systems which are generated from (13) and proved that they are definite or positive definite, finding the classical orthogonal systems which had been derived in [2] and some new definite systems.

In [4] the recursion formulae for all positive-definite systems have been computed in the following way. Let $\{\mathbf{P}_k\}_{k=0,1,\dots}$ be a definite orthogonal system with respect to \mathcal{J} . Multiplying (12) by \mathbf{P}_{k-1}^T , \mathbf{P}_k^T , and \mathbf{P}_{k+1}^T , respectively, and applying \mathcal{J} , we obtain

$$\begin{aligned} C_k M_k &= \mathcal{J}[x \mathbf{P}_k \mathbf{P}_k^T], \quad D_k M_{k-1} = \mathcal{J}[x \mathbf{P}_k \mathbf{P}_{k-1}^T] = M_k L_k^T, \\ \bar{C}_k M_k &= \mathcal{J}[y \mathbf{P}_k \mathbf{P}_k^T], \quad \bar{D}_k M_{k-1} = \mathcal{J}[y \mathbf{P}_k \mathbf{P}_{k-1}^T] = M_k F_k^T. \end{aligned}$$

By means of these identities the moment matrices can be computed by induction. Indeed, let $G_k = \text{diag}\{[2, E_{k-2}]\}$ and $\bar{G}_k = \text{diag}\{[E_{k-2}, 2]\}$; then

$$2E_k = L_k^T G_k L_k + F_k^T \bar{G}_k F_k,$$

and consequently,

$$2M_k = M_k L_k^T G_k L_k + M_k F_k^T \bar{G}_k F_k = D_k M_{k-1} G_k L_k + \bar{D}_k M_{k-1} \bar{G}_k F_k.$$

If one sets $M_0 = 1$, the last equation allows us to compute M_k from M_{k-1} , $k \in \mathbb{N}$. Based on [2], Verlinden [91] has computed explicit recursion formulae for classical two-dimensional integrals, too. So we refer to [91,4], if explicit recursion formulae are needed for standard integrals.

Not all two-dimensional orthogonal systems of interest can be obtained from (13). For further systems we refer to Koornwinder [38] and the references given there.

Kowalski in [39] presented a n -dimensional recursion formula and characterised it in [40,41]; Xu [93] refined this characterisation by dropping one condition. We will briefly outline these results. For a more complete insight into this development of a general theory of orthogonal polynomials in n dimensions we refer to the excellent survey by Xu [98].

Let \mathcal{J}^n be given, and let

$$M_k = \mathcal{J}^n[\mathbf{P}_k \mathbf{P}_k^T] \in \mathbb{R}^{M(n-1,k) \times M(n-1,k)}$$

be the moment matrix for \mathcal{J}^n . Then the recursion formula can be stated as follows.

Theorem 3. For $k = 0, 1, \dots$ there are matrices

$$A_{k,i} \in \mathbb{R}^{M(n-1,k) \times M(n-1,k+1)}, \quad B_{k,i} \in \mathbb{R}^{M(n-1,k) \times M(n-1,k)},$$

and

$$C_{k,i} \in \mathbb{R}^{M(n-1,k) \times M(n-1,k-1)},$$

such that

$$x_i \mathbf{P}_k = A_{k,i} \mathbf{P}_{k+1} + B_{k,i} \mathbf{P}_k + C_{k,i} \mathbf{P}_{k-1}, \quad i = 1, 2, \dots, n, \quad k = 0, 1, \dots,$$

where $\mathbf{P}_{-1} = 0$ and for all $i = 1, 2, \dots, n$ and all k

$$A_{k,i} M_{k+1} = \mathcal{J}^n[x_i \mathbf{P}_k \mathbf{P}_{k+1}^T],$$

$$B_{k,i} M_k = \mathcal{J}^n[x_i \mathbf{P}_k \mathbf{P}_k^T],$$

$$A_{k,i} M_{k+1} = M_k C_{k+1,i}^T.$$

Furthermore, there are matrices

$$D_{k,i}, G_k \in \mathbb{R}^{M(n-1,k+1) \times M(n-1,k)}, \quad H_k \in \mathbb{R}^{M(n-1,k+1) \times M(n-1,k)}$$

such that

$$\mathbf{P}_{k+1} = \sum_{i=1}^n x_i D_{k,i} \mathbf{P}_k + G_k \mathbf{P}_k + H_k \mathbf{P}_{k-1},$$

where

$$\sum_{i=1}^n D_{k,i} A_{k,i} = E_{M(n-1,k+1) \times M(n-1,k+1)}$$

and

$$\sum_{i=1}^n D_{k,i} B_{k,i} = -G_k, \quad \sum_{i=1}^n D_{k,i} C_{k,i} = -H_k.$$

We will denote the fundamental set of orthonormal polynomials (with respect to \mathcal{J}^n) of degree k by \mathbf{p}_k . The recursion for orthonormal polynomials is given by Xu [95]. We reuse the notations $A_{k,i}$, $B_{k,i}$. In the following, these matrices will refer to the recursion for orthonormal matrices.

Theorem 4. For $k = 0, 1, \dots$ there are matrices

$$A_{k,i} \in \mathbb{R}^{M(n-1,k) \times M(n-1,k+1)}, \quad B_{k,i} \in \mathbb{R}^{M(n-1,k) \times M(n-1,k)}$$

such that

$$x_i \mathbf{p}_k = A_{k,i} \mathbf{p}_{k+1} + B_{k,i} \mathbf{p}_k + A_{k-1,i}^\top \mathbf{p}_{k-1}, \quad i = 1, 2, \dots, n, \quad k = 0, 1, \dots,$$

where $\mathbf{p}_{-1} = 0$, $A_{-1,i} = 0$ and

$$\text{rank}(A_k) = \text{rank}([A_{k,1}^\top | A_{k,2}^\top | \dots | A_{k,n}^\top]^\top) = M(n-1, k+1).$$

For $i, j = 1, 2, \dots, n$, $i \neq j$, and $k \geq 0$, the following matrix equations hold for the coefficient matrices:

- (i) $A_{k,i} A_{k+1,j} = A_{k,j} A_{k+1,i}$,
- (ii) $A_{k,i} B_{k+1,j} + B_{k,i} A_{k,j} = B_{k,j} A_{k,i} + A_{k,j} B_{k+1,i}$,
- (iii) $A_{k-1,i}^\top A_{k-1,j} + B_{k,i} B_{k,j} + A_{k,i} A_{k,j}^\top = A_{k-1,j}^\top A_{k-1,i} + B_{k,j} B_{k,i} + A_{k,j} A_{k,i}^\top$.

In order to characterise Gaussian cubature formulae, see Section 7.1.4; the use of orthonormal systems gives more insight and often is easier to apply.

4.3. Common zeros

A direct analog of the Gaussian approach for $n \geq 2$ suggests considering the common zeros of all orthogonal polynomials of degree k as nodes of a formula of degree $2k - 1$. So the behaviour of common zeros of all orthogonal polynomials of degree k is of interest.

The following theorem, due to Mysovskikh [60,66], holds for (not necessarily orthogonal or real) fundamental systems of polynomials; it turned out to be essential.

Theorem 5. Let

$$R_m = \mathbf{x}^m + Q_m, \quad \text{deg}(Q_m) \leq m - 1, \quad |\mathbf{m}| = m,$$

be a fundamental system of degree m . Then the following is true.

- (i) The polynomials R_m have at most $\dim \mathbb{P}_{m-1}^n$ common zeros.
- (ii) No polynomial of degree $m - 1$ vanishes at the common zeros of the R_m , if and only if the R_m have exactly $\dim \mathbb{P}_{m-1}^n$ common pairwise distinct zeros.

We will briefly derive the main properties of the zeros of fundamental systems of orthogonal polynomials. Orthonormalising the monomials $\{\varphi_j(\mathbf{x})\}_{j=1}^\infty$ with respect to \mathcal{J}^n , e.g., by the Gram–Schmidt procedure, we obtain

$$\{F_j(\mathbf{x})\}_{j=1}^\infty \quad \text{where } \mathcal{J}^n[F_i F_j] = \delta_{ij}.$$

The reproducing kernel in \mathbb{P}_m^n is a polynomial in $2n$ variables,

$$K_m(\mathbf{u}, \mathbf{x}) = \sum_{j=1}^\mu F_j(\mathbf{u}) F_j(\mathbf{x}), \quad \mu = M(n, m), \tag{14}$$

having the property

$$\mathcal{J}^n[K_m(\mathbf{u}, \mathbf{x}) f(\mathbf{x})] = f(\mathbf{u}) \quad \text{for all } f \in \mathbb{P}_m^n. \tag{15}$$

Lemma 6. For an $\mathbf{a} \in \mathbb{C}^n$ let l be a linear polynomial such that $l(\mathbf{a}) = 0$. Then $R = l(\mathbf{x})K_m(\mathbf{a}, \mathbf{x})$ is quasi-orthogonal. Whenever \mathbf{a} is a common zero of \mathbf{P}_{m+1} , then R is orthogonal.

Proof. If $Q \in \mathbb{P}_{m-1}^n$ we obtain by (15)

$$\mathcal{I}^n[l(\mathbf{x})K_m(\mathbf{a}, \mathbf{x})Q(\mathbf{x})] = l(\mathbf{a})Q(\mathbf{a}) = 0.$$

If \mathbf{a} is a common zero of \mathbf{P}_{m+1} , then

$$F_{M(n-1,m)+i}(\mathbf{a}) = 0, \quad i = 1, 2, \dots, M(n-1, m+1),$$

and thus $K_m(\mathbf{a}, \mathbf{x}) = K_{m+1}(\mathbf{a}, \mathbf{x})$. Hence

$$R(\mathbf{x}) = l(\mathbf{x})K_{m+1}(\mathbf{a}, \mathbf{x}) = l(\mathbf{x})K_m(\mathbf{a}, \mathbf{x})$$

is orthogonal to \mathbb{P}_m^n . Assuming $\deg(l(\mathbf{x})K_m(\mathbf{a}, \mathbf{x})) \leq m$, we obtain that R is zero, in contradiction to

$$K_m(\mathbf{a}, \bar{\mathbf{a}}) = \sum_{i=1}^{\mu} |F_i(\mathbf{a})|^2 > 0, \quad \mu = M(n, m). \quad \square$$

The following theorem was proved in [61,65].

Theorem 7. The zeros of \mathbf{P}_{m+1} are real and simple, and they belong to the interior of the convex hull of Ω . Furthermore, \mathbf{P}_{m+1} and \mathbf{P}_m have no zeros in common.

Proof. Let $\mathbf{a} \in \mathbb{C}^n$ be a common zero of \mathbf{P}_{m+1} . By Lemma 6 the polynomials

$$(x_i - a_i)K_m(\mathbf{a}, \mathbf{x}), \quad i = 1, 2, \dots, n, \tag{16}$$

are orthogonal to all polynomials of degree m . Because of property (3) in Theorem 2, the linear factor $x_i - a_i$ is real, hence $\mathbf{a} \in \mathbb{R}^n$. The Jacobian matrix of (16) in \mathbf{a} is diagonal with elements $K_m(\mathbf{a}, \mathbf{a}) > 0$. This implies that \mathbf{a} is simple. If \mathbf{a} is not an interior point of the convex hull of Ω , there is a separating hyperplane $l(\mathbf{x})$ through \mathbf{a} , e.g., $l(\mathbf{x}) \geq 0$ for all \mathbf{x} in the interior of the convex hull. Since $l(\mathbf{x})$ is a real factor of $l(\mathbf{x})K_m(\mathbf{a}, \mathbf{x})$, this is a contradiction to property (5) in Theorem 2. Finally, \mathbf{a} is no common zero of \mathbf{P}_m since by Lemma 6 the degree of (16) is $m + 1$, hence $\deg(K_m(\mathbf{a}, \mathbf{x})) = m$. \square

Using the matrices presented in Theorem 4, Xu [97] defines infinite tridiagonal block Jacobi matrices of the form

$$T_i = \begin{bmatrix} B_{0,i} & A_{0,i} & 0 & 0 & \dots & 0 \\ A_{0,i}^T & B_{1,i} & A_{1,i} & 0 & \dots & 0 \\ 0 & A_{1,i}^T & B_{1,i} & A_{2,i} & \dots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \end{bmatrix}, \quad i = 1, 2, \dots, n,$$

and truncated versions of these. He found a relation between an eigenvalue problem for these matrices and the zeros of all orthogonal polynomials of a fixed degree. These results and their relation to cubature formulae are further elaborated in [94].

5. Lower bounds

5.1. Numerical characteristics

Mysovskikh [56] proved that Radon’s formulae are minimal whenever (8) holds. In [67] an integral is constructed where the matrix in (7) is zero and a formula of degree 5 with 6 nodes can be constructed. Applying Radon’s method to formulae of degree 3, Mysovskikh [59] found that such formulae with 4 nodes exist if and only if

$$\mathcal{I}[P_0^2 P_2^2 - P_1^2 P_1^2] \neq 0; \tag{17}$$

otherwise the formula has only 3 nodes. This has been further studied by Günther [28,29]. Fritsch [23] gave an example of an integral for which $\mathcal{Q}(n, 3, n + 1)$ exists. Cernicina [9] constructed a region in \mathbb{R}^n , $3 \leq n \leq 8$, admitting minimal formulae of type $\mathcal{Q}(n, 4, (n + 1)(n + 2)/2)$; for $n = 2$ a formula $\mathcal{Q}(2, 5, 6)$ is obtained. Stroud [90] extended (6) in the following way:

$$B = [\mathcal{I}[P_i^k P_j^k - P_\nu^k P_\mu^k]]_{i+j=\nu+\mu, \mu \neq i \neq \nu, 0 \leq i, j, \mu, \nu \leq k}, \tag{18}$$

in order to obtain the lower bound in Theorem 10.

Mysovskikh [60] generalised (5) and (6) (in order to study the case which Radon did not further pursue) by defining for given k and \mathcal{I} the following matrices:

$$M_{k-1}^\star = [\mathcal{I}[P_{j+1}^k P_i^k - P_j^k P_{i+1}^k]]_{i, j=0, 1, \dots, k-1}, \tag{19}$$

– note that M_k^\star is skew-symmetric – and

$$A = \frac{1}{2}[\mathcal{I}[P_{i+1}^k P_{j-1}^k - 2P_i^k P_j^k - P_{i-1}^k P_{j+1}^k]]_{i, j=1, 2, \dots, k-1}.$$

The elements of these matrices characterise the behaviour of the orthogonal polynomials with respect to \mathcal{I} ; so they were called *numerical characteristics*.

Theorem 8. *The following are equivalent:*

- (i) *the matrix A vanishes,*
- (ii) *the matrix M_{k-1}^\star vanishes,*
- (iii) *the orthogonal basis of degree k has $k(k + 1)/2$ common pairwise distinct real zeros,*
- (iv) *a cubature formula of degree $2k - 1$ with the lowest possible number of nodes exists. Its nodes are the common zeros of the orthogonal basis of degree k.*

The proof in [66, p. 189], is based on Theorem 5 and the following considerations. The polynomials

$$Q_i = yP_i^k - xP_{i+1}^k, \quad i = 0, 1, \dots, k - 1, \tag{20}$$

are of degree k ; this is Radon’s equation (5). Hence if the common zeros of all P_i^k are the nodes of a formula of degree $2k - 1$, then the Q_i are orthogonal polynomials of degree k . This implies $M_{k-1}^\star = 0$. Evidently, $M_{k-1}^\star = 0$ implies $A = 0$. On the other hand, if $A = 0$, then M_{k-1}^\star is of Hankel type, and, since M_k^\star is skew-symmetric, this implies $M_{k-1}^\star = 0$. The existence of integrals admitting the conditions of Theorem 8 was studied by Kuzmenkov in [44–46].

The articles based on Mysovskikh’s results prefer to work with M_{k-1}^\star , and it turns out that this matrix in many ways characterises the behaviour of the associated orthogonal polynomials.

In order to generalise Theorem 8 to n dimensions, Eq. (20) has to be studied for all possible variables. By means of the recursion formulae for orthonormal systems, n -dimensional numerical characteristics can be defined. By condition (ii) in Theorem 4,

$$A_{k-1,j}x_i p_k - A_{k-1,i}x_j p_k$$

can be computed under the condition that these polynomials are orthogonal to \mathbb{P}_{k-1}^n . This leads to the matrices

$$M_{k-1}^\star(i, j) = A_{k-1,i}A_{k-1,j}^\top - A_{k-1,j}A_{k-1,i}^\top, \quad i, j = 1, 2, \dots, n, \quad i \neq j, \tag{21}$$

which are representing the numerical characteristics of orthogonal polynomials in n dimensions.

5.2. Lower bounds

To settle the question of minimal formulae, lower bounds for the number of nodes are needed. The one-dimensional result can be generalised directly to find the following result, which seems to be folklore.

Theorem 9. *If $\mathcal{Q}(n, m, N)$ is a cubature sum for an integral \mathcal{I}^n , then*

$$N \geq \dim \mathbb{P}_{\lfloor m/2 \rfloor}^n = M(n, \lfloor m/2 \rfloor). \tag{22}$$

As we have seen in Section 3, this lower bound is not sharp for $n = 2$ and $m = 5$. A simple consequence of Theorem 8 is

Theorem 10. *If $\mathcal{Q}(2, 2k - 1, N)$ is a cubature sum for an integral \mathcal{I} for which $\text{rank}(M_{k-1}^\star) > 0$, then*

$$N \geq \dim \mathbb{P}_{k-1} + 1.$$

Stroud [90] showed this under the condition that B in (18) does not vanish.

Considerable progress was made by Möller [49], who improved the lower bound for $n = 2$.

Theorem 11. *If $\mathcal{Q}(2, 2k - 1, N)$ is a cubature sum for an integral \mathcal{I} , then*

$$N \geq \dim \mathbb{P}_{k-1} + \frac{1}{2} \text{rank}(M_{k-1}^\star). \tag{23}$$

Proof. If a cubature sum $\mathcal{Q}(2, 2k - 1, N)$ is given, then no polynomial in \mathbb{P}_{k-1} vanishes at all nodes. If no polynomial of degree k vanishes at all nodes, then $N \geq \dim \mathbb{P}_k > \dim \mathbb{P}_{k-1} + \frac{1}{2} \text{rank}(M_{k-1}^\star)$, since $M_{k-1}^\star \in \mathbb{R}^{k \times k}$. So Möller assumed the existence of s orthogonal polynomials Q_i of degree k which vanish at the nodes and first searched for a bound on s . Note that Q_i, xQ_i, yQ_i belong to an ideal which does not contain any polynomial of \mathbb{P}_{k-1} . Let

$$\mathcal{W} = \text{span}\{Q_i, xQ_i, yQ_i, i = 1, 2, \dots, s\};$$

then

$$3s - \eta = \dim \mathcal{W} \leq k + 2 + s,$$

where η is the number of those xQ_i, yQ_i which can be dropped without diminishing the dimension of \mathcal{W} . These dependencies in \mathcal{W} are of the form

$$x \sum_{i=1}^k a_i P_i^k - y \sum_{i=0}^{k-1} a_{i+1} P_i^k = \sum_{i=0}^k b_i P_i^k.$$

By orthogonality this leads to

$$\sum_{i=0}^{k-1} a_{i+1} \mathcal{I}[P_j^k P_{i+1}^k - P_{j+1}^k P_i^k] = 0, \quad j = 0, 1, \dots, k-1,$$

i.e.,

$$M_{k-1}^\star(a_1, a_2, \dots, a_k)^\top = 0.$$

Thus we get $\eta \leq k - \text{rank}(M_{k-1}^\star)$, from which we finally obtain

$$s \leq k + 1 - \frac{1}{2} \text{rank}(M_{k-1}^\star). \quad \square$$

For all classes of integrals for which the rank of M_{k-1}^\star has been computed, it turned out that either the rank is zero (cf. [82]) or

$$\text{rank}(M_{k-1}^\star) = 2 \lfloor k/2 \rfloor.$$

Classes of integrals for which the second rank condition holds have been already given by Möller [49]. He showed this for product integrals and integrals enjoying central symmetry. This includes the standard regions $C_2, S_2, H_2, E_2^{r^2}$ and E_2^r . Further classes with the same rank were detected by Rasputin [73], Berens and Schmid [3]. These include the standard region T_2 .

Another important fact was observed by Möller. If (23) is attained, then the polynomials xQ_i, yQ_i form a fundamental set of degree $k + 1$.

The improved lower bound, in general, is not sharp. Based on a characterisation of cubature sums $\mathcal{Q}(2, 4k + 1, 2(k + 1)^2 - 1)$ for circularly symmetric integrals in [92], it was shown in [16] that for all $k \in \mathbb{N} \setminus \{1\}$ the integrals

$$\int_{\mathbb{R}^2} f(x, y)(x^2 + y^2)^{\alpha-1} e^{-x^2-y^2} dx dy, \quad \alpha > 0,$$

and for $\alpha, \beta > -1$ the integrals

$$\int_{S_2} f(x, y)(x^2 + y^2)^\alpha (1 - x^2 - y^2)^\beta dx dy$$

admit cubature sums $\mathcal{Q}(2, 4k + 1, N)$ where at least $N \geq 2(k + 1)^2$. Note that this includes the standard regions S_2 and $E_2^{r^2}$. This result can however not be generalised to all circularly symmetric integrals. In [92] the existence of a circularly symmetric integral admitting a cubature sum $\mathcal{Q}(2, 9, 17)$ has been proven.

The n -dimensional version of Theorem 11 was stated in [51]. An explicit form of the matrices involved was given in [97], using (21), which allows us to formulate (23) as follows.

Theorem 12. *If $\mathcal{Q}(n, 2k - 1, N)$ is a cubature sum for an integral \mathcal{I}^n , then*

$$N \geq \dim \mathbb{P}_{k-1}^n + \frac{1}{2} \max\{\text{rank}(M_{k-1}^\star(i, j)): i, j = 1, 2, \dots, n\}. \tag{24}$$

Let us denote by \mathcal{G}_{2m} the linear space of all even polynomials in \mathbb{P}_{2m}^n and by \mathcal{G}_{2m-1} the linear space of all odd polynomials in \mathbb{P}_{2m-1}^n . For integrals \mathcal{I}^n which are centrally symmetric, i.e., for which

$$\mathcal{I}^n[Q] = 0 \quad \text{if } Q \in \mathcal{G}_{2m-1}, \quad m \in \mathbb{N},$$

holds, another lower bound is known, which is not based on orthogonality.

Theorem 13. *If $\mathcal{Q}(n, 2k-1, N)$ is a cubature sum for a centrally symmetric integral \mathcal{I}^n , then*

$$N \geq 2 \dim \mathcal{G}_{k-1} - \begin{cases} 1, & \text{if } 0 \text{ is a node and } k \text{ is even,} \\ 0, & \text{else.} \end{cases}$$

This bound was given for degree 3 by Mysovskikh [55]; the general case is due to Möller [47,51] and Mysovskikh [64]. Möller proved that cubature formulae attaining the bound of Theorem 13 (having the node 0, if k is even) are centrally symmetric, too. For $n \geq 3$ and \mathcal{I}^n centrally symmetric, the bound of Theorem 13 is better than the one of Theorem 12. For $n=2$ and \mathcal{I}^n centrally symmetric, they coincide.

To conclude this section, we remark that cubature formulae with all nodes real and attaining the bounds of Theorem 9 or Theorem 13 are known to have all weights positive [58,90,47,12].

6. Methods of construction

6.1. Interpolation

Let $\Omega \subseteq \mathbb{R}^n$ be given and assume that Ω contains interior points. By virtue of the linear independence of $\{\varphi_j(\mathbf{x})\}_{j=1}^{\infty}$ we can find for each m exactly $\mu = M(n, m)$ points from Ω such that they generate a regular Vandermonde matrix. We remark that v points, $v < \mu$, are always contained in an algebraic manifold of degree m , hence μ is the minimal number of points which do not belong to such a manifold. We denote by

$$V_m = [\varphi_1(\mathbf{x}^{(j)}), \varphi_2(\mathbf{x}^{(j)}), \dots, \varphi_{\mu}(\mathbf{x}^{(j)})]_{j=1}^{\mu}, \quad \mu = M(n, m), \quad (25)$$

the Vandermonde matrix defined by $\mathbf{x}^{(j)}$, $j = 1, 2, \dots, \mu$.

Theorem 14. *The points $\mathbf{x}^{(j)}$, $j = 1, 2, \dots, \mu$, do not lie on an algebraic manifold of degree m if and only if $\det V_m \neq 0$.*

A natural way to construct a cubature formula is interpolation. Choose μ points $\mathbf{x}^{(j)} \in \mathbb{R}^n$ which do not lie on a manifold of degree m . Because of the nonsingularity of the corresponding Vandermonde matrix we can construct the interpolating polynomial of f :

$$P_m(\mathbf{x}) = \sum_{j=1}^{\mu} L_j^{(m)}(\mathbf{x}) f(\mathbf{x}^{(j)}),$$

where

$$L_j^{(m)}(\mathbf{x}^{(i)}) = \delta_{ij}, \quad i, j = 1, 2, \dots, \mu.$$

Substituting P_m for f in (1), we obtain

$$\mathcal{I}[f] = \sum_{j=1}^{\mu} w_j f(\mathbf{x}^{(j)}) + R[f], \tag{26}$$

where

$$w_j = \int_{\Omega} L_j^{(m)}(\mathbf{x}) \omega(\mathbf{x}) \, d\mathbf{x}. \tag{27}$$

A cubature formula obtained in this way is obviously interpolatory, see Theorem 1.

6.2. Reproducing kernels

The method of reproducing kernel was introduced in [58] in order to construct cubature formulae of degree $2k$ with a minimal number of nodes $N = M(n, k)$. Most often the method will produce cubature formulae with more nodes. By means of the orthonormal basis such cubature formulae may be constructed by inserting $f = F_l F_m$ in (2) and studying

$$\sum_{j=1}^N w_j F_l(\mathbf{x}^{(j)}) F_m(\mathbf{x}^{(j)}) = \delta_{lm}, \quad l, m = 1, 2, \dots, N. \tag{28}$$

Introducing the $N \times N$ matrices

$$F = [F_1(\mathbf{x}^{(j)}), F_2(\mathbf{x}^{(j)}), \dots, F_N(\mathbf{x}^{(j)})]_{j=1}^N$$

and $C = \text{diag}\{w_1, w_2, \dots, w_N\}$, we can write Eq. (28) as

$$F^T C F = E.$$

This can be written as $FF^T = C^{-1}$, i.e.,

$$\sum_{i=1}^N F_i(\mathbf{x}^{(r)}) F_i(\mathbf{x}^{(s)}) = w_r^{-1} \delta_{rs}, \quad r, s = 1, 2, \dots, N.$$

If we are using (14), this can be rewritten as

$$K_k(\mathbf{x}^{(r)}, \mathbf{x}^{(s)}) = w_r^{-1} \delta_{rs}, \quad r, s = 1, 2, \dots, N. \tag{29}$$

If we assume that (28) will lead to a cubature formula, then the nodes and coefficients can be determined by (29).

Let $\mathbf{a}^{(i)}$, $i = 1, 2, \dots, n$, be pairwise distinct nodes of such a formula. We denote by \mathcal{H}_i the algebraic manifold defined by the polynomial $K_k(\mathbf{a}^{(i)}, \mathbf{x})$. From (29) we obtain

$$K_k(\mathbf{a}^{(i)}, \mathbf{a}^{(j)}) = b_i \delta_{ij}, \quad b_i = w_i^{-1}, \quad i, j = 1, 2, \dots, n. \tag{30}$$

The remaining nodes of the formula belong to $\bigcap_{i=1}^n \mathcal{H}_i$ and can be computed by solving for the unknown variables \mathbf{x} from

$$K_k(\mathbf{a}^{(i)}, \mathbf{x}) = 0, \quad i = 1, 2, \dots, n.$$

Since the nodes of the cubature sum $\mathcal{Q}(n, 2k, M(n, k))$ are not known, we proceed in the following way. The nodes $\mathbf{a}^{(i)}$ are chosen (whenever possible) in Ω but different from any of the common zeros of the fundamental system of orthogonal polynomials of degree k . So the order of the manifold \mathcal{H}_i generated by $K_k(\mathbf{a}^{(i)}, \mathbf{x})$ is k .

If $\mathbf{a}^{(1)}$ is fixed, then $\mathbf{a}^{(2)}$ will be chosen on \mathcal{H}_1 , and, if possible in Ω . If $\mathbf{a}^{(i)}$, $i = 1, 2, \dots, t - 1$, are fixed, the next node $\mathbf{a}^{(t)}$ is chosen on $\bigcap_{i=1}^{t-1} \mathcal{H}_i$, if possible in Ω . The $\mathbf{a}^{(i)}$, $i = 1, 2, \dots, n$, constructed in this way satisfy (30). If all nodes are chosen in \mathbb{R}^n , then $b_i > 0$; in fact,

$$b_i = \sum_{j=1}^N F_j^2(\mathbf{a}^{(i)}) > 0,$$

since the $\mathbf{a}^{(i)}$ are no zeros of the fundamental system of orthogonal polynomials of degree k .

If there are no points at infinity on $\mathcal{H} = \bigcap_{i=1}^n \mathcal{H}_i$, then \mathcal{H} consists of r points $\mathbf{x}^{(j)}$. Thus we obtain

$$\int_{\Omega} f(\mathbf{x})\omega(\mathbf{x}) \, d\mathbf{x} \cong \mathcal{Q}(n, 2k, n + r) = \sum_{j=1}^n A_j f(\mathbf{a}^{(j)}) + \sum_{j=1}^r B_j f(\mathbf{x}^{(j)}). \tag{31}$$

The coefficients A_i can be computed from (31) since the formula is exact for $K_k(\mathbf{a}^{(i)}, \mathbf{x})$, i.e.,

$$\int_{\Omega} K_k(\mathbf{a}^{(i)}, \mathbf{x})\omega(\mathbf{x}) \, d\mathbf{x} = \sum_{j=1}^n A_j K_k(\mathbf{a}^{(i)}, \mathbf{a}^{(j)}) = A_i K_k(\mathbf{a}^{(i)}, \mathbf{a}^{(i)}),$$

or, by using (15) with $f \equiv 1$,

$$A_i = \frac{1}{b_i} = \frac{1}{K_k(\mathbf{a}^{(i)}, \mathbf{a}^{(i)})}.$$

If $n + r = N = M(n, k)$, the coefficients B_j can be computed in an analogous way; if $n + r > N$, the B_j are determined by the condition for (31) to be of degree $2k$.

The method of reproducing kernels can be applied to regions in \mathbb{R}^n without inner points, see [36,52]. The method was applied in [58,7,8,25] to construct cubature formulae of degree 4 for a variety of regions and in [47] to construct a cubature formula of degree 9 for the region S_2 .

Möller [47] and Gegel' [26] proved

Theorem 15. *If $\mathbf{a}^{(i)}$, $i = 1, 2, \dots, n$, satisfy (30) where $b_i \neq 0$, and if $\bigcap_{i=1}^n \mathcal{H}_i$ consists of pairwise distinct nodes $\mathbf{x}^{(j)}$, $j = 1, 2, \dots, k^n$, then*

$$\int_{\Omega} f(\mathbf{x})\omega(\mathbf{x}) \, d\mathbf{x} \cong \mathcal{Q}(m, 2k, n + k^n) = \sum_{i=1}^n \frac{1}{b_i} f(\mathbf{a}^{(i)}) + \sum_{j=1}^{k^n} w_j f(\mathbf{x}^{(j)}),$$

where $b_i = K_k(\mathbf{a}^{(i)}, \mathbf{a}^{(i)})$.

Möller modified this for centrally symmetric integrals by using the following important observation. For these integrals, the orthogonal polynomials of degree m are even (odd) polynomials, if m is even (odd). For the linear space $\tilde{\mathbb{P}}_k^n$ of all even (odd) polynomials of degree $\leq k$ if k is even (odd)

the reproducing kernel

$$\tilde{K}_k(\mathbf{u}, \mathbf{x}) = \sum_{j=t}^N F_j(\mathbf{u})F_j(\mathbf{x}), \quad t = k - 2\lfloor k/2 \rfloor + 1, \quad N = M(n, k),$$

is considered. Here \sum' denotes summation over all even (odd) polynomials F_j if j is even (odd).

Again, nodes $\mathbf{a}^{(i)}$, $i = 1, 2, \dots, n$, are chosen (whenever possible) in Ω but different from any of the common zeros of the fundamental system of orthogonal polynomials of degree k .

The manifolds corresponding to $\tilde{K}_k(\mathbf{a}^{(i)}, \mathbf{x})$ will be denoted by $\tilde{\mathcal{H}}_i$. If $\mathbf{a}^{(i)}$, $i = 1, 2, \dots, t - 1$, are already selected, the node $\mathbf{a}^{(t)}$ is chosen on $\bigcap_{i=1}^{t-1} \tilde{\mathcal{H}}_i$, if possible in Ω . These nodes satisfy

$$\tilde{K}_k(\mathbf{a}^{(i)}, \mathbf{a}^{(j)}) = b_i \delta_{ij}, \quad i, j = 1, 2, \dots, n, \tag{32}$$

where $b_i > 0$ since $\mathbf{a}^{(i)} \in \mathbb{R}^n$.

We remark that the nodes in the modified method are chosen as $\mathbf{a}^{(i)}, -\mathbf{a}^{(i)}$, $i = 1, 2, \dots, n$. By central symmetry it follows that

$$\tilde{K}_k(\mathbf{a}^{(i)}, -\mathbf{a}^{(j)}) = (-1)^k \tilde{K}_k(\mathbf{a}^{(i)}, \mathbf{a}^{(j)}),$$

hence by (32), if $b_i \neq 0$, we get $\mathbf{a}^{(i)} \neq -\mathbf{a}^{(j)}$ if $i \neq j$. So the $\mathbf{a}^{(i)}, -\mathbf{a}^{(i)}$ are pairwise distinct, if $\mathbf{a}^{(i)} \neq 0$, $i = 1, 2, \dots, n$. If k is odd, this is satisfied; if k is even, the number of pairwise distinct nodes $\mathbf{a}^{(i)}$ and $-\mathbf{a}^{(i)}$ may be $2n$ or $2n - 1$. In [47] the following is derived.

Theorem 16. *Let the integral be centrally symmetric. If the nodes $\mathbf{a}^{(i)}$, $i = 1, 2, \dots, n$, satisfy (32) where $b_i \neq 0$, and $\bigcap_{i=1}^n \tilde{H}_i$ consists of pairwise distinct points $\mathbf{x}^{(j)}$, $j = 1, 2, \dots, k^n$, then*

$$\begin{aligned} \int_{\Omega} f(\mathbf{x})\omega(\mathbf{x}) \, d\mathbf{x} &\cong \mathcal{Q}(n, 2k + 1, 2n + k^n) \\ &= \sum_{i=1}^n \frac{1}{2b_i} [f(\mathbf{a}^{(i)}) + f(-\mathbf{a}^{(i)})] + \sum_{j=1}^{k^n} w_j f(\mathbf{x}^{(j)}), \end{aligned}$$

where $b_i = \tilde{K}_k(\mathbf{a}^{(i)}, \mathbf{a}^{(i)})$.

6.3. Ideal theory

Let

$$X = \{\mathbf{x}^{(j)}, j = 1, 2, \dots, N\} \subset \mathbb{R}^n$$

be a finite set of points, and define the subspace

$$\mathcal{W} = \{P \in \mathbb{P}_m^n : P(\mathbf{x}) = 0 \text{ for all } \mathbf{x} \in X\} \subset \mathbb{P}^n.$$

Sobolev [83] proved

Theorem 17. *The points X are the nodes of $\mathcal{Q}(n, m, N)$ for \mathcal{S}^n if and only if*

$$P \in \mathcal{W} \text{ implies } \mathcal{S}^n[P] = 0.$$

An English rendering of the proof can be found in [10].

The relationship of orthogonal polynomials and cubature formulae was studied since 1967 by Mysovskikh [57,59,61–63] and Stroud [87–90]; in particular they introduced elements from algebraic geometry.

Möller [47] recognised that this connection can be represented more transparently by using ideal theory, and that this theory will help in determining common zeros of orthogonal polynomials. E.g., Theorem 5 follows easily from this theory. Let $\mathcal{Q}(n, m, N)$ be given such that

$$X = \{\mathbf{x}^{(j)}, j = 1, 2, \dots, N\} \subset \mathbb{R}^n$$

is the finite set of nodes, and define the polynomial ideal

$$\mathfrak{A} = \{P \in \mathbb{P}^n : P(\mathbf{x}) = 0 \text{ for all } \mathbf{x} \in X\} \subset \mathbb{P}^n.$$

Then we obtain for each $P \in \mathfrak{A} \cap \mathbb{P}_m^n$ the orthogonality condition $\mathcal{I}^n[PQ] = 0$, whenever $PQ \in \mathbb{P}_m^n$. Möller introduced the notion of m -orthogonality. A set of polynomials is said to be m -orthogonal if for every element P we have $\mathcal{I}^n[PQ] = 0$, when $PQ \in \mathbb{P}_m^n$. Hence, orthogonal polynomials of degree m are $(2m - 1)$ -orthogonal, while quasi-orthogonal polynomials of degree m are $(2m - 2)$ -orthogonal.

The main problem is the selection of a suitable basis. It turns out that an H -basis suits best. $\{P_1, P_2, \dots, P_s\}$ is such a basis, if every $Q \in \mathfrak{A}$ can be written as

$$Q = \sum_{i=1}^s Q_i P_i \quad \text{where } \deg(Q_i P_i) \leq \deg(Q).$$

The ideal then is written as $\mathfrak{A} = (P_1, P_2, \dots, P_s)$.

Theorem 18. *Let $Q_i, i = 1, 2, \dots, s$, be an H -basis of a zero-dimensional ideal \mathfrak{A} . Then the following are equivalent:*

- (i) *The Q_i are m -orthogonal with respect to \mathcal{I}^n .*
- (ii) *There is a $\mathcal{Q}(n, m, N)$ using the N common zeros of \mathfrak{A} as nodes if no multiple nodes appear.*

For multiple nodes, function derivatives can be used; this was proposed in [62,63]. Möller called formulae of this type *generalised cubature formulae* of algebraic degree. This was further developed in [48–50].

In this ideal-theoretic setting, condition (5) can be interpreted as syzygy. If an H -basis of \mathfrak{A} is fixed, then syzygies of higher order will occur; e.g., if $P_1, P_2 \in \mathfrak{A}$ are of degree m , then it is possible that

$$Q_1 P_1 - Q_2 P_2 \in \mathbb{P}_{m-1}^n \quad \text{for } Q_i \in \mathbb{P}^n.$$

Möller found that such syzygies will occur in an H -basis and that they impose restrictions on the polynomials which can be used constructively to compute a suitable ideal. Furthermore, the Hilbert function can be used to study the number of common zeros. For the connection to Gröbner bases we refer to [53,13].

However, Theorem 18 allows nodes to be in \mathbb{C}^n . Schmid [78] proposed to avoid this by considering real ideals.

If the common zeros of an ideal \mathfrak{A} are denoted by $\mathcal{V}(\mathfrak{A})$ and the ideal of all polynomials which vanish at a finite set $X \subset \mathbb{R}^n$ by \mathfrak{A}_X , then

$$X \subseteq \mathcal{V}(\mathfrak{A}_X).$$

An ideal \mathfrak{A} is called real if

$$X = \mathcal{V}(\mathfrak{A}_X).$$

So m -orthogonal real ideals characterise cubature formulae, and real ideals are characterised by the following theorem due to Dubois et al. (cf. [18,19,75,76]).

Theorem 19. *The following are equivalent:*

- (i) \mathfrak{A} is a real ideal,
- (ii) the common zeros of \mathfrak{A} are pairwise distinct and real,
- (iii) P vanishes on $\mathcal{V}(\mathfrak{A})$ if and only if $P \in \mathfrak{A}$,
- (iv) for all $M \in \mathbb{N}$ and all $Q_i \in \mathbb{P}^n$, $i = 1, 2, \dots, M$,

$$\sum_{i=1}^M Q_i^2 \in \mathfrak{A} \text{ implies } Q_i \in \mathfrak{A}, \quad i = 1, 2, \dots, M.$$

By combining Möller’s results and the conditions which can be derived from Theorem 19 it is possible to give a complete characterisation of cubature formulae. However, if the degree of the formula m is fixed, the conditions which have to be satisfied strongly depend on the number of nodes. Indeed, the number of nodes influences the number of polynomials in the ideal basis and their degree. The conditions derived from Theorem 19 depend on the structure of the ideal basis, and their complexity therefore increases with m .

In [79] Theorem 5 is extended by using Theorem 19 and applying it to ideals containing a fundamental set of an arbitrary degree. It was then applied to construct cubature formulae for the regions C_2, S_2, T_2 .

Theorem 20. *Let R_i , $i = 1, 2, \dots, t$, be linearly independent polynomials in \mathbb{P}_m^n containing a fundamental system of degree m . If $\mathfrak{A} = (R_1, R_2, \dots, R_t)$, then*

- (i) $\mathcal{V}(\mathfrak{A}) \leq N = \dim \mathbb{P}_m^n - t$,
- (ii) $\mathcal{V}(\mathfrak{A}) = N$ if and only if \mathfrak{A} is a real ideal.

6.3.1. Even-degree formulae

By applying the syzygies of first order to quasi-orthogonal polynomials it is possible to characterise all even-degree formulae attaining the lower bound in (22).

Theorem 21. *Let*

$$R_i = P_i^k + \sum_{j=0}^{k-1} \gamma_{ij} P_j^{k-1}, \quad i = 0, 1, \dots, k,$$

be quasi-orthogonal polynomials generating the ideal \mathfrak{A} . A cubature formula $\mathcal{Q}(2, 2k-2, \dim \mathbb{P}_{k-1})$ with all weights positive exists if and only if the parameters γ_{ij} can be chosen such that

$$yR_i - xR_{i+1} \in \text{span}\{R_j, j = 0, 1, \dots, k\}, \quad i = 0, 1, \dots, k-1, \quad (33)$$

holds. If (33) holds, then the nodes of the formula are given by $\mathcal{V}(\mathfrak{A})$, and \mathfrak{A} is real.

Morrow and Patterson [54] proved this by applying Möller's Theorem 18 and using the Hilbert function to count the common zeros, counting multiplicities.

Schmid [77] applied Theorem 19 to prove that (33) is necessary and sufficient for \mathfrak{A} to be a real ideal. From the work in [54] a classical integral is known for which all even-degree minimal formulae can be computed, see Section 7.1.

The complexity of (33) can be realised by considering the equivalent matrix equation given in [81] for integrals having central symmetry. The quadratic matrix equation

$$0 = M_{k-1}^{\star} + \Gamma_k M_k^{-1} M_k^{\star} M_k^{-1} \Gamma_k^T$$

has to be solved. Here $M_k = [\mathcal{J}[P_i^k P_j^k]]_{i,j=0,1,\dots,k}$ is the moment matrix and M_{k-1}^{\star} the matrix of the numerical characteristics. Γ_k is a $k \times k+1$ Hankel matrix, which has to be determined; from its coefficients the γ_{ij} 's can be computed.

The straightforward generalisation to the n -dimensional case has been studied in [79,74]; however, only moderate-degree formulae could be constructed for C_n , $n = 2, 3, 4, 5$.

6.3.2. Odd-degree formulae

Stroud and Mysovskikh [88,59] proved that $\mathcal{Q}(2, 2k-1, k^2)$ can be constructed if two orthogonal polynomials of degree k can be found having exactly k^2 common pairwise distinct real zeros. Franke [21] derived sufficient conditions implying the existence of $\mathcal{Q}(2, 2k-1, N)$, where $N < k^2$, for special integrals over planar regions. Further generalisations were obtained in [62,63] by admitting point evaluations of derivatives and preassigning nodes.

We recall Theorem 8 in the following form.

Theorem 22. $\mathcal{Q}(n, 2k-1, \dim \mathbb{P}_{k-1})$ exists if and only if the nodes are the zeros of \mathbf{P}_k .

For the standard regions, such formulae exist for $n = 1$ and $k = 1, 2, \dots$ or $k = 1$ and $n = 1, 2, \dots$; for $n \geq 2$, $k \geq 2$, such formulae do not exist. The existence of $M(n, k-1)$ common roots of the polynomials gathered in \mathbf{P}_k can be reduced to the solution of a nonlinear system in n unknowns; however, the number of equations is larger than n , since for $n, k \geq 2$, we have

$$M(n-1, k) \geq M(n-1, 2) = \frac{n(n+1)}{2} \geq n+1.$$

The existence of special regions for which Theorem 22 holds for moderate k have been discussed in Section 5.2. A class of integrals for which Theorem 22 holds for arbitrary k was presented in [82] for $n = 2$, and in [5] for n arbitrary.

In order to find cubature sums $\mathcal{Q}(2, 2k - 1, N)$ where N attains the improved lower bound (23), Möller derived the following necessary conditions:

Theorem 23. *If $\mathcal{Q}(2, 2k - 1, N)$ exists where $N = \dim \mathbb{P}_{k-1} + \frac{1}{2} \text{rank}(M_{k-1}^{\star})$, then there are $s = k + 1 - \frac{1}{2} \text{rank}(M_{k-1}^{\star})$ orthogonal polynomials P_i of degree k vanishing at the nodes of the formula and satisfying the following conditions.*

- (i) *Whenever orthogonal polynomials of degree k satisfy $xQ_1 - yQ_2 = Q_3$, then $Q_i \in \text{span}\{P_i, i = 1, 2, \dots, s\}$.*
- (ii) *xP_i, yP_i form a fundamental set of degree $k + 1$.*
- (iii) *There are $2k - \frac{3}{2} \text{rank} M_{k-1}^{\star}$ linearly independent vectors $a \in \mathbb{R}^{3(k+1)}$ such that*

$$x^2 \sum_{i=0}^k a_i P_i + xy \sum_{i=0}^k a_{k+1+i} P_i + y^2 \sum_{i=0}^k a_{2k+2+i} P_i = \sum_{i=1}^s L_i P_i,$$

where L_i are linear polynomials.

These conditions are almost sufficient, too.

Theorem 24. *If there are $s = k + 1 - \frac{1}{2} \text{rank}(M_{k-1}^{\star})$ orthogonal polynomials P_i of degree k satisfying the conditions (i), (ii), and (iii) in Theorem 23, then these polynomials have $N = \dim \mathbb{P}_{k-1} + \frac{1}{2} \text{rank}(M_{k-1}^{\star})$ affine common zeros. If they are pairwise distinct and real, then a cubature sum $\mathcal{Q}(2, 2k - 1, N)$ exists.*

The surprising result from this theorem was the construction of $\mathcal{Q}(2, 9, 17)$ for C_2 , the square with constant weight function. Franke [22] expected that 20 would be the lowest possible number of nodes for such a formula. Haegemans and Piessens [70,33] conjectured that 18 would be lowest possible.

Again, by applying Theorem 19 one can determine further conditions which guarantee that the polynomials P_i generate a real ideal, i.e., have pairwise distinct real zeros. To check this, choose $U_i, i = 1, 2, \dots, k + 1 - s$, such that P_i, U_i are a fundamental system of degree k . By virtue of condition (ii) of Theorem 23 there are polynomials R_{ij} and $P \in \text{span}\{P_i, i = 1, 2, \dots, s\}$ such that $U_i U_j - R_{ij} P \in \mathbb{P}_{k+1}$. If, in addition, the P_i are chosen such that

$$\mathcal{I}[U^2 - RP] > 0$$

for all $U \in \text{span}\{U_i, i = 1, 2, \dots, k + 1 - s\}$, $P \in \text{span}\{P_i, i = 1, 2, \dots, s\}$, and R such that $U^2 - RP \in \mathbb{P}_{k+1}$, then the ideal (P_1, P_2, \dots, P_s) is real.

This holds in the n -dimensional case, too, even if we admit ideals with a fundamental system of maximal degree $m + 1$ [79].

Theorem 25. *Let $R_i, i = 1, 2, \dots, t$, be an m -orthogonal fundamental set of degree $m + 1$ of linearly independent polynomials in \mathbb{P}^n , and let $\mathfrak{A} = (R_1, R_2, \dots, R_t)$ and $\mathcal{W} = \text{span}\{R_1, R_2, \dots, R_t\}$. Let $\mathcal{U}, \dim \mathcal{U} = N$, be an arbitrary, but fixed, complement of \mathcal{W} such that $\mathbb{P}_{m+1}^n = \mathcal{W} \oplus \mathcal{U}$. Then the following are equivalent:*

- (i) *A positive $\mathcal{Q}(n, m, N)$ for \mathcal{I}^n exists with nodes in $\mathcal{V}(\mathfrak{A})$.*

- (ii) \mathfrak{A} and \mathcal{U} are characterised by
- (a) $\mathfrak{A} \cap \mathcal{U} = (0)$,
 - (b) $\mathcal{I}^n[Q^2 - R^+] > 0$ for all $Q \in \mathcal{U}$, where R^+ is chosen such that $Q^2 - R^+ \in \mathbb{P}_m^n$.
- (iii) \mathfrak{A} is a real ideal with a zero-set of N pairwise distinct real points, which are the nodes of the cubature formula of degree m .

6.4. Formulae characterised by three orthogonal polynomials

The nodes of a Gauss quadrature formula are the zeros of one particular polynomial. The nodes of a Gauss product cubature formula in n dimensions are the common zeros of n polynomials in n variables. Franke [21] derived conditions for planar product regions implying the existence of cubature sums $\mathcal{Q}(2, 2k - 1, N)$ where $N < k^2$, see Section 6.3.2. This is based on the common zeros of two orthogonal polynomials.

Huelsman [35] proved that for fully symmetric regions, $\mathcal{Q}(2, 7, 10)$ cannot exist. Franke [22] proved that for these regions, and also for symmetric product regions, a cubature sum $\mathcal{Q}(2, 7, 11)$ cannot exist. He observed that from Stroud's characterisation [90] there follows that a cubature sum $\mathcal{Q}(2, 7, 12)$ is characterised by three orthogonal polynomials of degree 4, and he exploited this to construct some formulae.

In [70,71], Piessens and Haegemans observed that there are actually three orthogonal polynomials of degree k that vanish in the nodes of their cubature formulae of degree $2k - 1$ for $k = 5, 6$. Following this observation, and using earlier results of Radon and Franke, in a series of articles [30,32,33] they constructed cubature formulae for a variety of planar regions whose nodes are the common zeros of three orthogonal polynomials in two variables. They restricted their work to regions that are symmetric with respect to both coordinate axes and noticed that Radon's cubature formulae for these regions have the same symmetry.

At first sight, it may look strange that Radon, Franke, Haegemans and Piessens characterised cubature formulae in two dimensions as the common zeros of three polynomial equations in two unknowns, i.e., as an overdetermined system of nonlinear equations. We now know, see Section 5.2, that for centrally symmetric regions there are $\lfloor \frac{k}{2} \rfloor + 1$ linearly independent orthogonal polynomials of degree k that vanish in the nodes of a cubature formula of degree $2k - 1$ that attains the lower bound of Theorem 11. We thus know that formulae of degree 5 and 7 that attain this bound are fully characterised by three such polynomials. Formulae of higher degrees $2k - 1$ that attain this bound will have even more than three linearly independent orthogonal polynomials of degree k that vanish in their nodes.

Franke, Haegemans and Piessens proceeded as follows. They assumed the existence of three linearly independent orthogonal polynomials of the form

$$\phi_i = \sum_{j=0}^k a_{ij} P_j^k, \quad i = 1, 2, 3.$$

The first set of conditions on the unknowns a_{ij} is obtained by demanding that whenever a node (α_i, β_i) is a common zero of ϕ_1 , ϕ_2 , and ϕ_3 , then also $(\pm\alpha_i, \pm\beta_i)$ is. A second set of conditions is obtained by demanding that these three polynomials have sufficiently many common zeros. Obtaining these conditions requires much labour, and a computer algebra system was used to derive some of these. For higher degrees, the result contains some free parameters, and consequently a continuum

Table 1
 Number of nodes in known cubature formulae [22,30,32,33]^a

| Degree | C_2 | S_2 | $E_2^{r^2}$ | E_2^r | H_2 |
|--------|---|---|---|----------------------------------|---|
| 7 | 12(∞) | 12(∞) | 12(∞) | 12(∞) | 12(∞) |
| 9 | 19(∞) 18(2) | 19(∞) 18(1) | 19(∞) 18(1) | 19(∞) | 19(∞) 18(1) |
| 11 | 28(∞) 26(∞) 25(2) | 28(∞) 26(∞) 25(1) | 28(∞) 26(∞) 25(1) | 28(∞) 26(∞) | 28(∞) 26(∞) 25(1) |

^aIn parentheses the number of such cubature formulae is given.

of cubature formulae was obtained. In such a continuum Haegemans and Piessens searched for the formula with the lowest number of nodes, e.g., by searching for a formula with a weight equal to zero. An overview of the cubature formulae for the symmetric standard regions C_2 , S_2 , $E_2^{r^2}$, E_2^r , and H_2 obtained in this way is presented in Table 1.

This approach was also used to construct cubature formulae of degree 5 for the four standard symmetric regions in three dimensions [31]. A continuum of formulae with 21 nodes is obtained. It is mentioned that this continuum contains formulae with 17, 15, 14 and 13 nodes, the last being the lowest possible.

7. Cubature formulae of arbitrary degree

For an overview of all known minimal formulae, we refer to [10]. In this final section we present those integrals for which minimal cubature formulae for an arbitrary degree of exactness were constructed by using orthogonal polynomials. Though these examples are limited, they illustrate that all lower bounds which have been discussed will be attained for special integrals and that the construction methods based on orthogonal polynomials can be applied. Indirectly this shows that improving these bounds will require more information about the given integral to be taken into account. The symmetry of the region Ω and the weight function ω is not enough!

7.1. Minimal formulae for the square with special weight functions

Two-dimensional integrals with an infinite number of minimal cubature formulae have been presented by Morrow and Patterson [54]. They studied

$$\mathcal{I}_{1/2}[f] = \int_{-1}^1 \int_{-1}^1 f(x, y)(1 - x^2)^{1/2}(1 - y^2)^{1/2} dx dy.$$

The associated fundamental orthogonal system of degree k , U_i^k , $i = 0, 1, \dots, k$, is gathered in

$$U_k = (U_0^k, U_1^k, \dots, U_k^k)^T.$$

Similarly, they studied

$$\mathcal{J}_{-1/2}[f] = \int_{-1}^1 \int_{-1}^1 f(x, y)(1 - x^2)^{-1/2}(1 - y^2)^{-1/2} dx dy,$$

where the associated fundamental orthogonal system of degree k , T_i^k , $i = 0, 1, \dots, k$, is gathered in

$$\mathbf{T}_k = (T_0^k, T_1^k, \dots, T_k^k)^T.$$

7.1.1. Even-degree formulae for $\mathcal{J}_{1/2}$

A minimal cubature sum $\mathcal{Q}(2, 2k - 2, \dim \mathbb{P}_{k-1})$ has been derived in [54]; the nodes are the common zeros of

$$\mathbf{U}_k + 1/2F_k^T \mathbf{U}_{k-1},$$

where $F_k = [0 \ E_k]$. This is the special case $\sigma = 1$ from the following result [80,81]:

For $k \geq 6$, up to symmetries, all minimal cubature sums $\mathcal{Q}(2, 2k - 2, \dim \mathbb{P}_{k-1})$ are generated by the common zeros of

$$\mathbf{U}_k + 1/2\Gamma_k^T \mathbf{U}_{k-1},$$

where Γ_k is a Hankel matrix of the form

$$\Gamma_k = \begin{bmatrix} \gamma_0 & \sigma\gamma_0 & \sigma^2\gamma_0 & \cdots & \sigma^{k-1}\gamma_0 & 1/\sigma \\ \sigma\gamma_0 & \sigma^2\gamma_0 & \sigma^3\gamma_0 & \cdots & 1/\sigma & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ \sigma^{k-1}\gamma_0 & 1/\sigma & 0 & \cdots & 0 & 0 \end{bmatrix}, \quad \gamma_0 = \frac{1 - \sigma^2}{\sigma^{k+1}}, \quad 0 \neq \sigma \in \mathbb{R}.$$

7.1.2. Odd-degree formulae for $\mathcal{J}_{1/2}$

Up to symmetries, all minimal cubature sums $\mathcal{Q}(2, 2k - 1, \dim \mathbb{P}_{k-1} + \lfloor k/2 \rfloor)$, k odd, for $\mathcal{J}_{1/2}$ are generated by the common zeros of

$$(E_k + \Gamma_k)\mathbf{U}_k,$$

where Γ_k is an orthogonal Hankel matrix of the form

$$\Gamma_k = \begin{bmatrix} \gamma_0 & \sigma\gamma_0 & \dots & \sigma^{k-1}\gamma_0 & \sigma^k\gamma_0 - \sigma \\ \sigma\gamma_0 & \sigma^2\gamma_0 & \dots & \sigma^k\gamma_0 - \sigma & \gamma_0 \\ \vdots & \vdots & & \vdots & \vdots \\ \sigma^{k-1}\gamma_0 & \sigma^k\gamma_0 - \sigma & \dots & \sigma^{k-3}\gamma_0 & \sigma^{k-2}\gamma_0 \\ \sigma^k\gamma_0 - \sigma & \gamma_0 & \dots & \sigma^{k-2}\gamma_0 & \sigma^{k-1}\gamma_0 \end{bmatrix}, \tag{34}$$

where

$$\gamma_0 = 2/(k + 1), \quad \sigma^2 = 1, \quad \text{or } \gamma_0 = \frac{\sigma^2 - 1}{\sigma^{k+1} - 1}, \quad \sigma^2 \neq 1, \quad \sigma \in \mathbb{R}.$$

Note that there are redundancies in (34), $\text{rank}(E_k + \Gamma_k) = \lfloor k/2 \rfloor + 2$. The general form is obtained in [81], special cases having been known long before: for $\sigma = 0$, $\gamma_0 = 1$ see [78], for $\sigma = 1$ and $\sigma = -1$ see [15].

For odd-degree formulae, k even, no general formula is known. However, there are minimal cubature sums $\mathcal{Q}(2, 2k - 1, \dim \mathbb{P}_{k-1} + k/2)$, k even, for $\mathcal{S}_{1/2}$, generated by the common zeros of

$$(E_k + \Gamma_k)U_k,$$

where Γ_k is an orthogonal Hankel matrix of the form (34), where

$$\gamma_0 = 2/(k + 1), \quad \sigma = 1, \quad \text{or} \quad \gamma_0 = \frac{\sigma^2 - 1}{\sigma^{k+1} - 1}, \quad \sigma \neq 1, \quad \sigma \in \mathbb{R}.$$

The case $\sigma = -1$, $\gamma_0 = 0$ was stated in [54]. The result for $\sigma = 1$ is obtained in [15], for $\sigma \neq 1$ it is obtained in [81].

7.1.3. Odd-degree formulae for $\mathcal{S}_{-1/2}$

If k is even, a minimal formula of degree $2k - 1$ exists, the nodes being the common zeros of

$$T_i^k + T_{k-i}^k, \quad i = 0, 1, \dots, k/2,$$

this result is due to [54]. Minimal formulae of degree $2k - 1$, k odd or even, were derived in [15], the nodes are the common zeros of

$$T_i^k - T_{k-i}^k, \quad i = 0, 1, \dots, \lfloor k/2 \rfloor, \quad T_0^k + T_1^k + \dots + T_{k-1}^k + T_k^k.$$

A third formula of degree $2k - 1$ for k even is given in [15], the nodes are the common zeros of

$$T_i^k - T_{k-i}^k, \quad i = 0, 1, \dots, k/2 - 1, \quad T_0^k + T_2^k + \dots + T_{k-2}^k + T_k^k.$$

7.1.4. Gaussian formulae

Cubature formulae attaining the lower bound (22) for even and odd degree are often called formulae of *Gaussian type* or *Gaussian formulae*. They exist for a class of (nonstandard) integrals, which will be shown in this section. This result is due to [82].

Let $\omega(x)$ be a nonnegative function on $I \subseteq \mathbb{R}$ and let $\{p_s\}$ be the orthonormal polynomials with respect to ω . Koornwinder [38] introduced bivariate orthogonal polynomials as follows.

For given $s \in \mathbb{N}$ let $u = x + y$ and $v = xy$ and define

$$P_i^{s,(-1/2)}(u, v) = \begin{cases} p_s(x)p_i(y) + p_s(y)p_i(x) & \text{if } i < s, \\ \sqrt{2}p_s(x)p_s(y) & \text{if } i = s, \end{cases}$$

and

$$P_i^{s,(1/2)}(u, v) = \frac{p_{s+1}(x)p_i(y) - p_{s+1}(y)p_i(x)}{x - y}.$$

Then $P_i^{s,(\pm 1/2)}$ are polynomials of total degree s . Koornwinder showed that they form a bivariate orthogonal system with respect to the weight function

$$(u^2 - 4v)^{\pm 1/2}W(u, v).$$

Let $x_{i,s}$ be the zeros of the quasi-orthogonal polynomial $p_s + \rho p_{s-1}$ where $\rho \in \mathbb{R}$ is arbitrary but fixed. The roots are ordered by $x_{1,s} < \dots < x_{s,s}$. Let $u = x + y$ and $v = xy$, and define $W(u, v) = \omega(x)\omega(y)$.

Then we have the following Gaussian cubature formula of degree $2k - 2$:

$$\iint_{\Omega} f(u, v)W(u, v)(u^2 - 4v)^{-1/2} du dv \cong \sum_{i=1}^k \sum_{j=1}^i \omega_{i,j} f(x_{i,k} + x_{j,k}, x_{i,k}x_{j,k}),$$

and

$$\iint_{\Omega} f(u, v)W(u, v)(u^2 - 4v)^{1/2} du dv \cong \sum_{i=1}^{k+1} \sum_{j=1}^{i-1} \omega_{i,j} f(x_{i,k+1} + x_{j,k+1}, x_{i,k+1}x_{j,k+1}),$$

where

$$\Omega = \{(u, v): (x, y) \in I \times I \text{ and } x < y\}.$$

If $\rho = 0$, then a uniquely determined formula of degree $2k - 1$ will be obtained.

So there are classes of two-dimensional integrals for which the one-dimensional result of Gaussian quadrature formulae can be regained. The lower bound (22) will be attained for odd and even degree, the common zeros of

$$\mathbf{P}_k + \rho \Gamma_k \mathbf{P}_{k-1}, \quad \Gamma_k \in \mathbb{R}^{k+1 \times k}, \quad \rho \in \mathbb{R},$$

are the nodes of the formula, where Γ_k is determined from commuting properties in the orthonormal recursion formula in Theorem 4 and a matrix equation which follows from (33) in Theorem 21.

These examples have been extended to the n -dimensional case in [5].

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