Applied Numerical Mathematics 61 (2011) 929–945

Contents lists available at ScienceDirect

Applied Numerical Mathematics

www.elsevier.com/locate/apnum

Symbolic–numeric Gaussian cubature rules

Annie Cuyt[a,*], Brahim Benouahmane[b], Hamsapriye[a], Irem Yaman[a]

[a] Departement Wis-Inf, Universiteit Antwerpen, Middelheimlaan 1, B-2020 Antwerpen-Wilrijk, Belgium

[b] Faculté des Sciences et Techniques, Université Hassan II, BP 146 Yasmina, 20650 Mohammadia, Morocco

ARTICLE INFO

Article history:
Received 22 June 2010
Received in revised form 11 March 2011
Accepted 14 March 2011
Available online 2 April 2011

Keywords:
Multidimensional integration
Gaussian cubature
Symbolic–numeric
Orthogonal polynomials

ABSTRACT

It is well known that Gaussian cubature rules are related to multivariate orthogonal polynomials. The cubature rules found in the literature use common zeroes of some linearly independent set of products of basically univariate polynomials. We show how a new family of multivariate orthogonal polynomials, so-called spherical orthogonal polynomials, leads to symbolic–numeric Gaussian cubature rules in a very natural way. They can be used for the integration of multivariate functions that in addition may depend on a vector of parameters and they are exact for multivariate parameterized polynomials. Purely numeric Gaussian cubature rules for the exact integration of multivariate polynomials can also be obtained.

We illustrate their use for the symbolic–numeric solution of the partial differential equations satisfied by the Appell function F_2, which arises frequently in various physical and chemical applications. The advantage of a symbolic–numeric formula over a purely numeric one is that one obtains a continuous extension, in terms of the parameters, of the numeric solution. The number of symbolic–numeric nodes in our Gaussian cubature rules is minimal, namely m for the exact integration of a polynomial of homogeneous degree $2m-1$.

In Section 1 we describe how the symbolic–numeric rules are constructed, in any dimension and for any order. In Sections 2, 3 and 4 we explicit them on different domains and for different weight functions. An illustration of the new formulas is given in Section 5 and we show in Section 6 how numeric cubature rules can be derived for the exact integration of multivariate polynomials. From Section 7 it is clear that there is a connection between our symbolic–numeric cubature rules and numeric cubature formulae with a minimal (or small) number of nodes.

1. Introduction

1.1. Classical orthogonal polynomials and Gaussian quadrature

Let $\mathbb{R}[z]$ denote the linear space of polynomials in the variable z with real coefficients and let the linear functional γ associate with z^i the moment c_i on the standard interval $[-1,1]$ for the weight function $w(z)$:

$$\gamma\left(z^i\right) = c_i = \int_{-1}^{1} w(z) z^i \, dz, \qquad \int_{-1}^{1} w(z)\, dz > 0.$$

* Corresponding author.
E-mail address: annie.cuyt@ua.ac.be (A. Cuyt).

0168-9274/$30.00 © 2011 IMACS. Published by Elsevier B.V. All rights reserved.
doi:10.1016/j.apnum.2011.03.003

In general, for an integrable function $f(z)$,

$$\gamma\big(f(z)\big) = \int_{-1}^{1} w(z) f(z)\,dz.$$

A sequence of orthogonal polynomials $V_m(z)$, $m \geqslant 0$, can be defined by requiring that the polynomial

$$V_m(z) = \sum_{i=0}^{m} b_{m-i} z^i, \quad \deg V_m = m,$$

satisfies the conditions

$$\gamma\big(z^i V_m(z)\big) = 0, \quad i = 0, \ldots, m-1. \tag{1}$$

If we introduce the inner product

$$\big\langle f(z), g(z)\big\rangle = \int_{-1}^{1} w(z) f(z) g(z)\,dz$$

then condition (1) amounts to the orthogonality requirements

$$\big\langle z^i, V_m(z)\big\rangle = 0, \quad i = 0, \ldots, m-1.$$

Up to a normalization, the orthogonal polynomial $V_m(z)$ can be computed from the linear system

$$\sum_{j=0}^{m} c_{i+j} b_{m-j} = 0, \quad i = 0, \ldots, m-1, \tag{2}$$

which is directly obtained from (1). Condition (2) allows us to write down explicit determinant formulas for the orthogonal polynomials $V_m(z)$ in terms of the Hankel determinants

$$H_m = \begin{vmatrix} c_0 & \cdots & c_{m-1} \\ \vdots & & \\ & & \vdots \\ c_{m-1} & \cdots & c_{2m-2} \end{vmatrix}, \quad m \geqslant 1, \qquad H_0 = 1.$$

Namely, when requiring $V_m(z)$ to be monic, we can write

$$V_m(z) = \frac{1}{H_m} \begin{vmatrix} c_0 & \cdots & c_{m-1} & c_m \\ \vdots & & & \vdots \\ c_{m-1} & & \cdots & c_{2m-1} \\ 1 & z & \cdots & z^m \end{vmatrix}, \qquad V_0(z) = 1.$$

It is well known that, if γ is positive definite, the zeroes of the orthogonal polynomials $V_m(z)$ can be used as nodes in so-called Gaussian quadrature rules. If we denote the zeroes of $V_m(z)$ by $\phi_i^{(m)}$, $i = 1, \ldots, m$, and

$$A_i^{(m)} := \gamma\left(\frac{V_m(z)}{(z - \phi_i^{(m)}) V_m'(\phi_i^{(m)})}\right),$$

then for every polynomial $p(z)$ of degree $2m-1$ we find

$$\gamma\big(p(z)\big) = \int_{-1}^{1} w(z) p(z)\,dz = \sum_{i=1}^{m} A_i^{(m)} p\big(\phi_i^{(m)}\big).$$

For more information we refer the reader, among many works on orthogonal polynomials, to [5,4].

1.2. Spherical orthogonal polynomials

The orthogonal polynomials under discussion were first introduced in [2] in a different form and later in [3] in the current form. Originally they were not termed spherical orthogonal polynomials because of a lack of insight into the mechanism behind the definition. In Section 3.6 we point out the difference with other definitions of multivariate orthogonal polynomials.

In dealing with multivariate polynomials and functions we often prefer to switch from the Cartesian to the spherical coordinate system. The Cartesian coordinates $X = (x_1, \ldots, x_n) \in \mathbb{R}^n$ are then replaced by $X = (x_1, \ldots, x_n) = (\lambda_1 z, \ldots, \lambda_n z)$ with $\lambda_k, z \in \mathbb{R}$ where the directional vector $\lambda = (\lambda_1, \ldots, \lambda_n)$ belongs for instance (but not necessarily) to the unit sphere $S_n = \{\lambda\colon \|\lambda\|_p = 1\}$. Here $\|\cdot\|_p$ denotes one of the usual ℓ_p-norms. A normalization such as $\|\lambda\|_p = 1$ only serves the purpose of avoiding redundant representations. While λ contains the directional information of X, the variable z contains the (signed) distance information. With the multi-index $\kappa = (\kappa_1, \ldots, \kappa_n) \in \mathbb{N}^n$ the notations X^κ, $\kappa!$ and $|\kappa|$ respectively denote

$$X^\kappa = x_1^{\kappa_1} \ldots x_n^{\kappa_n},$$
$$\kappa! = \kappa_1! \ldots \kappa_n!,$$
$$|\kappa| = \kappa_1 + \cdots + \kappa_n.$$

Two directional vectors can generate X, and hence z can be positive as well as negative. For given X, we choose the directional vector λ such that $z = \mathrm{sd}(X)$ where the signed distance function $\mathrm{sd}(X)$ is defined by

$$\mathrm{sd}(X) = \mathrm{sgn}(x_k)\|X\|_p, \quad k = \min\{j\colon x_j \neq 0\}.$$

For the sequel of the discussion we need some more notation. We denote by $\mathbb{R}[\lambda] = \mathbb{R}[\lambda_1, \ldots, \lambda_n]$ the linear space of n-variate polynomials in λ_k with real coefficients, by $\mathbb{R}(\lambda) = \mathbb{R}(\lambda_1, \ldots, \lambda_n)$ the commutative field of rational functions in λ_k with real coefficients, by $\mathbb{R}[\lambda][z]$ the linear space of polynomials in the variable z with coefficients from $\mathbb{R}[\lambda]$ and by $\mathbb{R}(\lambda)[z]$ the linear space of polynomials in the variable z with coefficients from $\mathbb{R}(\lambda)$.

Let us introduce the linear functional Γ acting on the variable z, as

$$\Gamma\big(z^i\big) = c_i(\lambda)$$

where $c_i(\lambda)$ is a homogeneous expression of degree i in the parameters λ_k:

$$c_i(\lambda) = \sum_{|\kappa|=i} c_\kappa \lambda^\kappa. \tag{3}$$

For our purpose

$$c_\kappa = \frac{|\kappa|!}{\kappa!} \int \cdots \int_{\|X\|_p \leqslant 1} w\big(\|X\|_p\big) X^\kappa \, dX \tag{4}$$

where $dX = dx_1 \ldots dx_n$. Hence

$$\Gamma\big(z^i\big) = c_i(\lambda) = \int \cdots \int_{\|X\|_p \leqslant 1} w\big(\|X\|_p\big) \left(\sum_{k=1}^n x_k \lambda_k\right)^i dX$$

and $\Gamma(z^i)$ can rightfully be called a parameterized multidimensional moment. The n-variate polynomials under investigation are of the form

$$V_m(X) = \mathcal{V}_m(\lambda; z) = \sum_{i=0}^m b_{m^2-i}(\lambda) z^i, \tag{5a}$$

$$b_{m^2-i}(\lambda) = \sum_{|\kappa|=m^2-i} b_\kappa \lambda^\kappa. \tag{5b}$$

The function $V_m(X)$ is a polynomial of degree m in z with polynomial coefficients from $\mathbb{R}[\lambda]$. The coefficients $b_{m(m-1)}(\lambda), \ldots, b_{m^2}(\lambda)$ are homogeneous polynomials in the parameters λ_k. The function $V_m(X)$ does itself not belong to $\mathbb{R}[X]$ but since $V_m(X) = \mathcal{V}_m(\lambda; z)$, it belongs to $\mathbb{R}[\lambda][z]$. Therefore the function $V_m(X)$ is given the name spherical polynomial: with every $\lambda \in S_n$ a parameterized polynomial $V_m(X) = \mathcal{V}_m(\lambda; z)$ is associated which is a polynomial of degree m in the variable $z = \mathrm{sd}(X)$.

Imposing the orthogonality conditions

$$\Gamma\big(z^i \mathcal{V}_m(\lambda; z)\big) = 0, \quad i = 0, \ldots, m-1, \tag{6}$$

implies that $\mathcal{V}_m(\lambda; z)$ satisfies for $i = 0, \ldots, m-1$,

$$\begin{aligned}\Gamma\big(z^i \mathcal{V}_m(\lambda; z)\big) &= \sum_{j=0}^{m} b_{m^2-j}(\lambda)\Gamma\big(z^{i+j}\big)\\ &= \int \cdots \int_{\|X\|_p \leqslant 1} \sum_{j=0}^{m} b_{m^2-j}(\lambda) w\big(\|X\|_p\big)\left(\sum_{k=1}^{n} x_k\lambda_k\right)^{i+j} dX\\ &= \int \cdots \int_{\|X\|_p \leqslant 1} w\big(\|X\|_p\big)\left(\sum_{k=1}^{n} x_k\lambda_k\right)^{i} \mathcal{V}_m\left(\lambda; \sum_{k=1}^{n} x_k\lambda_k\right) dX = 0.\end{aligned}$$

With (6) we can also associate the inner product

$$\big\langle z^i, \mathcal{V}_m(\lambda; z)\big\rangle = \int \cdots \int_{\|X\|_p \leqslant 1} w\big(\|X\|_p\big)\left(\sum_{k=1}^{n} x_k\lambda_k\right)^{i} \mathcal{V}_m\left(\lambda; \sum_{k=1}^{n} x_k\lambda_k\right) dX.$$

Hence (6) is equivalent to

$$\big\langle z^i, \mathcal{V}_m(\lambda; z)\big\rangle = 0, \quad i = 0, \ldots, m-1. \tag{7}$$

Essentially, the orthogonality conditions (7) represent a parameterized orthogonality, expressed in the spherical variable z that lives on each straight line spanned by λ, but with multidimensional moments (4).

In addition, the orthogonality conditions translate to the parameterized linear system

$$\sum_{j=0}^{m} c_{i+j}(\lambda) b_{m^2-j}(\lambda) = 0, \quad i = 0, \ldots, m-1.$$

As in the univariate case the orthogonality conditions (6) only determine $\mathcal{V}_m(\lambda; z)$ up to a kind of normalization: $m+1$ polynomial coefficients $b_{m^2-i}(\lambda)$ must be determined from the m parameterized conditions (6). How this is done, is shown now. For more information on this issue we refer to [3,6].

With the $c_i(\lambda)$ we define the polynomial Hankel determinants

$$H_m(\lambda) = \begin{vmatrix} c_0(\lambda) & \cdots & c_{m-1}(\lambda)\\ \vdots & & \\ & & \vdots\\ c_{m-1}(\lambda) & \cdots & c_{2m-2}(\lambda)\end{vmatrix}, \qquad H_0(\lambda) = 1.$$

We call the functional Γ definite if

$$H_m(\lambda) \not\equiv 0, \quad m \geqslant 0.$$

In what follows we assume that $\mathcal{V}_m(\lambda; z)$ satisfies (6) and that Γ is a definite functional. Also we assume that $\mathcal{V}_m(\lambda; z)$, as given by (5a)–(5b) is primitive, meaning that its polynomial coefficients $b_{m^2-i}(\lambda)$ are relatively prime. This last condition can always be satisfied, because for a definite functional Γ a solution of (6) is given by [3]

$$\mathcal{V}_m(\lambda; z) = \frac{1}{p_m(\lambda)}\begin{vmatrix} c_0(\lambda) & \cdots & c_{m-1}(\lambda) & c_m(\lambda)\\ \vdots & & & \vdots\\ c_{m-1}(\lambda) & & \cdots & c_{2m-1}(\lambda)\\ 1 & z & \cdots & z^m\end{vmatrix}, \qquad \mathcal{V}_0(\lambda; z) = 1, \tag{8}$$

where the polynomial $p_m(\lambda)$ is a polynomial greatest common divisor of the polynomial coefficients of the powers of z in this determinant expression. In the sequel we use both the notation $V_m(X)$ and $\mathcal{V}_m(\lambda; z)$ interchangeably to refer to (5a)–(5b).

1.3. Symbolic–numeric cubature rules

Let us now fix $\lambda = \lambda^*$ and take a look at the projected spherical polynomials

$$\mathcal{V}_m\big(\lambda^*; z\big) = V_m\big(\lambda_1^* z, \ldots, \lambda_n^* z\big) \tag{9}$$

on the slice $X = z\lambda^*$. From the definition of $V_m(X)$ it is clear that for each λ^* the functions $\mathcal{V}_m(\lambda^*; z)$ are polynomials of degree m in z. Are these projected polynomials themselves orthogonal? If so, what is their relationship to the classical univariate orthogonal polynomials? The answer to these questions is given in Theorem 1 and further elaborated in the next sections.

Let us introduce the (univariate) linear functional c^* acting on the variable z, by

$$c^*(z^i) = c_i(\lambda^*) = \Gamma(z^i)\big|_{\lambda=\lambda^*}. \tag{10}$$

In what follows we use the notation $V_m(z)$ to denote the univariate polynomials of degree m orthogonal with respect to the linear functional c^*. The reader should not confuse these polynomials with the $\mathcal{V}_m(\lambda; z)$ or the $V_m(X)$. Note that the $V_m(z)$ are computed from orthogonality conditions with respect to c^*, which is a particular projection of Γ, while the $\mathcal{V}_m(\lambda^*; z)$ introduced in (9) are a particular instance of the spherical polynomials orthogonal with respect to Γ.

Theorem 1. *Let the monic univariate polynomials $V_m(z)$ satisfy the orthogonality conditions*

$$c^*(z^i V_m(z)) = 0, \quad i = 0, \dots, m-1,$$

with c^* given by (10)*, and let the multivariate functions $V_m(X) = \mathcal{V}_m(\lambda; z)$ satisfy the orthogonality conditions* (6)*. Then*

$$\begin{aligned} H_m(\lambda^*)V_m(z) &= p_m(\lambda^*)\mathcal{V}_m(\lambda^*; z) \\ &= p_m(\lambda^*)V_m(X^*), \quad X^* = (\lambda_1^* z, \dots, \lambda_n^* z). \end{aligned}$$

Proof. The proof consists of an easy verification. From (8) we know that

$$\mathcal{V}_m(\lambda^*; z) = \frac{1}{p_m(\lambda^*)} \begin{vmatrix} c_0(\lambda^*) & \cdots & c_{m-1}(\lambda^*) & c_m(\lambda^*) \\ \vdots & & & \vdots \\ c_{m-1}(\lambda^*) & & \cdots & c_{2m-1}(\lambda^*) \\ 1 & z & \cdots & z^m \end{vmatrix}$$

while $V_m(z)$ computed using the functional defined in (10) is given by

$$\frac{1}{H_m(\lambda^*)} \begin{vmatrix} c_0(\lambda^*) & \cdots & c_{m-1}(\lambda^*) & c_m(\lambda^*) \\ \vdots & & & \vdots \\ c_{m-1}(\lambda^*) & & \cdots & c_{2m-1}(\lambda^*) \\ 1 & z & \cdots & z^m \end{vmatrix}$$

as outlined in Section 1. Hence

$$H_m(\lambda^*)V_m(z) = p_m(\lambda^*)\mathcal{V}_m(\lambda^*; z). \qquad \square$$

In words, Theorem 1 says that the $V_m(z)$ and $\mathcal{V}_m(\lambda^*; z)$ coincide up to a normalizing factor $p_m(\lambda^*)/H_m(\lambda^*)$. Or reformulated in yet another way, it says that the orthogonality conditions and the projection operator commute.

With respect to the projection property it is important to point out that $c^*(z^i)$ does not coincide with the one-dimensional version of c_κ given by (4), meaning (4) for $n = 1$ and $\kappa = i$. While in the one-dimensional situation, the linear functional

$$c(z^i) = c_i = \int_{-1}^{1} w(|x|)x^i \, dx \tag{11}$$

gives rise to the classical orthogonal polynomials, we do not immediately retrieve these classical polynomials from the projection, because the projected functional c^* given by (10) does not coincide with the functional c given by (11). More on this can also be found in Section 3.6.

If the functional Γ is positive definite, meaning that

$$\forall \lambda \in \mathbb{R}^2 \setminus \{(0,0)\}: \quad H_m(\lambda) > 0, \quad m \geqslant 0,$$

then the zeroes $z_i^{(m)}$ can be viewed as a holomorphic function of λ, namely $z_i^{(m)} = \phi_i^{(m)}(\lambda)$. Let us denote

$$A_i^{(m)}(\lambda) = \Gamma\left(\frac{\mathcal{V}_m(\lambda; \phi_i^{(m)}(\lambda))}{(z - \phi_i^{(m)}(\lambda))\mathcal{V}_m'(\lambda; \phi_i^{(m)}(\lambda))}\right). \tag{12}$$

Then the following cubature formula can rightfully be called a Gaussian cubature formula. The proof can be found in [1].

Theorem 2. *Let $\mathcal{P}(\lambda; z)$ be a polynomial of degree $2m-1$ belonging to $\mathbb{R}(\lambda)[z]$, the set of polynomials in the variable z with coefficients from the space of multivariate rational functions in the real λ_k with real coefficients. Let the functional Γ be positive definite. Then*

$$\int\limits_{\|X\|_p \leqslant 1} w\big(\|X\|_p\big)\mathcal{P}\big(\lambda; \lambda^T X\big)\,dX = \sum_{i=1}^{m} A_i^{(m)}(\lambda)\mathcal{P}\big(\lambda; \phi_i^{(m)}(\lambda)\big), \quad \lambda^T X = \sum_{k=1}^{n} \lambda_k x_k.$$

The combination of both symbolic and numeric features in this Gaussian cubature formula is not easy to grasp because of the conceptual differences between analytical and numerical methods. We illustrate in Section 5 how this symbolic–numeric cubature rule can be used. The principle is the same as with classical numeric Gaussian quadrature, the difference being here that the integration is multidimensional and that we integrate an entire parameterized family of functions in one sweep.

While Theorem 2 immediately allows the exact multidimensional numerical integration of a family of multivariate parameterized polynomials of degree $2m-1$ in the variable $\lambda^T X$, we show in Section 6 that the result can easily be extended to the exact integration of any multivariate polynomial of homogeneous degree $2m-1$. So Theorem 2 has a larger impact than at first sight. Next we point out in Section 7 that there is a connection with purely numeric (not symbolic!) Gaussian cubature rules with minimal nodes. This observation forms the basis of our future search for numeric cubature rules for different degrees and in all dimensions.

The difference between our spherical orthogonal polynomials and the multivariate orthogonal polynomials in, for instance, [7], although the weight functions are related, is that the latter are polynomial functions in the x_i while the former are parameterized polynomials in z, meaning that $\mathcal{V}_m(\lambda; z)$ is a univariate polynomial on each straight line $X = \lambda z$. But the functions $\mathcal{V}_m(\lambda; z)$ are not polynomial in the x_i.

In the next sections we present different families of spherical orthogonal polynomials, on different domains and for different weight functions.

2. Integration over the hypercube

2.1. Spherical Legendre polynomials (ℓ_∞)

When the weight function is $w(\|X\|_\infty) = 1$, then the spherical orthogonal polynomials can be called spherical Legendre polynomials and we denote them by $\mathcal{L}_m(\lambda; z)$. We now give explicit formulas for the moments c_κ, the first few polynomials $\mathcal{L}_m(\lambda; z)$ and the nodes $\zeta_i^{(m)}(\lambda)$ and weights $A_i^{(m)}(\lambda)$ stemming from the use of these polynomials. With the norm $\|X\|_\infty$ the domain is the hypercube $[-1, 1]^n$ and we have

$$\begin{aligned}
c_0(\lambda) &= 2^n,\\
c_i(\lambda) &= \int \cdots \int\limits_{\|X\|_\infty \leqslant 1} \left(\sum_{k=1}^{n} x_k \lambda_k\right)^i dX\\
&= \sum_{j_2=0}^{i} \sum_{j_3=0}^{j_2} \cdots \sum_{j_n=0}^{j_{n-1}} i!\, \frac{1+(-1)^{i-j_2}}{(i-j_2+1)!}\, \frac{1+(-1)^{j_2-j_3}}{(j_2-j_3+1)!} \cdots \frac{1+(-1)^{j_n}}{(j_n+1)!} \lambda_1^{i-j_2} \lambda_2^{j_2-j_3} \ldots \lambda_n^{j_n}.
\end{aligned}$$

The spherical Legendre polynomials on the hypercube (we omit appending the norm to the notation because it should be clear from the context when using the polynomials) are given by

$$\begin{aligned}
&\mathcal{L}_0(z) = 1, \qquad \mathcal{L}_1(z) = z,\\
&\mathcal{L}_2(z) = z^2 - \frac{1}{3}\sum_{i=1}^{n} \lambda_i^2,\\
&\mathcal{L}_3(z) = \left(5\sum_{i=1}^{n} \lambda_i^2\right) z^3 - \left(3\sum_{i=1}^{n} \lambda_i^4 + 10\sum_{i=1}^{n} \sum_{j>i} \lambda_i^2 \lambda_j^2\right) z.
\end{aligned}$$

2.2. Legendre nodes and weights (ℓ_∞)

The zero curves $\zeta_i^{(m)}(\lambda)$ of the polynomials $\mathcal{L}_m(z)$ occur in symmetric pairs. For $n = 2$ each pair coincides with one of the level curves shown in Fig. 1. For m odd $z = 0$ is always a zero. In Theorem 2 the spherical orthogonal polynomials are used with $z = \lambda^T X$. The zeroes of $\mathcal{L}_m(\lambda^T X)$ with $\|\lambda\|_\infty = 1$ and $n = 2$ fill up a region similar to the one shown in Fig. 2.

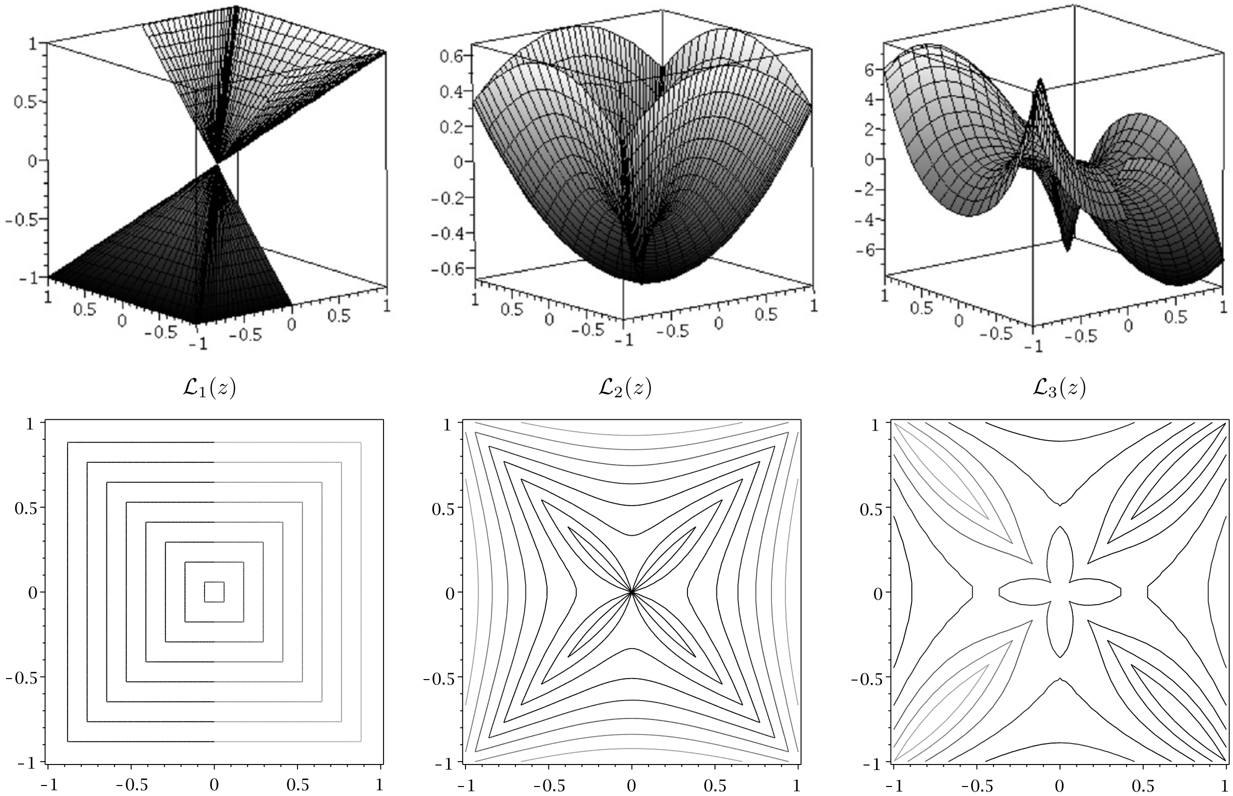

Fig. 1. Surface plots and contour lines.

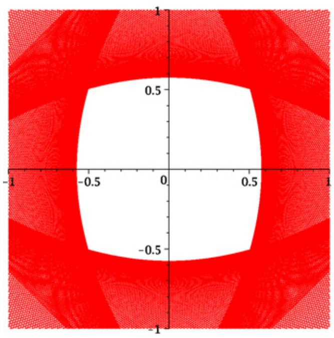

Fig. 2. Zeroes of $\mathcal{L}_2(\lambda^T X)$ with $\|\lambda\|_\infty = 1$.

We list the first few nodes and weights for integration over the hypercube:

$$\zeta_m^{(2m-1)}(\lambda) = 0, \quad m = 1, 2, \ldots,$$

$$\zeta_{1,2}^{(2)}(\lambda) = \mp\sqrt{\frac{\sum_{i=1}^n \lambda_i^2}{3}},$$

$$\zeta_{1,3}^{(3)}(\lambda) = \mp\sqrt{\frac{3\sum_{i=1}^n \lambda_i^4 + 10\sum_{i=1}^n \sum_{j>i} \lambda_i^2 \lambda_j^2}{5\sum_{i=1}^n \lambda_i^2}},$$

$$A_1^{(1)}(\lambda) = 2^n, \qquad A_{1,2}^{(2)}(\lambda) = 2^{n-1},$$

$$A_2^{(3)}(\lambda) = 2^n\left(1 - \frac{\sum_{i=1}^n \lambda_i^2}{3(\zeta_3^{(3)}(\lambda))^2}\right), \qquad A_{1,3}^{(3)}(\lambda) = 2^{n-1}\frac{\sum_{i=1}^n \lambda_i^2}{3(\zeta_3^{(3)}(\lambda))^2}.$$

3. Integration over the hyperball

Now the norm in use is $\|X\|_2$ and hence the domain of integration is the unit hyperball. We remark that the moments (and therefore the further formulas) depend on the dimension n. However, with $\|\lambda\|_2 = 1$ they do not depend on λ anymore and this allows to obtain more formulas.

3.1. Spherical Chebyshev polynomials

Let us first consider the weight function $w(\|X\|_2) = 1/\sqrt{1-\|X\|_2^2}$. We give the first few spherical Chebyshev polynomials $\mathcal{T}_m(\lambda; z)$, their zeroes and the cubature weights. They are given by

$$c_i(\lambda) = \begin{cases} \frac{1-(-1)^{n+i-1}}{2}\pi^{(n+1)/2}\frac{\Gamma((n+i)/2)}{\Gamma((n+i+1)/2)}\frac{(i-1)!!2^{(n-2)/2}}{(n+i-2)!!}(\sum_{k=1}^n \lambda_k^2)^{i/2}, & n \geqslant 2,\ n \text{ even}, \\ \frac{1+(-1)^{n+i-1}}{2}\pi^{n/2}\frac{\Gamma((n+i)/2)}{\Gamma((n+i+1)/2)}\frac{(i-1)!!2^{(n-1)/2}}{(n+i-2)!!}(\sum_{k=1}^n \lambda_k^2)^{i/2}, & n \geqslant 3,\ n \text{ odd}. \end{cases}$$

The polynomials are

$$\begin{aligned}
\mathcal{T}_0(z) &= 1, \\
\mathcal{T}_1(z) &= z, \\
\mathcal{T}_2(z) &= z^2 - \frac{1}{n+1}\sum_{i=1}^n \lambda_i^2, \\
\mathcal{T}_3(z) &= z^3 - \frac{3}{n+3}\left(\sum_{i=1}^n \lambda_i^2\right)z,
\end{aligned}$$

and, more generally [3], they satisfy

$$\mathcal{T}_{m+1}(z) = z\mathcal{T}_m(z) - \frac{m(n+m-2)}{(n+2m-3)(n+2m-1)}\left(\sum_{i=1}^n \lambda_i^2\right)\mathcal{T}_{m-1}(z), \quad m \geqslant 1.$$

3.2. Chebyshev nodes and weights

The zero curves of the polynomials $\mathcal{T}_m(z)$ form circles because they occur in symmetric pairs both when m is even and odd. For m odd $z = 0$ is always a zero. The zeroes of $\mathcal{T}_m(\lambda^T X)$ fill up the region $\{z\colon \min_{i=1,\ldots,m} |\zeta_i^{(m)}(\lambda)| \leqslant \|z\|_2 \leqslant 1\}$.

We list the first few nodes and weights for integration over the unit hyperball:

$$\begin{aligned}
\zeta_m^{(2m-1)}(\lambda) &= 0, \quad m = 1, 2, \ldots, \\
\zeta_{1,2}^{(2)}(\lambda) &= \mp\sqrt{\frac{\sum_{i=1}^n \lambda_i^2}{n+1}}, \\
\zeta_{1,3}^{(3)}(\lambda) &= \mp\sqrt{\frac{3\sum_{i=1}^n \lambda_i^2}{n+3}}, \\
A_1^{(1)}(\lambda) &= \begin{cases} \frac{(2\pi)^{n/2}}{(n-1)!!}, & n \text{ even}, \\ \frac{(2\pi)^{(n+1)/2}}{2(n-1)!!}, & n \text{ odd}, \end{cases} \\
A_{1,2}^{(2)}(\lambda) &= \begin{cases} \frac{(2\pi)^{n/2}}{2(n-1)!!}, & n \text{ even}, \\ \frac{(2\pi)^{(n+1)/2}}{4(n-1)!!}, & n \text{ odd}, \end{cases} \\
A_2^{(3)}(\lambda) &= \begin{cases} \frac{(2\pi)^{n/2}}{(n-1)!!} - \frac{(2\pi)^{n/2}\sum_{i=1}^n \lambda_i^2}{(n+1)!!(\zeta_3^{(3)}(\lambda))^2}, & n \text{ even}, \\ \frac{(2\pi)^{(n+1)/2}}{2(n-1)!!} - \frac{(2\pi)^{(n+1)/2}\sum_{i=1}^n \lambda_i^2}{2(n+1)!!(\zeta_3^{(3)}(\lambda))^2}, & n \text{ odd}, \end{cases} \\
A_{1,3}^{(3)}(\lambda) &= \begin{cases} \frac{(2\pi)^{n/2}\sum_{i=1}^n \lambda_i^2}{2(n+1)!!(\zeta_3^{(3)}(\lambda))^2}, & n \text{ even}, \\ \frac{(2\pi)^{(n+1)/2}\sum_{i=1}^n \lambda_i^2}{4(n+1)!!(\zeta_3^{(3)}(\lambda))^2}, & n \text{ odd}. \end{cases}
\end{aligned}$$

3.3. Spherical Legendre polynomials (ℓ_2)

When the weight function is $w(\|X\|_2) = 1$, then the moments and spherical orthogonal polynomials for the hyperball are given by

$$c_i(\lambda) = \begin{cases} \frac{1-(-1)^{n+i-1}}{n+i} \pi^{n/2} \frac{(i-1)!!2^{(n-2)/2}}{(n+i-2)!!} (\sum_{k=1}^n \lambda_k^2)^{i/2}, & n \geqslant 2,\ n \text{ even}, \\ \frac{1+(-1)^{n+i-1}}{n+i} \pi^{(n-1)/2} \frac{(i-1)!!2^{(n-1)/2}}{(n+i-2)!!} (\sum_{k=1}^n \lambda_k^2)^{i/2}, & n \geqslant 3,\ n \text{ odd}, \end{cases}$$

$$\mathcal{L}_0(z) = 1,$$

$$\mathcal{L}_1(z) = z,$$

$$\mathcal{L}_2(z) = z^2 - \frac{1}{n+2} \sum_{i=1}^n \lambda_i^2,$$

$$\mathcal{L}_3(z) = z^3 - \frac{3}{n+4} \left(\sum_{i=1}^n \lambda_i^2 \right) z,$$

$$\mathcal{L}_{m+1}(z) = z\mathcal{L}_m(z) - \frac{m(n+m-1)}{(n+2m-2)(n+2m)} \left(\sum_{i=1}^n \lambda_i^2 \right) \mathcal{L}_{m-1}(z), \quad m \geqslant 1.$$

3.4. Legendre nodes and weights (ℓ_2)

The zero curves of the polynomials $\mathcal{L}_m(z)$ form circles because they occur in symmetric pairs both when m is even and odd. For m odd $z = 0$ is always a zero. The zeroes of $\mathcal{L}_m(\lambda^T X)$ fill up the region $\{z\colon \min_{i=1,\ldots,m} |\zeta_i^{(m)}(\lambda)| \leqslant \|z\|_2 \leqslant 1\}$.

The first few nodes and weights for integration over the hyperball are given by:

$$\zeta_m^{(2m-1)}(\lambda) = 0, \quad m = 1, 2, \ldots,$$

$$\zeta_{1,2}^{(2)}(\lambda) = \mp \sqrt{\frac{\sum_{i=1}^n \lambda_i^2}{n+2}},$$

$$\zeta_{1,3}^{(3)}(\lambda) = \mp \sqrt{\frac{3\sum_{i=1}^n \lambda_i^2}{n+4}},$$

$$A_1^{(1)}(\lambda) = \begin{cases} \frac{(2\pi)^{n/2}}{n!!}, & n \text{ even}, \\ \frac{2(2\pi)^{(n-1)/2}}{n!!}, & n \text{ odd}, \end{cases}$$

$$A_{1,2}^{(2)}(\lambda) = \begin{cases} \frac{(2\pi)^{n/2}}{2n!!}, & n \text{ even}, \\ \frac{(2\pi)^{(n-1)/2}}{n!!}, & n \text{ odd}, \end{cases}$$

$$A_2^{(3)}(\lambda) = \begin{cases} \frac{(2\pi)^{n/2}}{n!!} - \frac{(2\pi)^{n/2} \sum_{i=1}^n \lambda_i^2}{(n+2)!!(\zeta_3^{(3)}(\lambda))^2}, & n \text{ even}, \\ \frac{2(2\pi)^{(n-1)/2}}{n!!} - \frac{2(2\pi)^{(n-1)/2} \sum_{i=1}^n \lambda_i^2}{(n+2)!!(\zeta_3^{(3)}(\lambda))^2}, & n \text{ odd}, \end{cases}$$

$$A_{1,3}^{(3)}(\lambda) = \begin{cases} \frac{(2\pi)^{n/2} \sum_{i=1}^n \lambda_i^2}{2(n+2)!!(\zeta_3^{(3)}(\lambda))^2}, & n \text{ even}, \\ \frac{(2\pi)^{(n-1)/2} \sum_{i=1}^n \lambda_i^2}{(n+2)!!(\zeta_3^{(3)}(\lambda))^2}, & n \text{ odd}. \end{cases}$$

3.5. Computing the zeroes of $\mathcal{T}_m(z)$ and $\mathcal{L}_m(z)$

Let B_{m+1} be the tridiagonal $(m+1) \times (m+1)$ matrix

$$B_{m+1} = \begin{pmatrix} b_{11} & b_{12} & & & & \\ b_{21} & b_{22} & b_{23} & & & \\ & b_{32} & b_{33} & b_{34} & & \\ & & \ddots & \ddots & \ddots & \\ & & & & & b_{m\,m+1} \\ & & & & b_{m+1\,m} & b_{m+1\,m+1} \end{pmatrix}$$

and let B_k denote its k-th principal minor, that is the submatrix formed by the first k rows and columns. Then

$$\det B_{m+1} = b_{m+1\,m+1} \det B_m - b_{m+1\,m} b_{m\,m+1} \det B_{m-1}.$$

Applying this to the matrix $zI_{m+1} - J_{m+1}$ where I_{m+1} is the $(m+1) \times (m+1)$ identity matrix and

$$J_{m+1} = \begin{pmatrix} 0 & 1 & & & & \\ \beta_0 & 0 & 1 & & & \\ & \beta_1 & 0 & 1 & & \\ & \ddots & \ddots & \ddots & & \\ & & & & & 1 \\ & & & & \beta_{m-1} & 0 \end{pmatrix}, \qquad \beta_k = \frac{(k+1)(n+k)}{(n+2k)(n+2k+2)}, \quad k = 0, \dots, m-1,$$

gives us the 3-term recurrence for the spherical Legendre polynomials in the hyperball. With

$$\beta_k = \frac{(k+1)(n+k-1)}{(n+2k-1)(n+2k+1)}$$

we get the 3-term recurrence for the spherical Chebyshev polynomials in the hyperball. Consequently the zeroes $z_i^{(m)}$ of the spherical orthogonal polynomial of degree m equal the eigenvalues of the tridiagonal matrix J_m. While for the hyperball the matrix entries β_k are simple and independent of the parameter λ, on the hypercube and the hypersimplex no simple form for the coefficients in the 3-term recurrence [3] has been obtained.

3.6. Connection with univariate polynomials

For given ν, and with $P_0^{(\nu)}(z) = 1$ and $P_1^{(\nu)}(z) = z$, the well-known univariate monic orthogonal Gegenbauer polynomials $P_m^{(\nu)}(z)$ satisfy the 3-term recurrence

$$P_{m+1}^{(\nu)}(z) = zP_m^{(\nu)}(z) - \frac{m(m+2\nu-1)}{(2m+2\nu)(2m+2\nu-2)} P_{m-1}^{(\nu)}(z).$$

With $2\nu = n-1$ the Gegenbauer polynomials in the single variable $z = \mathrm{sd}(X)$ apparently coincide with our spherical Chebyshev polynomials. With $2\nu = n$ they coincide with our spherical Legendre polynomials. The univariate Gegenbauer polynomials are orthogonal on the interval $[-1, 1]$ for the weight function $w(z) = (1-z^2)^{(2\nu-1)/2}$:

$$\int_{-1}^{1} z^i P_m^{(\nu)}(z) \left(1-z^2\right)^{(2\nu-1)/2} dz = 0, \quad i = 0, \dots, m-1.$$

So the spherical orthogonal polynomials in the hyperball coincide with a different sequence of univariate Gegenbauer polynomials, where the weight function depends on the dimension n. In terms of $X = (x_1, \dots, x_n)$ we have

$$w(X) = \left(1 - \|X\|_2^2\right)^{(2\nu-1)/2}.$$

4. Integration over the hypersimplex

4.1. Spherical Legendre polynomials (ℓ_1)

With the norm $\|X\|_1$ the moments and spherical Legendre polynomials are given by

$$c_0(\lambda) = 2^n/n!,$$

$$c_i(\lambda) = \sum_{j_2=0}^{i} \sum_{j_3=0}^{j_2} \cdots \sum_{j_n=0}^{j_{n-1}} \frac{1+(-1)^{i-j_2}}{i+1} \cdots \frac{1+(-1)^{j_{n-1}-j_n}}{i+n-1} \frac{1+(-1)^{j_n}}{i+n} \lambda_1^{i-j_2} \dots \lambda_{n-1}^{j_{n-1}-j_n} \lambda_n^{j_n},$$

$$\mathcal{L}_0(z) = 1, \qquad \mathcal{L}_1(z) = z,$$

$$\mathcal{L}_2(z) = z^2 - \frac{2}{(n+1)(n+2)} \sum_{i=1}^{n} \lambda_i^2,$$

$$\mathcal{L}_3(z) = \left(\sum_{i=1}^{n} \lambda_i^2\right) z^3 - \frac{12}{(n+3)(n+4)} \left(\sum_{i=1}^{n} \lambda_i^4 + \sum_{i=1}^{n} \sum_{j>i} \lambda_i^2 \lambda_j^2\right) z.$$

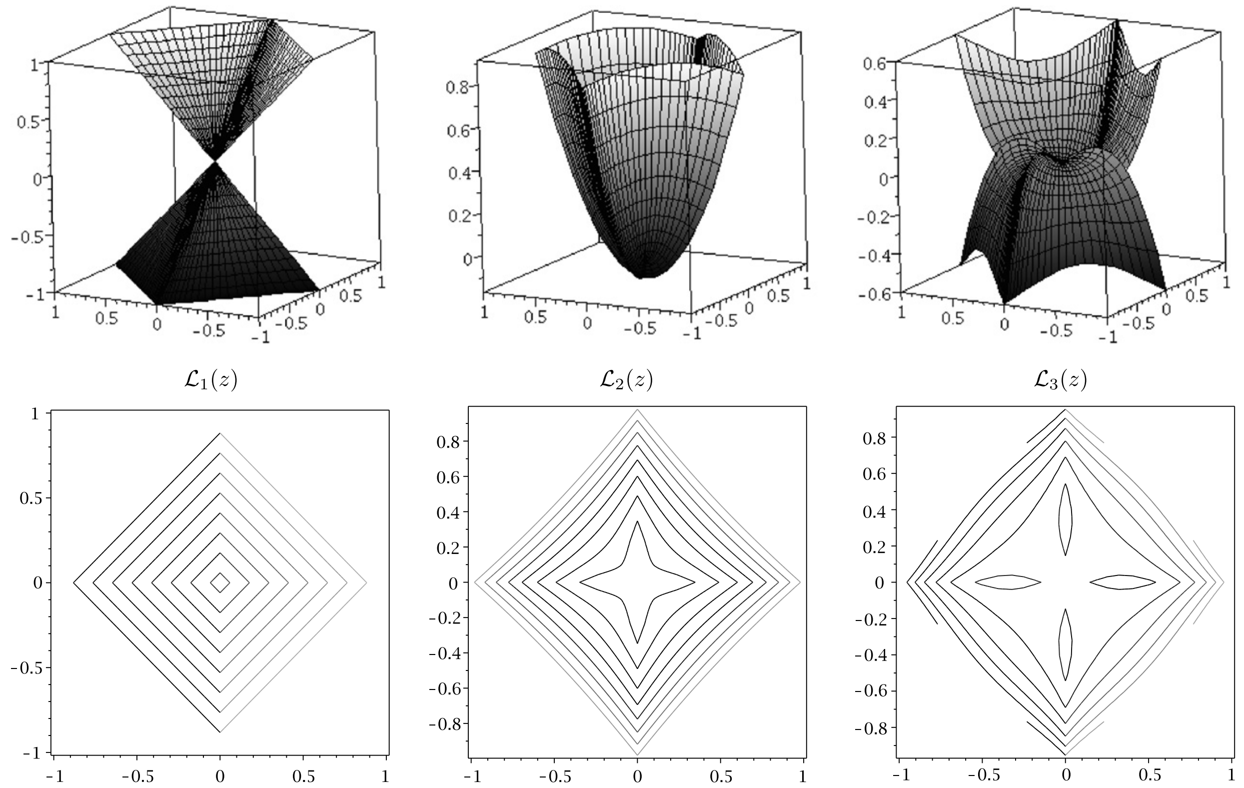

Fig. 3. Surface plots and contour lines.

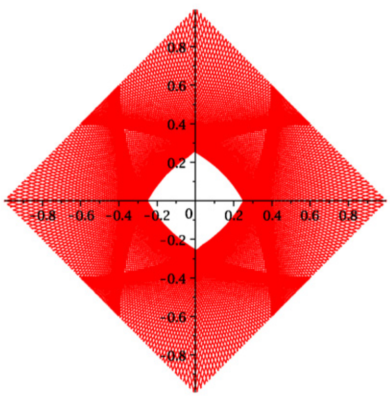

Fig. 4. Zeroes of $\mathcal{L}_2(\lambda^T X)$ with $\|\lambda\|_1 = 1$.

4.2. Legendre nodes and weights (ℓ_1)

The zero curves $\zeta_i^{(m)}(\lambda)$ of the polynomials $\mathcal{L}_m(z)$ occur in symmetric pairs. For $n = 2$ each pair coincides with one of the level curves shown in Fig. 3. For m odd $z = 0$ is always a zero. In Theorem 2 the spherical orthogonal polynomials are used with $z = \lambda^T X$. The zeroes of $\mathcal{L}_m(\lambda^T X)$ with $\|\lambda\|_1 = 1$ and $n = 2$ fill up a region similar to the one shown in Fig. 4.

The first few nodes and weights for integration over the hypersimplex are given by:

$$\zeta_m^{(2m-1)}(\lambda) = 0, \quad m = 1, 2, \ldots,$$

$$\zeta_{1,2}^{(2)}(\lambda) = \mp\sqrt{\frac{2\sum_{i=1}^{n} \lambda_i^2}{(n+1)(n+2)}},$$

$$\zeta_{1,3}^{(3)}(\lambda) = \mp 2\sqrt{\frac{3}{(n+3)(n+4)}}\sqrt{\frac{\sum_{i=1}^{n}\lambda_i^4 + \sum_{i=1}^{n}\sum_{j>i}\lambda_i^2\lambda_j^2}{\sum_{i=1}^{n}\lambda_i^2}},$$

$$A_1^{(1)}(\lambda) = \frac{2^n}{n!}, \qquad A_{1,2}^{(2)}(\lambda) = \frac{2^{n-1}}{n!},$$

$$A_2^{(3)}(\lambda) = 2^n\left(\frac{1}{n!} - \frac{2\sum_{i=1}^{n}\lambda_i^2}{(n+2)!(\zeta_3^{(3)}(\lambda))^2}\right), \qquad A_{1,3}^{(3)}(\lambda) = \frac{2^n\sum_{i=1}^{n}\lambda_i^2}{(n+2)!(\zeta_3^{(3)}(\lambda))^2}.$$

5. Integration of multivariate parameterized functions

An obvious application of Theorem 2 is the symbolic–numeric multidimensional integration of parameterized functions. Take for instance the integral appearing in the Appell function

$$F_2(\alpha,1,1;2,2;\lambda_1,\lambda_2) = \int_0^1\int_0^1 (1-\lambda_1 x - \lambda_2 y)^{-\alpha}\,dx\,dy$$

which satisfies the partial differential equations

$$x(1-x)\frac{\partial^2 F_2}{\partial x^2} - xy\frac{\partial^2 F_2}{\partial x\partial y} + \bigl(2-(\alpha+2)x\bigr)\frac{\partial F_2}{\partial x} - y\frac{\partial F_2}{\partial y} - \alpha F_2 = 0$$

and similarly with the role of x and y interchanged. The Appell function F_2 arises frequently in various physical and chemical applications, among which the evaluation of radiation field integrals [9,8]. We restrict ourselves to the domain $\lambda_1 < 1$, $\lambda_2 < 1$, $\lambda_1 + \lambda_2 < 1$ where the integral is real-valued. By a change of variable this integral can be written as

$$F_2(\alpha,1,1;2,2;\lambda_1,\lambda_2) = \int_{-1}^{1}\int_{-1}^{1} f(\lambda;\lambda_1 x + \lambda_2 y)\,dx\,dy$$

with

$$f(\lambda;z) = \frac{1}{4}\left(1 - \frac{\lambda_1+\lambda_2+z}{2}\right)^{-\alpha}.$$

Hence we can approximate

$$F_2(\alpha,1,1;2,2;\lambda_1,\lambda_2) \approx G_3(\lambda_1,\lambda_2) := \sum_{i=1}^{3} A_i^{(3)}(\lambda) f\bigl(\lambda;\zeta_i^{(3)}(\lambda)\bigr)$$

with $A_i^{(3)}(\lambda)$ and $\zeta_i^{(3)}(\lambda)$ taken from Section 2. This leads to the symbolic approximation formula

$$\begin{aligned}G_3(\lambda_1,\lambda_2) = \frac{1}{6(3\lambda_1^4+10\lambda_1^2\lambda_2^2+3\lambda_2^4)}\Biggl(& 2^{\alpha+3}(2-\lambda_1-\lambda_2)^{-\alpha}\bigl(\lambda_1^4+5\lambda_1^2\lambda_2^2+\lambda_2^4\bigr)\\ &+ 2^{\alpha}5\bigl(\lambda_1^2+\lambda_2^2\bigr)^2\left(2-\lambda_1-\lambda_2-\frac{\sqrt{5}}{5}\sqrt{\frac{3\lambda_1^4+10\lambda_1^2\lambda_2^2+3\lambda_2^4}{\lambda_1^2+\lambda_2^2}}\right)^{-\alpha}\\ &+ 2^{\alpha}5\bigl(\lambda_1^2+\lambda_2^2\bigr)^2\left(2-\lambda_1-\lambda_2+\frac{\sqrt{5}}{5}\sqrt{\frac{3\lambda_1^4+10\lambda_1^2\lambda_2^2+3\lambda_2^4}{\lambda_1^2+\lambda_2^2}}\right)^{-\alpha}\Biggr).\end{aligned}$$

To illustrate the quality of this approximation we compute a few evaluations of $G_3(\lambda_1,\lambda_2)$ for $\alpha = \log(2), \log(3/2), 1/8, 1/16$ and $(\lambda_1,\lambda_2) = r(\cos(j\pi/k), \sin(j\pi/k))$ with $j,k \in \mathbb{N}$. We compare these with the numerical results obtained using Radon's 7-point degree 5 ($m=3$) cubature formula on the square $[-1,1]\times[-1,1]$, computed for each individual combination of α and (λ_1,λ_2), which we denote by R_3 [10]. In Tables 1 and 2 one finds the exact value of $F_2(\alpha,1,1;2,2;\lambda_1,\lambda_2)$ together with the errors $F_2 - G_3$ and $F_2 - R_3$. It is clear that both approximations have the same accuracy. But expression $G_3(\lambda_1,\lambda_2)$ provides a continuous extension, in terms of the parameters, in addition to the numeric values.

Note that the symmetry

$$F_2(\alpha,1,1;2,2;\lambda_1,\lambda_2) = F_2(\alpha,1,1;2,2;\lambda_2,\lambda_1)$$

is preserved by the symbolic integration rule, but not by Radon's cubature formula. For $\lambda_2 = 0$ the symbolic and Radon's cubature formula coincide.

Table 1
$F_2(\alpha, 1, 1; 2, 2; r\cos j\pi/k, r\sin j\pi/k)$ with $\alpha = \log 2$ and $\alpha = \log 3/2$.

α	r	j	k	$F_2(\alpha, 1, 1; 2, 2; r\cos j\pi/k, r\sin j\pi/k)$	$F_2 - G_3$	$F_2 - R_3$
$\log 2$	1/2	0	1	$1.24878542341637 \times 10^{0}$	2.0×10^{-5}	2.0×10^{-5}
	1/2	1	2	$1.24878542341637 \times 10^{0}$	2.0×10^{-5}	-6.3×10^{-6}
	1/2	1	1	$8.63536332176800 \times 10^{-1}$	5.8×10^{-7}	5.8×10^{-7}
	1/2	3	4	$1.01276420123863 \times 10^{0}$	8.9×10^{-6}	7.1×10^{-6}
	1	0	1	$3.25889070928323 \times 10^{0}$	9.8×10^{-1}	9.8×10^{-1}
	1	1	2	$3.25889070928323 \times 10^{0}$	9.8×10^{-1}	2.3×10^{-1}
	1	1	1	$7.72377702823892 \times 10^{-1}$	1.2×10^{-5}	1.2×10^{-5}
	1	2	3	$1.26581509450621 \times 10^{0}$	4.9×10^{-3}	4.8×10^{-3}
	1	5	4	$7.02555439039178 \times 10^{-1}$	1.7×10^{-5}	1.3×10^{-5}
	1	7	4	$1.05976599939755 \times 10^{0}$	9.9×10^{-4}	8.2×10^{-4}
	5	5	4	$3.77604178657645 \times 10^{-1}$	7.6×10^{-4}	6.3×10^{-4}
	10	5	4	$2.60473326815451 \times 10^{-1}$	1.5×10^{-3}	1.2×10^{-3}
$\log 3/2$	1/2	0	1	$1.13615560548628 \times 10^{0}$	6.4×10^{-6}	6.4×10^{-6}
	1/2	1	2	$1.13615560548628 \times 10^{0}$	6.4×10^{-6}	-2.0×10^{-6}
	1/2	1	1	$9.17024069560555 \times 10^{-1}$	2.2×10^{-7}	2.2×10^{-7}
	1/2	3	4	$1.00615026516751 \times 10^{0}$	3.1×10^{-6}	2.5×10^{-6}
	1	0	1	$1.68198704527817 \times 10^{0}$	1.3×10^{-1}	1.3×10^{-1}
	1	1	2	$1.68198704527817 \times 10^{0}$	1.3×10^{-1}	-1.8×10^{-2}
	1	1	1	$7.72377702823892 \times 10^{-1}$	4.9×10^{-6}	4.9×10^{-6}
	1	2	3	$1.26581509450621 \times 10^{0}$	1.5×10^{-3}	1.4×10^{-3}
	1	5	4	$8.11948001089517 \times 10^{-1}$	6.9×10^{-6}	5.5×10^{-6}
	1	7	4	$1.02793906532740 \times 10^{0}$	3.3×10^{-4}	2.7×10^{-4}
	5	5	4	$5.60944616658580 \times 10^{-1}$	3.9×10^{-4}	3.2×10^{-4}
	10	5	4	$4.49648935245511 \times 10^{-1}$	8.4×10^{-4}	7.2×10^{-4}

Table 2
$F_2(\alpha, 1, 1; 2, 2; r\cos j\pi/k, r\sin j\pi/k)$ with $\alpha = 1/8$ and $\alpha = 1/16$.

α	r	j	k	$F_2(\alpha, 1, 1; 2, 2; r\cos j\pi/k, r\sin j\pi/k)$	$F_2 - G_3$	$F_2 - R_3$
1/8	1/2	0	1	$1.03941973413604 \times 10^{0}$	1.0×10^{-6}	1.0×10^{-6}
	1/2	1	2	$1.03941973413604 \times 10^{0}$	1.0×10^{-6}	-3.3×10^{-7}
	1/2	1	1	$9.73416542767547 \times 10^{-1}$	4.1×10^{-8}	4.1×10^{-8}
	1/2	3	4	$1.00150741213994 \times 10^{0}$	5.5×10^{-7}	4.4×10^{-7}
	1	0	1	$1.14285714496901 \times 10^{0}$	1.1×10^{-2}	1.1×10^{-2}
	1	1	2	$1.14285714496901 \times 10^{0}$	1.1×10^{-2}	-3.9×10^{-3}
	1	1	1	$9.53152098789471 \times 10^{-1}$	9.5×10^{-7}	9.5×10^{-7}
	1	2	3	$1.03657602454864 \times 10^{0}$	2.3×10^{-4}	2.2×10^{-4}
	1	5	4	$9.37292569668350 \times 10^{-1}$	1.4×10^{-6}	1.1×10^{-6}
	1	7	4	$1.00667220285694 \times 10^{0}$	5.6×10^{-5}	4.6×10^{-5}
	5	5	4	$8.34745461087668 \times 10^{-1}$	9.8×10^{-5}	8.1×10^{-5}
	10	5	4	$7.78937606474670 \times 10^{-1}$	2.4×10^{-4}	2.1×10^{-4}
1/16	1/2	0	1	$1.01944130080770 \times 10^{0}$	4.5×10^{-7}	4.5×10^{-7}
	1/2	1	2	$1.01944130080770 \times 10^{0}$	4.5×10^{-7}	-1.4×10^{-7}
	1/2	1	1	$9.86592532406697 \times 10^{-1}$	1.8×10^{-8}	1.8×10^{-8}
	1/2	3	4	$1.00071082742536 \times 10^{0}$	2.4×10^{-7}	1.9×10^{-7}
	1	0	1	$1.06666666856784 \times 10^{0}$	4.3×10^{-3}	4.3×10^{-3}
	1	1	2	$1.06666666856784 \times 10^{0}$	4.3×10^{-3}	-1.6×10^{-3}
	1	1	1	$9.76220334133076 \times 10^{-1}$	4.3×10^{-7}	4.3×10^{-7}
	1	2	3	$1.01778196026324 \times 10^{0}$	9.7×10^{-5}	9.4×10^{-5}
	1	5	4	$9.68081140952200 \times 10^{-1}$	6.3×10^{-7}	5.1×10^{-7}
	1	7	4	$1.00312956738424 \times 10^{0}$	2.4×10^{-5}	2.0×10^{-5}
	5	5	4	$9.13408320640060 \times 10^{-1}$	4.7×10^{-5}	3.8×10^{-5}
	10	5	4	$8.82255628091554 \times 10^{-1}$	1.2×10^{-4}	1.0×10^{-4}

6. Exact integration of multivariate polynomials

Theorem 2 can also be used for the exact numerical integration of any multivariate polynomial

$$P(X) = \sum_{|\kappa|=0}^{d} a_\kappa X^\kappa.$$

It suffices to rewrite $P(X)$ in the form

$$P(X) = \sum_{|\kappa|=0}^{d} b_\kappa \left\langle \frac{\kappa}{\|\kappa\|_p}, X \right\rangle^{|\kappa|}, \qquad \langle \kappa, X \rangle = \sum_{i=1}^{n} \kappa_i x_i.$$

Take m such that $2m-1$ is the smallest odd integer larger than or equal to the degree of $P(X)$ and integrate

$$\begin{aligned}\int\limits_{\|X\|_p\leqslant 1} w\bigl(\|X\|_p\bigr)P(X)\,dX &= \sum_{k=0}^{d}\sum_{|\kappa|=k} b_\kappa \int\limits_{\|X\|_p\leqslant 1} w\bigl(\|X\|_p\bigr)\left(\frac{\langle\kappa,X\rangle}{\|\kappa\|_p}\right)^k dX\\ &= \sum_{k=0}^{d}\sum_{|\kappa|=k} b_\kappa \sum_{i=1}^{m} A_i^{(m)}(\lambda)\bigl(\phi_i^{(m)}(\lambda)\bigr)^k, \quad \lambda=\kappa/\|\kappa\|_p. \end{aligned} \tag{13}$$

Then Theorem 2 applies with $\lambda=\kappa/\|\kappa\|_p$. The coefficients b_κ of $P(X)$ in the new basis $\langle\kappa,X\rangle^{|\kappa|}$ can be found from the linear system

$$\frac{|\kappa|!}{\kappa_1!\dots\kappa_n!}\sum_{j_1+\cdots+j_n=|\kappa|} b_{j_1\dots j_n} j_1^{\kappa_1}\dots j_n^{\kappa_n} = a_{\kappa_1\dots\kappa_n}, \quad |\kappa|=0,\dots,d. \tag{14}$$

This linear system of equations has a particularly interesting structure which makes it extremely easy to obtain the coefficients $b_{j_1\dots j_n}$ from the $a_{\kappa_1\dots\kappa_n}$. In order to explore this structure we partition the index set $K=\{(0,\dots,0)\}\cup\{\kappa\colon 1\leqslant|\kappa|\leqslant d\}$ into

$$\begin{aligned}&K_0^{(k,n)} = \bigl\{\kappa\colon |\kappa|=k,\ \kappa_i\neq 0,\ i=1,\dots,n\bigr\}, \quad k=1,\dots,d,\\ &K_{k_1,\dots,k_q}^{(k,n)} = \bigl\{\kappa\colon |\kappa|=k,\ \kappa_{k_1}=\cdots=\kappa_{k_q}=0,\ \kappa_i\neq 0,\ i\neq k_\ell,\ \ell=1,\dots,q\bigr\},\\ &\quad k=1,\dots,d,\ 1\leqslant k_1<\cdots<k_q\leqslant n,\ 1\leqslant q\leqslant n-1,\\ &K_{1,\dots,n}^{(k,n)} = \bigl\{(0,\dots,0)\bigr\}.\end{aligned}$$

For each $|\kappa|=k=0,\dots,d$ we group the equations in the linear system (14) in the same way as the indices in K: clearly $b_{0\dots0}=a_{0\dots0}$, then first the equations indexed by $K_0^{(k,n)}$, then those by the different $K_{k_1}^{(k,n)}$ and so on. The equations indexed by $K_0^{(k,n)}$ only involve unknown coefficients indexed by $K_0^{(k,n)}$. The equations indexed by a set $K_{k_1}^{(k,n)}$ only involve unknowns indexed by $K_{k_1}^{(k,n)}\cup K_0^{(k,n)}$. Since the unknowns indexed by $K_0^{(k,n)}$ have already been computed, these can be substituted. Moreover, all systems indexed by one of the sets $K_{k_1}^{(k,n)}$ have the same coefficient matrix and hence it suffices to perform only one LU decomposition for one set $K_{k_1}^{(k,n)}$. Let us illustrate this by means of an example. Take $n=3$ and $k=4$. The linear subsystem of equations determining the coefficients $b_{j_1j_2j_3}$ with $j_1+j_2+j_3=4$ from the $a_{\kappa_1\kappa_2\kappa_3}$ with $\kappa_1+\kappa_2+\kappa_3=4$, when ordered as described above (to make the coefficient matrix fraction-free we have taken $\lambda=\kappa$ in (13) instead of $\lambda=\kappa/\|\kappa\|_p$ and have avoided redundancy in the λ in another way), looks like:

$$\begin{aligned}
&\begin{pmatrix}24&24&48\\24&48&24\\48&24&24\end{pmatrix}\begin{pmatrix}b_{112}\\b_{121}\\b_{211}\end{pmatrix}=\begin{pmatrix}a_{211}\\a_{121}\\a_{112}\end{pmatrix},\\
&\begin{pmatrix}12&64&108\\54&96&54\\108&64&12\end{pmatrix}\begin{pmatrix}b_{130}\\b_{220}\\b_{310}\end{pmatrix}+\begin{pmatrix}4&8&32\\6&24&24\\4&32&8\end{pmatrix}\begin{pmatrix}b_{112}\\b_{121}\\b_{211}\end{pmatrix}=\begin{pmatrix}a_{310}\\a_{220}\\a_{130}\end{pmatrix},\\
&\begin{pmatrix}12&64&108\\54&96&54\\108&64&12\end{pmatrix}\begin{pmatrix}b_{103}\\b_{202}\\b_{301}\end{pmatrix}+\begin{pmatrix}8&4&32\\24&6&24\\32&4&8\end{pmatrix}\begin{pmatrix}b_{112}\\b_{121}\\b_{211}\end{pmatrix}=\begin{pmatrix}a_{301}\\a_{202}\\a_{103}\end{pmatrix},\\
&\begin{pmatrix}12&64&108\\54&96&54\\108&64&12\end{pmatrix}\begin{pmatrix}b_{013}\\b_{022}\\b_{031}\end{pmatrix}+\begin{pmatrix}8&32&4\\24&24&6\\32&8&4\end{pmatrix}\begin{pmatrix}b_{112}\\b_{121}\\b_{211}\end{pmatrix}=\begin{pmatrix}a_{031}\\a_{022}\\a_{013}\end{pmatrix},\\
&256b_{400}+\begin{pmatrix}1&16&81&1&16&81\end{pmatrix}\begin{pmatrix}b_{130}\\b_{220}\\b_{310}\\b_{103}\\b_{202}\\b_{301}\end{pmatrix}+\begin{pmatrix}1&1&16\end{pmatrix}\begin{pmatrix}b_{112}\\b_{121}\\b_{211}\end{pmatrix}=a_{400},\\
&256b_{040}+\begin{pmatrix}81&16&1&1&16&81\end{pmatrix}\begin{pmatrix}b_{130}\\b_{220}\\b_{310}\\b_{013}\\b_{022}\\b_{031}\end{pmatrix}+\begin{pmatrix}1&16&1\end{pmatrix}\begin{pmatrix}b_{112}\\b_{121}\\b_{211}\end{pmatrix}=a_{040},
\end{aligned}$$

$$256b_{004}+(81\quad 16\quad 1\quad 81\quad 16\quad 1)\begin{pmatrix}b_{103}\\b_{202}\\b_{301}\\b_{013}\\b_{022}\\b_{031}\end{pmatrix}+(16\quad 1\quad 1)\begin{pmatrix}b_{112}\\b_{121}\\b_{211}\end{pmatrix}=a_{004}.$$

Let us analyze how many different λ really appear in (13). In case of integration over the unit ball in one of the ℓ_p norms, then $\phi_i^{(m)}(\lambda_1,\dots,\lambda_n)=\phi_i^{(m)}(\nu_1,\dots,\nu_n)$ where the ν_j are merely a permutation of the λ_j. Hence the number of different nonzero λ is given by the cardinality of the set

$$\{(1,0,\dots,0)\}\cup\{\kappa\colon\ 2\leqslant|\kappa|\leqslant d,\ \kappa_1\geqslant\kappa_2\geqslant\cdots\geqslant\kappa_n,\ 1\leqslant\kappa_i\leqslant d/n,\ \mathrm{GCD}(\kappa_1,\dots,\kappa_n)=1\}.$$

We illustrate the above procedure with the integration of the following fifth-degree ($d=5$, $m=3$) bivariate polynomial ($n=2$) over the unit hypercube (ℓ_∞-norm):

$$\begin{aligned}P(x,y)&=\sum_{i+j=0}^{5}a_{ij}x^iy^j\\&=1+x+y+2xy-6x^3+18xy^2+15y^3+3x^2y^2+5x^3y^2+4x^4y+x^5.\end{aligned}$$

The integral is easy enough to obtain exactly,

$$\int_{-1}^{1}\int_{-1}^{1}P(x,y)\,dx\,dy=\frac{16}{3},$$

but the example is given here to illustrate the principle of these new symbolic–numeric cubature rules. After rewriting $P(x,y)$ as

$$\begin{aligned}P(x,y)={}&1+x+y-x^2+(x+y)^2-y^2+2(x+2y)^3-(2x+y)^3\\&+\frac{13}{6}x^4-\frac{1}{24}(3x+y)^4+\frac{5}{64}(2x+2y)^4-\frac{1}{24}(x+3y)^4+\frac{13}{6}y^4\\&+\frac{353}{240}x^5-\frac{49}{15\,000}(4x+y)^5+\frac{199}{15\,000}(3x+2y)^5\\&-\frac{83}{7500}(2x+3y)^5+\frac{137}{30\,000}(x+4y)^5-\frac{289}{120}y^5\end{aligned}$$

we can distinguish 6 polynomials of degree 5 to which Theorem 2 applies:

$$\begin{aligned}&\mathcal{P}_1(z)=1+2z-2z^2+\frac{13}{3}z^4-\frac{15}{16}z^5,\quad \lambda^{(1)}=(1,0),\ z=X^T\lambda^{(1)},\\&\mathcal{P}_2(z)=z^2+\frac{5}{4}z^4,\quad \lambda^{(2)}=(1,1),\ z=X^T\lambda^{(2)},\\&\mathcal{P}_3(z)=8z^3,\quad \lambda^{(3)}=(1,1/2),\ z=X^T\lambda^{(3)},\\&\mathcal{P}_4(z)=-\frac{27}{4}z^4,\quad \lambda^{(4)}=(1,1/3),\ z=X^T\lambda^{(4)},\\&\mathcal{P}_5(z)=\frac{3008}{375}z^5,\quad \lambda^{(5)}=(1,1/4),\ z=X^T\lambda^{(5)},\\&\mathcal{P}_6(z)=\frac{5913}{1000}z^5,\quad \lambda^{(6)}=(1,2/3),\ z=X^T\lambda^{(6)}.\end{aligned}$$

Here we have made use of the fact that

$$\int_{-1}^{1}\int_{-1}^{1}\mathcal{P}(\lambda;\lambda_1x+\lambda_2y)\,dx\,dy=\int_{-1}^{1}\int_{-1}^{1}\mathcal{P}(\lambda;\lambda_2x+\lambda_1y)\,dx\,dy$$

or more generally

$$\int\cdots\int_{\|X\|_p\leqslant 1}w(\|X\|_p)\mathcal{F}(\lambda;\lambda^TX)\,dX=\int\cdots\int_{\|X\|_p\leqslant 1}w(\|X\|_p)\mathcal{F}(\lambda;\lambda_P^TX)\,dX$$

where the vector λ_P is a permutation of the vector λ. Hence the symbolic–numeric nodes and weights $\phi_i^{(3)}(\lambda)$ and $A_i^{(3)}(\lambda)$ need to be evaluated in 6 specific λ in order to obtain numeric nodes for the integration of $P(x,y)$. In practice only $\phi_2^{(3)}(\lambda)$ and $A_2^{(3)}(\lambda)$ need to be evaluated since $\phi_1^{(3)}(\lambda)=0$ independently of λ, $\phi_3^{(3)}(\lambda)=-\phi_2^{(3)}(\lambda)$ and $A_3^{(3)}(\lambda)=A_2^{(3)}(\lambda)$ (see Section 2 for the nodes and weights):

$$\int_{-1}^{1}\int_{-1}^{1} P(x,y)\,dx\,dy = \sum_{\ell=1}^{6}\int_{-1}^{1}\int_{-1}^{1}\mathcal{P}_\ell\big(\lambda_1^{(\ell)}x+\lambda_2^{(\ell)}y\big)\,dx\,dy$$
$$= A_1^{(3)}\big(\lambda^{(1)}\big)P(0,0)+\sum_{\ell=1}^{6}A_2^{(3)}\big(\lambda^{(\ell)}\big)\big(\mathcal{P}_\ell\big(\phi_2^{(3)}\big(\lambda^{(\ell)}\big)\big)+\mathcal{P}_\ell\big(-\phi_2^{(3)}\big(\lambda^{(\ell)}\big)\big)\big)$$
$$= \frac{16}{3}.$$

7. Minimal numeric cubature rules

From the above it is clear that cubature rules for the exact symbolic–numeric integration of polynomials of the form $\mathcal{P}(\lambda;\lambda^T X)$ of degree $2m-1$ also form the basis of cubature rules for the exact numeric integration of multivariate polynomials $P(X)$ of degree $2m-1$. The relationship is even tighter. When we take a look at existing minimal numeric cubature formulae, the distribution of the nodes is similar to that of the zero curves of the spherical orthogonal polynomials. The nodes appear on semicircles and are mirrored with respect to the origin. To illustrate our believe that these spherical orthogonal polynomials are a good departure point for the construction of numeric Gaussian cubature formulae, we take a closer look at the 7-point degree 5 Radon formula on the disk (ℓ_2-norm) [10]:

$$\iint_{x^2+y^2\leqslant 1} P_5(x,y)\,dx\,dy = \frac{\pi}{8}\Bigg(2P_5(0,0)+P_5\bigg(\frac{1}{\sqrt{2}},\frac{1}{\sqrt{6}}\bigg)+P_5\bigg(\frac{-1}{\sqrt{2}},-1\sqrt{6}\bigg)+P_5\bigg(\frac{1}{\sqrt{2}},-1\sqrt{6}\bigg)$$
$$+P_5\bigg(\frac{-1}{\sqrt{2}},1\sqrt{6}\bigg)+P_5\bigg(0,\sqrt{\frac{2}{3}}\bigg)+P_5\bigg(0,-\sqrt{\frac{2}{3}}\bigg)\Bigg). \tag{15}$$

This Radon formula can be deduced from the exact symbolic–numeric integration rule for degree 5 polynomials ($m=3$) of the form $\mathcal{P}_5(\lambda;\lambda_1 x+\lambda_2 y)$ as follows. Take the bivariate polynomial $P_5(x,y)$ with constant coefficients a_i defined by

$$P_5(x,y)=\sum_{i=0}^{5}a_i(\lambda_1 x+\lambda_2 y)^i$$

and apply the 7-point numeric Radon formula (15) to

$$I=\iint_{x^2+y^2\leqslant 1} P_5(x,y)\,dx\,dy.$$

This numeric formula is exact for I which equals

$$I=\frac{\pi}{8}(8a_0+2a_2+a_4).$$

It is easy to verify, by means of a computer algebra system, that with $(\lambda_1,\lambda_2)=(\cos\theta,\sin\theta)$ and

$$\mathcal{P}_5(\lambda;z)=\sum_{i=0}^{5}a_i z^i,$$

the application of Radon's formula is equivalent to the 7-point evaluation

$$I=\frac{\pi}{8}\Bigg(2\mathcal{P}_5(\lambda;0)+\mathcal{P}_5\bigg(\lambda;\sqrt{\frac{2}{3}}\cos(\pi/6-\theta)\bigg)+\mathcal{P}_5\bigg(\lambda;-\sqrt{\frac{2}{3}}\cos(\pi/6-\theta)\bigg)$$
$$+\mathcal{P}_5\bigg(\lambda;\sqrt{\frac{2}{3}}\cos(-\pi/6-\theta)\bigg)+\mathcal{P}_5\bigg(\lambda;-\sqrt{\frac{2}{3}}\cos(-\pi/6-\theta)\bigg)$$
$$+\mathcal{P}_5\bigg(\lambda;\sqrt{\frac{2}{3}}\cos(\pi/2-\theta)\bigg)+\mathcal{P}_5\bigg(\lambda;-\sqrt{\frac{2}{3}}\cos(\pi/2-\theta)\bigg)\Bigg). \tag{16}$$

The latter expression is actually independent of θ. The choice $\theta = 0$ identifies the application of Radon's formula with the symbolic–numeric formula

$$I = \frac{\pi}{8}\left(4\mathcal{P}_5(\lambda; 0) + 2\mathcal{P}_5\left(\lambda; \frac{1}{\sqrt{2}}\right) + 2\mathcal{P}_5\left(\lambda; \frac{-1}{\sqrt{2}}\right)\right)$$

which uses the zeroes of $\mathcal{L}_3(z)$ listed in Section 3.3. In a future work we expect to prove that from a symbolic cubature formula of the form

$$\iint\limits_{x^2+y^2\leqslant 1} \mathcal{P}_{2m-1}(\lambda; \lambda_1 x + \lambda_2 y)\,dx\,dy = \sum_{i=0}^{n(m)} A_i^{(m)} \mathcal{P}_{2m-1}(\lambda; \lambda_1 x_i + \lambda_2 y_i)$$

a numeric cubature formula of the form

$$\iint\limits_{x^2+y^2\leqslant 1} P_{2m-1}(x, y)\,dx\,dy = \sum_{i=0}^{n(m)} A_i^{(m)} P_{2m-1}(x_i, y_i)$$

can be deduced. Applying this principle, for instance, to the above expression brings us directly from (16) back to (15) since with $\lambda_1 = \cos\theta$ and $\lambda_2 = \sin\theta$,

$$\sqrt{\frac{2}{3}}\cos(\pi/6 - \theta) = \frac{1}{\sqrt{2}}\lambda_1 + \frac{1}{\sqrt{6}}\lambda_2 \to (x_1, y_1) = \left(\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{6}}\right),$$
$$\sqrt{\frac{2}{3}}\cos(\pi/2 - \theta) = \sqrt{\frac{2}{3}}\lambda_2 \to (x_5, y_5) = \left(0, \sqrt{\frac{2}{3}}\right).$$

The conjectured principle has also been verified for the 12-point degree 7 Radon rule on the disk.

8. Conclusion

The number of symbolic–numeric nodes in the Gaussian cubature rules from Theorem 2 is minimal, namely m for a polynomial of degree $2m - 1$. Furthermore we have conjectured in Section 7 how to construct purely numeric cubature rules with a minimal (or small) number of nodes. The proof of this conjecture and the search for cubature rules for general multidimensional integrands with a minimal number of discrete numeric nodes is the subject of further investigation.

References

[1] S. Becuwe, A. Cuyt, Multivariate Padé approximants: homogeneous or not, that's the question, in: Michel Deville, Robert Owens (Eds.), Abstract Book of the 16th IMACS World Congress 2000 (Lausanne), IMACS, 2000, p. 362.
[2] B. Benouahmane, Approximants de Padé et polynômes orthogonaux à deux variables, Thèse de doctorat, Rouen, 1992.
[3] B. Benouahmane, A. Cuyt, Properties of multivariate homogeneous orthogonal polynomials, J. Approx. Theory 113 (2001) 1–20.
[4] C. Brezinski, Padé Type Approximation and General Orthogonal Polynomials, ISNM, vol. 50, Birkhäuser Verlag, Basel, 1980.
[5] T.S. Chihara, An Introduction to Orthogonal Polynomials, Gordon and Breach, New York, 1978.
[6] A. Cuyt, Padé Approximants for Operators: Theory and Applications, LNM, vol. 1065, Springer-Verlag, Berlin, 1984.
[7] C. Dunkl, Y. Xu, Orthogonal Polynomials of Several Variables, Encyclopedia of Mathematics and Its Applications, vol. 81, Cambridge University Press, 2001.
[8] L. Galué, Unification of generalized radiation field integrals involving confluent hypergeometric functions, Radiat. Phys. Chem. 66 (2003) 269–273.
[9] S.B. Opps, N. Saad, H.M. Srivastava, Recursion formulas for Appell's hypergeometric function f_2 with some applications to radiation field problems, Appl. Math. Comp. 207 (2009) 545–558.
[10] J. Radon, Zur mechanischen kubatur, Monatsh. Math. 52 (4) (1948) 286–300.