Multivariate orthogonal polynomials, homogeneous Padé approximants and Gaussian cubature

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The connection between orthogonal polynomials, Padé approximants and Gaussian quadrature is well known and will be repeated in section 1. In the past, several generalizations to the multivariate case have been suggested for all three concepts [4,6,9,...], however without reestablishing a fundamental and clear link. In sections 2 and 3 we will elaborate definitions for multivariate Padé and Padé-type approximation, multivariate polynomial orthogonality and multivariate Gaussian integration in order to bridge the gap between these concepts. We will show that the new m-point Gaussian cubature rules allow the exact integration of homogeneous polynomials of degree $2m-1$, in any number of variables. A numerical application of the new integration rules can be found in sections 4 and 5.

Keywords: orthogonal polynomials, Gaussian quadrature, Padé approximation, cubature, multivariate

1. Padé approximation, orthogonality conditions and numerical quadrature

The Padé approximation problem of a function $f(z)$ consists in finding a rational function $W_n(z)/V_m(z)$ that matches the formal Taylor series development of $f(z)$ as well as can be. In detail, for f given and for W_n of degree n and V_m of degree m, their coefficients are determined from

$$\begin{aligned} f(z) &= c_0 + c_1 z + c_2 z^2 + \cdots, \\ W_n(z) &= a_0 + \cdots + a_n z^n, \\ V_m(z) &= b_0 + \cdots + b_m z^m, \\ (fV_m - W_n)(z) &= \sum_{i=0}^{\infty} d_i z^i \Rightarrow d_i = 0, \quad i = 0, \ldots, n+m. \end{aligned} \tag{1}$$

It can be proven [7] that all solutions $W_n(z)$ and $V_m(z)$ of the above problem reduce to the same irreducible form which will be denoted by $[n/m]^f(z)$ and which is called the Padé approximant of order (n,m) for f.

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Instead of constructing the Padé approximant, one can prefer in some circumstances, for instance when one wants to have full control over the poles of the rational approximant, to compute a Padé-type approximant. Then one proceeds as follows. With the sequence $\{c_i\}_{i\in\mathbb{N}}$ from (1) one associates a linear functional c defined on the space of polynomials $\mathbb{C}[t]$ by

$$c\left(t^i\right) = c_i, \quad i = 0, 1, \ldots.$$

In this way

$$f(z) = c(1) + c(t)z + c\left(t^2\right)z^2 + \cdots = c\left(\frac{1}{1-tz}\right).$$

Let us now choose a polynomial $V_m(z)$ of degree m and let us construct the associated polynomial $W_{m-1}(z)$ by

$$W_{m-1}(z) = c\left(\frac{V_m(t) - V_m(z)}{t-z}\right).$$

It can be proven [2, p. 10] that W_{m-1} is of degree $m-1$ and, hence, we can define the polynomials

$$\begin{aligned} \widetilde{W}_{m-1}(z) &= z^{m-1} W_{m-1}\left(\frac{1}{z}\right), \\ \widetilde{V}_m(z) &= z^m V_m\left(\frac{1}{z}\right), \end{aligned}$$

which appear to satisfy [2, p. 11]

$$\left(f\widetilde{V}_m - \widetilde{W}_{m-1}\right)(z) = \sum_{i=m}^{\infty} d_i z^i. \tag{2}$$

The rational approximant $\widetilde{W}_{m-1}/\widetilde{V}_m$ clearly does not approximate the Taylor series development of f up to the same degree as the Padé approximant does, but it will play an important role in explaining the connection between Padé approximants, orthogonal polynomials and Gaussian quadrature formulae. We denote it by $(m-1/m)^f(z)$ and call it a Padé-type approximant.

If the polynomial $V_m(z)$ in the above construction is not chosen randomly, but if it is computed from the orthogonality conditions

$$c\left(t^i V_m(t)\right) = 0, \quad i = 0, \ldots, m-1, \tag{3}$$

with respect to the linear functional c, then (2) improves to

$$\left(f\widetilde{V}_m - \widetilde{W}_{m-1}\right)(z) = \sum_{i=2m}^{\infty} d_i z^i.$$

Hence, adding orthogonality conditions to the generating polynomial of the Padé-type approximation delivers the Padé approximant $[m-1/m]^f(z)$. This explains the well-known fact that denominators of Padé approximants are in a way orthogonal polynomials.

With the sequence $\{c_i\}_{i\in\mathbb{N}}$ we can also define the Hankel determinants

$$H_m^{(0)} = \begin{vmatrix} c_0 & \dots & c_{m-1} \\ \vdots & \ddots & c_m \\ & & \vdots \\ c_{m-1} & \dots & c_{2m-2} \end{vmatrix}, \qquad H_0^{(0)} = 1.$$

The linear functional c is called definite if

$$H_m^{(0)} \neq 0, \quad m \geqslant 0.$$

For a definite functional c, the roots of the orthogonal polynomial V_m satisfying (3) all differ from those of W_{m-1} and those of V_{m+1}. Let us denote these m zeroes of $V_m(z)$ by $z_1^{(m)}, \dots, z_m^{(m)}$ and let us for now assume that these zeroes are distinct. Let us then compute the interpolating polynomial $p(z,t)$ of degree $m-1$ for the function $1/(1-tz)$ through the interpolation points $z_1^{(m)}, \dots, z_m^{(m)}$, where z is treated as a parameter and t is the complex variable. Then we can consider yet another approximation to $f(z)$, namely,

$$f(z) = c\left(\frac{1}{1-tz}\right) \approx c\bigl(p(z,t)\bigr) = c\left(\sum_{i=1}^{m} \frac{V_m(t)}{(t - z_i^{(m)})V_m'(z_i^{(m)})} \frac{1}{1 - z_i^{(m)} z}\right). \tag{4}$$

With

$$A_i^{(m)} = \frac{W_{m-1}(z_i^{(m)})}{V_m'(z_i^{(m)})}$$

formula (4) can be written as

$$c\left(\frac{1}{1-tz}\right) \approx \sum_{i=1}^{m} A_i^{(m)} \left(\frac{1}{1 - z_i^{(m)} z}\right).$$

If the values c_i are moments,

$$c_i = \int_{-1}^{1} t^i \,\mathrm{d}t, \quad i = 0, 1, \dots,$$

then (4) becomes

$$f(z) = \int_{-1}^{1} \frac{1}{1-tz} \,\mathrm{d}t \approx \int_{-1}^{1} p(z,t) \,\mathrm{d}t = \sum_{i=1}^{m} A_i^{(m)} \left(\frac{1}{1 - z_i^{(m)} z}\right).$$

It can be proven [2, p. 62] that the approximation 4, which is a Gaussian quadrature rule for the integration of $1/(1-tz)$, satisfies

$$\sum_{i=1}^{m} A_i^{(m)}\left(\frac{1}{1-z_i^{(m)}z}\right) = [m-1/m]^f(z).$$

This establishes a clear link between Padé approximation and Gaussian integration, namely, that a Gaussian quadrature formula can be considered as a Padé approximant for the particular function $c(1/(1-tz))$, where t is the complex variable and z is treated as a parameter:

$$\boxed{\begin{aligned} f(z) = c\left(\frac{1}{1-tz}\right) &= \int_{-1}^{1}\frac{1}{1-tz}\,\mathrm{d}t \\ \approx \textstyle\sum_{i=1}^{m} A_i^{(m)}\left(\frac{1}{1-z_i^{(m)}z}\right) &= c\big(p(z,t)\big) = [m-1/m]^f(z). \end{aligned}}$$

Let us now try to generalize all the above to higher dimensions. For the sake of simplicity and without loss of generality, we will write down all formulas for the case of two variables x and y. Because of the great similarity with the univariate case, readers have been confused in the past when we used the usual multi-index notation.

2. Homogeneous Padé and Padé-type approximation

Assume we are given a formal series representation

$$f(x,y) = \sum_{i,j=0}^{\infty} c_{ij}x^i y^j,$$

which we rewrite as

$$f(x,y) = \sum_{k=0}^{\infty} C_k(x,y),$$

where

$$C_k(x,y) = \sum_{i+j=k} c_{ij}x^i y^j.$$

The homogeneous Padé approximation problem of $f(x,y)$ consists in finding polynomials $W_n(x,y)$ and $V_m(x,y)$ of the form

$$W_n(x,y) = \sum_{k=0}^{n}\left[\sum_{i+j=nm+k} a_{ij}x^i y^j\right] = \sum_{k=0}^{n} A_k(x,y),$$

$$V_m(x,y) = \sum_{k=0}^{m}\left[\sum_{i+j=nm+k} b_{ij}x^i y^j\right] = \sum_{k=0}^{m} B_k(x,y),$$

such that

$$(fq - p)(x, y) = \sum_{i+j \geqslant nm+n+m+1} d_{ij} x^i y^j. \tag{5}$$

Note the fact that the homogeneous degrees in W_n, V_m and (5) are shifted by nm, the necessity of which is explained in [5, pp. 16–18]. It can again be proven that all polynomials satisfying (5) reduce to the same irreducible rational function, which is now denoted by $[n/m]^f_{\mathrm{H}}(x, y)$ and which is called the homogeneous Padé approximant of order (n, m) to f.

Before continuing, we switch to a spherical coordinate system. We introduce the directional vector λ and the homogeneous function $c_k(\lambda)$ by

$$(x, y) = (\lambda_1 z, \lambda_2 z), \quad x, y, z \in \mathbb{C}, \quad \lambda = (\lambda_1, \lambda_2) \in \mathbb{C}^2 \setminus \{(0, 0)\}$$

and

$$c_k(\lambda) = \sum_{j=0}^{k} c_{k-j,j} \lambda_1^{k-j} \lambda_2^j.$$

Here the norm is one of the usual Minkowski-norms

$$\|(\lambda_1, \lambda_2)\|_k = \left(\lambda_1^k + \lambda_2^k\right)^{1/k}$$

and to avoid redundancy when selecting λ the condition $||\lambda|| = 1$ can be added. In this coordinate system our given function f reduces to

$$f(x, y) = \sum_{k=0}^{\infty} C_k(x, y) = \sum_{k=0}^{\infty} c_k(\lambda) z^k.$$

If we project f onto the one-dimensional subspace spanned by the vector $\lambda = \lambda^*$,

$$f_{\lambda^*}(z) = f\left(\lambda_1^* z, \lambda_2^* z\right)$$

and if we do the same with the homogeneous Padé approximant $[n/m]^f_{\mathrm{H}}$, then one can prove that [3]

$$[n/m]^f_{\mathrm{H}}\left(\lambda_1^* z, \lambda_2^* z\right) = [n/m]^{f_{\lambda^*}}(z).$$

We want to emphasize the fact that the form of the projected $[n/m]^f_{\mathrm{H}}$ is

$$[n/m]^f_{\mathrm{H}}(\lambda_1 z, \lambda_2 z) = \frac{\sum_{k=0}^{n} (\sum_{i+j=nm+k} a_{ij} \lambda_1^i \lambda_2^j) z^k}{\sum_{k=0}^{m} (\sum_{i+j=nm+k} b_{ij} \lambda_1^i \lambda_2^j) z^k}$$

and that it belongs to $\mathbb{C}[\lambda_1, \lambda_2](z)$, the space of rational functions in the variable z with coefficients being complex-valued bivariate polynomials in λ_1 and λ_2. For fixed $\lambda = \lambda^*$, it coincides with the univariate Padé approximant for the projected function f_{λ^*}, and this for each λ^*, which is a very strong projection property. The shift of nm in the homogeneous degrees of all the polynomial expressions involved has, of course, an effect on the definition of the so-called homogeneous Padé-type approximants which we want to repeat now.

Let us introduce the functional Γ defined on the space $\mathbb{C}[t]$ by

$$\Gamma(t^i) = c_i(\lambda)$$

and let us choose a function $V_m(x,y)$ of the form

$$V_m(x,y) = \mathcal{V}_m(z) = \sum_{i=0}^{m} B_{m^2-i}(\lambda) z^i,$$

where $B_{m^2-i}(\lambda)$ is a homogeneous expression of degree $m^2 - i$ in λ_1 and λ_2. For the associated function $W_{m-1}(x,y)$ defined by

$$W_{m-1}(x,y) = \mathcal{W}_{m-1}(z) = \Gamma\left(\frac{\mathcal{V}_m(t) - \mathcal{V}_m(z)}{t-z}\right)$$

one can show [1] that it is a polynomial of degree $m-1$ in z, but not that it is a polynomial in x and y. Instead it belongs to $\mathbb{C}[\lambda_1, \lambda_2][z]$ and has the form

$$W_{m-1}(x,y) = \mathcal{W}_{m-1}(z) = \sum_{i=0}^{m-1} A_{m^2-1-i}(\lambda) z^i.$$

For the polynomials $\widetilde{V}_m(x,y)$ and $\widetilde{W}_{m-1}(x,y)$ defined by

$$\begin{aligned}
\widetilde{V}_m(x,y) &= \widetilde{\mathcal{V}}_m(z) = z^{m^2}\mathcal{V}_m(z^{-1}) = \sum_{k=0}^{m} \widetilde{B}_{m(m-1)+k}(\lambda) z^{m(m-1)+k} \\
&= \sum_{k=0}^{m}\left(\sum_{i+j=m(m-1)+k} \tilde{b}_{ij} x^i y^j\right), \\
\widetilde{W}_{m-1}(x,y) &= \widetilde{\mathcal{W}}_{m-1}(z) = z^{m^2-1}\mathcal{W}_{m-1}(z^{-1}) = \sum_{k=0}^{m-1} \widetilde{A}_{m(m-1)+k}(\lambda) z^{m(m-1)+k} \\
&= \sum_{k=0}^{m-1}\left(\sum_{i+j=m(m-1)+k} \tilde{a}_{ij} x^i y^j\right)
\end{aligned}$$

and belonging to $\mathbb{C}[x,y]$, holds

$$\begin{aligned}
\left(f\widetilde{V}_m - \widetilde{W}_{m-1}\right)(x,y) &= \left(f\widetilde{\mathcal{V}}_m - \widetilde{\mathcal{W}}_{m-1}\right)(z) = \sum_{i=m^2}^{\infty} d_i(\lambda) z^i \\
&= \sum_{i=m^2}^{\infty}\left(\sum_{j=0}^{i} d_{i-j,j} x^{i-j} y^j\right). \qquad (6)
\end{aligned}$$

Since $\widetilde{V}_m$ and $\widetilde{W}_{m-1}$ are respectively of homogeneous degree $(m-1)m+m$ and $(m-1)m+m-1$ and since the order of $f\widetilde{V}_m - \widetilde{W}_{m-1}$ equals $m^2 = (m-1)m+m-1+1$, the rational function $\widetilde{W}_{m-1}/\widetilde{V}_m$ can be called a homogeneous Padé-type approximant of order $(m-1,m)$ for $f(x,y)$. We denote it by $(m-1/m)^f_{\mathrm{H}}$. For more detailed information we refer to [1].

3. Multivariate orthogonality conditions and Gaussian cubature formulae

Instead of choosing the function $V_m(x,y)$ freely, we can impose the λ-parameterized orthogonality conditions [1]

$$\Gamma\big(t^i \mathcal{V}_m(t)\big) = 0, \quad i = 0,\dots,m-1, \tag{7}$$

and thus improve (6) to become

$$\begin{aligned}\big(f\widetilde{V}_m(x,y) - \widetilde{W}_m(x,y)\big) = \big(f\widetilde{\mathcal{V}}_m - \widetilde{\mathcal{W}}_m\big)(z) &= \sum_{k=m(m-1)+2m}^{\infty} d_k(\lambda) z^k \\ &= \sum_{k=m(m-1)+2m}^{\infty} \left(\sum_{j=0}^{k} d_{k-j,j} x^{k-j} y^j\right).\end{aligned}$$

In this way we generalize the conclusion that denominators of Padé approximants (evaluated in z) are orthogonal polynomials (evaluated in $1/z$) with respect to a linear functional. Apparently it is also the case that, when adding orthogonality conditions to the generating function $V_m(x,y)$, the multivariate rational approximant $(\widetilde{W}_{m-1}/\widetilde{V}_m)(x,y)$ becomes a homogeneous Padé approximant with $z^{m^2}\mathcal{V}_m(1/z)$ in the denominator. These multivariate orthogonal functions were discussed in detail in [1]. For the moment we want to focus on their use in integration.

With the homogeneous polynomial expressions $c_k(\lambda)$, we define the λ-parameterized Hankel determinants

$$H_m^{(0)}(\lambda) = \begin{vmatrix} c_0(\lambda) & \dots & c_{m-1}(\lambda) \\ \vdots & \ddots & c_m(\lambda) \\ & & \vdots \\ c_{m-1}(\lambda) & \dots & c_{2m-2}(\lambda) \end{vmatrix}, \qquad H_0^{(0)} = 1.$$

We call the functional Γ definite if

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

Let us again fix $\lambda = \lambda^*$ and work with the projected functions $f_{\lambda^*}(z)$ and

$$\mathcal{V}_{m,\lambda^*}(z) = V_m\big(\lambda_1^* z, \lambda_2^* z\big).$$

With $\Gamma(t^k) = c_k(\lambda^*)$ as defined above, the function $f_{\lambda^*}(z)$ can be rewritten as

$$f_{\lambda^*}(z) = \sum_{k=0}^{\infty} c_k\big(\lambda^*\big)z^k = \sum_{k=0}^{\infty} \Gamma\big(t^k\big)z^k = \Gamma\left(\frac{1}{1-tz}\right).$$

We know that the orthogonal function $V_m(x,y) = \mathcal{V}_m(z)$ is only a polynomial of degree m in z, not in x and y, and that it coincides, for fixed $\lambda = \lambda^*$, on the one-dimensional subspace spanned by λ^*, with the univariate orthogonal polynomial with respect to the functional c_{λ^*} associated with the sequence

$$\big\{c_k\big(\lambda^*\big)\big\}_{k\in\mathbb{N}}.$$

Hence, this functional c_{λ^*} acting on the space $\mathbb{C}[t]$ is defined by

$$c_{\lambda^*}\big(t^k\big) = c_k\big(\lambda^*\big) = \Gamma\big(t^k\big)\big|_{\lambda=\lambda^*}.$$

Let us denote the m zeroes of $V_m(\lambda_1^* z, \lambda_2^* z)$ by $z_1^{(m)}(\lambda^*), \ldots, z_m^{(m)}(\lambda^*)$ and let us compute the Hermite interpolating polynomial $p_{\lambda^*}(z,t)$ of degree $m-1$ for the function $f_{\lambda^*}(z)$ through these interpolation points, where again z is treated as a parameter. Remember that λ is fixed. This interpolating polynomial can be written as

$$\begin{aligned} p_{\lambda^*}(z,t) &= \sum_{i=1}^{m} \frac{V_m(\lambda_1^* t, \lambda_2^* t)}{(t-z_i^{(m)})V_m'(\lambda_1^* z_i^{(m)}, \lambda_2^* z_i^{(m)})}\left(\frac{1}{1-z_i^{(m)}z}\right) \\ &= \sum_{i=1}^{m} \frac{\mathcal{V}_{m,\lambda^*}(t) - \mathcal{V}_{m,\lambda^*}(z_i^{(m)})}{t-z_i^{(m)}} \frac{1}{\mathcal{V}_{m,\lambda^*}'(z_i^{(m)})}\left(\frac{1}{1-z_i^{(m)}z}\right). \end{aligned}$$

By applying the functional c_{λ^*}, which is Γ with λ fixed, to both sides of this last equation, we obtain

$$\begin{aligned} \Gamma\big(p_{\lambda^*}(z,t)\big) = c_{\lambda^*}\big(p_{\lambda^*}(z,t)\big) &= \sum_{i=1}^{m} \frac{\mathcal{W}_{m-1,\lambda^*}(z_i^{(m)})}{\mathcal{V}_{m,\lambda^*}'(z_i^{(m)})}\left(\frac{1}{1-z_i^{(m)}z}\right) \\ &= \frac{1}{z}\frac{\mathcal{W}_{m-1,\lambda^*}(z^{-1})}{\mathcal{V}_{m,\lambda^*}(z^{-1})} = \frac{\widetilde{\mathcal{W}}_{m-1,\lambda^*}(z)}{\widetilde{\mathcal{V}}_{m,\lambda^*}(z)} \end{aligned} \tag{8}$$

and, hence, we see that for each $\lambda = \lambda^*$

$$\Gamma\big(p_{\lambda^*}(z,t)\big) = [m-1/m]^{f_{\lambda^*}} = [m-1/m]_{\mathrm{H}}^{f}\big(\lambda_1^* z, \lambda_2^* z\big).$$

As in the univariate case, we introduce the notation

$$A_i^{(m)}\big(\lambda^*\big) = \frac{\mathcal{W}_{m-1,\lambda^*}(z_i^{(m)})}{\mathcal{V}_{m,\lambda^*}'(z_i^{(m)})}.$$

Let us now consider the case that the $c_k(\lambda)$ are moments, for instance,

$$c_{i-j,j} = \binom{i}{j} \iint_{||(r,s)||\leqslant 1} r^{i-j}s^j \,\mathrm{d}r\,\mathrm{d}s \tag{9}$$

with as before

$$c_i(\lambda) = \sum_{j=0}^{i} c_{i-j,j} \lambda_1^{i-j} \lambda_2^j,$$

where the norm is one of the usual Minkowski-norms. Then for $x = \lambda_1 z,\ y = \lambda_2 z$ and $t = \lambda_1 r + \lambda_2 s$,

$$\begin{aligned}\iint_{||(r,s)||\leqslant 1} \frac{1}{1 - xr - ys}\,\mathrm{d}r\,\mathrm{d}s &= \iint_{||(r,s)||\leqslant 1} \frac{1}{1 - (\lambda_1 r + \lambda_2 s)z}\,\mathrm{d}r\,\mathrm{d}s \\ &= \sum_{k=0}^{\infty} c_i(\lambda) z^i = \Gamma\left(\frac{1}{1 - tz}\right),\end{aligned}$$

from which we can conclude

$$\boxed{\begin{aligned}f_\lambda(z) = \Gamma\left(\frac{1}{1 - tz}\right) &= \iint_{||(r,s)||\leqslant 1} \frac{1}{1 - (\lambda_1 r + \lambda_2 s)z}\,\mathrm{d}r\,\mathrm{d}s \\ &\approx \sum_{i=1}^{m} A_i^{(m)}(\lambda)\left(\frac{1}{1 - z_i^{(m)}(\lambda)z}\right) = \Gamma\big(p_\lambda(z,t)\big) = [m-1/m]_{\mathrm{H}}^{f}(\lambda_1 z, \lambda_2 z).\end{aligned}} \tag{10}$$

This establishes a link between homogeneous Padé approximation and Gaussian integration, in a very similar way as in the univariate situation.

Let us carry out some more computations in order to transform the above relationship into a useful Gaussian cubature formula. We assume from now on that the functional Γ is positive definite, meaning that [1]

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

In this case, for each λ, the zeroes $z_i^{(m)}$ of $V_m(\lambda_1 z, \lambda_2 z) = \mathcal{V}_m(z)$ are real and simple [2, pp. 58–59] because the functional c_λ is positive definite. Then according to the implicit function theorem [8], there exists for each $z_i^{(m)}$ a unique holomorphic function $\phi_i^{(m)}(\lambda_1, \lambda_2)$ such that in a neighbourhood of $z_i^{(m)}$,

$$\mathcal{V}_m(z) = 0 \Longleftrightarrow z = \phi_i^{(m)}(\lambda_1, \lambda_2).$$

Since this is true for each λ because Γ is positive definite, this implies that for each $i = 1, \ldots, m$ the zeroes $z_i^{(m)}$ can be viewed as a holomorphic function of λ, namely, $z_i^{(m)} = \phi_i^{(m)}(\lambda_1, \lambda_2)$. If we denote in (8)

$$A_i^{(m)}(\lambda) = \frac{\mathcal{W}_{m-1,\lambda}(z_i^{(m)})}{\mathcal{V}'_{m,\lambda}(z_i^{(m)})} = \frac{\mathcal{W}_{m-1}(\phi_i^{(m)}(\lambda))}{\mathcal{V}'_m(\phi_i^{(m)}(\lambda))}, \tag{11}$$

then (8) and (10) can for $t = \lambda_1 r + \lambda_2 s$ be written as

$$\iint_{||(r,s)||\leqslant 1} \frac{1}{1-(\lambda_1 r + \lambda_2 s)z}\,\mathrm{d}r\,\mathrm{d}s \approx \sum_{i=1}^{m} A_i^{(m)}(\lambda)\left(\frac{1}{1-\phi_i^{(m)}(\lambda_1,\lambda_2)z}\right)$$

and the Gaussian cubature formula

$$\iint_{||(x,y)||\leqslant 1} g(\lambda_1 x + \lambda_2 y)\,\mathrm{d}x\,\mathrm{d}y \approx \sum_{i=1}^{m} A_i^{(m)}(\lambda) g\big(\phi_i^{(m)}(\lambda)\big) \tag{12}$$

can be proposed. In order ro rightfully talk about a Gaussian cubature formula we prove the property that the formula exactly integrates homogeneous polynomials of degree $2m-1$.

Theorem 1. Let $\mathcal{P}(z)$ be a polynomial of degree $2m-1$ belonging to $\mathbb{C}(\lambda_1,\lambda_2)[z]$, the set of polynomials in the variable z with coefficients from the space of bivariate rational functions in λ_1 and λ_2 with complex coefficients. Let the functions $\phi_i^{(m)}(\lambda_1,\lambda_2)$ be given as above and be such that

$$\forall \lambda \in \mathbb{R}^2 \setminus \big\{(0,0)\big\}\colon\ j \neq i \Rightarrow \phi_j^{(m)}(\lambda) \neq \phi_i^{(m)}(\lambda).$$

Then for $z = \lambda_1 x + \lambda_2 y$ holds

$$\iint_{||(x,y)||\leqslant 1} \mathcal{P}(\lambda_1 x + \lambda_2 y)\,\mathrm{d}x\,\mathrm{d}y = \sum_{i=1}^{m} A_i^{(m)}(\lambda)\mathcal{P}\big(\phi_i^{(m)}(\lambda)\big).$$

Proof. The polynomial $\mathcal{P}$ is of the form

$$\mathcal{P}(z) = \sum_{i=0}^{2m-1} \pi_i(\lambda_1,\lambda_2) z^i$$

with $\pi_i(\lambda_1,\lambda_2) \in \mathbb{C}(\lambda_1,\lambda_2)$. Let us consider for $z = \lambda_1 x + \lambda_2 y$ the functional

$$\Gamma(\mathcal{P}) = \iint_{||(x,y)||\leqslant 1} \mathcal{P}(\lambda_1 x + \lambda_2 y)\,\mathrm{d}x\,\mathrm{d}y.$$

Then

$$\Gamma(\mathcal{P}) = \sum_{i=0}^{2m-1} \pi(\lambda_1,\lambda_2) c_i(\lambda) = c_\lambda\big(\mathcal{P}(z)\big)$$

and from hereon the proof is a λ-parameterized version of the univariate proof. Let $\mathcal{V}_m(z)$ satisfy (7) with zeroes given by $\phi_i^{(m)}(\lambda),\ i = 1,\ldots,m$. Then

$$\mathcal{P}(z) = \mathcal{Q}(z)\mathcal{V}_m(z) + \mathcal{R}(z)$$

with $\mathcal{Q}(z)$ and $\mathcal{R}(z)$ belonging to $\mathbb{C}(\lambda_1,\lambda_2)[z]$ and of degree at most $m-1$ in z. Also

$$\Gamma(\mathcal{P}) = \Gamma(\mathcal{Q}\mathcal{V}_m) + \Gamma(\mathcal{R}) = \Gamma(\mathcal{R}).$$

The polynomial $\mathcal{R}(z)$ equals its Lagrange interpolant of degree $m-1$ through the interpolation points $\phi_i^{(m)}(\lambda)$, which is given by

$$\mathcal{R}(z) = \sum_{i=1}^{m} \frac{\mathcal{V}_m(z)}{z-\phi_i^{(m)}(\lambda)} \frac{\mathcal{R}(\phi_i^{(m)}(\lambda))}{\mathcal{V}_m'(\phi_i^{(m)}(\lambda))}.$$

When applying the functional Γ to both sides of this equation, one obtains

$$\begin{aligned}\Gamma(\mathcal{P}) = \Gamma(\mathcal{R}) &= \sum_{i=1}^{m} \frac{\mathcal{W}_{m-1}(\phi_i^{(m)}(\lambda))}{\mathcal{V}_m'(\phi_i^{(m)}(\lambda))} \mathcal{R}\bigl(\phi_i^{(m)}(\lambda)\bigr) \\ &= \sum_{i=1}^{m} \frac{\mathcal{W}_{m-1}(\phi_i^{(m)}(\lambda))}{\mathcal{V}_m'(\phi_i^{(m)}(\lambda))} \mathcal{P}\bigl(\phi_i^{(m)}(\lambda)\bigr) = \sum_{i=1}^{m} A_i^{(m)}(\lambda) \mathcal{P}\bigl(\phi_i^{(m)}(\lambda)\bigr),\end{aligned}$$

which completes the proof. □

Let us illustrate theorem 1 with an example to render the achieved result more understandable. Take

$$\mathcal{P}(z) = \mathcal{P}(\lambda_1 x + \lambda_2 y) = \sum_{i=0}^{3} \binom{3}{i} \left(\frac{\lambda_1}{\lambda_2}\right)^{3-i} (\lambda_1 x + \lambda_2 y)^i$$

and consider the ℓ_2-norm

$$\bigl\|(x,y)\bigr\| = \sqrt{x^2+y^2}, \quad (x,y) \in \mathbb{R}^2.$$

Then

$$\iint_{\|(x,y)\| \leqslant 1} \mathcal{P}(\lambda_1 x + \lambda_2 y)\, \mathrm{d}x\, \mathrm{d}y = \frac{\pi \lambda_1}{4\lambda_2^3} \bigl(4\lambda_1^2 + 3\lambda_1^2\lambda_2^2 + 3\lambda_2^4\bigr). \tag{13}$$

For the ℓ_2-norm the expressions $c_i(\lambda)$ given by (9) equal

$$\begin{aligned} c_0(\lambda) &= \pi, \\ c_1(\lambda) &= 0, \\ c_2(\lambda) &= \frac{\pi}{4}\bigl(\lambda_1^2 + \lambda_2^2\bigr), \\ c_3(\lambda) &= 0, \\ &\vdots \end{aligned}$$

When we want to apply the exact integration rule proved in theorem 1, then we have to choose $m=2$. From the orthogonal function $V_2(x,y) = \mathcal{V}_2(z)$ the zeroes

$$\begin{aligned} \phi_1^{(2)}(\lambda) &= \frac{1}{2}\sqrt{\lambda_1^2 + \lambda_2^2}, \\ \phi_2^{(2)}(\lambda) &= -\frac{1}{2}\sqrt{\lambda_1^2 + \lambda_2^2} \end{aligned}$$

and the weights

$$A_1^{(2)}(\lambda) = A_2^{(2)}(\lambda) = \frac{\pi}{2}$$

are obtained. The integration rule

$$A_1^{(2)}\mathcal{P}\big(\phi_1^{(2)}(\lambda)\big) + A_2^{(2)}\mathcal{P}\big(\phi_2^{(2)}(\lambda)\big)$$

then yields the same result as (13). For the ℓ_1- and ℓ_∞-norm similar computations can be performed: after obtaining the $c_i(\lambda)$ for these norms, the orthogonal polynomial $\mathcal{V}_2(z)$ constructed from the $c_i(\lambda)$ delivers all necessary ingredients for the application of the Gaussian cubature rule.

4. Interpolatory cubature rules

Another application of the above results can be found in the derivation of some other new multidimensional integration rules, now of interpolatory type. Let us take

$$\begin{aligned}
\mathcal{V}_m(z) &= \gamma_0(\lambda)\prod_{i=1}^{m}\big(z-\gamma_i(\lambda)\big), \\
\gamma_i(\lambda) &= \alpha_i\lambda_1 + \beta_i\lambda_2, \qquad \alpha_i,\beta_i \in \mathbb{R}, \quad i=1,\ldots,m, \\
\gamma_0(\lambda) &= \sum_{j=0}^{m(m-1)} \delta_j \lambda_1^j \lambda_2^{m(m-1)-j}, \qquad \delta_j \in \mathbb{R}.
\end{aligned} \tag{14}$$

Then the interpolatory cubature rule

$$\iint_{||(x,y)||\leqslant 1} g(\lambda_1 x + \lambda_2 y)\,\mathrm{d}x\,\mathrm{d}y \approx \sum_{i=1}^{m} A_i^{(m)}(\lambda) g(\alpha_i\lambda_1 + \beta_i\lambda_2) \tag{15}$$

can be constructed. The difference with the Gaussian cubature rule being that $\mathcal{V}_m(z)$ does not satisfy the orthogonality conditions (7), but is chosen freely. In other words, $\widetilde{\mathcal{V}}_m(z)$ is the denominator of a Padé-type approximant and not that of a Padé approximant and hence its zeroes are fixed beforehand and must not be computed. In order to rightfully call this a cubature formula of interpolatory type, we now prove that it integrates polynomials of degree m exactly.

Theorem 2. Let $\mathcal{P}(z)$ be a polynomial of degree m belonging to $\mathbb{C}(\lambda_1,\lambda_2)[z]$. Let the functions $\phi_i^{(m)}(\lambda_1,\lambda_2)$, $i=1,\ldots,m$, for each λ give the m distinct zeroes of the polynomial $\mathcal{V}_m(z)$. Then for $z=\lambda_1 x+\lambda_2 y$ holds

$$\iint_{||(x,y)||\leqslant 1} \mathcal{P}(\lambda_1 x + \lambda_2 y)\,\mathrm{d}x\,\mathrm{d}y = \sum_{i=1}^{m} A_i^{(m)}(\lambda)\mathcal{P}\big(\phi_i^{(m)}(\lambda)\big).$$

Proof. We compute the interpolating polynomial $\mathcal{R}(z)$ of degree m for $\mathcal{P}(z)$ through the interpolation points $z_i^{(m)} = \phi_i^{(m)}(\lambda_1, \lambda_2)$. Using the Lagrange formula, it is given by

$$\mathcal{R}(z) = \sum_{i=1}^{m} \frac{\mathcal{V}_m(z)}{z - \phi_i^{(m)}(\lambda)} \frac{\mathcal{P}(\phi_i^{(m)}(\lambda))}{\mathcal{V}'_m(\phi_i^{(m)}(\lambda))}.$$

The theorem is then a consequence of the fact that, on the one hand,

$$\Gamma(\mathcal{R}) = \sum_{i=1}^{m} A_i^{(m)}(\lambda)\mathcal{P}\big(\phi_i^{(m)}(\lambda)\big)$$

and, on the other hand, $\mathcal{P}(z) = \mathcal{R}(z)$. □

An example of such an integration rule is for instance (15) with $\phi_i^{(m)}(\lambda) = \gamma_i(\lambda)$ as given by (14) and $A_i^{(m)}(\lambda)$ still given by (11).

5. Numerical example

Let us apply the new cubature rules (12) and (15) to the integration of

$$\int_0^1 \int_0^1 \big(1 + \mathrm{e}^{-\lambda_1 x - \lambda_2 y} \sin(4\lambda_1 x + 4\lambda_2 y)\big)\,\mathrm{d}x\,\mathrm{d}y. \tag{16}$$

Some simple computations reveal that

$$\begin{aligned}
c_0(\lambda) &= 1,\\
c_1(\lambda) &= \frac{1}{2}(\lambda_1 + \lambda_2),\\
c_2(\lambda) &= \frac{1}{3}\lambda_1^2 + \frac{1}{2}\lambda_1\lambda_2 + \frac{1}{3}\lambda_2^2,\\
c_3(\lambda) &= \frac{1}{4}\lambda_1^3 + \frac{1}{2}\lambda_1\lambda_2(\lambda_1 + \lambda_2) + \frac{1}{4}\lambda_2^3,\\
&\ \ \vdots
\end{aligned}$$

and that for $\mathcal{V}_2(z)$ orthogonal with respect to Γ

$$\begin{aligned}
\phi_1^{(2)}(\lambda) &= \frac{1}{6}\big(3\lambda_1 + 3\lambda_2 - \sqrt{3}\big(\lambda_1^2 + \lambda_2^2\big)\big),\\
\phi_2^{(2)}(\lambda) &= \frac{1}{6}\big(3\lambda_1 + 3\lambda_2 + \sqrt{3}\big(\lambda_1^2 + \lambda_2^2\big)\big),\\
A_1^{(2)}(\lambda) &= \frac{c_1(\lambda) - \phi_2^{(2)}(\lambda)}{\phi_1^{(2)}(\lambda) - \phi_2^{(2)}(\lambda)},\\
A_2^{(2)}(\lambda) &= \frac{\phi_1^{(2)}(\lambda) - c_1(\lambda)}{\phi_1^{(2)}(\lambda) - \phi_2^{(2)}(\lambda)}.
\end{aligned}$$

Table 1

λ	Formula (12)	Exact value
$(1,0)$	1.29985	1.30825
$(1/10,0)$	1.184699	1.184705
$(\sqrt{2}/2,\sqrt{2}/2)$	1.1896	1.1645
$(\sqrt{2}/20,\sqrt{2}/20)$	1.25543	1.25544
$(\sqrt{3}/2,1/2)$	1.209	1.189
$(\sqrt{3}/20,1/20)$	1.24744	1.24745

The use of (12) for different choices of λ yields the results presented in table 1.

When applying (15) to the computation of (16) we choose a polynomial of degree 4 in z in order to obtain a comparable accuracy. For

$$\begin{aligned}\mathcal{V}_4(z) &= \left(z-\frac{1}{2}\lambda_1\right)\left(z-\lambda_1-\frac{1}{2}\lambda_2\right)\left(z-\frac{1}{2}\lambda_1-\lambda_2\right)\left(z-\frac{1}{2}\lambda_2\right)\\ &= \prod_{i=1}^{4}\left(z-\phi_i^{(4)}(\lambda)\right)\end{aligned}$$

the associated polynomial $\mathcal{W}_3(z)$ is given by

$$\mathcal{W}_3(z)=\Gamma\left(\frac{\mathcal{V}_4(z)-\mathcal{V}_4(t)}{z-t}\right)=\sum_{i=0}^{3}\left[c_{3-i}(\lambda)+\sum_{j=0}^{3-i-1}\mu_{3-i-j}(\lambda)c_j(\lambda)\right]z^i$$

with

$$\begin{aligned}\mu_1(\lambda) &= -\sum_{i=1}^{4}\phi_i^{(4)}(\lambda),\\ \mu_2(\lambda) &= \sum_{\substack{i,j=1\\ i<j}}^{4}\phi_i^{(4)}(\lambda)\phi_j^{(4)}(\lambda),\\ \mu_3(\lambda) &= -\sum_{\substack{i,j,k=1\\ i<j<k}}^{4}\phi_i^{(4)}(\lambda)\phi_j^{(4)}(\lambda)\phi_k^{(4)}(\lambda),\\ \mu_4(\lambda) &= \prod_{i=1}^{4}\phi_i^{(4)}(\lambda).\end{aligned}$$

The use of (15) for different choices of λ then almost produces the same results as above, when rounded to the same number of digits as above, the only exception being that, for $\lambda = (\sqrt{3}/2,1/2)$, the approximation computed using formula (15) equals 1.204.

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