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Numerical quadratures and orthogonal polynomials

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Abstract. Orthogonal polynomials of different kinds as the basic tools play very important role in construction and analysis of quadrature formulas of maximal and nearly maximal algebraic degree of exactness. In this survey paper we give an account on some important connections between orthogonal polynomials and Gaussian quadratures, as well as several types of generalized orthogonal polynomials and corresponding types of quadratures with simple and multiple nodes. Also, we give some new results on a direct connection of generalized Birkhoff-Young quadratures for analytic functions in the complex plane with multiple orthogonal polynomials.

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1. Introduction

Let $\mathcal{P}_n$ be the set of all algebraic polynomials of degree at most n and $d\sigma$ be a finite positive Borel measure on the real line $\mathbb{R}$ such that its support $\operatorname{supp}(d\sigma)$ is an infinite set, and all its moments $\mu_k = \int_{\mathbb{R}} t^k \, d\sigma(t)$, $k = 0, 1, \ldots$, exist and are finite.

The n-point quadrature formula

$$\int_{\mathbb{R}} f(t) d\sigma(t) = \sum_{k=1}^{n} \sigma_k f(\tau_k) + R_n(f), \tag{1.1}$$

which is exact on the set $\mathcal{P}_{2n-1}$ is known as the Gauss-Christofell quadrature formula (cf. [14, p. 29], [20, p. 324]). It is a quadrature formula of the maximal algebraic degree of exactness, i.e., $R_n(\mathcal{P}_{d_{\max}}) = 0$, where $d_{\max} = 2n - 1$.

This famous method of numerical integration, for the Legendre measure $d\sigma(t) = dt$ on $[-1, 1]$, was discovered in 1814 by C.F. Gauss [11], using his theory of continued fractions associated with hypergeometric series. It is interesting to mention that Gauss determined numerical values of quadrature parameters, the nodes τ_k and the weights σ_k, $k = 1, \ldots, n$, for all $n \leq 7$. An elegant alternative derivation of this method was provided by Jacobi, and a significant generalization to arbitrary measures was given by Christoffel. The error term $R_n(f)$ and convergence were proved by Markov and Stieltjes, respectively. A nice survey of Gauss-Christoffel quadrature formulae was written by Gautschi [12].

In this survey paper we give an account on some important connections between orthogonal polynomials and Gaussian quadratures, as well as several types of generalized orthogonal polynomials and corresponding types of quadratures. The paper is organized as follows. Section 2 is devoted to quadratures of Gaussian type (with maximal or nearly maximal degree of exactness) and quasi-orthogonal polynomials. A connection between s- and *σ-orthogonal polynomials* and quadratures with multiple nodes is presented in Section 3. Finally, in Section 4 we consider the so-called *multiple orthogonal polynomials* and give two applications. First, we show a direct connection of Borges quadratures [3] with multiple orthogonal polynomial. Second application is related to a generalization of the Birkhoff-Young quadratures [2] for analytic functions in the complex plane. We give a characterization of such generalized quadratures in terms of multiple orthogonal polynomials and prove the existence and uniqueness of these quadratures.

2. Orthogonal and quasi-orthogonal polynomials and Gaussian type of quadratures

The construction of quadrature formulae of the maximal (Gauss-Christoffel), or nearly maximal, algebraic degree of exactness for integrals involving a positive measure $d\sigma$ is closely connected to polynomials orthogonal on the real line with respect to the inner product

$$(f, g) = (f, g)_{d\sigma} = \int_{\mathbb{R}} f(t)g(t)\, d\sigma(t) \quad (f, g \in L^2(d\sigma)). \tag{2.1}$$

The monic polynomials $\pi_\nu = \pi_\nu(d\sigma; \cdot\,)$, $\nu = 0, 1, \ldots$, orthogonal with respect to (2.1) satisfy the three-term recurrence relation (cf. [20, p. 97])

$$\begin{aligned} \pi_{\nu+1}(t) &= (t - \alpha_\nu)\pi_\nu(t) - \beta_\nu \pi_{\nu-1}(t), \quad \nu = 0, 1, \ldots, \\ \pi_0(t) &= 1, \ \pi_{-1}(t) = 0, \end{aligned} \tag{2.2}$$

with recurrence coefficients $\alpha_\nu = \alpha_\nu(d\sigma)$ and $\beta_\nu = \beta_\nu(d\sigma) > 0$, and $\beta_0 = \mu_0 = \int_{\mathbb{R}} d\sigma(t)$ (by definition).

The following theorem is due to Jacobi (cf. [20, p. 322]):

Theorem 2.1. *Given a positive integer m ($\leq n$), the quadrature formula* (1.1) *has degree of exactness $d = n - 1 + m$ if and only if the following conditions are satisfied:*

1° *Formula* (1.1) *is interpolatory;*

2° *The node polynomial* $q_n(t) = (t-\tau_1)(t-\tau_2)\cdots(t-\tau_n)$ *satisfies*

$$(\forall p \in \mathcal{P}_{m-1}) \qquad (p, q_n) = \int_{\mathbb{R}} p(t) q_n(t)\, d\sigma(x) = 0.$$

According to this theorem, an n-point quadrature formula (1.1) has the maximal degree of exactness $2n-1$, i.e., $m = n$ is optimal, because the higher m $(> n)$ is impossible. Namely, the condition 2° in Theorem 2.1 for $m = n+1$ requires the orthogonality $(p, q_n) = 0$ for all $p \in \mathcal{P}_n$, which is impossible when $p = q_n$.

Thus, in the case $m = n$, the orthogonality condition 2° from Theorem 2.1 shows that the node polynomial q_n must be (monic) orthogonal polynomial with respect to the measure $d\sigma$, and therefore the nodes τ_k must be zeros of the polynomial $q_n(t) = \pi_n(d\sigma; t)$. The corresponding weights σ_k (Christoffel numbers) can be expressed in terms of orthogonal polynomials as values of the Christoffel function $\lambda_n(d\sigma; t)$ at these zeros (cf. [20, p. 324]).

Computationally, today there are very stable methods for generating Gauss-Christoffel rules. The most popular of them is one due to Golub and Welsch [18]. Their method is based on determining the eigenvalues and the first components of the eigenvectors of a symmetric tridiagonal Jacobi matrix $J_n(d\sigma)$, with elements formed from the coefficients in the three-term recurrence relation (2.2).

Theorem 2.2. *The nodes τ_k in the Gauss-Christoffel quadrature rule* (1.1)*, with respect to a positive measure $d\sigma$, are the eigenvalues of the n-th order Jacobi matrix*

$$J_n(d\sigma) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & \mathrm{O} \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \sqrt{\beta_2} & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \sqrt{\beta_{n-1}} \\ \mathrm{O} & & & \sqrt{\beta_{n-1}} & \alpha_{n-1} \end{bmatrix},$$

where α_ν and β_ν, $\nu = 0, 1, \ldots, n-1$, are the coefficients in the three-term recurrence relation for the monic orthogonal polynomials $\pi_\nu(d\sigma;\,\cdot\,)$, and the weights σ_k are given by

$$\sigma_k = \beta_0 v_{k,1}^2, \qquad k = 1, \ldots, n,$$

where $\beta_0 = \mu_0 = \int_{\mathbb{R}} d\sigma(t)$ and $v_{k,1}$ is the first component of the normalized eigenvector $\mathbf{v}_k$ corresponding to the eigenvalue τ_k,

$$J_n(d\sigma)\mathbf{v}_k = \tau_k \mathbf{v}_k, \qquad \mathbf{v}_k^{\mathrm{T}}\mathbf{v}_k = 1, \qquad k = 1, \ldots, n.$$

If we put a smaller value of m, say $m = n - r$, in Theorem 2.1, the node polynomial can be expressed in terms of orthogonal polynomials π_ν as

$$q_n(t) = q_{n,r}(t) = \pi_n(t) + \varrho_1 \pi_{n-1}(t) + \cdots + \varrho_r \pi_{n-r}(t), \tag{2.3}$$

where $\varrho_1, \ldots, \varrho_r$ are real numbers and $n > r$. For $r = 0$ we put $q_{n,0} = \pi_n$.

Such polynomials $\{q_{n,r}\}$ are known as *quasi-orthogonal* polynomials and they play very important role in the study of interpolatory quadratures with exactness $d = 2n - r - 1$, $0 \leq r < n$. Notice that for $r = n$, i.e., $m = 0$, the quadrature (1.1) is only interpolatory, without the orthogonality condition 2° in Theorem 2.1.

It is clear if τ_k, $k = 1, \ldots, n$, are nodes of the quadrature formula (1.1), with exactness $d = 2n-r-1$, then these nodes are zeros of a quasi-polynomial of the form (2.3). Contrary, if a quasi-polynomial $q_{n,r}$ has n real distinct zeros τ_k, $k = 1, \ldots, n$, then there exists a quadrature rule of the form (1.1), with exactness $d = 2n - r - 1$ and non-zero weights σ_k, $k = 1, \ldots, n$. Such kind of quadratures have been studied by several authors (cf. [4, 5, 10, 21, 43]). Quadratures with positive weigts are of particular interest and they are known as *positive quadrature formulae*. Their convergence and some characterizations were studied by several authors (cf. [10, 26, 27, 44]). For example, Xu [44] showed that the quasi-orthogonal polynomials that lead to the positive quadratures can all be expressed as characteristic polynomials of a symmetric tridiagonal matrix with positive subdiagonal entries. Also, as a consequence, for a fixed n, Xu [44] obtained that every positive quadrature is a Gaussian quadrature formula for some another nonnegative measure.

Positive quadrature formulas on the real line with the highest degree of exactness and with one or two prescribed nodes anywhere on the interval of integration have been recently characterized in [5]. The simplest kinds of such formulas are well known Gauss-Radau and Gauss-Lobatto quadratures with one or both (finite) endpoints being fixed nodes, respectively (cf. [20, p. 328]). Their nodes and weights can be obtained by a little modification of the Golub-Welsch Theorem 2.2. Also, some cases with one or two additional prescribed nodes inside the interval of integration can be analyzed by considering certain modified Jacobi matrices (see [5]).

3. Power orthogonality and quadrature with multiple nodes

The first idea of numerical integration involving multiple nodes appeared in the middle of the last century (Chakalov [6, 7, 8], Turán [40], Popoviciu [28], Ghizzetti and Ossicini [15, 16], etc.).

Let $\eta_1, \ldots, \eta_m$ $(\eta_1 < \cdots < \eta_m)$ be given *fixed* (or *prescribed*) nodes, with multiplicities $m_1, \ldots, m_m$, respectively, and $\tau_1, \ldots, \tau_n$ $(\tau_1 < \cdots < \tau_n)$ be *free* nodes, with given multiplicities $n_1, \ldots, n_n$, respectively. Interpolation quadrature formulae of a general form

$$I(f) = \int_{\mathbb{R}} f(t)\, d\sigma(t) \cong \sum_{\nu=1}^{n} \sum_{i=0}^{n_\nu - 1} A_{i,\nu} f^{(i)}(\tau_\nu) + \sum_{\nu=1}^{m} \sum_{i=0}^{m_\nu - 1} B_{i,\nu} f^{(i)}(\eta_\nu), \quad (3.1)$$

with an algebraic degree of exactness at least $M + N - 1$, were investigated by Stancu [31, 35, 38].

Using fixed and free nodes we introduce two polynomials

$$q_M(t) \colon = \prod_{\nu=1}^{m} (t - \eta_\nu)^{m_\nu} \quad \text{and} \quad Q_N(t) \colon = \prod_{\nu=1}^{n} (t - \tau_\nu)^{n_\nu},$$

where $M = \sum_{\nu=1}^{m} m_\nu$ and $N = \sum_{\nu=1}^{n} n_\nu$. Choosing the free nodes to increase the degree of exactness leads to the so-called Gaussian type of quadratures. If the free (or *Gaussian*) nodes $\tau_1, \ldots, \tau_n$ are such that the quadrature rule (3.1) is exact for each $f \in \mathcal{P}_{M+N+n-1}$, then we call it the *Gauss-Stancu formula*. Stancu [36] proved that $\tau_1, \ldots, \tau_n$ *are the Gaussian nodes if and only if*

$$\int_{\mathbb{R}} t^k Q_N(t) q_M(t)\, d\sigma(t) = 0, \quad k = 0, 1, \ldots, n-1. \tag{3.2}$$

Under some restrictions of node polynomials $q_M(t)$ and $Q_N(t)$ on the support interval of the measure $d\sigma(t)$ we can give sufficient conditions for the existence of Gaussian nodes (cf. Stancu [36] and [17]). For example, *if the multiplicities of the Gaussian nodes are odd, e.g., $n_\nu = 2s_\nu + 1$, $\nu = 1, \ldots, n$, and if the polynomial with fixed nodes $q_M(t)$ does not change its sign in the support interval of the measure $d\sigma(t)$, then, in this interval, there exist real distinct nodes τ_ν, $\nu = 1, \ldots, n$.*

The last condition for the polynomial $q_M(t)$ means that the multiplicities of the internal fixed nodes must be even. Defining a new (nonnegative) measure $d\hat{\sigma}(t) := |q_M(t)|\, d\sigma(t)$, the "orthogonality conditions" (3.2) can be expressed in a simpler form

$$\int_{\mathbb{R}} t^k Q_N(t)\, d\hat{\sigma}(t) = 0, \quad k = 0, 1, \ldots, n-1.$$

This means that the general quadrature problem (3.1), under these conditions, can be reduced to a problem with only Gaussian nodes, but with respect to another modified measure. Computational methods for this purpose are based on Christoffel's theorem and described in details in [13] (see also [17]).

Let $\pi_n(t)\colon = \prod_{\nu=1}^{n}(t - \tau_\nu)$. Since $Q_N(t)/\pi_n(t) = \prod_{\nu=1}^{n}(t-\tau_\nu)^{2s_\nu} \geq 0$ over the support interval, we can make an additional reinterpretation of the "orthogonality conditions" (3.2) in the form

$$\int_{\mathbb{R}} t^k \pi_n(t)\, d\mu(t) = 0, \quad k = 0, 1, \ldots, n-1, \tag{3.3}$$

where

$$d\mu(t) = \left(\prod_{\nu=1}^{n} (t - \tau_\nu)^{2s_\nu} \right) d\hat{\sigma}(t). \tag{3.4}$$

This means that $\pi_n(t)$ is a polynomial orthogonal with respect to the new nonnegative measure $d\mu(t)$ and, therefore, all zeros $\tau_1, \ldots, \tau_n$ are simple, real, and belong to the support interval. As we see the measure $d\mu(t)$ involves the nodes $\tau_1, \ldots, \tau_n$, i.e., the unknown polynomial $\pi_n(t)$, which is implicitly defined. This polynomial $\pi_n(t)$ belongs to the class of the so-called *σ-orthogonal polynomials* $\{\pi_{n,\sigma}(t)\}_{n\in\mathbb{N}_0}$, which correspond to the sequence $\sigma = (s_1, s_2, \ldots)$ connected with multiplicities of Gaussian nodes. Namely, the solution $(\hat{\tau}_1, \ldots, \hat{\tau}_n)$ of the previous (nonlinear) system of equations (3.3) gives the σ-orthogonal polynomial

$$\pi_n(t) = \pi_{n,\sigma}(t) = (t - \hat{\tau}_1) \cdots (t - \hat{\tau}_n),$$

which is also the unique solution of the extremal problem

$$\min_{\tau_1<\cdots<\tau_n} \int_{\mathbb{R}} |t-\tau_1|^{2s_1+2}\cdots|t-\tau_n|^{2s_n+2}d\hat{\sigma}(t) = \int_{\mathbb{R}} |\pi_{n,\sigma}(t)|^2 d\hat{\mu}(t), \qquad (3.5)$$

where $d\hat{\mu}$ is of the form (3.4) with $\hat{\tau}_\nu$ instead of τ_ν, $\nu = 1,\ldots,n$.

If $\sigma = (s,s,\ldots)$, these polynomials reduce to the *s-orthogonal polynomials* and the corresponding extremal problem (3.5) becomes

$$\min_{p\in\mathcal{P}_{n-1}} \int_{\mathbb{R}} |t^n+p(t)|^{2s+2}d\hat{\sigma}(t) = \int_{\mathbb{R}} |\pi_n(t)|^2 d\hat{\mu}(t) = \|\pi_n\|^2_{d\hat{\mu}},$$

where $d\hat{\mu}(t) = \pi_n(t)^{2s}d\hat{\sigma}(t)$. (For details see Milovanović [22].)

Quadratures with only Gaussian nodes ($m = 0$),

$$\int_{\mathbb{R}} f(t)\,d\sigma(t) = \sum_{\nu=1}^{n}\sum_{i=0}^{2s_\nu} A_{i,\nu} f^{(i)}(\tau_\nu) + R(f),$$

which are exact for all algebraic polynomials of degree at most $d_{\max} = 2\sum_{\nu=1}^{n} s_\nu + 2n - 1$, are known as *Chakalov-Popoviciu quadrature formulas* (see [6, 7, 8], [28]). A deep theoretical progress in this subject was made by Stancu (see [38] and [32]–[37]). In the special case of the Legendre measure on $[-1,1]$, when all multiplicities are mutually equal, these formulas reduce to the well-known *Turán quadrature* [40]. A connection between quadratures, s and σ-orthogonality and moment-preserving approximation with defective splines was given in survey paper [22]. A very efficient method for constructing quadratures with multiple nodes was given recently by Milovanović, Spalević and Cvetković [24]. We mention also a nice recent book by Shi [30].

4. Multiple orthogonality

In this section we consider applications of multiple orthogonal polynomials to some special type of quadratures. Otherwise, multiple orthogonal polynomials are intimately related to Hermite-Padé approximants and, because of that, they are known as Hermite-Padé polynomials. A nice survey on these polynomials, as well as some their applications to various fields of mathematics (number theory, special functions, etc.) and in the study of their analytic, asymptotic properties, was given by Aptekarev [1].

4.1. Multiple orthogonal polynomials

Multiple orthogonal polynomials are a generalization of standard orthogonal polynomials in the sense that they satisfy m orthogonality conditions.

Let $m \geq 1$ be an integer and let w_j, $j = 1,\ldots,m$, be weight functions on the real line so that the support of each w_j is a subset of an interval E_j. Let $\vec{n} = (n_1, n_2, \ldots, n_m)$ be a vector of m nonnegative integers, which is called a *multi-index* with the length $|\vec{n}| = n_1 + n_2 + \cdots + n_m$. There are two types of multiple orthogonal polynomials, but here we consider only the so-called *type II multiple orthogonal polynomials* $\pi_{\vec{n}}(t)$ of degree $|\vec{n}|$. Such monic polynomials are defined by the m orthogonality relations

$$\left.\begin{aligned} \int_{E_1} \pi_{\vec{n}}(t)\, t^{\ell} w_1(t)\, dt = 0, &\qquad \ell = 0,1,\ldots,n_1-1,\\ \int_{E_2} \pi_{\vec{n}}(t)\, t^{\ell} w_2(t)\, dt = 0, &\qquad \ell = 0,1,\ldots,n_2-1,\\ &\vdots\\ \int_{E_m} \pi_{\vec{n}}(t)\, t^{\ell} w_m(t)\, dt = 0, &\qquad \ell = 0,1,\ldots,n_m-1. \end{aligned}\right\} \tag{4.1}$$

Evidently, for $m = 1$ they reduce to the ordinary orthogonal polynomials.

The conditions (4.1) give $|\vec{n}|$ linear equations for the $|\vec{n}|$ unknown coefficients $a_{k,\vec{n}}$ of the polynomial $\pi_{\vec{n}}(t) = \sum_{k=0}^{|\vec{n}|} a_{k,\vec{n}}\, t^k$, where $a_{|\vec{n}|,\vec{n}} = 1$. However, the matrix of coefficients of this system of equations can be singular and we need some additional conditions on the m weight functions to provide the uniqueness of the multiple orthogonal polynomials. If the polynomial $\pi_{\vec{n}}(t)$ is unique, then we say that $\vec{n}$ is a *normal multi-index* and if all multi-indices are normal then we have a *complete system.*

One important complete system is the *AT* system, in which all weight functions are supported on the same interval E $(= E_1 = E_2 = \cdots = E_m)$ and the following $|\vec{n}|$ functions:

$$\begin{gathered} w_1(t),\, tw_1(t),\, \ldots,\, t^{n_1-1}w_1(t),\quad w_2(t),\, tw_2(t),\, \ldots,\, t^{n_2-1}w_2(t),\\ \ldots,\, w_m(t),\, tw_m(t),\, \ldots,\, t^{n_m-1}w_m(t) \end{gathered}$$

form a *Chebyshev system* on E for each multi-index $\vec{n}$. This means that every linear combination

$$\sum_{j=1}^{m} Q_{n_j-1}(t) w_j(t),$$

where Q_{n_j-1} is a polynomial of degree at most $n_j - 1$, has at most $|\vec{n}| - 1$ zeros on E.

In 2001 Van Assche and Coussement [42] proved the following result:

Theorem 4.1. *In an AT system the type II multiple orthogonal polynomial $\pi_{\vec{n}}(x)$ has exactly $|\vec{n}|$ zeros on E.*

For these multiple orthogonal polynomials with *nearly diagonal multi-index* there is an interesting recurrence relation of order $m + 1$. Let $n \in \mathbb{N}$ and write it as $n = km + j$, with $k = [n/m]$ and $0 \le j < m$. The nearly diagonal multi-index $\vec{s}(n)$ corresponding to n is given by

$$\vec{s}(n) = (\underbrace{k+1, k+1, \ldots, k+1}_{j\ \text{times}}, \underbrace{k, k, \ldots, k}_{m-j\ \text{times}}).$$

Denote the corresponding type II multiple (monic) orthogonal polynomials by $\pi_n(t) = \pi_{\vec{s}(n)}(t)$. Then, the following recurrence relation

$$x\pi_k(t) = \pi_{k+1}(t) + \sum_{i=0}^{m} \alpha_{k,m-i}\pi_{k-i}(t)\,, \quad k \ge 0, \tag{4.2}$$

holds, with initial conditions $\pi_0(t) = 1$ and $\pi_i(t) = 0$ for $i = -1, -2, \ldots, -m$ (see [41]).

Setting $k = 0, 1, \ldots, n-1$ in the recurrence relation (4.2), we get

$$t\begin{bmatrix} \pi_0(t) \\ \pi_1(t) \\ \vdots \\ \pi_{n-1}(t) \end{bmatrix} = H_n \begin{bmatrix} \pi_0(t) \\ \pi_1(t) \\ \vdots \\ \pi_{n-1}(t) \end{bmatrix} + \pi_n(t)\begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{bmatrix},$$

i.e.,

$$H_n\mathbf{p}_n(t) = t\,\mathbf{p}_n(t) - \pi_n(t)\mathbf{e}_n, \tag{4.3}$$

where

$$\mathbf{p}_n(t) = \begin{bmatrix}\pi_0(t) & \pi_1(t) & \ldots & \pi_{n-1}(t)\end{bmatrix}^T, \qquad \mathbf{e}_n = [0 \;\; 0 \;\; \ldots \;\; 0 \;\; 1]^T,$$

and $H_n = [h_{ij}]_{i,j=1}^{n}$ is a lower (banded) Hessenberg matrix of order n, where

$$\begin{aligned} h_{i,i+1} &= 1, \quad i = 1, \ldots, n-1; \\ h_{i,i-r} &= \alpha_{i-1,m-r}, \quad i = r+1, \ldots, n, \; r = 0, 1, \ldots, m. \end{aligned}$$

It is easy to see that $\pi_n(t) = \det(tI_n - H_n)$, where I_n is the identity matrix of the order n. In [25] we presented an effective numerical method for constructing the Hessenberg matrix H_n using a form of the discretized Stieltjes-Gautschi procedure.

These multiple orthogonal polynomials can be applied to some kinds of quadratures. Here, we consider such two applications.

4.2. Quadratures of C.F. Borges

In 1994 Borges [3] considered a problem that arises in evaluation of computer graphics illumination models. Starting with that problem, he examined the problem of numerically evaluating a set of m definite integrals taken with respect to distinct weight functions w_j, $j = 1, 2, \ldots, m$, but related by a common integrand and interval of integration

$$\int_E f(t)w_j(t)\,dt, \quad j = 1, 2, \ldots, m.$$

It was shown that it is not efficient to use a set of m Gauss-Christoffel quadrature formulas because valuable information is wasted.

In [3] Borges introduced a performance ratio as

$$R = \frac{\text{Overall degree of exactness} + 1}{\text{Number of integrand evaluation}}\,.$$

For example, for a set of m Gauss-Christoffel n-point quadrature formulas, this performance index gives

$$R = \frac{(2n-1)+1}{mn} = \frac{2}{m},$$

i.e., $R < 1$ for all $m > 2$.

Borges [3] proposed quadratures of the following form

$$\int_E f(t)\, w_j(t)\, dt \approx \sum_{\nu=1}^{n} A_{j,\nu} f(\tau_\nu), \quad j = 1, 2, \ldots, m. \tag{4.4}$$

If $A_{j,\nu}$ are determined so that (4.4) are interpolatory quadratures (degree of exactness $\leq n-1$), then $R = n/n = 1$. However, this performance ratio can be improved taking an AT system of the weights $W = \{w_1, w_2, \ldots, w_m\}$ supported on the same interval E. For a multi-index $\vec{n} = (n_1, n_2, \ldots, n_m)$ we put $n = |\vec{n}|$.

Following [3, Definition 3] an optimal set of quadratures with respect to $(W, \vec{n})$ was introduced in [25]. In that sense, the Borges set of quadratures (4.4) is optimal if and only if their weight coefficients $A_{j,\nu}$ and nodes τ_ν satisfy the following system of equations

$$\sum_{\nu=1}^{n} A_{j,\nu}\, \tau_\nu^k = \int_E t^k w_j(t)\, dt, \quad k = 0, 1, \ldots, n + n_j - 1,$$

for $j = 1, 2 \ldots, m$.

Regarding this facts, the following characterization of Borges quadratures in terms of multiple orthogonal polynomials can be given (see [25]):

Theorem 4.2. *Let W be an AT system of weight functions supported on the interval E, $\vec{n} = (n_1, n_2, \ldots, n_m)$, and $n = |\vec{n}|$. The Borges quadrature formulae* (4.4) *form an optimal set with respect to* $(W, \vec{n})$ *if and only if:*

1° *They are exact for all polynomials of degree $\leq n-1$;*

2° *The node polynomial $q_n(t) = (t-\tau_1)(t-\tau_2)\cdots(t-\tau_n)$ is the type II multiple orthogonal polynomial $\pi_{\vec{n}}$ with respect to W.*

Notice that the performance ratio for such quadratures is $R > 1$. Evidently, the nodes τ_ν, $\nu = 1, \ldots, n$, as a zeros of the type II multiple orthogonal polynomial $\pi_{\vec{n}}$, are distinct and located in E (see Theorem 4.1). The weight coefficients satisfy m systems of linear equations with Vandermonde matrix

$$V(\tau_1, \tau_2, \ldots, \tau_n) \begin{bmatrix} A_{j,1} \\ A_{j,2} \\ \vdots \\ A_{j,n} \end{bmatrix} = \begin{bmatrix} \mu_0^{(j)} \\ \mu_1^{(j)} \\ \vdots \\ \mu_{n-1}^{(j)} \end{bmatrix}, \quad j = 1, 2, \ldots, m,$$

where

$$\mu_\nu^{(j)} = \int_E t^\nu w_j(t)\, dt, \quad \nu = 0, 1, \ldots, n-1.$$

This Vandermonde matrix is non-singular and each of the previous systems always has the unique solution.

For the case of the nearly diagonal multi-indices $\vec{s}(n)$ we can compute the nodes τ_ν, $\nu = 1, \ldots, n$, as eigenvalues of the corresponding banded Hessenberg matrix H_n. Then, from (4.3) it follows that the eigenvector associated with τ_ν is given by $\mathbf{p}_n(\tau_\nu)$, where $\mathbf{p}_n(t) = \big[\pi_0(t) \;\; \pi_1(t) \;\; \ldots \;\; \pi_{n-1}(t)\big]^T$. We can use now this fact to compute the weight coefficients $A_{j,\nu}$ by requiring that each rule correctly generate the first n modified moments

$$\hat{\mu}_\nu^{(j)} = \int_E \pi_\nu(t) w_j(t)\, dt, \quad \nu = 0, 1, \ldots, n-1.$$

Let V_n be the matrix of the eigenvectors of matrix H_n, each normalized so that the first component is equal to 1, i.e.,

$$V_n = \big[\mathbf{p}_n(\tau_1) \; \mathbf{p}_n(\tau_2) \; \ldots \; \mathbf{p}_n(\tau_n)\big].$$

Thus, for determining the weight coefficients we should solve the following m systems of equations

$$V_n \begin{bmatrix} A_{j,1} \\ A_{j,2} \\ \vdots \\ A_{j,n} \end{bmatrix} = \begin{bmatrix} \hat{\mu}_0^{(j)} \\ \hat{\mu}_1^{(j)} \\ \vdots \\ \hat{\mu}_{n-1}^{(j)} \end{bmatrix}, \quad j = 1, 2, \ldots, m.$$

This efficient and stable algorithm for constructing Borges quadratures, as well as several numerical examples, were given in [25].

4.3. Birkhoff-Young quadratures and improvements

For numerical integration of analytic functions over a line segment in the complex plane, Birkhoff and Young [2] proposed a quadrature formula of the form

$$\begin{aligned} I(f) \;\; &= \int_{z_0-h}^{z_0+h} f(z)\, dz = \frac{h}{15}\big\{24 f(z_0) + 4\,[f(z_0+h) + f(z_0-h)] \\ &\qquad - [f(z_0+\mathrm{i}h) + f(z_0-\mathrm{i}h)]\big\} + R_5^{BY}(f). \end{aligned} \tag{4.5}$$

For the error term $R_5^{BY}(f)$ the following estimate [45] (see also Davis and Rabinowitz [9, p. 136])

$$|R_5^{BY}(f)| \le \frac{|h|^7}{1890} \max_{z\in S} |f^{(6)}(z)|$$

holds, where S denotes the square with vertices $z_0 + \mathrm{i}^k h$, $k = 0, 1, 2, 3$. This error estimate is about four tenths as large as the corresponding error $R_5^{ES}(f)$ for the so-called extended Simpson's rule (cf. [29, p. 124])

$$I(f) \approx \frac{h}{90}\big\{114 f(z_0) + 34\big[f(z_0+h) + f(z_0-h)\big] - \big[f(z_0+2h) + f(z_0-2h)\big]\big\},$$

for which we have

$$|R_5^{ES}(f)| \sim \frac{|h|^7}{756} |f^{(6)}(\zeta)|, \qquad 0 < \frac{\zeta - (z_0 - 2h)}{4h} < 1.$$

Without loss of generality we can consider the integration over $[-1,1]$ for analytic functions in a unit disk $\Omega = \{z : |z| \le 1\}$, so that the previous Birkhoff-Young formula (4.5) becomes

$$\int_{-1}^{1} f(z)\,dz = \frac{8}{5}f(0) + \frac{4}{15}\big[f(1)+f(-1)\big] - \frac{1}{15}\big[f(\mathrm{i})+f(-\mathrm{i})\big] + R_5(f). \quad (4.6)$$

In 1976 Lether [19] pointed out that the three point Gauss-Legendre quadrature

$$\int_{-1}^{1} f(z)\,dz = \frac{8}{9}f(0) + \frac{5}{9}\big[f(\sqrt{3/5}) + f(-\sqrt{3/5})\big] + R_3(f), \qquad (4.7)$$

which is also exact for all polynomials of degree at most five, is more precise than (4.6) and he recommended it for numerical integration. However, Tošić [39] improved the quadrature (4.6) in the form

$$\int_{-1}^{1} f(z)\,dz = Af(0) + B\big[f(r)+f(-r)\big] + C\big[f(\mathrm{i}r)+f(-\mathrm{i}r)\big] + R_5^T(f;r), \quad (4.8)$$

where

$$A = 2\left(1 - \frac{1}{5r^4}\right), \quad B = \frac{1}{6r^2} + \frac{1}{10r^4}, \quad C = -\frac{1}{6r^2} + \frac{1}{10r^4}, \quad 0 < r < 1,$$

and the error-term is given by the expression

$$R_5^T(f;r) = \left(-\frac{2}{3}r^4 + \frac{2}{7}\right)\frac{f^{(6)}(0)}{6!} + \left(-\frac{2}{5}r^4 + \frac{2}{9}\right)\frac{f^{(8)}(0)}{8!} + \cdots. \qquad (4.9)$$

Evidently, for $r = 1$ this formula reduces to (4.6) and for $r = \sqrt{3/5}$ to the Gauss-Legendre formula (4.7) (then $C = 0$). Moreover, for $r = \sqrt[4]{3/7}$ the first term on the right-hand side in (4.9) vanishes and (4.8) reduces to the modified Birkhoff-Young formula of maximum accuracy (named *MF* in [39]), with the coefficients

$$A = \frac{16}{15}, \quad B = \frac{1}{6}\left(\frac{7}{5} + \sqrt{\frac{7}{3}}\right), \quad C = \frac{1}{6}\left(\frac{7}{5} - \sqrt{\frac{7}{3}}\right),$$

and with the error-term

$$R_5^{MF}(f) = R_5^T(f; \sqrt[4]{3/7}) = \frac{1}{793800}f^{(8)}(0) + \frac{1}{61122600}f^{(10)}(0) + \cdots.$$

This formula was extended by Milovanović and Đorđević [23] to the following quadrature formula of interpolatory type

$$\begin{aligned}\int_{-1}^{1} f(z)\,dz = Af(0) &+ C_{11}\big[f(r_1)+f(-r_1)\big] + C_{12}\big[f(\mathrm{i}r_1)+f(-\mathrm{i}r_1)\big]\\ &+ C_{21}\big[f(r_2)+f(-r_2)\big] + C_{22}\big[f(\mathrm{i}r_2)+f(-\mathrm{i}r_2)\big] + R_9(f;r_1,r_2),\end{aligned}$$

where $0 < r_1 < r_2 < 1$. They proved that for

$$r_1 = r_1^* = \sqrt[4]{\frac{63 - 4\sqrt{114}}{143}} \quad \text{and} \quad r_2 = r_2^* = \sqrt[4]{\frac{63 + 4\sqrt{114}}{143}},$$

this formula reduces to a quadrature rule of the algebraic exactness $p = 13$, with the error-term

$$R_9(f; r_1^*, r_2^*) = \frac{1}{28122661066500} f^{(14)}(0) + \cdots \approx 3.56 \cdot 10^{-14} f^{(14)}(0).$$

4.4. Generalized Birkhoff-Young quadratures

In this subsection we consider a kind of generalized Birkhoff-Young quadrature formulas and give a connection with multiple orthogonal polynomials. We introduce N-point quadrature formula for weighted integrals of analytic functions in $\Omega = \{z : |z| \le 1\}$,

$$I(f) := \int_{-1}^{1} f(z)w(z)\,dz = Q_N(f) + R_N(f),$$

where $w : (-1,1) \to \mathbb{R}^+$ is an *even* positive weight function, for which all moments $\mu_k = \int_{-1}^{1} z^k w(z)\,dz$, $k = 0, 1, \ldots$, exist.

For a given fixed integer $m \ge 1$ and for each $N \in \mathbb{N}$, we put $N = 2mn+\nu$, where $n = [N/2m]$ and $\nu \in \{0, 1, \ldots, 2m-1\}$. We define the node polynomial

$$\omega_N(z) = z^\nu p_{n,\nu}(z^{2m}) = z^\nu \prod_{k=1}^{n} (z^{2m} - r_k), \quad 0 < r_1 < \cdots < r_n < 1, \tag{4.10}$$

and consider the corresponding interpolatory quadrature rule Q_N of the form

$$Q_N(f) = \sum_{j=0}^{\nu-1} C_j f^{(j)}(0) + \sum_{k=1}^{n} \sum_{j=1}^{m} A_{k,j} \left[f\left(x_k e^{\mathrm{i}\theta_j}\right) + f\left(-x_k e^{\mathrm{i}\theta_j}\right) \right],$$

where

$$x_k = \sqrt[2m]{r_k}, \quad k = 1, \ldots, n; \quad \theta_j = \frac{(j-1)\pi}{m}, \quad j = 1, \ldots, m.$$

If $\nu = 0$, the first sum in $Q_N(f)$ is empty.

Theorem 4.3. *Let m be a fixed positive integer and w be an even positive weight function w on $(-1,1)$, for which all moments $\mu_k = \int_{-1}^{1} z^k w(z)\,dz$, $k \ge 0$, exist. For any $N \in \mathbb{N}$ there exists a unique interpolatory quadrature $Q_N(f)$ with a maximal degree of exactness $d_{\max} = 2(m+1)n + s$, where*

$$n = \left[\frac{N}{2m}\right], \quad \nu = N - 2mn, \quad s = \begin{cases} \nu - 1, & \nu \ \text{even}, \\ \nu, & \nu \ \text{odd}. \end{cases} \tag{4.11}$$

The node polynomial (4.10) *is characterized by the following orthogonality relations*

$$\int_0^1 t^k p_{n,\nu}(t^m) t^{s/2} w(\sqrt{t})\,dt = 0, \quad k = 0, 1 \ldots, n-1. \tag{4.12}$$

Proof. For a given $N \in \mathbb{N}$ and a fixed $m \in \mathbb{N}$, suppose that $f \in \mathcal{P}_d$, where $d \ge N = 2mn + \nu$, with $n = [N/2m]$ and $\nu = N - 2mn$. Then, it can be expressed in the form

$$f(z) = u(z)\omega_N(z) + v(z) = u(z) z^\nu p_{n,\nu}(z^{2m}) + v(z), \quad u \in \mathcal{P}_{d-N},\ v \in \mathcal{P}_{N-1},$$

from which, by an integration with respect to the weight function w, we get

$$I(f) = \int_{-1}^{1} u(z) z^{\nu} p_{n,\nu}(z^{2m}) w(z)\, dz + I(v).$$

Since our quadrature is interpolatory and $v(z) = f(z)$ at the zeros of ω_N, we have $I(v) = Q_N(v) = Q_N(f)$. Thus, the quadrature formula $Q_N(f)$ has a maximal degree of precision if and only if

$$\int_{-1}^{1} u(z) z^{\nu} p_{n,\nu}(z^{2m}) w(z)\, dz = 0$$

for a maximal degree of the polynomial $u \in \mathcal{P}_{d-N}$. According to the values of ν, this “orthogonality condition” can be represented in the form

$$\int_{-1}^{1} h(z^2) z^{s+1} p_{n,\nu}(z^{2m}) w(z)\, dz = 0, \quad h \in \mathcal{P}_{n-1}, \tag{4.13}$$

which means that the maximal degree of the polynomial $u \in \mathcal{P}_{d-N}$ is

$$d_{\max} - N = \begin{cases} 2n-1, & \nu \text{ is even}, \\ 2n, & \nu \text{ is odd}, \end{cases}$$

i.e., $d_{\max} = 2(m+1)n + s$, where s is defined by (4.11).

Finally, by substitution $z^2 = t$, the orthogonality conditions (4.13) can be expressed in the form (4.12). □

Regarding (4.12) the polynomial $t \mapsto p_{n,\nu}(t^m)$ (of degree mn) is orthogonal to $\mathcal{P}_n$ with respect to the weight function $t^{s/2} w(\sqrt{t})$ on $(0,1)$, and it can be interpreted in terms of multiple orthogonal polynomials.

Theorem 4.4. *Under conditions of the previous theorem, for any $N \in \mathbb{N}$ there exists a unique interpolatory quadrature $Q_N(f)$, with a maximal degree of exactness $d_{\max} = 2(m+1)n + s$, if and only if the polynomial $p_{n,\nu}(t)$ is the type II multiple orthogonal polynomial $\pi_{\vec{n}}(t)$, with respect to the weights $w_j(t) = t^{(s+2j)/(2m)-1} w(t^{1/(2m)})$, with $n_j = 1 + \left[\frac{n-j}{m}\right]$, $j = 1, \ldots, m$.*

Proof. Evidently, the conditions (4.12) are equivalent to

$$\int_0^1 t^{k/m} p_{n,\nu}(t) t^{(s+2)/(2m)-1} w(t^{1/(2m)})\, dt = 0, \quad k = 0, 1, \ldots, n-1.$$

Now, putting $k = m\ell + j - 1$, $\ell = [k/m]$, we get for each $j = 1, \ldots, m$,

$$\int_0^1 t^{\ell} p_{n,\nu}(t) w_j(t)\, dt = 0, \quad \ell = 0, 1 \ldots, n_j - 1,$$

where

$$w_j(t) = t^{(s+2j)/(2m)-1} w(t^{1/(2m)}) \quad \text{and} \quad n_j = 1 + \left[\frac{n-j}{m}\right].$$

Notice that these weight functions, defined on the same interval $E_1 = E_2 = \cdots = E_m = E = (0,1)$, can be expressed in the form $w_j(t) = t^{(j-1)/m} w_1(t)$, $j = 1, \ldots, m$, where $w_1(t) = t^{(s+2)/(2m)-1} w(t^{1/(2m)})$. Since the Müntz system $\{t^{k+(j-1)/m}\}$, $k = 0, 1, \ldots, n_j - 1$; $j = 1, \ldots, m$, is a Chebyshev system on $[0,\infty)$, and also on $E=(0,1)$, and $w_1(t)>0$ on E, we conclude that $\{w_j,\, j=1,\ldots,m\}$ is an AT system on E.

Therefore, according to Theorem 4.1, the unique type II multiple orthogonal polynomial $p_{n,\nu}(t)=\pi_{\vec{n}}(t)$ has exactly

$$|\vec{n}| := \sum_{j=1}^{m} n_j = \sum_{j=1}^{m}\left(1+\left[\frac{n-j}{m}\right]\right)=n$$

zeros in $(0,1)$. □

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