QUADRATURE WITH MULTIPLE NODES, POWER ORTHOGONALITY, AND MOMENT-PRESERVING SPLINE APPROXIMATION, PART II

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The paper deals with new contributions to the theory of the Gauss quadrature formulas with multiple nodes that are published after 2001, including numerical construction, error analysis and applications. The first part was published in *Numerical analysis 2000, Vol. V, Quadrature and orthogonal polynomials* (W. Gautschi, F. Marcellan, and L. Reichel, eds.) [J. Comput. Appl. Math. **127** (2001), no. 1-2, 267–286].

1. INTRODUCTION

Gauss quadrature is a popular approach to approximate the value of an integral

$$I(f) = \int_{\mathbb{R}} f(t) \, d\lambda(t), \tag{1}$$

where $d\lambda(t)$ is a given nonnegative measure with support on the real axis, such that

$$\langle f, g \rangle = I(fg)$$

is an inner product on $\mathcal{P}$, the space of algebraic polynomials with real coefficients. The formula

$$I(f) = \sum_{\nu=1}^{n} A_\nu f(\tau_\nu) + R(f) \tag{2}$$

is called the Gauss quadrature if its (algebraic) degree of exactness is $2n-1$, i.e., if $R(f) = 0$ for all f from $\mathcal{P}_{2n-1}$, the space of polynomials of degree at most $2n-1$. It is easy to see that a degree of exactness of the quadrature (2) cannot be larger than $2n-1$.

This approach can be generalized in several directions. For example, to approximate an arbitrary linear functional on $\mathcal{P}$, or to be exact on certain space of rational functions. Here we consider the following generalization of the Gauss quadrature: Instead of (2), we use the formula of the form

$$(3) \qquad Q_n(f) = \sum_{\nu=1}^{n} \sum_{i=0}^{m_\nu - 1} A_{i,\nu} f^{(i)}(\tau_\nu)$$

to approximate $I(f)$. In other words, we assume that the nodes

$$\tau_1 < \tau_2 < \cdots < \tau_n$$

may have multiplicities larger than one. Naturally, we ask the question what is the maximal possible degree of exactness for the formula (3). For any choice of (different) nodes τ_ν, $\nu = 1, \ldots, n$, and their multiplicities m_ν, such that $m_1 + \cdots + m_n = \ell$, it is possible to achieve that the quadrature (3) is exact for any f from $\mathcal{P}_{\ell-1}$. As shown in [**11**, Theorem 5.1], it is necessary and sufficient to take

$$(4) \qquad A_{i,\nu} = I(h_{i,\nu}),$$

where $h_{i,\nu}$ are polynomials from $\mathcal{P}_{\ell-1}$ such that

$$h_{i,\nu}^{(t)}(\tau_k) = 1 \quad \text{for } \tau_k = \tau_\nu \text{ and } t = i,$$
$$h_{i,\nu}^{(t)}(\tau_k) = 0 \quad \text{for } \tau_k \neq \tau_\nu \text{ or } t \neq i,$$

with $k = 1, 2, \ldots, n$, and $t = 0, 1, \ldots, m_\nu - 1$. In this case we say that the quadrature (3) is *interpolatory*, since it can be obtained by applying the integral I on the generalized (Hermite) interpolating polynomial for the integrand f at the nodes τ_ν of the multiplicities m_ν. The degree of exactness of the interpolatory quadrature (3) is $\ell - 1 + k$ if and only if the polynomial

$$(5) \qquad \omega_\ell(t) = (t - \tau_1)^{m_1}(t - \tau_2)^{m_2} \ldots (t - \tau_n)^{m_n}$$

is orthogonal to $\mathcal{P}_{k-1}$, i.e.,

$$I(t^j \omega_\ell(t)) = 0, \quad j = 0, 1, \ldots, k - 1.$$

Indeed, any polynomial q from $\mathcal{P}_{\ell+k-1}$ can be written as $q(t) = r(t)\omega_\ell(t) + s(t)$, with $r \in \mathcal{P}_{k-1}$ and $s \in \mathcal{P}_{\ell-1}$. The orthogonality condition $\omega_\ell \perp \mathcal{P}_{k-1}$ implies

$$I(q) = I(r\omega_\ell + s) = I(s) = Q(s) = Q(s + r\omega_\ell) = Q(q).$$

On the other hand, if $I(q) = Q(q)$ for all q from $\mathcal{P}_{\ell+k-1}$, then

$$I(t^j \omega_\ell(t)) = Q(t^j \omega_\ell(t)) = 0, \quad j = 0, 1, \ldots, k-1.$$

Recalling the fact that $\langle f, g \rangle = I(fg)$ is an inner product on $\mathcal{P}$, the largest possible value of k is m, where m is number of odd numbers among m_ν, $\nu = 1, \ldots, n$. For example, if only m_n is even, then ω_ℓ cannot be orthogonal to the polynomial $\prod_{i=1}^{n-1}(t - \tau_i)$.

Remark. The quadrature formula (3) can be also used to approximate integrals $\int_{\mathbb{R}} f(t) \, d\lambda(t)$, where $d\lambda(t)$ is not a positive measure. In such a case, the degree of exactness can be larger than $\ell + m - 1$.

Definition 1.1. We say that the quadrature formula with real weights $A_{i,\nu}$ and real nodes $\tau_1 < \cdots < \tau_n$ with preassigned multiplicities $m_1, \ldots, m_n$

$$(6) \qquad \int_{\mathbb{R}} f(t) \, d\lambda(t) = \sum_{\nu=1}^{n} \sum_{i=0}^{m_\nu - 1} A_{i,\nu} f^{(i)}(\tau_\nu) + R(f)$$

is a Gauss quadrature with multiple nodes if

$$R(f) = 0, \quad f \in \mathcal{P}_{\ell+m-1},$$

where $d\lambda$ is an arbitrary measure, $\ell = m_1 + \cdots + m_n$, and m is a number of odd multiplicities m_ν.

For obvious reasons, particular attention is paid to the case when all multiplicities are odd:

$$(7) \qquad I(f) = \sum_{\nu=1}^{n} \sum_{i=0}^{2s_\nu} A_{i,\nu} f^{(i)}(\tau_\nu) + R(f),$$

$$R(f) = 0, \quad f \in \mathcal{P}_{\ell+n-1}, \quad \ell = 2(s_1 + \cdots + s_n) + n.$$

The quadrature (7) is called a Chakalov-Popoviciu quadrature, in honor of Chakalov and Popoviciu who first considered such quadratures independently of each other; see [6], [7], [86]. The special case $s = s_1 = \cdots = s_n$ of (7), i.e.,

$$(8) \qquad I(f) = \sum_{\nu=1}^{n} \sum_{i=0}^{2s} A_{i,\nu} f^{(i)}(\tau_\nu) + R(f) \quad (s \geq 0),$$

is usually referred to as a Gauss-Turán quadrature [97].

If some of the nodes in (3) are preassigned, then the interpolatory quadrature (3) has the form

$$(9) \qquad \widetilde{Q}(f) = \sum_{\nu=1}^{n_1} \sum_{i=0}^{m_\nu - 1} A_{i,\nu} f^{(i)}(\tau_\nu) + \sum_{\mu=1}^{n_2} \sum_{j=0}^{r_\mu - 1} B_{j,\mu} f^{(j)}(\alpha_\mu),$$

where $\alpha_1, \ldots, \alpha_{n_2}$ are preassigned nodes and $n = n_1 + n_2$. Let

$$m = m_1 + \cdots + m_{n_1}, \qquad r = r_1 + \cdots + r_{n_2},$$

and

(10)
$$\widetilde{\omega}_m(t) = \prod_{\nu=1}^{n_1} (t - \tau_\nu)^{m_\nu}, \quad \varphi_r(t) = \prod_{\mu=1}^{n_2} (t - \alpha_\mu)^{r_\mu}.$$

We have $I(f) = \widetilde{Q}(f)$ for all $f \in \mathcal{P}_{m+r-1+k}$ if and only if

(11)
$$\int_{\mathbb{R}} t^j \widetilde{\omega}_m(t) \varphi_r(t) \, \mathrm{d}\lambda(t) = 0, \quad j = 0, \ldots, k-1.$$

If we define the new measure $\mathrm{d}\mu(t) = \varphi_r(t) \, \mathrm{d}\lambda(t)$, then the orthogonality conditions (11) can be written in the form

(12)
$$\int_{\mathbb{R}} t^j \widetilde{\omega}_m(t) \, \mathrm{d}\mu(t) = 0, \quad j = 0, 1, \ldots, k-1.$$

Usually, $\mathrm{d}\mu$ is not a positive measure. If we require $k \geq n_1$, then we refer to (9) as the Gauss-Stancu quadrature. The special case of the Gauss-Stancu quadrature when $n_1 = n_2 + 1$, $r_1 = \cdots = r_{n_2} = 2s + 1$ and $\varphi_r \perp \mathcal{P}_{n_2-1}$ with respect to $\mathrm{d}\lambda$ is known as the Kronrod extension of the Gauss-Turan quadrature

$$\sum_{\mu=1}^{n_2} \sum_{j=0}^{2s} C_{j,\mu} f^{(j)}(\alpha_\mu).$$

This paper is written as a follow-up of [47] published in 2001, where a survey of the Gauss quadrature with multiple nodes was given, including many historical remarks. Thus we will not repeat them here, but rather focus on the results published after 2001. The paper is organized as follows. For completeness, we discuss in Section 2 the question of existence and uniqueness of the Gauss quadrature with multiple nodes. This is closely related to the theory of so-called σ-orthogonal polynomials. In Section 3 we present a numerical procedure for computing the nodes and weights in (7). Section 4 is devoted to the error term $R(f)$ for an analytic function f. Most of results about Gauss quadrature with multiple nodes published after 2001 deal with analytically derived error bounds (estimates). They are presented in Section 5. Some applications, particularly those to moment-preserving spline approximation, are presented in Section 6.

2. σ-ORTHOGONAL POLYNOMIALS

Existence and uniqueness of Chakalov-Popoviciu quadrature (7) for integrals with a positive measure is shown by Ghizzetti and Ossicini in [25]. It means that the following problem has an unique solution.

Problem I: Given a positive measure $\mathrm{d}\lambda$ such that $\langle f, g \rangle = \int_{\mathbb{R}} f g \, \mathrm{d}\lambda$ is an inner product on $\mathcal{P}$, and a sequence of nonnegative integers $\sigma = (s_1, s_2, \ldots)$, find n real numbers $\tau_1^{(n,\sigma)} < \tau_2^{(n,\sigma)} < \cdots < \tau_n^{(n,\sigma)}$ satisfying

$$(13) \qquad \int_{\mathbb{R}} t^j \left[\prod_{i=1}^{n} \left(t - \tau_i^{(n,\sigma)} \right) \right]^{2s_i + 1} \mathrm{d}\lambda(t) = 0, \quad j = 0, 1, \ldots, n-1.$$

The solution of Problem I defines the nth degree polynomial

$$\pi_{n,\sigma}(t) = \prod_{i=1}^{n} \left(t - \tau_i^{(n,\sigma)} \right), \quad n = 1, 2, \ldots,$$

that is known as the σ-orthogonal polynomial.

Thus, σ-orthogonal polynomials are unique when $\tau_1^{(n,\sigma)} < \tau_2^{(n,\sigma)} < \cdots < \tau_n^{(n,\sigma)}$ is imposed, with corresponding multiplicities $m_i = 2s_i + 1$, $i = 1, \ldots, n$. Otherwise, the number of distinct σ-polynomials is

$$\frac{n!}{k_1! k_2! \cdots k_q!}$$

for some q $(1 \le q \le n)$, where k_i is the number of nodes of multiplicity $m_j = i$, each node counted exactly once, $\sum_{i=1}^{q} k_i = n$. For example, in the case $n = 4$, with multiplicities $3, 3, 3, 5$, we have four different σ-polynomials, which correspond to $\sigma = (1, 1, 1, 2)$, $(1, 1, 2, 1)$, $(1, 2, 1, 1)$, and $(2, 1, 1, 1)$.

The special case $s = s_1 = s_2 = \cdots$ gives so-called s-orthogonal polynomials $\pi_{n,s}$ satisfying

$$(14) \qquad \int_{\mathbb{R}} \pi_{j,s}(t) [\pi_{n,s}(t)]^{2s+1} \, \mathrm{d}\lambda(t) = 0, \quad j = 0, 1, \ldots, n-1.$$

For $s = 0$, (14) reduces to the standard orthogonality conditions.

In the definition of σ-orthogonal polynomials it is tacitly assumed that all their zeros are real and simple. In other words, polynomials with complex or multiple zeros are disqualified to be σ-orthogonal by definition. This is not the case if (14) is used as a definition of s-orthogonal polynomials. However, it cannot lead to confusion since the monic nth degree polynomial whose zeros are the solution of the proper version of Problem I is the only monic nth degree polynomial satisfying (14). As in the case of standard orthogonal polynomials, the zeros of $\pi_{n,s}$ and $\pi_{n+1,s}$ interlace. For more properties of s-orthogonal polynomials see [**47**, Section 2]. There are only a couple of measures when explicit formulas for corresponding s-orthogonal polynomials are known. All these measures are of the form $\mathrm{d}\lambda(t) = w(t) \, \mathrm{d}t$ on $[-1, 1]$:

- If $w_1(t) = (1 - t^2)^{-1/2}$, then for all s, $\pi_{n,s}(t) = \widehat{T}_n(t) = 2^{1-n} T_n(t)$, where $T_n(t) = \cos(n \arccos t)$ is the Chebyshev polynomial of the first kind; see [**1**].

- If $w_2(t) = (1 - t^2)^{1/2+s}$, then $\pi_{n,s} = \widehat{U}_n(t) = 2^{-n}U_n(t)$, where $U_n(\cos\theta) = \sin(n+1)\theta/\sin\theta$ is the Chebyshev polynomial of the second kind; see [**74**].

- If $w_3(t) = (1 - t)^{-1/2}(1 + t)^{1/2+s}$, then $\pi_{n,s} = \widehat{V}_n(t) = 2^{-n}V_n(t)$, where $V_n(\cos\theta) = \cos(n + \frac{1}{2})\theta/\cos\frac{1}{2}\theta$ is the Chebyshev polynomial of the third kind; see [**74**].

- If $w_4(t) = (1 + t)^{-1/2}(1 - t)^{1/2+s}$, then $\pi_{n,s} = \widehat{W}_n(t) = 2^{-n}W_n(t)$, where $W_n(\cos\theta) = \sin(n + \frac{1}{2})\theta/\sin\frac{1}{2}\theta$ is the Chebyshev polynomial of the fourth kind; see [**74**].

- If $w_{n,\mu}(t) = |U_{n-1}(t)/n|^{2\mu+1}(1 - t^2)^\mu$, with $\mu > -1$, then $\pi_{n,s}(t) = \widehat{T}_n(t) = 2^{1-n}T_n(t)$ for all s; see [**31**].

We refer to the weight functions w_1, w_2, w_3 and w_4 as the Chebyshev weight functions of the first, second, third and fourth kind. Note that w_2, w_3 and w_4 depend on s. The weight functions $w_{n,\mu}$ do not depend on s, but depend on n. This class of weight functions is known as Gori-Micchelli weight functions. As for the σ-orthogonal polynomials, the corresponding theory is not yet developed.

The previous discussion cannot be applied to the Gauss-Stancu quadrature since, in general, the measure $d\mu$ in (12) is not positive, i.e., $\langle f, g \rangle = \int_{\mathbb{R}} fg\,d\mu$ is not an inner product on $\mathcal{P}$. Even if the polynomial $\widetilde{\omega}_m$ satisfying (12) for $k = n_1$ exists, all its zeros are not necessarily real. This happens, for example, in the case of the standard Gauss-Kronrod quadrature with Gegenbauer weight function $(1-t^2)^{\ell-1/2}$ for $\ell > 3$; see [**84**]. However, if φ_r does not change sign on the support of $d\lambda$ and all numbers m_ν are odd, then we can claim the existence and uniqueness of Gauss-Stancu quadrature. It can be done in the case of the Lobatto extension of the Chakalov-Popoviciu quadrature

$$(15) \quad \int_{-1}^{1} f(t)w(t)\,dt = \sum_{j=0}^{r_1-1} C_j f^{(j)}(-1) + \sum_{\nu=1}^{n-2}\sum_{i=0}^{m_\nu-1} A_{i,\nu} f^{(i)}(\tau_\nu) + \sum_{j=0}^{r_2-1} B_j f^{(j)}(1),$$

where we assume that $d\lambda$ is an absolutely continuous measure on $[-1, 1]$, and w is corresponding weight function. If we omit in (15) the first or the third sum on the right-hand side, i.e., if we preassign only one endpoint of the interval $(-1, 1)$, we get the Radau extension of the Chakalov-Popoviciu quadrature.

3. NUMERICAL CONSTRUCTION

In this section we consider the numerical construction of s- and σ-orthogonal polynomials, as well as the calculation the coefficients $A_{i,\nu}$ in the quadrature with multiple nodes (6), i.e., in the Gauss-Turán and the Chakalov-Popoviciu quadrature formulas (8) and (7). These methods have enabled progress in the theory of quadratures with multiple nodes.

3.1. Construction of s- and σ-orthogonal polynomials

The first attempt in the numerical construction of s-orthogonal polynomials with respect to an even weight function on a symmetric interval $(-c, c)$ was given by Vincenti in 1986 [**100**], describing an iterative process for computing their coefficients. This process was applied to Legendre s-orthogonal polynomials and corresponding numerical results for coefficients were obtained only for low degrees of polynomials n and relatively small values of s, because the process becomes numerically unstable when n and s increase.

At the Third Conference on Numerical Methods and Approximation Theory (Niš, 18–21 August, 1987) (see [**45**]) one of us presented a stable method for numerically constructing s-orthogonal polynomials and their zeros. It uses an iterative method with quadratic convergence based on a discretized Stieltjes-Gautschi procedure and the Newton-Kantorovič method. This approach opened the door to the numerical construction of not only s and σ-orthogonal polynomials, but also to the quadrature rules of Gauss-Turán and other generalized rules with multiple nodes, mentioned in the previous sections.

The basic idea of this method for constructing s-orthogonal polynomials with respect to the measure $\mathrm{d}\lambda(t)$ on the real line $\mathbb{R}$ is a reinterpretation of the "*orthogonality conditions*," given by (14) or (13), i.e.,

$$\int_{\mathbb{R}} t^j [\pi_{n,s}(t)]^{2s+1} \, \mathrm{d}\lambda(t) = 0, \quad j = 0, 1, \ldots, n-1,$$

in the following form

(16)
$$\int_{\mathbb{R}} t^j \pi_{n,s}(t) \, \mathrm{d}\mu_{n,s}(t) = 0, \quad j = 0, 1, \ldots, n-1,$$

where $\mathrm{d}\mu_{n,s}(t) = [\pi_{n,s}(t)]^{2s} \, \mathrm{d}\lambda(t)$ is a new positive measure, implicitly defined for given n and s. It is clear that for such a measure $\mathrm{d}\mu_{n,s}(t)$ (n and s are fixed), there exists a unique sequence of (monic) polynomials $\{\pi_k^{(n,s)}\}_{k\geq 0}$ $(\deg \pi_k^{(n,s)} = k)$, such that

(17)
$$\int_{\mathbb{R}} t^j \pi_k^{(n,s)}(t) \, \mathrm{d}\mu_{n,s}(t) = 0, \quad j = 0, 1, \ldots, k-1.$$

Thus, $\{\pi_k^{(n,s)}\}_{k\geq 0}$ is a sequence of standard monic polynomials orthogonal with respect to the measure $\mathrm{d}\mu_{n,s}(t)$ on $\mathbb{R}$. Due to the unicity of this sequence, by comparing (17) with (16), we conclude that its nth member must be the s-orthogonal polynomial, i.e.,

$$\pi_{n,s}(t) = \pi_n^{(n,s)}(t).$$

For a given $s \in \mathbb{N}$ and each $n = 0, 1, 2, \ldots$, this construction is presented in Table 1, whose diagonal (boxed) elements are, in fact, the s-orthogonal polynomials, i.e., $\pi_n^{(n,s)} = \pi_{n,s}$, $n = 0, 1, 2, \ldots$.

Table 1: Construction of s-orthogonal polynomials

n	$\mathrm{d}\mu_{n,s}(t)$	Orthogonal polynomials				
0	$[\pi_{0,s}(t)]^{2s}\,\mathrm{d}\lambda(t)$	$\boxed{\pi_0^{(0,s)}}$				
1	$[\pi_{1,s}(t)]^{2s}\,\mathrm{d}\lambda(t)$	$\pi_0^{(1,s)}$	$\boxed{\pi_1^{(1,s)}}$			
2	$[\pi_{2,s}(t)]^{2s}\,\mathrm{d}\lambda(t)$	$\pi_0^{(2,s)}$	$\pi_1^{(2,s)}$	$\boxed{\pi_2^{(2,s)}}$		
3	$[\pi_{3,s}(t)]^{2s}\,\mathrm{d}\lambda(t)$	$\pi_0^{(3,s)}$	$\pi_1^{(3,s)}$	$\pi_2^{(3,s)}$	$\boxed{\pi_3^{(3,s)}}$	
4	$[\pi_{4,s}(t)]^{2s}\,\mathrm{d}\lambda(t)$	$\pi_0^{(4,s)}$	$\pi_1^{(4,s)}$	$\pi_2^{(4,s)}$	$\pi_3^{(4,s)}$	$\boxed{\pi_4^{(4,s)}}$
$\vdots$						

As we can see, for a fixed n, the polynomials π_k ($\equiv \pi_k^{(n,s)}$), $k = 0, 1, \ldots$, from one row in Table 1, are implicitly defined, because the measure $\mathrm{d}\mu_{n,s}(t)$ depends on $\pi_{n,s}(t)$. However, they satisfy the usual three-term recurrence relation with coefficients α_k ($\equiv \alpha_k(n,s)$) and β_k ($\equiv \beta_k(n,s)$), $k \geq 0$, i.e.,

$$
\begin{aligned}
(18) \qquad \pi_{k+1}(t) &= (t - \alpha_k)\pi_k(t) - \beta_k \pi_{k-1}(t), \quad k = 0, 1, \ldots, \\
\pi_{-1}(t) &= 0, \quad \pi_0(t) = 1,
\end{aligned}
$$

where, because of orthogonality,

$$
(19) \qquad \alpha_k = \frac{(t\pi_k, \pi_k)}{(\pi_k, \pi_k)}, \quad \beta_k = \frac{(\pi_k, \pi_k)}{(\pi_{k-1}, \pi_{k-1})},
$$

where

$$
(20) \qquad (p, q) = (p, q)_{\mathrm{d}\mu_{n,s}} = \int_{\mathbb{R}} p(t)q(t)\,\mathrm{d}\mu_{n,s}(t),
$$

and, by convention, $\beta_0 = (1, 1) = \int_{\mathbb{R}} \mathrm{d}\mu_{n,s}(t)$.

Knowing the coefficients α_k and β_k, for $k = 0, 1, \ldots, n-1$, gives us access to the first $n + 1$ orthogonal polynomials $\pi_0, \pi_1, \ldots, \pi_n$. Here, we are interested only in the last one, i.e., $\pi_n \equiv \pi_{n,s}$. Unfortunately, in this case the discretized Stieltjes-Gautschi procedure cannot be applied directly, because the measure $\mathrm{d}\mu_{n,s}(t)$ involves the unknown s-orthogonal polynomial $\pi_{n,s}$. However, these recurrence coefficients for $k \leq n - 1$ are solutions of the following system of nonlinear equations

$$
\begin{aligned}
(21) \qquad f_{2k+1} &\equiv \int_{\mathbb{R}} (\alpha_k - t)\pi_k^2(t)\pi_n^{2s}(t)\,\mathrm{d}\lambda(t) = 0, && k = 0, 1, \ldots, n-1, \\
f_{2k} &\equiv \int_{\mathbb{R}} \left[\beta_k \pi_{k-1}^2(t) - \pi_k^2(t)\right]\pi_n^{2s}(t)\,\mathrm{d}\lambda(t) = 0, && k = 1, 2, \ldots, n-1,
\end{aligned}
$$

obtained from Darboux's formulae (19).

The previous reinterpretation of the "*orthogonality conditions*" (14) in terms of the ordinary orthogonality, as well as the method for solving the system of $2n$ nonlinear equations (21), using the Newton-Kantorovič method, were given in [**45**]. All these integrals in (21), as well as the ones in the elements of the Jacobian, can be computed exactly, except for rounding errors, by using a Gauss-Christoffel quadrature formula with respect to the measure $d\lambda(t)$, taking $N = (s+1)n$ nodes. Notice that the partial derivatives $a_{k,\nu} = \partial\pi_k/\partial\alpha_\nu$ and $b_{k,\nu} = \partial\pi_k/\partial\beta_\nu$ satisfy the the same recurrence relation as π_k, but with other (delayed) initial values.

Thus, for all calculations we use only the fundamental three-term recurrence relation (18) and the Gauss-Christoffel quadrature rule with respect to the measure $d\lambda(t)$.

As usual, the main problem are starting values for $\alpha_k^{[0]} = \alpha_k^{[0]}(n, s)$ and $\beta_k^{[0]} = \beta_k^{[0]}(n, s)$ in the Newton-Kantorovič iterative process. In [**45**] (see also [**19**] and [**47**]) we proposed to take the values obtained for $n-1$, i.e., $\alpha_k^{[0]} = \alpha_k(n-1, s)$ and $\beta_k^{[0]} = \beta_k(n-1, s)$, $k \le n-2$, and the corresponding extrapolated values for $\alpha_{n-1}^{[0]}$ and $\beta_{n-1}^{[0]}$. In the case $n = 1$ we have only one nonlinear equation $\int_{\mathbb{R}}(t - \alpha_0)^{2s+1}\,d\lambda(t) = 0$.

In the case of the Laguerre and Hermite weight functions, Gautschi [**16**] recently presented procedures and corresponding Matlab software for generating Gauss-Turán quadrature rules to arbitrarily high accuracy. The initial approximations have been taken sufficiently accurate to be capable of producing n-point quadrature formulae for n as large as 42 in the case of the Laguerre weight function, and 90 in the case of the Hermite weight function.

In the general case, a more convenient procedure for solving (21) is to apply a method of continuation in relation to the corresponding problem with $s = 0$ (or even better in relation to the problem with some smaller s, for example $s - 1$).

Following the previous idea, Gori, Lo Cascio and Milovanović [**33**] developed the corresponding iterative method for the construction of σ-orthogonal polynomials. In this case, the corresponding reinterpretation of the "*orthogonality conditions*" (13) leads to the conditions

$$(22) \qquad \int_{\mathbb{R}} t^j \pi_k^{(n,\sigma)}(t)\,d\mu^{(n,\sigma)}(t) = 0, \quad j = 0, 1, \ldots, k-1,$$

where

$$(23) \qquad d\mu^{(n,\sigma)}(t) = \prod_{\nu=1}^{n}(t - \tau_\nu^{(n,\sigma)})^{2s_\nu}\,d\lambda(t),$$

and we conclude that $\{\pi_k^{(n,\sigma)}\}$ is a sequence of (standard) orthogonal polynomials with respect to the measure $d\mu^{(n,\sigma)}(t)$, so that $\pi_n^{(n,\sigma)}(\cdot)$ is the desired σ-orthogonal polynomial $\pi_{n,\sigma}(\cdot)$. Unfortunately, the same procedure as in the case of s-orthogonal polynomials cannot be applied. Namely, the determination of the Jacobian requires the partial derivatives of the zeros $\tau_k^{(n,\sigma)}$ with respect to α_ν and

β_ν, which is not possible in an analytic form. Therefore in [**33**], it was replaced by a discrete analogue of the Newton-Kantorovič method (a version of the secant method). The convergence of such a method is superlinear and strongly depends on the choice of the starting points.

An alternative approach with quadratic convergence was given in 2004 by Milovanović, Spalević and Cvetković [**64**] (see also [**88**]). It can be used in constructions for measures with the bounded and unbounded supports.

For a given sequence $\sigma = (s_1, s_2, \ldots)$, the orthogonality conditions (22) can be rewritten as the following system of nonlinear equations

$$(24) \qquad F_j(\tau_1, \ldots, \tau_n) \equiv \int_{\mathbb{R}} p_{j-1}(t)\pi_{n,\sigma}(t)\, \mathrm{d}\mu^{(n,\sigma)}(t) = 0, \quad j = 1, \ldots, n,$$

where the measure $\mathrm{d}\mu^{(n,\sigma)}(t)$ is given by (23), and, instead of monomials $\{1, t, \ldots\}$, we take the sequence of orthonormal polynomials $\{p_j\}$, with respect to the measure $\mathrm{d}\lambda(t)$ on $\mathbb{R}$, which satisfy the three-term recurrence relation

$$\sqrt{\beta_{j+1}}\, p_{j+1}(t) + \alpha_j p_j(t) + \sqrt{\beta_j}\, p_{j-1}(t) = t p_j(t), \quad j = 0, 1, \ldots,$$

with $p_{-1}(t) = 0$ and $p_0(t) = 1/\sqrt{\beta_0}$, where $\beta_0 = \int_{\mathbb{R}} \mathrm{d}\lambda(t)$.

The nonlinear system of equations (24) can be written in matrix form as

$$\mathbf{F}(\mathbf{t}) = \begin{bmatrix} \mathbf{F}_1(\mathbf{t}) & \ldots & \mathbf{F}_n(\mathbf{t}) \end{bmatrix}^T = \mathbf{0},$$

where $\mathbf{t} = [\tau_1 \ \ldots \ \tau_n]^T$. If

$$W = W(\mathbf{t}) = \begin{bmatrix} w_{j,k} \end{bmatrix}_{n \times n} = \left[\frac{\partial F_j}{\partial \tau_k} \right]_{n \times n}$$

is the corresponding Jacobian of $\mathbf{F}(\mathbf{t})$, then for finding the zeros of the σ-orthogonal polynomial $\pi_{n,\sigma}(t)$ we can apply the Newton-Kantorovič method [**44**, p. 239]

$$(25) \qquad \mathbf{t}^{(m+1)} = \mathbf{t}^{(m)} - W^{-1}(\mathbf{t}^{(m)})\mathbf{F}(\mathbf{t}^{(m)}), \quad m = 0, 1, \ldots,$$

where $\mathbf{t}^{(m)} = \begin{bmatrix} \tau_1^{(m)} & \ldots & \tau_n^{(m)} \end{bmatrix}^T$.

The elements of the Jacobian, in this case, are

$$w_{j,k} = \frac{\partial F_j}{\partial \tau_k} = -(2s_k + 1) \int_{\mathbb{R}} \frac{p_{j-1}(t)}{t - \tau_k} \left(\prod_{\nu=1}^{n} (t - \tau_\nu)^{2s_\nu + 1} \right) \mathrm{d}\lambda(t), \quad j, k = 1, \ldots, n,$$

and they can be calculated by the recurrence relation [**64**]

$$\sqrt{\beta_{j+1}}\, w_{j+2,k} = (\tau_k - \alpha_j)w_{j+1,k} - \sqrt{\beta_j}\, w_{j,k} - (2s_k + 1)F_{j+1}, \quad j = 0, 1, \ldots, n-2,$$

where $w_{0.k} = 0$ and

$$(26) \qquad w_{1,k} = -\frac{2s_k + 1}{\sqrt{\beta_0}} \int_{\mathbb{R}} (t - \tau_k)^{2s_k} \left(\prod_{\nu=1, \nu \neq k}^{n} (t - \tau_\nu)^{2s_\nu + 1} \right) \mathrm{d}\lambda(t).$$

Thus, for calculating the elements of the Jacobian by the previous recurrence relation we only need to know F_j and $w_{1,j}$ for each $j = 1, \dots, n$. All of the integrals in (24) and (26) can be calculated exactly, except for rounding errors, for example, by using a Gauss-Christoffel quadrature rule with respect to the measure $\mathrm{d}\lambda(t)$,

$$\int_{\mathbb{R}} g(t)\, \mathrm{d}\lambda(t) = \sum_{\nu=1}^{N} A_\nu^{(N)} g\big(\tau_\nu^{(N)}\big) + R_N(g),$$

taking $N = \sum_{\nu=1}^{n} s_\nu + n$ nodes. Such a formula is exact for all polynomials of degree at most $2N - 1 = 2\sum_{\nu=1}^{n} s_\nu + 2n - 1$, which is enough in this case. Numerical experiments with respect to several different measures are considered in [64].

3.2. Calculation of coefficients

A stable method for determining the coefficients $A_{i,\nu}$ in the Gauss–Turán quadrature formula (8) was given by Gautschi and Milovanović [19]. Some alternative methods were proposed earlier by Stroud and Stancu [96] (see also [95]), Golub and Kautsky [27], and Milovanović and Spalević [50]. A generalization of the method from [19] to the general case of Chakalov-Popoviciu quadrature formulas (7) has been derived in [51]. These methods have enabled further progress in the theory of quadratures with multiple nodes.

Here, we shortly present the basic idea of the method for the general case when $s_\nu \in \mathbb{N}_0$, $\nu = 1, \dots, n$. Let $\tau_\nu = \tau_\nu^{(n,\sigma)}$, $\nu = 1, \dots, n$, be corresponding zeros of the σ-orthogonal polynomial $\pi_{n,\sigma}(t)$.

For each $1 \leq j \leq n$ we first define

$$\Omega_j(t) = \prod_{i \neq j} (t - \tau_i)^{2s_i + 1},$$

as well as the polynomials

$$f_{k,j}(t) = (t - \tau_j)^k \Omega_j(t) = (t - \tau_j)^k \prod_{i \neq j} (t - \tau_i)^{2s_i + 1} \quad (0 \leq k \leq 2s_j).$$

Since the Chakalov-Popoviciu quadrature formula (7) is exact for all polynomials of degree at most $\ell + n - 1 = 2(s_1 + \cdots + s_n) + 2n - 1$ and

$$\deg f_{k,j}(t) = k + \sum_{i \neq j} (2s_i + 1) \leq 2(s_1 + \cdots + s_n) + n - 1,$$

we conclude that the integration by (7) is exact for each of the polynomials $f_{k,j}(t)$, $0 \leq k \leq 2s_j$, i.e.,

$$(27) \qquad \int_{\mathbb{R}} f_{k,j}(t)\, \mathrm{d}\lambda(t) = \sum_{\nu=1}^{n} \sum_{i=0}^{2s_\nu} A_{i,\nu} f_{k,j}^{(i)}(\tau_\nu).$$

On the other hand $f_{k,j}^{(i)}(\tau_\nu) = 0$, $0 \le i \le 2s_\nu$, for each $\nu \ne j$. Therefore, for each $j = 1, \ldots, n$, (27) becomes

$$\sum_{i=0}^{2s_j} A_{i,j} f_{k,j}^{(i)}(\tau_j) = \mu_{k,j}, \quad k = 0, 1, \ldots, 2s_j,$$

or in the matrix form

$$(28) \quad \begin{bmatrix} f_{0,j}(\tau_j) & f_{0,j}'(\tau_j) & \cdots & f_{0,\nu}^{(2s_\nu)}(\tau_\nu) \\ & f_{1,j}'(\tau_j) & \cdots & f_{1,j}^{(2s_j)}(\tau_j) \\ & & \ddots & \\ & & & f_{2s_j,j}^{(2s_j)}(\tau_j) \end{bmatrix} \begin{bmatrix} A_{0,j} \\ A_{1,j} \\ \vdots \\ A_{2s_j,j} \end{bmatrix} = \begin{bmatrix} \mu_{0,j} \\ \mu_{1,j} \\ \vdots \\ \mu_{2s_j,j} \end{bmatrix},$$

where we put

$$\mu_{k,j} = \int_{\mathbb{R}} f_{k,j}(t)\,\mathrm{d}\lambda(t) = \int_{\mathbb{R}} (t - \tau_j)^k \prod_{i \ne \nu} (t - \tau_i)^{2s_i+1}\,\mathrm{d}\lambda(t).$$

Thus, for each zero τ_j of the σ-orthogonal polynomial $\pi_{n,\sigma}(t)$, $j = 1, \ldots, n$, the corresponding upper triangular system of equations (28) gives the weight coefficients (generalized Cotes numbers) $A_{i,j}$, $i = 0, 1, \ldots, 2s_j$, in the Chakalov-Popoviciu quadrature formula (7). The moments $\mu_{k,j}$ can be computed exactly, except for rounding errors, by using the same Gauss–Christoffel formula as in the construction of σ-orthogonal polynomials in the previous subsection, with $N = \sum_{\nu=1}^{n} s_\nu + n$ nodes. Recurrence formulas for the generalized Cotes numbers have been derived in [**51**], after some normalizations in systems of equations (28).

A software implementation for constructing s- and σ-orthogonal polynomials and the corresponding quadrature formulas with multiple nodes is given in the MATHEMATICA package `OrthogonalPolynomials` ([**8**], [**48**]), which is freely downloadable from the Web Site: `http://www.mi.sanu.ac.rs/~gvm/`.

4. The REMAINDER TERM

An elementary and old technique of deriving derivative-free representation of the remainder term in quadrature rules is based on Cauchy's integral formula. This technique has already been used in 1878 by Hermite [**35**], and in 1881 by Heine [**34**], to derive an error term for polynomial interpolation; these, when integrated, yield a remainder term for interpolatory quadrature rules.

Assume that the support of the measure $\mathrm{d}\lambda$ in (1) is an interval, say $[-1, 1]$, Γ is a simple closed curve in the complex plane surrounding the interval $[-1, 1]$ and D is its interior. If the integrand f is an *analytic function* on D, then the remainder term $R(f)$ in (6) admits the contour integral representation

$$(29) \quad R(f) = R(f; \lambda) = \frac{1}{2\pi i} \oint_\Gamma K(z; \lambda) f(z)\,\mathrm{d}z.$$

The *kernel* is given by

$$(30) \qquad K(z;\lambda) = K_n(z;\lambda) = \frac{q(z;\lambda)}{\omega_\ell(z)} \ , \qquad z \notin [-1,1],$$

where

$$q(z;\lambda) = \int_{-1}^{1} \frac{\omega_\ell(t)}{z-t} \ d\lambda(t),$$

and ω_ℓ is given by (5).

Note that in the case of Gauss-Stancu quadrature (9)

$$\omega_\ell = \tilde{\omega}_m \, \varphi_r,$$

with $\tilde{\omega}_m$ and φ_r given by (10).

The integral representation (29) leads to a general error estimate, by using Hölder's inequality,

$$|R(f;\lambda)| \quad = \quad \frac{1}{2\pi} \left| \oint_\Gamma K(z;\lambda)f(z) \ dz \right|$$

$$(31) \qquad \leq \quad \frac{1}{2\pi} \left(\oint_\Gamma |K(z;\lambda)|^r |dz| \right)^{1/r} \left(\oint_\Gamma |f(z)|^{r'} |dz| \right)^{1/r'},$$

i.e.,

$$(32) \qquad |R(f;\lambda)| \leq \frac{1}{2\pi} \|K\|_r \|f\|_{r'},$$

where $1 \leq r \leq +\infty$, $1/r + 1/r' = 1$, and

$$\|f\|_r := \begin{cases} \left(\oint_\Gamma |f(z)|^r |dz| \right)^{1/r}, & 1 \leq r < +\infty, \\ \\ \max_{z \in \Gamma} |f(z)|, & r = +\infty. \end{cases}$$

Important features of the estimate (32), besides being derivative-free, are its sharpness, its natural conduciveness to a comparison of different quadrature processes, and the neat separation it expresses between the influence of the quadrature rule (given by $\|K_n\|_r$) and the function to which it is applied (given by $\|f\|_{r'}$). The following choices of r are natural. The case $r = +\infty$ ($r' = 1$) gives

$$(33) \qquad |R(f;\lambda)| \leq \frac{1}{2\pi} \left(\max_{z \in \Gamma} |K(z;\lambda)| \right) \|f\|_1 \ ,$$

whereas for $r = 1$ ($r' = +\infty$) we have

$$(34) \qquad |R(f;\lambda)| \leq \frac{1}{2\pi} \left(\oint_\Gamma |K(z;\lambda)| |dz| \right) \|f\|_\infty \ .$$

The bounds in (33) and (34) depend on the contour Γ, while the contour Γ is arbitrary and $R(f;\lambda)$ does not depend on Γ. Therefore, there is a possibility for optimizing these bounds over suitable families of contours. Two choices of the contours Γ have been most frequently used: concentric circles

$$C_r = \big\{z \in \mathbb{C} : |z| = r\big\}, \quad r > 1,$$

and confocal ellipses

$$(35) \qquad \mathcal{E}_\varrho = \left\{z \in \mathbb{C} : z = \frac{1}{2}\left(u + u^{-1}\right), \ 0 \leq \theta \leq 2\pi\right\}, \quad u = \varrho e^{i\theta}, \ \varrho > 1,$$

having foci at ± 1 and the sum of semi-axes equal to ϱ. We limit ourselves to elliptic contours which we consider to be more flexible than circular ones. Indeed, they can be chosen to snuggle tightly around the interval $[-1,1]$ by selecting ρ sufficiently close to 1, thereby avoiding possible singularities or excessive growth of f. The circular contours are used in [56] and [60].

5. ANALYTICALLY DERIVED ERROR BOUNDS

We focus on the Gauss quadrature with multiple nodes in which the corresponding nodal polynomial ω_ℓ is known. Then, by (30), it is possible to derive an explicit formula for the kernel $K_n(z;\lambda)$, and investigate the values of $\max_{z \in \Gamma} |K_n(z;\lambda)|$ and $\oint_\Gamma |K_n(z;\lambda)||\,dz|$; see (33) and (34).

5.1. Gauss-Turán quadrature

In Section 2 we have already mentioned five cases when the nodes in the Gauss-Turán quadrature (8) are explicitly known.

(I) *The Chebyshev weight function of the first kind w_1.* This case was considered in [68], [53] and [55], where it is shown that

$$\max_{z \in \mathcal{E}_\rho} |K(z;w_1)| = \frac{2^{1-s}\pi}{\varrho^n} \cdot \frac{\displaystyle\sum_{k=0}^{s} \binom{2s+1}{k} \varrho^{-2n(s-k)}}{(a_2 - 1)^{1/2}(a_{2n} + 1)^{s+1/2}}, \quad n > n_0(w_1),$$

and

$$\frac{1}{2\pi} \oint_{\mathcal{E}_\rho} |K_{n,s}(z;w_1)|\,|\,dz| \leq \frac{\sqrt{\pi}}{2^{s-1/2}\varrho^{(s+1)n}} \left(\sum_{k=0}^{s} A_k\, J_k(a_{2n})\right)^{1/2},$$

where $n_0(w_1)$ is the largest zero of the function

$$F_{n,s}(\rho) := (a_{2n} + 1)^{2s+1} - \big[(a_2 - 1)n^2 + 2\big]$$
$$\times \left[\sum_{k=0}^{s} 4^k \binom{2s+1}{2k+1}(a_{2n} + 1)^{2s-2k} - \frac{1}{2}\sum_{k=1}^{s} 4^k \binom{2s+1}{2k}(a_{2n} + 1)^{2s-2k+1}\right],$$

$$a_j = a_j(\rho) = \frac{1}{2}\left(\rho^j + \rho^{-j}\right), \quad A_k = \frac{2}{\varrho^{2n(s-k)}} \sum_{\nu=0}^{s-k} \binom{2s+1}{\nu}\binom{2s+1}{\nu+k}\varrho^{4n\nu},$$

and

$$\begin{aligned}
J_k(a) &= \int_0^\pi \frac{\cos k\theta}{(a+\cos\theta)^{2s+1}}\,\mathrm{d}\theta \\
&= \frac{(-1)^k \pi 2^{2s+1} x^{s-(k-1)/2}}{(x-1)^{4s+1}} \sum_{\nu=0}^{2s} \binom{2s+\nu}{\nu}\binom{2s+k}{\nu+k}(x-1)^{2s-\nu},
\end{aligned}$$

where $a = (x+1)/(2\sqrt{x})$, $x > 1$.

(II) *The Chebyshev weight function of the second kind* w_2. The following results can be found in [68], [53] and [55]:

$$\max_{z\in\mathcal{E}_\rho}|K_{n,s}(z;w_2)| = \frac{\pi}{4^s \varrho^{n+1}}\cdot\frac{(a_2+1)^{s+1/2}}{(a_{2n+2}+(-1)^n)^s}\cdot\frac{\displaystyle\sum_{k=0}^{s}(-1)^{kn}\binom{2s+1}{s+k+1}\varrho^{-2(n+1)k}}{(a_{2n+2}+(-1)^n)^{1/2}},$$

for $n > n_0(w_2)$, and

$$\frac{1}{2\pi}\oint_{\mathcal{E}_\varrho}|K_{n,s}(z;w_2)||\,\mathrm{d}z| \le \frac{\sqrt{\pi}}{2^{2s+1/2}\varrho^{(s+1)(n+1)}}\left(M_{2s+2}(\varrho^2)\sum_{k=0}^{s}A_k\,J_k(a_{2n+2})\right)^{1/2},$$

where

$$M_n(\varrho) = (2\varrho)^{-n}\sum_{\nu=0}^{n}\binom{n}{\nu}^2\varrho^{2\nu}$$

and $n_0(w_2)$ is either zero (if n is odd) or the unique root of the equation

$$\frac{\rho+\rho^{-1}}{\rho^{n+1}+\rho^{-(n+1)}} = \frac{1}{n+1}.$$

(III) *The Chebyshev weight function of the third kind* w_3. In [68], [53] and [55] it is shown that

$$\max_{z\in\mathcal{E}_\rho}|K_{n,s}(z;w_3)| = \frac{2^{1-s}\pi}{\varrho^{n+1/2}}\cdot\frac{(a_1+1)^{s+1}\displaystyle\sum_{k=0}^{s}\binom{2s+1}{s+k+1}\varrho^{-(2n+1)k}}{(a_2-1)^{1/2}(a_{2n+1}+1)^{s+1/2}},$$

for $n > n_0(w_1) - 1/2$, and

$$\frac{1}{2\pi}\oint_{\mathcal{E}_\varrho}|K_{n,s}(z;w_3)||\,\mathrm{d}z| \le \frac{\sqrt{\pi}}{2^{s-1/2}\varrho^{(s+1)(n+1/2)}}\left(M_{2s+2}(\varrho)\sum_{k=0}^{s}A_k\,J_k(a_{2n+1})\right)^{1/2}.$$

(*IV*) *the Chebyshev weight function of the fourth kind* w_4. Note that $W_n(-t) = (-1)^n V_n(t)$ and the results for the weight function w_3 can be easily adjusted for this case.

(*V*) *The Gori-Micchelli weight function* $w_{n,\ell}$. The Gauss-Turán quadrature with the Gori-Micchelli weight function with $\mu = \ell - 1/2$, $\ell \in \mathbb{N}$, has been considered in [**72**]. It is shown that $|K(z; w_{n,\ell})|$, $z \in \mathcal{E}_\varrho$, attains its maximum on the real axis for sufficiently large ρ since

$$|K(z; w_{n,\ell})| \sim \frac{\pi F_{s,k}(0)}{n^{2k+2} 4^k \varrho^{2n(s+1)+1}} \left(1 + \frac{2\cos 2\theta}{\varrho^2}\right)^{1/2}, \quad \varrho \to \infty,$$

with

$$
\begin{aligned}
F_{s,k}(\lambda) &= \sum_{j+p=\lambda} (-1)^p \binom{2k+1}{k-p}\binom{2s+1}{s-j} \\
&+ \sum_{|p-j|=\lambda+1} (-1)^p \operatorname{sign}(p-j) \binom{2k+1}{k-p}\binom{2s+1}{s-j},
\end{aligned}
$$

$j = 0, 1, \ldots, s$; $p = 0, 1, \ldots, k$. In addition,

$$
\frac{1}{2\pi} \oint_{\mathcal{E}_\varrho} |K(z; w_{n,\ell})| \, |\mathrm{d}z| \le \frac{\pi^{1/2}}{2^{s+2\ell-1} n^{2\ell} \varrho^{n(s+\ell+1)}} \times
$$

$$
\times \left\{ \sum_{j=0}^{s+\ell-1} \bar{A}_j \left[a_{2n} J_j(a_{2n}) - \frac{1}{2}(J_{j+1}(a_{2n}) + J_{|j-1|}(a_{2n})) \right] \right\}^{1/2},
$$

where

$$
\bar{A}_0 = \frac{1}{\rho^{2n(s+k)}} \sum_{\nu=0}^{s+k} [F_{s,k}(s+k-\nu)]^2 \, \rho^{4n\nu},
$$

$$
\bar{A}_j = \frac{2}{\rho^{2n(s+k-j)}} \sum_{\nu=0}^{s+k-j} F_{s,k}(s+k-\nu)\, F_{s,k}(s+k-\nu-j)\, \rho^{4n\nu}, \quad j = 1, \ldots, s.
$$

5.2. Gauss-Turán quadrature of Lobatto (Radau) type

Here we mention two cases of the quadrature (15) with

$$\widehat{w}(t) = (1-t)^{k-1/2}(1+t)^{m-1/2}$$

on $(-1, 1)$ considered in [**54**].

(*I*) If we set $r_1 = s + 1 - m$, $r_2 = s + 1 - k$, $m_\nu = 2s + 1$ in (15), then the nodes $\tau_1, \ldots, \tau_{n-2}$ are the zeros of $U_{n-2}(t)$, and

$$|K_n(z; \widehat{w})| \le \left(\frac{2}{a_2 - 1}\right)^{s+1} (a_1 + 1)^{k+m} \max_{z \in \mathcal{E}_\varrho} |K_{n-2}(z; w_2)|,$$

where $K_{n-2}(z; w_2)$ is the kernel for the Gauss-Turán quadrature with $n-2$ nodes of multiplicities $2s+1$, with respect to the Chebyshev weight function of the second type.

(II) If we set $r_1 = s + 1 - m$, $r_2 = 0$, $m_\nu = 2s + 1$ in (15), then the nodes $\tau_1, \ldots, \tau_{n-2}$ are the zeros of $V_{n-2}(t)$, and

$$K_n(z; \widehat{w}) \leq \frac{1}{(a_1 - 1)^{s+1-m}} \max_{z \in \mathcal{E}_\varrho} \big| K_{n-2}(z; w_3) \big|,$$

where $K_{n-2}(z; w_3)$ is the kernel for the Gauss-Turán quadrature with $n-2$ nodes of multiplicities $2s + 1$, with respect to w_3.

5.3. Kronrod extension of the Gauss-Turán quadrature

Consider the special case of the Gauss-Stancu quadrature

$$(36) \qquad \int_{-1}^{1} f(t)w(t)\,\mathrm{d}t = \sum_{\mu=1}^{n} \sum_{j=0}^{2s} B_{j,\mu} f^{(j)}(\alpha_\mu) + \sum_{\nu=1}^{n+1} \sum_{i=0}^{m_\nu - 1} A_{i,\nu} f^{(i)}(\tau_\nu),$$

where $\prod_{\mu=1}^{n}(t - \alpha_\mu)$ is an s-orthogonal polynomial with respect to the weight function w.

(I) *The Chebyshev weight function of the first kind w_1.* If all the nodes τ_ν in (36) are simple, i.e., $m_\nu = 1$ for $\nu = 1 \ldots, n+1$, then $\tau_1, \ldots, \tau_{n+1}$ are the zeros of the polynomial $(t^2 - 1)U_{n-1}(t)$. The upper bound for $\frac{1}{2\pi} \oint_{\mathcal{E}_\rho} |K_n(z; w_1)| \, |\mathrm{d}z|$ is given in [**58**, Section 3.1].

(II) *The Chebyshev weight function of the second kind w_2.* If we set $m_\nu = 1$ for all ν in (36), then the nodes $\tau_1, \ldots, \tau_{n+1}$ are the zeros of the polynomial $T_{n+1}(t)$. The upper bound for $\frac{1}{2\pi} \oint_{\mathcal{E}_\rho} |K_{n,s}(z; w_1)| \, |\mathrm{d}z|$ is given in [**58**, Section 3.2].

(III) *The Chebyshev weight function of the third kind w_3.* If we set $m_\nu = 1$ for all ν in (36), then the nodes $\tau_1, \ldots, \tau_{n+1}$ are the zeros of the polynomial $(1-t)W_n(t)$. The upper bound for $\frac{1}{2\pi} \oint_{\mathcal{E}_\rho} |K_{n,s}(z; w_1)| \, |\mathrm{d}z|$ is given in [**58**, Section 3.3].

(IV) *The Gori-Micchelli weight function $w_{n\ell}$.* If we set $m_1 = m_{n+1} = s - \ell + 1$ and $m_2 = \cdots = m_n = 2(s - \ell) + 1$ in (36), then the free nodes $\tau_1, \ldots, \tau_{n+1}$ are the zeros of the polynomial $(t^2 - 1)U_{n_2-1}(t)$. The upper bound for $\max_{z \in \mathcal{E}_\rho} |K(z; w_{n,\ell})|$ is given in [**67**, Theorems 1 and 2], and the upper bound for $\frac{1}{2\pi} \oint_{\mathcal{E}_\rho} |K(z; w_{n,\ell})| \, |\mathrm{d}z|$ is given in [**65**, Theorem 4.1].

6. APPLICATIONS

Here we discuss how the Gauss quadrature with multiple nodes can be used to solve some classical mathematical problems, such as the approximation of functions by defective spline and computation of Fourier coefficients.

6.1. Moment preserving spline approximation

A spline function of degree $m \geq 2$ on the (finite or infinite) interval $[a,b]$ with n distinct knots τ_ν $(\nu = 1, \ldots, n)$ in the interior of $[a,b]$ having multiplicities m_ν $(\leq m)$, can be written in the form

$$(37) \qquad S_{n,m}(t) = p_m(t) + \sum_{\nu=1}^{n} \sum_{i=0}^{m_\nu - 1} \alpha_{i,\nu}(\tau_\nu - t)_+^{m-i},$$

where $\alpha_{i,\nu}$ are real numbers and $p_m(t)$ is a polynomial of degree $\leq m$. We discuss a problem of approximating a function f by the spline (37) on the interval $[0,1]$ and on the interval $[0, +\infty)$.

(*I*) *Spline-approximation on* $[0,1]$. We discuss the two following problems. Let $N = m_1 + \cdots + m_n$.

Problem AI. Determine $S_{n,m}$ in (37) such that

$$(38) \qquad \int_0^1 t^j S_{n,m}(t)\, \mathrm{d}t = \int_0^1 t^j f(t)\, \mathrm{d}t, \quad j = 0, 1, \ldots, N + n + m.$$

Problem AII. Determine $S_{n,m}$ in (37) such that

$$(39) \qquad S_{n,m}^{(k)}(1) = p_m^{(k)}(1) = f^{(k)}(1), \quad k = 0, 1, \ldots, m,$$

and such that (38) holds for $j = 0, 1, \ldots, N + n - 1$.

The following theorems give solutions for Problems AI and AII.

Theorem 6.1. *Let* $f \in C^{m+1}[0,1]$. *There exists a unique spline function* (37) *on* $[0,1]$ *satisfying* (38) *if and only if the measure*

$$(40) \qquad \mathrm{d}\psi(t) = \frac{(-1)^{m+1}}{m!} f^{(m+1)}(t)\, \mathrm{d}t$$

admits the quadrature of Lobatto type

$$(41) \quad \int_0^1 g(t)\, \mathrm{d}\psi(t) = \sum_{k=0}^{m} \left[\alpha_k g^{(k)}(0) + \beta_k g^{(k)}(1) \right] + \sum_{\nu=1}^{n} \sum_{i=0}^{m_\nu - 1} A_{i,\nu}^L g^{(i)}\left(\tau_\nu^{(n)}\right) + R(g),$$

satisfying

$$(42) \qquad R(g) = 0 \quad \text{for} \quad g \in \mathcal{P}_{N+n+2m+1},$$

with distinct zeros $\tau_\nu^{(n)}$, $\nu = 1, \ldots, n$, *all contained in the open interval* $(0,1)$. *The spline function* $S_{n,m}$ *is given by*

$$\tau_\nu = \tau_\nu^{(n)}, \quad a_{m-k,\nu} = \frac{m!}{(m-k)!} A_{k,\nu}^L; \quad \nu = 1, 2, \ldots, n, \ k = 0, 1, \ldots, m_\nu - 1,$$

and

$$p_m^{(j)}(1) = f^{(j)}(1) + (-1)^j m! \beta_{m-j}, \quad j = 0, 1, \ldots, m.$$

Theorem 6.2. *Let $f \in C^{m+1}[0,1]$. The spline function $S_{n,m}$ satisfying conditions of the problem AI exists and is unique if and only if the measure $d\psi(t)$ given by (40) admits the quadrature of Radau type*

$$(43) \qquad \int_0^1 g(t) \, d\psi(t) = \sum_{k=0}^m \alpha_k^* g^{(k)}(0) + \sum_{\nu=1}^n \sum_{i=0}^{2s_\nu} A_{i,\nu}^R g^{(i)}(\tau_\nu^{(n)*}) + R(g),$$

satisfying

$$R(g) = 0 \quad \text{for} \quad g \in \mathcal{P}_{N+n+m},$$

with distinct nodes $\tau_\nu^{(n)*}$, $\nu = 1, \ldots, n$, all contained in the open interval $(0,1)$. The spline $S_{n,m}$ is given by

$$\tau_\nu^* = \tau_\nu^{(n)*}, \quad a_{m-k,\nu}^* = \frac{m!}{(m-k)!} A_{k,\nu}^R; \quad \nu = 1, 2, \ldots, n, \ k = 0, 1, \ldots, 2s_\nu,$$

and

$$p_m^*(t) = \sum_{k=0}^m \frac{f^{(k)}(1)}{k!} (t-1)^k.$$

The special case $m_1 = \cdots = m_n = 1$ of Problems AI and AII was considered in [**13**], and generalized in [**12**] to the case $m_1 = \cdots = m_n = 2s$, $s \in \mathbb{N}$.

Interval $[0, +\infty)$. Similarly as in the previous case, we discuss two problems of approximating a function $f(t)$, $0 \le t < +\infty$, by the spline function (37).

Problem BI. Determine $S_{n,m}$ in (37) with $p_m(t) = 0$ such that $S_{n,m}^{(k)}(0) = f^{(k)}(0)$ $(k = 0, 1, \ldots, N + n - 1; \ m \ge N + n - 1)$.

Problem BII. Determine $S_{n,m}$ in (37 with $p_m(t) = 0$ such that $S_{n,m}^{(k)}(0) = f^{(k)}(0)$ $(k = 0, 1, \ldots, l; \ l \le m)$ and

$$\int_0^{+\infty} t^j S_{n,m}(t) \, dt = \int_0^{+\infty} t^j f(t) \, dt \qquad (j = 0, 1, \ldots, N + n - l - 2).$$

The next theorem gives the solution of Problem BII.

Theorem 6.3. *Let $f \in C^{m+1}[0, +\infty)$ and $\int_0^{+\infty} t^{N+n-l+m} |f^{(m+1)}(t)| \, dt < +\infty$. Then a spline function $S_{n,m}$ with positive knots τ_ν that satisfies the conditions of Problem BII exists and is unique if and only if the measure*

$$d\lambda(t) = \frac{(-1)^{m+1}}{m!} t^{m-l} f^{(m+1)}(t) \, dt$$

admits the quadrature

$$(44) \qquad \int_0^{+\infty} g(t)\,\mathrm{d}\lambda(t) = \sum_{\nu=1}^{n} \sum_{k=0}^{m_\nu-1} A_{k,\nu}^{(n)} g^{(k)}(\tau_\nu^{(n)}) + R(g),$$

with n distinct positive nodes $\tau_\nu^{(n)}$, satisfying $R(g) = 0$ for all $g \in \mathcal{P}_{N+n-1}$. The knots in (37) are given by $\tau_\nu = \tau_\nu^{(n)}$, and the coefficients $\alpha_{\nu,i}$ by the following triangular system:

$$A_{\nu,k}^{(n)} = \sum_{i=k}^{m_\nu-i} \frac{(m-i)!}{m!} \binom{i}{k} \left[D^{i-k} t^{m-l} \right]_{t=\tau_\nu} \alpha_{\nu,i} \qquad (k = 0, 1, \ldots, m_\nu - 1).$$

If we set $l = N + n - 1$, Theorem 6.3 gives also the solution of Problem BI. The case $m_1 = m_2 = \cdots = m_n = 1$, $l = -1$, was considered by Gautschi and Milovanović in [**18**].

      The error of the spline approximation can be expressed as the remainder term in (44), (43) or (41) for a particular function $\sigma_t(x) = x^{-(m-l)}(x - t)_+^m$ (see [**38**]). A generalization of these results can be found in [**90**].

6.2. Computation of Fourier coefficients

      Let $\{P_k\}_{k=0}^{\infty}$ be a system of orthonormal polynomials on $[a, b]$ with respect to a weight function w. The coefficients $a_k(f)$ in the Fourier series expansion

$$(45) \qquad f(x) = \sum_{k=0}^{\infty} a_k(f) P_k(x), \quad a_k(f) = \int_a^b w(t) P_k(t) f(t)\,\mathrm{d}t,$$

can be approximated by Gauss quadrature with multiple nodes

$$(46) \qquad \int_a^b f(t) P_k(t) w(t)\,\mathrm{d}t \approx \sum_{j=1}^{n} \sum_{i=0}^{\nu_j-1} c_{ji} f^{(i)}(x_j), \quad a < x_1 < \cdots < x_n < b.$$

The question of existence of the Gauss quadrature (46) can be answered by the following theorem from [**3**].

Theorem 6.4. *For any given sets of multiplicities $\bar{\mu} := (\mu_1, \ldots, \mu_k)$ and $\bar{\nu} := (\nu_1, \ldots, \nu_n)$, and nodes $y_1 < \cdots < y_k$, $x_1 < \cdots < x_n$, there exists a quadrature formula of the form*

$$(47) \qquad \int_a^b f(t) w(t) \prod_{m=1}^{k} (t - y_m)^{\mu_m}\,\mathrm{d}t \approx \sum_{j=1}^{n} \sum_{i=0}^{\nu_j-1} c_{ji} f^{(i)}(x_j),$$

having degree of exactness N if and only if there exists a quadrature formula of the form

$$(48) \qquad \int_a^b f(t) w(t)\,\mathrm{d}t \approx \sum_{m=1}^{k} \sum_{\lambda=0}^{\mu_m-1} b_{m\lambda} f^{(\lambda)}(y_m) + \sum_{j=1}^{n} \sum_{i=0}^{\nu_j-1} a_{ji} f^{(i)}(x_j),$$

which has degree of exactness $N + \mu_1 + \cdots + \mu_k$. In the case $y_m = x_j$ for some m and j, the corresponding terms in both sums combine in one term of the form

$$\sum_{\lambda=0}^{\mu_m+\nu_j-1} d_{m\lambda} f^{(\lambda)}(y_m).$$

For example, the existence of the Gauss-Turán quadrature (8) with respect to the Chebyshev weight function w_1 guarantees the existence of the following Gauss quadrature

$$\int_{-1}^{1} f(t) T_n(t) \frac{1}{\sqrt{1-t^2}} \, \mathrm{d}t \approx \sum_{i=1}^{n} \sum_{h=0}^{2s-1} \hat{A}_{hi} f^{(h)}(\tau_i).$$

In a similar way, several types of the Gauss quadrature for approximating coefficients in Fourier series in terms of the Chebyshev polynomials T_n, U_n, V_n and W_n are derived in [**62**]. Other approaches within the same topic can be found in [**41**], [**43**], [**2**]. Error bounds of the form (34) and (33) for some of these quadrature are considered in [**79**], [**80**], [**73**].

The quadrature (47) can be easily computed if we know the quadrature (48):

$$c_{ji} = \sum_{s=i}^{\nu_j-1} a_{js} \binom{s}{i} \left[\prod_{m=1}^{k} (t - y_m)^{\mu_m} \right]^{(s-i)} \Bigg|_{t=x_j}.$$

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