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Quadratures with multiple nodes, power orthogonality, and moment-preserving spline approximation ☆

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Abstract

Quadrature formulas with multiple nodes, power orthogonality, and some applications of such quadratures to moment-preserving approximation by defective splines are considered. An account on power orthogonality (s- and σ-orthogonal polynomials) and generalized Gaussian quadratures with multiple nodes, including stable algorithms for numerical construction of the corresponding polynomials and Cotes numbers, are given. In particular, the important case of Chebyshev weight is analyzed. Finally, some applications in moment-preserving approximation of functions by defective splines are discussed.

Keywords: Quadratures with multiple nodes; Gauss–Turán-type quadratures; Error term; Convergence; Orthogonal polynomials; s- and σ-orthogonal polynomials; Nonnegative measure; Extremal polynomial; Weights; Nodes; Degree of precision; Stieltjes procedure; Chebyshev polynomials; Spline function; Spline defect; Moments

1. Introduction

More than 100 years after Gauss published his famous method of approximate integration, which was enriched by significant contributions of Jacobi and Christoffel, there appeared the idea of numerical integration involving multiple nodes. Taking any system of n distinct points $\{\tau_1,\ldots,\tau_n\}$ and n nonnegative integers $m_1,\ldots,m_n$, and starting from the Hermite the interpolation formula, Chakalov (Tschakaloff in German transliteration) [8] in 1948 obtained the quadrature formula

$$\int_{-1}^{1} f(t)\,\mathrm{d}t = \sum_{\nu=1}^{n} [A_{0,\nu} f(\tau_\nu) + A_{1,\nu} f'(\tau_\nu) + \ldots + A_{m_\nu-1,\nu} f^{(m_\nu-1)}(\tau_\nu)], \tag{1.1}$$

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which is exact for all polynomials of degree at most $m_1 + \dots + m_n - 1$. Precisely, he gave a method for computing the coefficients $A_{i,v}$ in (1.1). Such coefficients (Cotes numbers of higher order) are evidently $A_{i,v} = \int_{-1}^{1} \ell_{i,v}(t)\,\mathrm{d}t$ $(v = 1,\dots,n;\ i = 0,1,\dots,m_v - 1)$, where $\ell_{i,v}(t)$ are the fundamental functions of Hermite interpolation.

In 1950, specializing $m_1 = \dots = m_n = k$ in (1.1), Turán [90] studied numerical quadratures of the form

$$\int_{-1}^{1} f(t)\,\mathrm{d}t = \sum_{i=0}^{k-1} \sum_{v=1}^{n} A_{i,v} f^{(i)}(\tau_v) + R_{n,k}(f). \tag{1.2}$$

Let $\mathscr{P}_m$ be the set of all algebraic polynomials of degree at most m. It is clear that formula (1.2) can be made exact for $f \in \mathscr{P}_{kn-1}$, for any given points $-1 \leqslant \tau_1 \leqslant \dots \leqslant \tau_n \leqslant 1$. However, for $k = 1$ formula (1.2), i.e.,

$$\int_{-1}^{1} f(t)\,\mathrm{d}t = \sum_{v=1}^{n} A_{0,v} f(\tau_v) + R_{n,1}(f)$$

is exact for all polynomials of degree at most $2n - 1$ if the nodes τ_v are the zeros of the Legendre polynomial P_n, and it is the well-known Gauss–Legendre quadrature rule.

Because of Gauss's result it is natural to ask whether nodes τ_v can be chosen so that the quadrature formula (1.2) will be exact for algebraic polynomials of degree not exceeding $(k + 1)n - 1$. Turán [90] showed that the answer is negative for $k = 2$, and for $k = 3$ it is positive. He proved that the nodes τ_v should be chosen as the zeros of the monic polynomial $\pi_n^*(t) = t^n + \dots$ which minimizes the integral $\int_{-1}^{1} [\pi_n(t)]^4\,\mathrm{d}t$, where $\pi_n(t) = t^n + a_{n-1}t^{n-1} + \dots + a_1 t + a_0$.

In the general case, the answer is negative for even, and positive for odd k, and then τ_v must be the zeros of the polynomial minimizing $\int_{-1}^{1} [\pi_n(t)]^{k+1}\,\mathrm{d}t$. When $k = 1$, then π_n is the monic Legendre polynomial $\hat{P}_n$.

Because of the above, we assume that $k = 2s + 1$, $s \geqslant 0$. Instead of (1.2), it is also interesting to consider a more general *Gauss–Turán-type* quadrature formula

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t) = \sum_{i=0}^{2s} \sum_{v=1}^{n} A_{i,v} f^{(i)}(\tau_v) + R_{n,2s}(f), \tag{1.3}$$

where $\mathrm{d}\lambda(t)$ is a given nonnegative measure on the real line $\mathbb{R}$, with compact or unbounded support, for which all moments $\mu_k = \int_{\mathbb{R}} t^k\,\mathrm{d}\lambda(t)$ $(k = 0,1,\dots)$ exist and are finite, and $\mu_0 > 0$. It is known that formula (1.3) is exact for all polynomials of degree not exceeding $2(s + 1)n - 1$, i.e., $R_{n,2s}(f) = 0$ for $f \in \mathscr{P}_{2(s+1)n-1}$. The nodes τ_v $(v = 1,\dots,n)$ in (1.3) are the zeros of the monic polynomial $\pi_{n,s}(t)$, which minimizes the integral

$$F(a_0, a_1, \dots, a_{n-1}) = \int_{\mathbb{R}} [\pi_n(t)]^{2s+2}\,\mathrm{d}\lambda(t), \tag{1.4}$$

where $\pi_n(t) = t^n + a_{n-1}t^{n-1} + \dots + a_1 t + a_0$. This minimization leads to the conditions

$$\frac{1}{2s + 2}\frac{\partial F}{\partial a_k} = \int_{\mathbb{R}} [\pi_n(t)]^{2s+1} t^k\,\mathrm{d}\lambda(t) = 0 \qquad (k = 0,1,\dots,n - 1). \tag{1.5}$$

These polynomials $\pi_n = \pi_{n,s}$ are known as *s-orthogonal* (or *s-self associated*) *polynomials* on $\mathbb{R}$ with respect to the measure $\mathrm{d}\lambda(t)$ (for more details see [15,62,65,66]. For $s = 0$ they reduce to the standard orthogonal polynomials and (1.3) becomes the well-known Gauss–Christoffel formula.

Using some facts about monosplines, Micchelli [47] investigated the sign of the Cotes coefficients $A_{i,v}$ in the Turán quadrature.

A generalization of the Turán quadrature formula (1.3) (for $\mathrm{d}\lambda(t)=\mathrm{d}t$ on (a,b)) to rules having nodes with arbitrary multiplicities was derived independently by Chakalov [9,10] and Popoviciu [74]. Important theoretical progress on this subject was made by Stancu [82,84] (see also [88]).

In this case, it is important to assume that the nodes τ_v are ordered, say

$$\tau_1 < \tau_2 < \ldots < \tau_n, \tag{1.6}$$

with multiplicities m_1, m_2, $\ldots$, m_n, respectively. A permutation of the multiplicities m_1, m_2, $\ldots$, m_n, with the nodes held fixed, in general yields a new quadrature rule.

It can be shown that the quadrature formula (1.1) is exact for all polynomials of degree less than $2\sum_{v=1}^{n}[(m_v+1)/2]$. Thus, the multiplicities m_v that are even do not contribute toward an increase in the degree of exactness, so that it is reasonable to assume that all m_v be odd integers, $m_v=2s_v+1$ $(v=1,2,\ldots,n)$. Therefore, for a given sequence of nonnegative integers $\sigma=(s_1,s_2,\ldots,s_n)$ the corresponding quadrature formula

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t)=\sum_{v=1}^{n}\sum_{i=0}^{2s_v} A_{i,v}f^{(i)}(\tau_v)+R(f) \tag{1.7}$$

has maximum degree of exactness

$$d_{\max}=2\sum_{v=1}^{n} s_v+2n-1 \tag{1.8}$$

if and only if

$$\int_{\mathbb{R}}\prod_{v=1}^{n}(t-\tau_v)^{2s_v+1}t^k\,\mathrm{d}\lambda(t)=0 \quad (k=0,1,\ldots,n-1). \tag{1.9}$$

The last *orthogonality conditions* correspond to (1.5) and they could be obtained by the minimization of the integral

$$\int_{\mathbb{R}}\prod_{v=1}^{n}(t-\tau_v)^{2s_v+2}\,\mathrm{d}\lambda(t).$$

The existence of such quadrature rules was proved by Chakalov [9], Popoviciu [74], Morelli and Verna [57], and existence and uniqueness (subject to (1.6)) by Ghizzetti and Ossicini [27].

Conditions (1.9) define a sequence of polynomials $\{\pi_{n,\sigma}\}_{n\in\mathbb{N}_0}$,

$$\pi_{n,\sigma}(t)=\prod_{v=1}^{n}(t-\tau_v^{(n,\sigma)}), \qquad \tau_1^{(n,\sigma)}<\tau_2^{(n,\sigma)}<\ldots<\tau_n^{(n,\sigma)},$$

such that

$$\int_{\mathbb{R}}\pi_{k,\sigma}(t)\prod_{v=1}^{n}(t-\tau_v^{(n,\sigma)})^{2s_v+1}\,\mathrm{d}\lambda(t)=0 \quad (k=0,1,\ldots,n-1). \tag{1.10}$$

Thus, we get now a general type of power orthogonality. These polynomials $\pi_{k,\sigma}$ are called σ-orthogonal polynomials, and they correspond to the sequence $\sigma=(s_1,s_2,\ldots)$. We will often write simple τ_ν or $\tau_\nu^{(n)}$ instead of $\tau_\nu^{(n,\sigma)}$. If we have $\sigma=(s,s,\ldots)$, the above polynomials reduce to the s-orthogonal polynomials.

This paper is devoted to quadrature formulas with multiple nodes, power orthogonality, and some applications of such quadrature formulas to moment-preserving approximation by defective splines. In Section 2, we give an account on power orthogonality, which includes some properties of s- and σ-orthogonal polynomials and their construction. Section 3 is devoted to some methods for constructing generalized Gaussian formulas with multiple nodes. The important case of Chebyshev weight is analyzed in Section 4. Finally, some applications to moment-preserving approximation by defective splines are discussed in Section 5.

2. Power orthogonality

This section is devoted to power-orthogonal polynomials. We give an account on theoretical results on this subject, and we also consider methods for numerical construction of such polynomials.

2.1. Properties of s- and σ-orthogonal polynomials

The orthogonality conditions for s-orthogonal polynomials $\pi_{n,s}=\pi_{n,s}(\,\cdot\,;\mathrm{d}\lambda)$ are given by (1.5) i.e.,

$$\int_{\mathbb{R}}[\pi_{n,s}(t)]^{2s+1}\pi_{k,s}(t)\,\mathrm{d}\lambda(t)=0 \qquad (k=0,1,\ldots,n-1). \tag{2.1}$$

These polynomials were investigated mainly by Italian mathematicians, especially the case $\mathrm{d}\lambda(t)=w(t)\,\mathrm{d}t$ on $[a,b]$ (e.g., Ossicini [62,63], Ghizzetti and Ossicini [23–27], Guerra [37,38], Ossicini and Rosati [67–69], Gori [29], Gori and Lo Cascio [30]). The basic result concerns related to zero distribution.

Theorem 2.1. *There exists a unique monic polynomial $\pi_{n,s}$ for which* (2.1) *is satisfied, and $\pi_{n,s}$ has n distinct real zeros which are all contained in the open interval* (a,b).

This result was proved by Turán [90] for $\mathrm{d}\lambda(t)=\mathrm{d}t$ on $[-1,1]$. It was also proved by Ossicini [62] (see also the book [24, pp. 74–75]) using different methods.

Usually, we assume that the zeros $\tau_\nu=\tau_\nu^{(n,s)}$ $(\nu=1,2,\ldots,n)$ of $\pi_{n,s}$ are ordered as in (1.6).

In the symmetric case $w(-t)=w(t)$ on $[-b,b]$ $(b>0)$, it is easy to see that $\pi_{n,s}(-t)=(-1)^n\pi_{n,s}(t)$. In the simplest case of Legendre s-orthogonal polynomials $P_{n,s}(t)=a_n\prod_{\nu=1}^{n}(t-\tau_\nu)$, where the normalization factor a_n is taken to have $P_{n,s}(1)=1$, Ghizzetti and Ossicini [23] proved that $|P_{n,s}(t)|\leqslant 1$, when $-1\leqslant t\leqslant 1$. Also, they determined the minimum in (1.4) in this case,

$$F_{n,s}=\int_{-1}^{1}[P_{n,s}(t)]^{2s+2}\,\mathrm{d}t=\frac{2}{1+(2s+2)n}.$$

Indeed, integration by parts gives

$$F_{n,s}=[tP_{n,s}(t)^{2s+2}]_{-1}^{1}-(2s+2)\int_{-1}^{1}tP_{n,s}(t)^{2s+1}P'_{n,s}(t)\,\mathrm{d}t=2-(2s+2)nF_{n,s}$$

because $tP'_{n,s}(t)=nP_{n,s}(t)+Q(t)$ $(Q\in\mathscr{P}_{n-2}$ in this symmetric case). It would be interesting to determine this minimum for other classical weights.

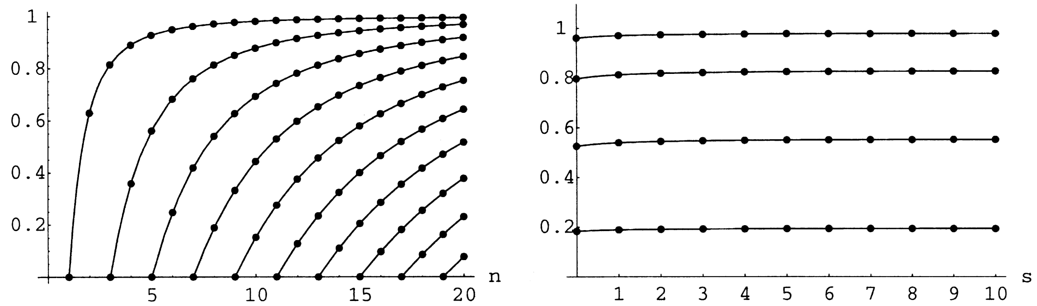

Fig. 1. Nonnegative zeros of $P_{n,s}(t)$ for $s=1$ and $n=1(1)20$ (left); Positive zeros of $P_{n,s}(t)$ for $n=8$ and $s=0(1)10$ (right).

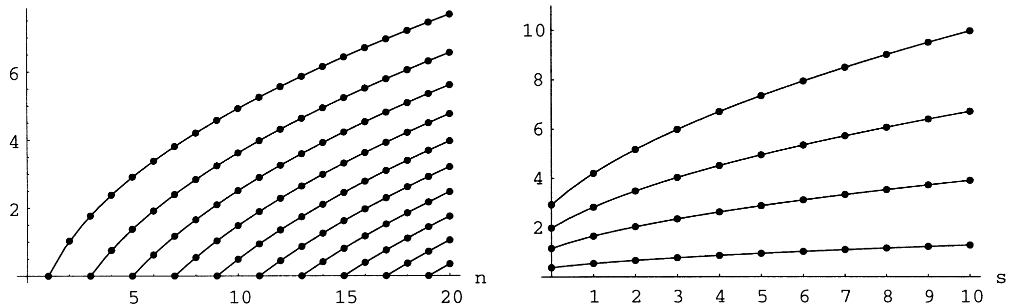

Fig. 2. Nonnegative zeros of $H_{n,s}(t)$ for $s=1$ and $n=1(1)20$ (left); Positive zeros of $H_{n,s}(t)$ for $n=8$ and $s=0(1)10$ (right).

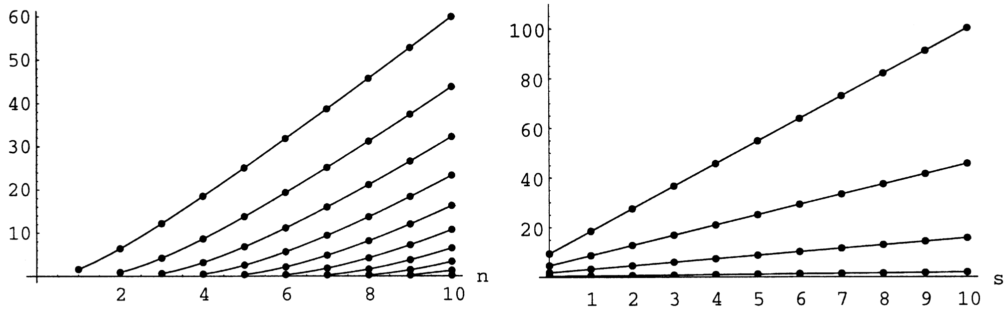

Fig. 3. Zeros of $L_{n,s}(t)$ for $s=1$ and $n=1(1)10$ (left) and for $n=4$ and $s=0(1)10$ (right).

In Fig. 1 we display the distribution of nonnegative zeros for Legendre s-orthogonal polynomials, taking $s=1$ and $n=1,2,\ldots,20$. Also, we present graphics when n is fixed ($n=8$) and s runs up to 10. The corresponding graphics for Hermite s-orthogonal polynomials $H_{n,s}$ are given in Fig. 2.

In Fig. 3 we present all zeros of Laguerre s-orthogonal polynomials for $s=1$ and $n \leqslant 10$, and also for $n=4$ and $s \leqslant 10$. Also, we give the corresponding zero distribution of generalized Laguerre s-orthogonal polynomial $L_{n,s}^{(\alpha)}$, when $\alpha \in (-1,5]$ ($n=4$, $s=1$) (see Fig. 4). Numerical experimentation suggests the following result.

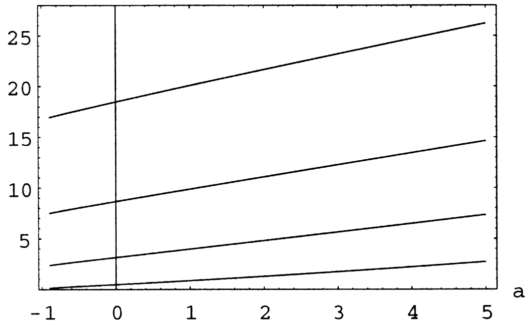

Fig. 4. Zero distribution of $L^{\alpha}_{n,s}(t)$ for $n=4$, $s=1$ and $-1<\alpha\leqslant 5$.

Theorem 2.2. *For every $s\in\mathbb{N}_0$, the zeros of $\pi_{n,s}$ and $\pi_{n+1,s}$ mutually separate each other.*

This interlacing property is well-known when $s=0$ (cf. [89, p. 46], [11, p. 28]). The proof of Theorem 2.2 can be obtained by applying a general result on interlacing properties of the zeros of the error functions in best L^p-approximations, given by Pinkus and Ziegler [73, Theorem 1.1]. Precisely, we put $u_\nu(t)=t^{\nu-1}$ $(\nu=1,\ldots,n+2)$, $p=2s+2$, and then use Corollary 1.1 from [73]. In the notation of this paper, $q_{n,p}=\pi_{n,s}$ and $q_{n+1,p}=\pi_{n+1,s}$, and their zeros strictly interlace for each $s\geqslant 0$.

A particularly interesting case is the Chebyshev measure

$$\mathrm{d}\lambda_1(t)=(1-t^2)^{-1/2}\mathrm{d}t.$$

In 1930, Bernstein [3] showed that the monic Chebyshev polynomial $\hat{T}_n(t)=T_n(t)/2^{n-1}$ minimizes all integrals of the form

$$\int_{-1}^{1}\frac{|\pi_n(t)|^{k+1}}{\sqrt{1-t^2}}\,\mathrm{d}t \qquad (k\geqslant 0).$$

Thus, the Chebyshev polynomials T_n are s-orthogonal on $[-1,1]$ for each $s\geqslant 0$. Ossicini and Rosati [65] found three other measures $\mathrm{d}\lambda_k(t)$ $(k=2,3,4)$ for which the s-orthogonal polynomials can be identified as Chebyshev polynomials of the second, third, and fourth kind: S_n, V_n, and W_n, which are defined by

$$S_n(\cos\theta)=\frac{\sin(n+1)\theta}{\sin\theta},\qquad V_n(\cos\theta)=\frac{\cos(n+\frac{1}{2})\theta}{\cos\frac{1}{2}\theta},\qquad W_n(\cos\theta)=\frac{\sin(n+\frac{1}{2})\theta}{\sin\frac{1}{2}\theta},$$

respectively (cf. [18]). However, these measures depend on s,

$$\mathrm{d}\lambda_2(t)=(1-t^2)^{1/2+s}\mathrm{d}t,\qquad \mathrm{d}\lambda_3(t)=\frac{(1+t)^{1/2+s}}{(1-t)^{1/2}}\mathrm{d}t,\qquad \mathrm{d}\lambda_4(t)=\frac{(1-t)^{1/2+s}}{(1+t)^{1/2}}\mathrm{d}t.$$

Notice that $W_n(-t)=(-1)^nV_n(t)$.

Considering the set of Jacobi polynomials $P_n^{(\alpha,\beta)}$, Ossicini and Rosati [69] showed that the only Jacobi polynomials which are s-orthogonal for a positive integer s are the Chebyshev polynomials of the first kind, which occur when $\alpha=\beta=-\frac{1}{2}$. Recently, Shi [77] (see also [78]) has proved that the Chebyshev weight $w(t) = (1 - t^2)^{-1/2}$ is the only weight (up to a linear transformation) having the property: *For each fixed n, the solutions of the extremal problem*

$$\int_{-1}^{1} \left(\prod_{v=1}^{n} (t - \tau_v) \right)^m w(t)\,\mathrm{d}t = \min_{\pi(t) = t^n + \cdots} \int_{-1}^{1} [\pi(t)]^m w(t)\,\mathrm{d}t \tag{2.2}$$

for every even m are the same. Precisely, he proved the following result.

Theorem 2.3. *Let w be a weight supported on* $[-1,1]$ *such that* $\int_{-1}^{1} w(t)\,\mathrm{d}t = 1$. *If* (2.2) *holds for the following pairs* (m,n):

$$m = m_1, m_2, \ldots, \ if\ n = 1,2,4, \quad and \quad m = 2,4,\ if\ n = 3,5,6,\ldots,$$

where $\{m_k\}_{k\in\mathbb{N}}$ *is a strictly increasing sequence of even natural numbers such that* $m_1 = 2$ *and* $\sum_{k=1}^{+\infty}(1/m_k) = +\infty$, *then there exist two numbers* α *and* β *such that* $w = v_{\alpha,\beta}$, *where*

$$v_{\alpha,\beta}(t) = \begin{cases} \dfrac{1}{\pi\sqrt{(t-\alpha)(\beta-t)}}, & t \in (\alpha,\beta), \\ 0, & t \notin (\alpha,\beta). \end{cases}$$

Recently, Gori and Micchelli [33] have introduced for each n a class of weight functions $\mathscr{W}_n$ defined on $[-1,1]$ for which explicit n-point Gauss–Turán quadrature formulas of all orders can be found. In other words, these classes of weight functions have the peculiarity that the corresponding s-orthogonal polynomials, of the same degree, are independent of s. The class $\mathscr{W}_n$ includes certain generalized Jacobi weight functions $w_{n,\mu}(t) = |S_{n-1}(t)/n|^{2\mu+1}(1-t^2)^{\mu}$, where $S_{n-1}(\cos\theta) = \sin n\theta/\sin\theta$ (Chebyshev polynomial of the second kind) and $\mu > -1$. In this case, the Chebyshev polynomials T_n appear as s-orthogonal polynomials. For $n = 2$ the previous weight function reduces to the weight $w_{2,\mu}(t) = |t|^{2\mu+1}(1-t^2)^{\mu}$, which was studied in [30,31,36].

Very little is known about σ-orthogonal polynomials. Except for Rodrigues' formula, which has an analogue for these polynomials (see [25,26]), no general theory is available. Some particular results on zeros of σ-orthogonal polynomials and their asymptotic behavior are known (cf. [59–61]). The Legendre case with $\sigma = (0,s)$ was considered by Morelli and Verna [59], and they proved that

$$\lim_{s\to+\infty} \tau_1 = -1 \quad \text{and} \quad \lim_{s\to+\infty} \tau_2 = 0.$$

2.2. Numerical construction of power-orthogonal polynomials

An iterative process for computing the coefficients of s-orthogonal polynomials in a special case, when the interval $[a,b]$ is symmetric with respect to the origin and the weight w is an even function, was proposed by Vincenti [93]. He applied his process to the Legendre case. When n and s increase, the process becomes numerically unstable.

At the Third Conference on Numerical Methods and Approximation Theory (Niš, August 18–21, 1987) (see [51]) we 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 procedure and the Newton–Kantorovič method.

Table 1

n	$d\mu^{(n,s)}(t)$	Orthogonal polynomials			
0	$(\pi_0^{(0,s)}(t))^{2s}d\lambda(t)$	$\boxed{\pi_0^{(0,s)}}$			
1	$(\pi_1^{(1,s)}(t))^{2s}d\lambda(t)$	$\pi_0^{(1,s)}$	$\boxed{\pi_1^{(1,s)}}$		
2	$(\pi_2^{(2,s)}(t))^{2s}d\lambda(t)$	$\pi_0^{(2,s)}$	$\pi_1^{(2,s)}$	$\boxed{\pi_2^{(2,s)}}$	
3	$(\pi_3^{(3,s)}(t))^{2s}d\lambda(t)$	$\pi_0^{(3,s)}$	$\pi_1^{(3,s)}$	$\pi_2^{(3,s)}$	$\boxed{\pi_3^{(3,s)}}$
$\vdots$					

The basic idea for our method to numerically construct s-orthogonal polynomials with respect to the measure $d\lambda(t)$ on the real line $\mathbb{R}$ is a reinterpretation of the "*orthogonality conditions*" (2.1). For given n and s, we put $d\mu(t) = d\mu^{(n,s)}(t) = (\pi_{n,s}(t))^{2s}d\lambda(t)$. The conditions can then be written as

$$\int_{\mathbb{R}} \pi_k^{(n,s)}(t)t^{\nu}d\mu(t) = 0 \quad (\nu = 0, 1, \ldots, k-1),$$

where $\{\pi_k^{(n,s)}\}$ is a sequence of monic orthogonal polynomials with respect to the new measure $d\mu(t)$. Of course, $\pi_{n,s}(\cdot) = \pi_n^{(n,s)}(\cdot)$. As we can see, the polynomials $\pi_k^{(n,s)}$ $(k = 0, 1, \ldots)$ are implicitly defined, because the measure $d\mu(t)$ depends of $\pi_n^{(n,s)}(t)$. A general class of such polynomials was introduced and studied by Engels (cf. [12, pp. 214–226]). We will write simply $\pi_k(\cdot)$ instead of $\pi_k^{(n,s)}(\cdot)$. These polynomials satisfy a three-term recurrence relation

$$\begin{aligned} &\pi_{\nu+1}(t) = (t - \alpha_\nu)\pi_\nu(t) - \beta_\nu\pi_{\nu-1}(t), \quad \nu = 0, 1, \ldots, \\ &\pi_{-1}(t) = 0, \quad \pi_0(t) = 1, \end{aligned} \tag{2.3}$$

where because of orthogonality

$$\begin{aligned} \alpha_\nu = \alpha_\nu(n,s) &= \frac{(t\pi_\nu, \pi_\nu)}{(\pi_\nu, \pi_\nu)} = \frac{\int_{\mathbb{R}} t\pi_\nu^2(t)\,d\mu(t)}{\int_{\mathbb{R}} \pi_\nu^2(t)\,d\mu(t)}, \\ \beta_\nu = \beta_\nu(n,s) &= \frac{(\pi_\nu, \pi_\nu)}{(\pi_{\nu-1}, \pi_{\nu-1})} = \frac{\int_{\mathbb{R}} \pi_\nu^2(t)\,d\mu(t)}{\int_{\mathbb{R}} \pi_{\nu-1}^2(t)\,d\mu(t)} \end{aligned} \tag{2.4}$$

and by convention, $\beta_0 = \int_{\mathbb{R}} d\mu(t)$.

The coefficients α_ν and β_ν are the fundamental quantities in the constructive theory of orthogonal polynomials. They provide a compact way of representing orthogonal polynomials, requiring only a linear array of parameters. The coefficients of orthogonal polynomials, or their zeros, in contrast need two-dimensional arrays. Knowing the coefficients α_ν, β_ν $(\nu = 0, 1, \ldots, n-1)$ gives us access to the first $n+1$ orthogonal polynomials $\pi_0, \pi_1, \ldots, \pi_n$. Of course, for a given n, we are interested only in the last of them, i.e., $\pi_n \equiv \pi_n^{(n,s)}$. Thus, for $n = 0, 1, \ldots,$ the diagonal (boxed) elements in Table 1 are our s-orthogonal polynomials $\pi_n^{(n,s)}$.

A stable procedure for finding the coefficients α_ν, β_ν is the discretized Stieltjes procedure, especially for infinite intervals of orthogonality (see [15,16,20]). Unfortunately, in our case this procedure cannot be applied directly, because the measure $d\mu(t)$ involves an unknown polynomial

$\pi_n^{(n,s)}$. Consequently, we consider the system of nonlinear equations in the unknowns $\alpha_0, \alpha_1, \ldots, \alpha_{n-1}$, $\beta_0, \beta_1, \ldots, \beta_{n-1}$

$$\begin{aligned} f_0 &\equiv \beta_0 - \int_{\mathbb{R}} \pi_n^{2s}(t)\, d\lambda(t) = 0, \\ f_{2v+1} &\equiv \int_{\mathbb{R}} (\alpha_v - t)\pi_v^2(t)\pi_n^{2s}(t)\, d\lambda(t) = 0 \quad (v = 0, 1, \ldots, n-1), \\ f_{2v} &\equiv \int_{\mathbb{R}} (\beta_v \pi_{v-1}^2(t) - \pi_v^2(t))\pi_n^{2s}(t)\, d\lambda(t) = 0 \quad (v = 1, \ldots, n-1), \end{aligned} \tag{2.5}$$

which follows from (2.4), and then we apply the Newton–Kantorovič method for determining the coefficients of the recurrence relation (2.3) (see [51,22]). If sufficiently good starting approximations are chosen, the convergence of this method is quadratic. The elements of the Jacobian can be easily computed using the recurrence relation (2.3), but with other (delayed) initial values (see [51,22]). All integrals in (2.5), as well as the integrals 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 $d\lambda(t)$:

$$\int_{\mathbb{R}} g(t)\, d\lambda(t) = \sum_{v=1}^{N} A_v^{(N)} g(\tau_v^{(N)}) + R_N(g), \tag{2.6}$$

taking $N = (s+1)n$ nodes. This formula is exact for all polynomials of degree at most $2N - 1 = 2(s+1)n - 1 = 2(n-1) + 2ns + 1$.

Thus, all calculations in this method are based on using only the fundamental three-term recurrence relation (2.3) and the Gauss–Christoffel quadrature formula (2.6). The problem of finding sufficiently good starting approximations for $\alpha_v^{[0]} = \alpha_v^{[0]}(n,s)$ and $\beta_v^{[0]} = \beta_v^{[0]}(n,s)$ is the most serious one. In [51,22] we proposed to take the values obtained for $n-1$, i.e., $\alpha_v^{[0]} = \alpha_v(s, n-1)$, $\beta_v^{[0]} = \beta_v(s, n-1)$, $v \leqslant n-2$, and the corresponding extrapolated values for $\alpha_{n-1}^{[0]}$ and $\beta_{n-1}^{[0]}$. In the case $n = 1$ we solve the equation

$$\phi(\alpha_0) = \phi(\alpha_0(s,1)) = \int_{\mathbb{R}} (t - \alpha_0)^{2s+1}\, d\lambda(t) = 0,$$

and then determine $\beta_0 = \beta_0(s,1) = \int_{\mathbb{R}} (t-\alpha_0)^{2s}\, d\lambda(t)$.

The zeros $\tau_v = \tau_v(n,s)$ $(v = 1, \ldots, n)$ of $\pi_n^{(n,s)}$, i.e., the nodes of the Gauss–Turán-type quadrature formula (1.3), can be obtained very easily as eigenvalues of a (symmetric tridiagonal) Jacobi matrix J_n using the QR algorithm, namely

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

where $\alpha_v = \alpha_v(n,s)$, $\beta_v = \beta_v(n,s)$ $(v = 0, 1, \ldots, n-1)$.

Table 2

σ	(1, 1, 3)	(1, 3, 1)	(3, 1, 1)
$\tau_1^{(3,\sigma)}$	−2.30298348189811	−2.26862030544612	−1.57815506119966
$\tau_2^{(3,\sigma)}$	−0.62210813435576	0	0.62210813435576
$\tau_3^{(3,\sigma)}$	1.57815506119966	2.26862030544612	2.30298348189811

An iterative method for the construction of σ-orthogonal polynomials was developed by Gori et al. [32]. In this case, the corresponding reinterpretation of the "*orthogonality conditions*" (1.10) leads to conditions

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

where

$$\mathrm{d}\mu(t) = \mathrm{d}\mu^{(n,\sigma)}(t) = \prod_{\nu=1}^{n} (t - \tau_\nu^{(n,\sigma)})^{2s_\nu} \, \mathrm{d}\lambda(t). \tag{2.7}$$

Therefore, we conclude that $\{\pi_k^{(n,\sigma)}\}$ is a sequence of (standard) orthogonal polynomials with respect to the measure $\mathrm{d}\mu(t)$. Evidently, $\pi_n^{(n,\sigma)}(\,\cdot\,)$ is the desired σ-orthogonal polynomial $\pi_{n,\sigma}(\,\cdot\,)$. Since $\mathrm{d}\mu(t)$ is given by (2.7), we cannot apply here the same procedure as in the case of s-orthogonal polynomials. Namely, the determination of the Jacobian requires the partial derivatives of the zeros $\tau_\nu^{(n,\sigma)}$ with respect to α_k and β_k, which is not possible in an analytic form. Because of that, in [32] a discrete analogue of the Newton–Kantorovič method (a version of the secant method) was used. The convergence of this method is superlinear and strongly depends on the choice of the starting points. Recently, Milovanović and Spalević [56] have considered an iterative method for determining the zeros of σ-orthogonal polynomials.

As we mentioned in Section 1, σ-orthogonal polynomials are unique when (1.6) is imposed, with corresponding multiplicities $m_1, m_2, \ldots, m_n$. Otherwise, the number of distinct σ-polynomials is $n!/(k_1!k_2!\cdots k_q!)$ for some q $(1 \leqslant q \leqslant n)$, 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 $n = 3$, with multiplicities 3, 3, 7, we have three different Hermite σ-polynomials ($w(t) = \mathrm{e}^{-t^2}$ on $\mathbb{R}$), which correspond to $\sigma = (1, 1, 3)$, $(1, 3, 1)$, and $(3, 1, 1)$ (see Table 2).

3. Generalized Gaussian quadrature with multiple nodes

3.1. A theoretical approach

In order to construct a quadrature formula of form (1.7), with multiple nodes τ_ν (whose multiplicities are $m_\nu = 2s_\nu + 1$), Stroud and Stancu [88] (see also Stancu [80,84]) considered ℓ distinct real numbers $\alpha_1, \ldots, \alpha_\ell$ and assumed that none of these coincide with any of the τ_ν. The Lagrange–Hermite interpolation polynomial for the function f at simple nodes α_μ and the multiple nodes τ_ν,

$$L(t;f) \equiv L\begin{pmatrix} \tau_1 \\ 2s_1+1 \end{pmatrix},\ldots,\begin{pmatrix}\tau_n \\ 2s_n+1,\end{pmatrix}\begin{pmatrix}\alpha_1 \\ 1\end{pmatrix},\ldots,\begin{pmatrix}\alpha_\ell \\ 1\end{pmatrix}; \; f|t$$

$$L(t;f) \equiv L\left(\begin{matrix} \tau_1 \\ 2s_1+1 \end{matrix},\ldots,\begin{matrix}\tau_n \\ 2s_n+1,\end{matrix}\begin{matrix}\alpha_1 \\ 1\end{matrix},\ldots,\begin{matrix}\alpha_\ell \\ 1\end{matrix}; \; f\Big|t\right)$$

can be expressed in the form

$$L(t;f) = \omega(t)L\left(\begin{matrix} \tau_1 \\ 2s_1+1 \end{matrix},\ldots,\begin{matrix}\tau_n \\ 2s_n+1\end{matrix}; \; f_1\Big|t\right) + \Omega(t)L\left(\begin{matrix}\alpha_1 \\ 1\end{matrix},\ldots,\begin{matrix}\alpha_\ell \\ 1\end{matrix}; \; f_2\Big|t\right),$$

where $\omega(t)=(t-\alpha_1)\cdots(t-\alpha_\ell)$, $\Omega(t)=(t-\tau_1)^{2s_1+1}\cdots(t-\tau_n)^{2s_n+1}$, and $f_1(t)=f(t)/\omega(t)$, $f_2(t)=f(t)/\Omega(t)$. Since the remainder $r(t;f)$ of the interpolation formula $f(t)=L(t;f)+r(t;f)$ can be expressed as a divided difference,

$$r(t;f) = \Omega(t)\omega(t)\left[\begin{matrix} \tau_1 \\ 2s_1+1 \end{matrix},\ldots,\begin{matrix}\tau_n \\ 2s_n+1\end{matrix},\begin{matrix}\alpha_1 \\ 1\end{matrix},\ldots,\begin{matrix}\alpha_\ell \\ 1\end{matrix},\begin{matrix} t \\ 1\end{matrix}; f\right], \tag{3.1}$$

we obtain the quadrature formula

$$\int_{\mathbb{R}} f(t)\,\mathrm{d}\lambda(t) = Q(f) + \varphi(f) + \varrho(f), \tag{3.2}$$

where $Q(f)$ is the quadrature sum in (1.7), $\varrho(f)=\int_{\mathbb{R}} r(t;f)\,\mathrm{d}\lambda(t)$ and $\varphi(f)$ has the form $\varphi(f)=\sum_{\mu=1}^{\ell} B_\mu f(\alpha_\mu)$. Since the divided difference in (3.1) is of order $M+\ell=\sum_{\nu=1}^{n}(2s_\nu+1)+\ell$, it follows that the quadrature formula (3.2) has degree of exactness $M+\ell-1$.

For arbitrary $\alpha_1,\ldots,\alpha_\ell$ it was proved [88] that it is possible to determine the nodes $\tau_1,\ldots,\tau_n$ (with the m_ν given) so that $B_1=\cdots=B_\ell=0$. For this, the *necessary and sufficient condition* is that $\Omega(t)$ be *orthogonal* to $\mathscr{P}_{\ell-1}$ with respect to the measure $\mathrm{d}\lambda(t)$, i.e.,

$$\int_{\mathbb{R}} t^k \Omega(t)\,\mathrm{d}\lambda(t) = 0 \quad (k=0,1,\ldots,\ell-1). \tag{3.3}$$

If $\ell=n$, system (3.3) has at least one real solution consisting of the n distinct real nodes $\tau_1,\ldots,\tau_n$. The case $\ell<n$ was considered by Stancu [85]. Stancu [81–86] also generalized the previous quadrature formulas using the quadrature sum with multiple Gaussian nodes τ_ν and multiple preassigned nodes α_μ in the form

$$Q(f) = \sum_{\nu=1}^{n}\sum_{i=0}^{m_\nu-1} A_{i,\nu} f^{(i)}(\tau_\nu) + \sum_{\mu=1}^{\ell}\sum_{j=0}^{k_\mu-1} B_{j,\mu} f^{(j)}(\alpha_\mu).$$

A particular case with simple Gaussian nodes and multiple fixed nodes was considered by Stancu and Stroud [87]. The existence and uniqueness of the previous quadratures exact for an extended complete Chebyshev (ETC) system were proved by Karlin and Pinkus [41,42] without using a variational principle. Barrow [2] gave a different proof using the topological degree of a mapping. On the other hand, Barrar et al. [1] obtained the results entirely via a variational principle. Namely, they considered the problem of finding the element of minimal L_p norm ($1 \leqslant p < +\infty$) from a family of generalized polynomials, where the multiplicities of the zeros are specified. As an application, they obtained Gaussian quadrature formulas exact for extended Chebyshev systems. The L_1 case was studied in [4,6] (see also [40]).

Using a result from [80], Stancu [84] determined the following expression for Cotes coefficients in (1.7):

$$A_{i,v} = \frac{1}{i!(2s_v - i)!}\left[\frac{1}{\Omega_v(t)}\int_{\mathbb{R}} \frac{\Omega(t) - \Omega(x)}{t - x}\,\mathrm{d}\lambda(x)\right]^{(2s_v - i)}_{t=\tau_v},$$

where $\Omega_v(t) = \Omega(t)/(t - \tau_v)^{2s_v+1}$. An alternative expression

$$A_{i,v} = \frac{1}{i!}\sum_{k=0}^{2s_v - i}\frac{1}{k!}\left[\frac{(t-\tau_v)^{2s_v+1}}{\Omega(t)}\right]^{(k)}_{t=\tau_v}\int_{\mathbb{R}}\frac{\Omega(t)}{(t-\tau_v)^{2s_v-i-k+1}}\,\mathrm{d}\lambda(t) \tag{3.4}$$

was obtained in [55].

Some properties of Cotes numbers in the Turán quadrature (1.3), as well as some inequalities related to zeros of s-orthogonal polynomials, were investigated by Ossicini and Rosati [68] (see also [46]).

The remainder term in formulas with multiple nodes was studied by Chakalov [9], Ionescu [39], Ossicini [63], Pavel [70–72]. For holomorphic functions f in the Turán quadrature (1.3) over a finite interval $[a,b]$, Ossicini and Rosati [65] found the contour integral representation

$$R_{n,2s}(f) = \frac{1}{2\pi \mathrm{i}}\oint_{\Gamma}\frac{\rho_{n,s}(z)}{[\pi_{n,s}(z)]^{2s+1}}f(z)\,\mathrm{d}z, \quad \rho_{n,s}(z) = \int_a^b \frac{[\pi_{n,s}(z)]^{2s+1}}{z-t}\,\mathrm{d}\lambda(t),$$

where $[a,b] \subset \operatorname{int}\Gamma$ and $\pi_{n,s} = \pi_{n,s}(\cdot;\mathrm{d}\lambda)$. Taking as Γ confocal ellipses (having foci at ± 1 and the sum of semiaxes equal to $\rho > 1$), Ossicini et al. [64] considered two special Chebyshev measures $\mathrm{d}\lambda_1(t)$ and $\mathrm{d}\lambda_2(t)$ (see Section 2.1) and determined estimates for the corresponding remainders $R_{n,2s}(f)$, from which they proved the convergence and rate of convergence of the quadratures, $R_{n,s}(f) = \mathrm{O}(\rho^{-n(2s+1)})$, $n \to +\infty$. Morelli and Verna [58] also investigated the convergence of quadrature formulas related to σ-orthogonal polynomials.

3.2. Numerical construction

A stable method for determining the coefficients $A_{i,v}$ in the Gauss–Turán quadrature formula (1.3) was given by Gautschi and Milovanović [22]. Some alternative methods were proposed by Stroud and Stancu [88] (see also [84]), Golub and Kautsky [28], and Milovanović and Spalević [54]. A generalization of the method from [22] to the general case when $s_v \in \mathbb{N}_0$ $(v = 1,\dots,n)$ was derived recently in [55]. Here, we briefly present the basic idea of this method.

First, we define as in the previous subsection $\Omega_v(t) = \prod_{i\neq v}(t-\tau_i)^{2s_i+1}$ and use the polynomials

$$f_{k,v}(t) = (t-\tau_v)^k\Omega_v(t) = (t-\tau_v)^k\prod_{i\neq v}(t-\tau_i)^{2s_i+1},$$

where $0 \leqslant k \leqslant 2s_v$ and $1 \leqslant v \leqslant n$. Notice that $\deg f_{k,v} \leqslant 2\sum_{i=1}^n s_i + n - 1$. This means that the integration (1.7) is exact for all polynomials $f_{k,v}$, i.e., $R(f_{k,v}) = 0$, when $0 \leqslant k \leqslant 2s_v$ and $1 \leqslant v \leqslant n$. Thus, we have

$$\sum_{j=1}^{n}\sum_{i=0}^{2s_j} A_{i,j} f_{k,v}^{(i)}(\tau_j) = \int_{\mathbb{R}} f_{k,v}(t)\,\mathrm{d}\lambda(t),$$

that is,

$$\sum_{i=0}^{2s_v} A_{i,v} f_{k,v}^{(i)}(\tau_v) = \mu_{k,v}, \tag{3.5}$$

because for every $j \neq v$ we have $f_{k,v}^{(i)}(\tau_j) = 0$ $(0 \leqslant i \leqslant 2s_j)$. Here, we have put

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

For each v we have in (3.5) a system of $2s_v + 1$ linear equations in the same number of unknowns, $A_{i,v}$ $(i = 0, 1, \ldots, 2s_v)$. It can be shown that each system (3.5) is upper triangular. Thus, once all zeros of the σ-orthogonal polynomial $\pi_{n,\sigma}$, i.e., the nodes of the quadrature formula (1.7), are known, the determination of its weights $A_{i,v}$ is reduced to solving the n linear systems of $2s_v + 1$ equations

$$\begin{bmatrix} f_{0,v}(\tau_v) & f'_{0,v}(\tau_v) & \ldots & f_{0,v}^{(2s_v)}(\tau_v) \\ & f'_{1,v}(\tau_v) & \ldots & f_{1,v}^{(2s_v)}(\tau_v) \\ & & \ddots & \\ & & & f_{2s_v,v}^{(2s_v)}(\tau_v) \end{bmatrix} \begin{bmatrix} A_{0,v} \\ A_{1,v} \\ \vdots \\ A_{2s_v,v} \end{bmatrix} = \begin{bmatrix} \mu_{0,v} \\ \mu_{1,v} \\ \vdots \\ \mu_{2s_v,v} \end{bmatrix}.$$

Using these systems and the normalized moments

$$\hat{\mu}_{k,v} = \frac{\mu_{k,v}}{\prod_{i \neq v} (\tau_v - t_i)^{2s_i+1}} = \int_{\mathbb{R}} (t-\tau_v)^k \prod_{i \neq v} \left(\frac{t-\tau_i}{\tau_v - \tau_i} \right)^{2s_i+1} \mathrm{d}\lambda(t),$$

we can prove [55]

Theorem 3.1. *For fixed v $(1 \leqslant v \leqslant n)$ the coefficients $A_{i,v}$ in the generalized Gauss–Turán quadrature formula* (1.7) *are given by*

$$b_{2s_v+1} = (2s_v)!\,A_{2s_v,v} = \hat{\mu}_{2s_v,v},$$

$$b_k = (k-1)!\,A_{k-1,v} = \hat{\mu}_{k-1,v} - \sum_{j=k+1}^{2s_v+1} \hat{a}_{k,j} b_j \quad (k = 2s_v, \ldots, 1),$$

where

$$\hat{a}_{k,k} = 1, \quad \hat{a}_{k,k+j} = -\frac{1}{j} \sum_{l=1}^{j} u_l \hat{a}_{l,j}, \quad u_l = \sum_{i \neq v} (2s_i + 1)(\tau_i - \tau_v)^{-l}.$$

The normalized moments $\hat{\mu}_{k,v}$ can be computed exactly, except for rounding errors, by using the same Gauss–Christoffel formula as in the construction of σ-orthogonal polynomials, i.e., (2.6) with $N = \sum_{v=1}^{n} s_v + n$ nodes. A few numerical examples can be found in [22,52,55]. Also, in [55] an alternative approach to the numerical calculation of the coefficients $A_{i,v}$ was given using expression (3.4).

4. Some remarks on the Chebyshev measure

From the remarks in Section 2 about s-orthogonal polynomials with Chebyshev measure, it is easy to see that the Chebyshev–Turán formula is given by

$$\int_{-1}^{1} \frac{f(t)}{\sqrt{1-t^2}}\,\mathrm{d}t = \sum_{i=0}^{2s}\sum_{v=1}^{n} A_{i,v} f^{(i)}(\tau_v) + R_n(f), \tag{4.1}$$

where $\tau_v = \cos((2v-1)\pi/2n)$ $(v=1,\ldots,n)$. It is exact for all polynomials of degree at most $2(s+1)n-1$. Turán stated the problem of explicit determination of the $A_{i,v}$ and their behavior as $n \to +\infty$ (see Problem XXVI in [91]). In this regard, Micchelli and Rivlin [49] proved the following characterization: *If* $f \in \mathscr{P}_{2(s+1)n-1}$ *then*

$$\int_{-1}^{1} \frac{f(t)}{\sqrt{1-t^2}}\,\mathrm{d}t = \frac{\pi}{n}\left\{\sum_{v=1}^{n} f(\tau_v) + \sum_{j=1}^{s} \alpha_j f'[\tau_1^{2j},\ldots,\tau_n^{2j}]\right\},$$

where

$$\alpha_j = \frac{(-1)^j}{2j4^{(n-1)j}}\binom{-1/2}{j} \quad (j=1,2,\ldots)$$

and $g[y_1^r,\ldots,y_m^r]$ *denotes the divided difference of the function* g, *where each* y_j *is repeated* r *times*. In fact, they obtained a quadrature formula of highest algebraic degree of precision for the Fourier–Chebyshev coefficients of a given function f, which is based on the divided differences of f' at the zeros of the Chebyshev polynomial T_n. A Lobatto type of Turán quadrature was considered by Micchelli and Sharma [50]. Recently, Bojanov [5] has given a simple approach to questions of the previous type and applied it to the coefficients in arbitrary orthogonal expansions of f. As an auxiliary result he obtained a new interpolation formula and a new representation of the Turán quadrature formula. Some further results can be found in [79].

For $s=1$, the solution of the Turán problem XXVI is given by

$$A_{0,v} = \frac{\pi}{n}, \quad A_{1,v} = -\frac{\pi\tau_v}{4n^3}, \quad A_{2,v} = \frac{\pi}{4n^3}(1-\tau_v^2).$$

In 1975 Riess [75], and in 1984 Varma [92], using very different methods, obtained the explicit solution of the Turán problem for $s=2$. One simple answer to Turán's question was given by Kis [43]. His result can be stated in the following form: *If* g *is an even trigonometric polynomial of degree at most* $2(s+1)n-1$, *then*

$$\int_0^{\pi} g(\theta)\,\mathrm{d}\theta = \frac{\pi}{n(s!)^2}\sum_{j=0}^{s}\frac{S_j}{4^j n^{2j}}\sum_{v=1}^{n} g^{(2j)}\left(\frac{2v-1}{2n}\pi\right),$$

where the S_{s-j} $(j=0,1,\ldots,s)$ *denote the elementary symmetric polynomials with respect to the numbers* $1^2,2^2,\ldots,s^2$, i.e., $S_s=1$, $S_{s-1}=1^2+2^2+\cdots+s^2,\ldots,S_0=1^2\cdot 2^2\cdots s^2$. Consequently,

$$\int_{-1}^{1} \frac{f(t)}{\sqrt{1-t^2}}\,\mathrm{d}t = \frac{\pi}{n(s!)^2}\sum_{j=0}^{s}\frac{S_j}{4^j n^{2j}}\sum_{v=1}^{n}[\mathrm{D}^{2j} f(\cos\theta)]_{\theta=((2v-1)/2n)\pi}.$$

An explicit expression for the coefficients $A_{i,v}$ was recently derived by Shi [76]. The remainder $R_n(f)$ in (4.1) was studied by Pavel [70].

5. Some remarks on moment-preserving spline approximation

Solving some problems in computational plasma physics, Calder and Laframboise [7] considered the problem of approximating the Maxwell velocity distribution by a step function, i.e., by a “multiple-water-bag distribution” in their terminology, in such a way that as many of the initial moments as possible of the Maxwell distribution are preserved. They used a classical method of reduction to an eigenvalue problem for Hankel matrices, requiring high-precision calculations because of numerical instability. A similar problem, involving Dirac’s δ-function instead of Heaviside’s step function, was treated earlier by Laframboise and Stauffer [45], using the classical Prony’s method. A stable procedure for these problems was given by Gautschi [17] (see also [19]), who found the close connection of these problems with Gaussian quadratures. This work was extended to spline approximation of arbitrary degree by Gautschi and Milovanović [21]. In this case, a spline $s_{n,m}$ of degree m with n knots is sought so as to faithfully reproduce the first $2n$ moments of a given function f. Under suitable assumptions on f, it was shown that the problem has a unique solution if and only if certain Gauss–Christoffel quadratures exist that correspond to a moment functional or weight distribution depending on f. Existence, uniqueness, and pointwise convergence of such approximations were analyzed. Frontini et al. [13] and Frontini and Milovanović [14] considered analogous problems on an arbitrary finite interval. If the approximations exist, they can be represented in terms of generalized Gauss–Lobatto and Gauss–Radau quadrature formulas relative to appropriate measures depending on f.

At the Singapore Conference on Numerical Mathematics (1988) we presented a moment-preserving approximation on $[0,+\infty)$ by defective splines of degree m, with odd defect (see [53]).

A spline function of degree $m \geqslant 1$ on the interval $0 \leqslant t < +\infty$, vanishing at $t = +\infty$, with variable positive knots τ_ν $(\nu = 1,\ldots,n)$ having multiplicities m_ν $(\leqslant m)$ $(\nu = 1,\ldots,n;\ n > 1)$ can be represented in the form

$$S_{n,m}(t) = \sum_{\nu=1}^{n} \sum_{i=0}^{m_\nu - 1} \alpha_{\nu,i} (\tau_\nu - t)_+^{m-i} \quad (0 \leqslant t < +\infty), \tag{5.1}$$

where $\alpha_{\nu,i}$ are real numbers. Under the conditions

$$\int_0^{+\infty} t^{j+d-1} S_{n,m}(t)\,\mathrm{d}t = \int_0^{+\infty} t^{j+d-1} f(t)\,\mathrm{d}t \quad (j = 0,1,\ldots,2(s+1)n-1)$$

in [53] we considered the problem of approximating a function $f(t)$ of the radial distance $t = \|x\|$ $(0 \leqslant t < +\infty)$ in $\mathbb{R}^d$ $(d \geqslant 1)$ by the spline function (5.1), where $m_\nu = 2s+1$ $(\nu = 1,\ldots,n;\ s \in \mathbb{N}_0)$. Under suitable assumptions on f, we showed that the problem has a unique solution if and only if certain generalized Turán quadratures exist corresponding to a measure depending on f. A more general case with variable defects was considered by Gori and Santi [34] and Kovačević and Milovanović [44] (see also [52]). In that case, the approximation problems reduce to quadratures of form (1.7) and σ-orthogonal polynomials.

Following [44], we discuss here two problems of approximating a function $f(t)$, $0 \leqslant t < +\infty$, by the defective spline function (5.1). Let N denote the number of the variable knots τ_ν $(\nu = 1,\ldots,n)$ of the spline function $S_{n,m}(t)$, counting multiplicities, i.e., $N = m_1 + \cdots + m_n$.

Problem 5.1. *Determine* $S_{n,m}$ *in* (5.1) *such that* $S_{n,m}^{(k)}(0)=f^{(k)}(0)$ $(k=0,1,\ldots,N+n-1;\ m \geqslant N+n-1)$.

Problem 5.2. *Determine* $S_{n,m}$ in (5.1) *such that* $S_{n,m}^{(k)}(0)=f^{(k)}(0)$ $(k=0,1,\ldots,l;\ l\leqslant m)$ *and*

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

The next theorem gives the solution of Problem 5.2.

Theorem 5.3. *Let* $f\in C^{m+1}[0,+\infty)$ *and* $\int_0^{+\infty} t^{N+n-l+m}|f^{(m+1)}(t)|\,\mathrm{d}t<+\infty$. *Then a spline function* $S_{n,m}$ *of form* (5.2), *with positive knots* τ_ν, *that satisfies the conditions of Problem* 5.2 *exists and is unique if and only if the measure*

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

admits a generalized Gauss–Turán quadrature

$$\int_0^{+\infty} g(t)\,\mathrm{d}\lambda(t)=\sum_{\nu=1}^{n}\sum_{k=0}^{m_\nu-1} A_{\nu,k}^{(n)}g^{(k)}(\tau_\nu^{(n)})+R_n(g;\mathrm{d}\lambda) \tag{5.2}$$

with n distinct positive nodes $\tau_\nu^{(n)}$, *where* $R_n(g;d\lambda)=0$ *for all* $g\in\mathscr{P}_{N+n-1}$. *The knots in* (5.1) *are given by* $\tau_\nu=\tau_\nu^{(n)}$, *and the coefficients* $\alpha_{\nu,i}$ *by the following triangular system*:

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

If we let $l=N+n-1$, this theorem gives also the solution of Problem 5.1. The case $m_1=m_2=\cdots=m_n=1$, $l=-1$, has been obtained by Gautschi and Milovanović [21]. The error of the spline approximation can be expressed as the remainder term in (5.2) for a particular function $\sigma_t(x)=x^{-(m-l)}(x-t)_+^m$ (see [44]).

Further extensions of the moment-preserving spline approximation on $[0,1]$ are given by Micchelli [48]. He relates this approximation to the theory of monosplines. A similar problem by defective spline functions on the finite interval $[0,1]$ has been studied by Gori and Santi [35] and solved by means of monosplines.

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