



Calculation of Gaussian-Type Quadratures with Multiple Nodes

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Abstract—A new algorithm for constructing quadrature formulas with multiple Gaussian nodes in the presence of certain fixed nodes is presented. It can be used in construction for measures with the bounded and infinite supports. The algorithm includes a simple and fast method for finding elements of the Jacobian matrix in an iterative process with quadratic convergence, which is based on using the fundamental three-term recurrence relation for the corresponding orthogonal polynomials with respect to a given measure. Numerical experiments with respect to several different measures are also included. Finally, a simple method for calculating weight coefficients (Cotes numbers of higher order) of Gaussian and prescribed nodes is presented. Numerical examples are included. © 2004 Elsevier Ltd. All rights reserved.

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1. INTRODUCTION AND PRELIMINARIES

Let $d\lambda(t)$ be a given nonnegative measure on the real line \mathbb{R} , with compact or unbounded support, for which all moments $\mu_k = \int_{\mathbb{R}} t^k d\lambda(t)$ $k = 0, 1, \dots$ exist and are finite, and $\mu_0 > 0$. With \mathcal{P}_k , we denote the set of all algebraic polynomials of degree at most k ($\in \mathbb{N}_0$).

Let η_1, \dots, η_m ($\eta_1 < \dots < \eta_m$) be given *fixed* (or *prescribed*) nodes, with multiplicities m_1, \dots, m_m , respectively, and τ_1, \dots, τ_n ($\tau_1 < \dots < \tau_n$) be *free* nodes, with given multiplici-

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ties n_1, \dots, n_n , respectively. Quadrature formulae of the form

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

where

$$Q(f) := \sum_{\nu=1}^n \sum_{i=0}^{n_\nu-1} A_{i,\nu} f^{(i)}(\tau_\nu) + \sum_{\nu=1}^m \sum_{i=0}^{m_\nu-1} B_{i,\nu} f^{(i)}(\eta_\nu) \tag{1.1}$$

were investigated by Stancu [1-3].

Using fixed and free nodes, we introduce two polynomials

$$q_M(t) := \prod_{\nu=1}^m (t - \eta_\nu)^{m_\nu} \quad \text{and} \quad Q_N(t) := \prod_{\nu=1}^n (t - \tau_\nu)^{n_\nu}, \tag{1.2}$$

where $M = \sum_{\nu=1}^m m_\nu$ and $N = \sum_{\nu=1}^n n_\nu$. The quadrature formula (1.1) is called *interpolatory* with an algebraic degree of exactness at least $M + N - 1$ if $I(f) = Q(f)$ for all polynomials of degree at most $M + N - 1$. Choosing the free nodes to increase the degree of exactness leads to so-called Gaussian type of quadratures. If the free (or *Gaussian*) nodes τ_1, \dots, τ_n are such that $I(f) = Q(f)$ for each $f \in \mathcal{P}_{M+N+n-1}$, the corresponding quadrature Q we call the *Gauss-Stancu formula*. The following characterization is well known (see [4]).

THEOREM 1.1. *Let the polynomials $q_M(t)$ and $Q_N(t)$ be given by (1.2). The nodes τ_1, \dots, τ_n are the Gaussian nodes if and only if*

$$\int_{\mathbb{R}} t^k Q_N(t) q_M(t) d\lambda(t) = 0, \tag{1.3}$$

for $k = 0, 1, \dots, n - 1$.

Under some restrictions of polynomials $q_M(t)$ and $Q_N(t)$ on the support interval of the measure $d\lambda(t)$ (the smallest interval containing $\text{supp}(d\lambda)$), we can give sufficient conditions for the existence of Gaussian nodes (cf. [4,5]).

THEOREM 1.2. *If the multiplicities of the Gaussian nodes are odd, e.g., $n_\nu = 2s_\nu + 1, \nu = 1, \dots, n$, and if the polynomial with fixed nodes $q_M(t)$ does not change its sign in the support interval of the measure $d\lambda(t)$, then, in this interval, there exist real distinct nodes $\tau_\nu, \nu = 1, \dots, n$.*

The condition for the polynomial $q_M(t)$ in the last theorem means that the multiplicities of the internal fixed nodes must be even. Defining a new (nonnegative) measure $d\hat{\lambda}(t)$ by

$$d\hat{\lambda}(t) = \gamma q_M(t) d\lambda(t), \quad \gamma = \text{sgn}(q_M(t)), \tag{1.4}$$

the ‘‘orthogonality conditions’’ (1.3) can be expressed in the simpler form

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

This means that the general quadrature problem (1.1), under conditions of Theorem 1.2, can be reduced to a problem with only Gaussian nodes, but with respect to another modified measure. Computational methods for this purpose are based on Christoffel’s theorem and described in detail in [6] (see also [5,7]).

Let $\pi_n(t) := \prod_{\nu=1}^n (t - \tau_\nu)$. Since $Q_N(t)/\pi_n(t) = \prod_{\nu=1}^n (t - \tau_\nu)^{2s_\nu} \geq 0$ over the support interval, we can make an additional reinterpretation of the ‘‘orthogonality conditions’’ (1.3) in the form

$$\int_{\mathbb{R}} t^k \pi_n(t) d\mu(t) = 0, \quad k = 0, 1, \dots, n - 1, \tag{1.5}$$

where

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

This means that $\pi_n(t)$ is a polynomial orthogonal with respect to the new nonnegative measure $d\mu(t)$, and therefore, all zeros τ_1, \dots, τ_n are simple, real, and belong to the support interval. As we see the measure $d\mu(t)$ involves the nodes τ_1, \dots, τ_n , i.e., the unknown polynomial $\pi_n(t)$, which is implicitly defined (see [8, pp. 214–226]). This polynomial $\pi_n(t)$ belongs to the class of so-called σ -orthogonal polynomials $\{\pi_{n,\sigma}(t)\}_{n \in \mathbb{N}_0}$, which correspond to the sequence $\sigma = (s_1, s_2, \dots)$ connected with multiplicities of Gaussian nodes (see Theorem 1.2). Namely, $\pi_n(t) = \pi_{n,\sigma}(t)$. If $\sigma = (s, s, \dots)$, the above polynomials reduce to the s -orthogonal polynomials. (For details, see for example, [9].)

For prescribed nodes η_1, \dots, η_m , we assumed that they are distinct. Under the conditions of Theorem 1.2, the Gaussian nodes τ_1, \dots, τ_n are also distinct, but some of them may coincide with some of the prescribed nodes. In that case, the quadrature Q must be adjusted in the following way (cf. [5]). If $\tau_i = \eta_j$, then η_j has to be removed from the list of fixed nodes and the multiplicity of the Gaussian node τ_i changed to $n_i + m_j = 2(s_i + r_j) + 1$. Note that such merging of nodes does not change the value of $M + N$.

Also, we mention here that the conditions of Theorem 1.2 are not necessary for the existence of Gauss-Stancu quadratures. As an interesting and important example, we mention the Gauss-Kronrod quadratures with simple prescribed internal nodes or, in general, with prescribed nodes of odd multiplicities.

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

$$\int_{\mathbb{R}} f(t) d\lambda(t) = \sum_{\nu=1}^n \sum_{i=0}^{2s_\nu} A_{i,\nu} f^{(i)}(\tau_\nu) + R(f), \quad (1.6)$$

which are exact for all algebraic polynomials of degree at most $d_{\max} = 2 \sum_{\nu=1}^n s_\nu + 2n - 1$, are known as *Chakalov-Popoviciu quadrature formulas* (see [10–12]). Deep theoretical progress in this subject was made by Stancu (see [3,13–17]). In the special case of the Legendre measure on $[-1, 1]$, when all multiplicities are mutually equal, these formulas reduce to the well-known *Turán quadrature* [18]. The case with a weight function $d\lambda(t) = w(t) dt$ on $[a, b]$ has been investigated by Italian mathematicians Ossicini, Ghizzetti, Guerra, and Rosati, and also by Chakalov, Stroud, Stancu, Ionescu, Pavel, etc. (see [9] for references).

In this paper, we consider only cases described by Theorem 1.2. In the numerical construction of such formulas, we deal with two tasks. The first task is a nonlinear algebraic problem of finding Gaussian nodes τ_1, \dots, τ_n , and the second one is a linear problem—the calculation of the coefficients $A_{i,\nu}$ and $B_{i,\nu}$ in (1.1). The first problem is treated in Sections 2–4. Some numerical experiments with respect to several different measures are considered in Section 5. A simple method for calculating weight coefficients (Cotes numbers of higher order) of Gaussian and prescribed nodes is presented in Section 6, including some numerical results. Finally, some concluding remarks are given in Section 7.

2. NUMERICAL PROCEDURE FOR FINDING GAUSSIAN NODES

Under conditions of Theorem 1.2, the problem of the construction of Gaussian nodes in (1.1) reduces to the corresponding problem for the Chakalov-Popoviciu quadrature formula (1.6) with respect to the modified measure $d\hat{\lambda}(t)$ given by (1.4). Therefore, without loss of generality, we consider only the problem of finding nodes τ_1, \dots, τ_n in (1.4). In fact, we need the zeros of σ -orthogonal (or s -orthogonal) polynomials.

An idea for finding s -orthogonal polynomials, i.e., their zeros τ_ν , solving the system of nonlinear equations (1.5) when $s_1 = \dots = s_n = s$, i.e.,

$$\int_{\mathbb{R}} t^k \pi_{n,s}(t)^{2s+1} d\lambda(t) = 0, \quad k = 0, 1, \dots, n-1 \quad (2.1)$$

in unknowns τ_1, \dots, τ_n , can be found in [8, pp. 214–226] (see also [19]).

Recently, this idea has been used in construction of an iterative method with quadratic convergence for finding the corresponding s - and σ -orthogonal polynomials (see [20]). This method was made in two parts; the first part constructs the s -orthogonal polynomial with the maximal value of s_k , i.e., for $\bar{s} = \max\{s_\nu \mid \nu = 1, \dots, n\}$, and the second one constructs the desired σ -orthogonal polynomial through several steps by reducing only one s_ν to $s_\nu - 1$ in each of the steps.

The first part of the method (construction of s -orthogonal polynomial with $s = \bar{s}$) starts with zeros of the σ -orthogonal polynomial for $\sigma = (0, 0, \dots, 0)$, i.e., with zeros τ_1, \dots, τ_n of the standard orthogonal polynomial. Then, applying one QR step with the shift τ_1 , we determine the starting vector in the nonlinear procedure for finding the zeros of σ -orthogonal polynomial for $\sigma = (1, 0, \dots, 0)$. Further, in each of the following steps, we raise only one s_ν to $s_{\nu+1}$ via the following path:

$$\begin{aligned} &(1, 0, 0, \dots, 0, 0), (1, 1, 0, \dots, 0, 0), \dots, (1, 1, 1, \dots, 1, 1), \\ &(1, 1, 1, \dots, 1, 2), (1, 1, 1, \dots, 2, 2), \dots, (2, 2, 2, \dots, 2, 2), \\ &(3, 2, 2, \dots, 2, 2), (3, 3, 2, \dots, 2, 2), \dots, (3, 3, 3, \dots, 3, 3), \\ &(3, 3, 3, \dots, 3, 4), \dots, \end{aligned} \quad (2.2)$$

until we get the desired s -orthogonal polynomial with $\sigma = \sigma_n = (s, s, s, \dots, s, s)$. In each step, except in the first one, the initial value for each of the zeros we determine by Lagrange extrapolating polynomial by using the values, obtained in the previous steps, for the corresponding zero.

This approach was mainly based on the behavior of the zeros of s -orthogonal polynomials for the Legendre, Laguerre, and Hermite measure, recently presented in [9, Figures 1–3]. One can see that behavior of the zeros, when the degree of the polynomial is fixed and s increases, is almost linear. The method is very successful, in particular for measures on the bounded support (e.g., for the Jacobi measure). In the case of measures on the unbounded support (e.g., for the Laguerre and Hermite measures), sometimes the computation can break down, so that the algorithm cannot be applied in such cases.

The main problem in the application of this method is a choice of the initial values of zeros, as well as a lot of computation via the above mentioned path (2.2) with ns steps. Notice that, in each step in this chain, we must solve a system of n nonlinear equations using an iterative procedure.

In this section, we give a new algorithm with at least three important improvements.

- The algorithm can be used in constructions for measures with the bounded and unbounded supports.
- Under certain initial values, the algorithm requires only $n - 3$ steps for constructing the polynomial $\pi_{n,s}(t)$ instead of ns steps in the chain (2.2).
- There is a simple and fast method for finding elements of the Jacobian matrix in the corresponding iterative process.

In the next sections, we describe only phases of the new algorithm which are different from one proposed in [20]. The iterative procedure for finding zeros of $\pi_{n,\sigma}(t)$ (or $\pi_{n,s}(t)$ in a special case) with quadratic convergence, under suitable starting values, is presented in Section 3. An important part of the new algorithm is a much simpler construction of the s -orthogonal polynomial $\pi_{n,s}(t)$ in only $n - 3$ steps. It is considered in Section 4, including a selection of the starting values in this process. Numerical experiments with several kinds of the classical and nonclassical measures are considered in Section 5.

3. ITERATIVE METHOD FOR ZEROS

In this section, we present a modification of the corresponding method from [20]. This iterative method for finding zeros of σ -polynomials can be applied for a wide class of the measures $d\lambda(t)$. We also derive a simple way for quickly finding elements of the corresponding Jacobian matrix.

For a given sequence $\sigma = \sigma_n = (s_1, s_2, \dots, s_n)$, we rewrite the orthogonality conditions (1.5) as the following system of nonlinear equations:

$$F_j(\mathbf{t}) \equiv \int_{\mathbb{R}} p_{j-1}(t) \left(\prod_{\nu=1}^n (t - \tau_\nu)^{2s_\nu+1} \right) d\lambda(t) = 0, \quad j = 1, \dots, n, \tag{3.1}$$

where $\mathbf{t} = (\tau_1, \tau_2, \dots, \tau_n)$ and $\{p_j\}_{j \in \mathbb{N}_0}$ is the sequence of orthonormal polynomials with respect to the measure $d\lambda(t)$ on \mathbb{R} . These polynomials satisfy the three-term recurrence relation

$$\sqrt{\beta_{j+1}} p_{j+1}(t) + \alpha_j p_j(t) + \sqrt{\beta_j} p_{j-1}(t) = t p_j(t), \quad j = 0, 1, \dots, \tag{3.2}$$

with $p_{-1}(t) = 0$ and $p_0(t) = 1/\sqrt{\beta_0}$, where $\beta_0 = \mu_0 = \int_{\mathbb{R}} d\lambda(t)$.

Notice that in equation (5.1) in [20], in (3.1), we used the monomials $\{t^{j-1}\}_{j=1}^n$ instead of these orthonormal polynomials $\{p_{j-1}\}_{j=1}^n$. Also, in our software implementation, we used alternatively the (modified) fundamental Lagrange polynomials $\{\ell_{n,1}(t), \dots, \ell_{n,n}(t)\}$, where $\ell_{n,j}(t) = \pi_n(t)/(t - \tau_j)$, $j = 1, \dots, n$, and $\pi_n(t) = (t - \tau_1) \cdots (t - \tau_n)$.

In order to solve the system of nonlinear equations (3.1), we use the matrix notation

$$\mathbf{t} = [\tau_1 \tau_2 \dots \tau_n]^\top, \quad \mathbf{t}^{(m)} = [\tau_1^{(m)} \tau_2^{(m)} \dots \tau_n^{(m)}]^\top, \quad m = 0, 1, \dots,$$

and

$$\mathbf{F}(\mathbf{t}) = [F_1(\mathbf{t}) F_2(\mathbf{t}) \dots F_n(\mathbf{t})]^\top.$$

If $W = W(\mathbf{t})$ is the corresponding Jacobian of $\mathbf{F}(\mathbf{t})$, we can apply the Newton-Kantorovič method

$$\mathbf{t}^{(m+1)} = \mathbf{t}^{(m)} - W^{-1}(\mathbf{t}^{(m)}) \mathbf{F}(\mathbf{t}^{(m)}), \quad m = 0, 1, 2, \dots, \tag{3.3}$$

for determining the zeros of the σ -orthogonal polynomial $\pi_{n,\sigma}$. If a sufficiently good approximation $\mathbf{t}^{(0)}$ is chosen, the convergence of the method (3.3) is quadratic.

The elements of the Jacobian

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

can be calculated by

$$w_{j,k} = \frac{\partial F_j}{\partial \tau_k} = -(2s_k + 1) \int_{\mathbb{R}} \frac{p_{j-1}(t)}{t - \tau_k} \left(\prod_{\nu=1}^n (t - \tau_\nu)^{2s_\nu+1} \right) d\lambda(t), \tag{3.4}$$

where $j, k = 1, \dots, n$.

THEOREM 2.1. *Let F_j be defined by (3.1), $w_{0,k} = 0$, and $w_{1,k}$, $k = 1, \dots, n$, be given by (3.4), i.e.,*

$$w_{1,k} = -\frac{2s_k + 1}{\sqrt{\beta_0}} \int_{\mathbb{R}} (t - \tau_k)^{2s_k} \left(\prod_{\substack{\nu=1 \\ \nu \neq k}}^n (t - \tau_\nu)^{2s_\nu+1} \right) d\lambda(t). \tag{3.5}$$

Then

$$\sqrt{\beta_{j+1}} w_{j+2,k} = (\tau_k - \alpha_j) w_{j+1,k} - \sqrt{\beta_j} w_{j,k} - (2s_k + 1) F_{j+1}, \tag{3.6}$$

for $j = 0, 1, \dots, n - 2$.

PROOF. Multiplying the three-term recurrence relation for orthonormal polynomials (3.2) by $-(2s_k + 1)(\prod_{\nu=1}^n (t - \tau_\nu)^{2s_\nu + 1}) / (t - \tau_k)$, and then integrating over \mathbb{R} with respect to the measure $d\lambda(t)$ and using (3.4) and (3.1), we obtain

$$\begin{aligned} \sqrt{\beta_{j+1}} w_{j+2,k} + \alpha_j w_{j+1,k} + \sqrt{\beta_j} w_{j,k} &= -(2s_k + 1) \int_{\mathbb{R}} \frac{tp_j(t)}{t - \tau_k} \left(\prod_{\nu=1}^n (t - \tau_\nu)^{2s_\nu + 1} \right) d\lambda(t) \\ &= -(2s_k + 1) F_{j+1} + \tau_k w_{j+1,k}, \end{aligned}$$

i.e., (3.6). ■

Thus, knowing only F_j and $w_{1,j}$ ($j = 1, \dots, n$), we calculate the elements of the Jacobian matrix by the nonhomogeneous recurrence relation (3.6). All of the integrals in (3.1) and (3.5) can be calculated exactly, except for rounding errors, by using a Gauss-Christoffel quadrature formula with respect to the measure $d\lambda(t)$ (see [21]),

$$\int_{\mathbb{R}} g(t) d\lambda(t) = \sum_{\nu=1}^L A_\nu^{(L)} g(\tau_\nu^{(L)}) + R_L(g), \tag{3.7}$$

taking $L = n + \sum_{\nu=1}^n s_\nu$ nodes. This formula is exact for all polynomials g of degree at most $2L - 1 = 2n - 1 + 2 \sum_{\nu=1}^n s_\nu$.

4. CONSTRUCTION OF s -ORTHOGONAL POLYNOMIALS

Let $\pi_{n,s}(t)$ be the s -orthogonal polynomial with respect to the measure $d\lambda(t)$, and let $\tau_\nu^{(n,s)}$, $\nu = 1, \dots, n$, be its zeros. The behavior of the zeros $\tau_\nu^{(n,s)}$ for a fixed s and when the degree of the polynomial n increases can be used in the construction of s -orthogonal polynomials. In Figure 1, we display the distribution of nonnegative zeros for Legendre and Hermite s -orthogonal polynomials, taking $s = 1$ and $n = 2, \dots, 15$. The solid lines connect the zeros $\tau_\nu^{(n,s)}$ with the same index ν . For the same values of s and n , the zeros of the generalized Laguerre polynomials $L_{n,s}^\alpha(t)$ for $\alpha = 0$ and $\alpha = 101/3$ are presented in Figure 2. If s is bigger than one, the corresponding graphics are quite similar to the previous one, especially for the generalized Laguerre measure.

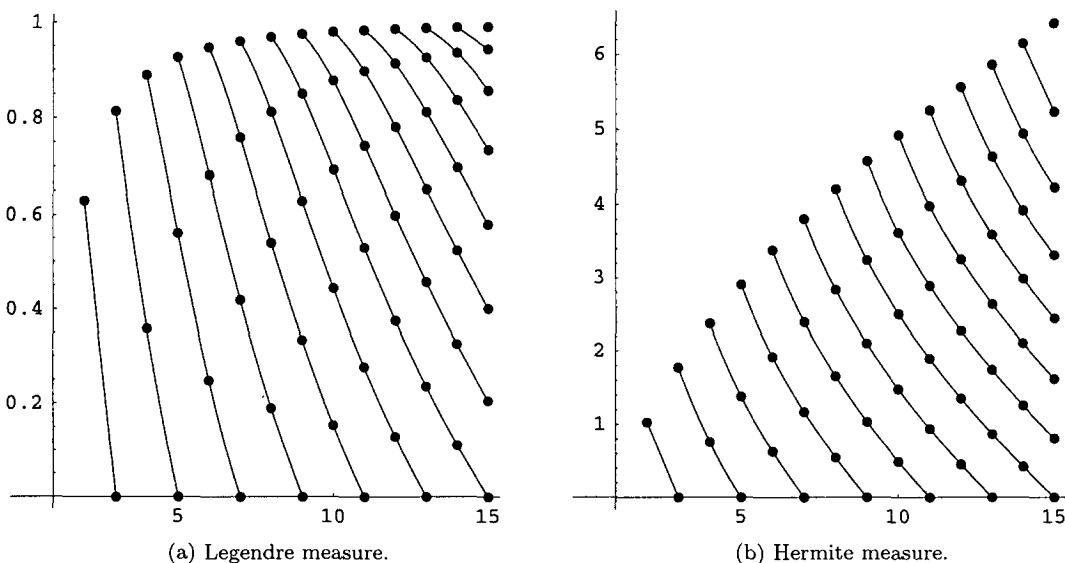


Figure 1. Nonnegative zeros of s -orthogonal polynomials for $s = 1$ and $n = 2(1)15$ for the Legendre measure (a) and the Hermite measure (b).

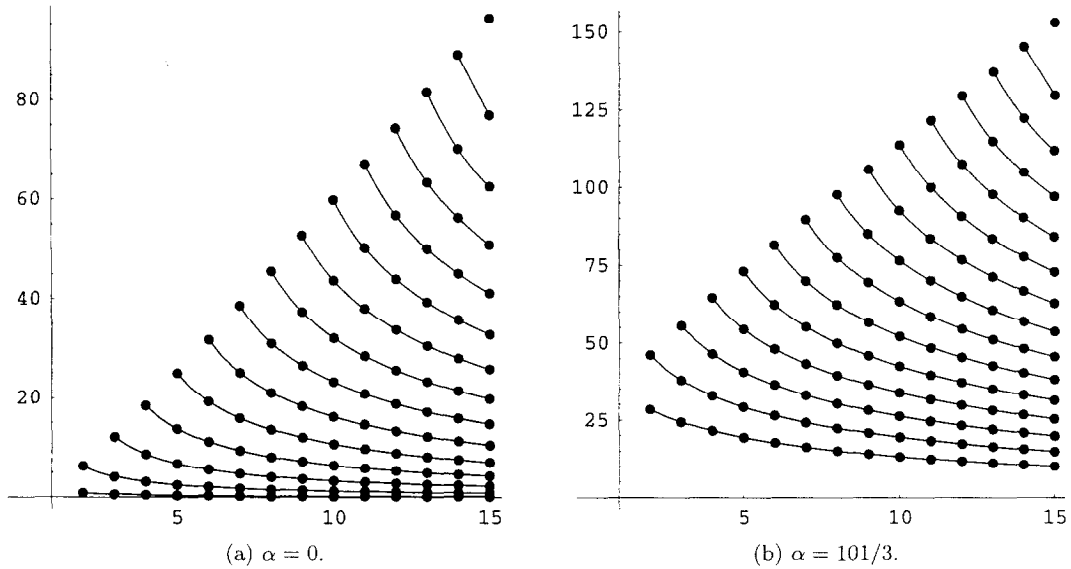


Figure 2. Zeros of the generalized Laguerre s -orthogonal polynomials $L_{ns}^\alpha(t)$ for $s = 1, n = 2(1)15$, and $\alpha = 0$ (a) and $\alpha = 101/3$ (b).

As we can see, the behavior of zeros is almost linear for the Hermite and Legendre case, but it is not true for the Laguerre case. This observation gives us an inspiration to construct an iterative algorithm for calculating zeros of s -orthogonal polynomials over the path when the degree of a polynomial increases, and s is a fixed number.

In this new approach, for a fixed s , we start from the zeros of s -orthogonal polynomials of degree two and three, usually obtained by the algorithm proposed in [20], and then we calculate the starting values for the method described in Section 3. Using this method, we determine the zeros of the s -orthogonal polynomial $\pi_{4,s}(t)$ of degree four.

In general, using the zeros of $\pi_{k-2,s}(t)$ and $\pi_{k-1,s}(t)$, i.e.,

$$\mathbf{t}_i = \left[\tau_1^{(i,s)} \tau_2^{(i,s)} \dots \tau_i^{(i,s)} \right]^\top, \quad i = k - 2, \quad k - 1,$$

we must determine at first the starting vector

$$\mathbf{t}_k^{(0)} = \left[\hat{\tau}_1^{(k,s)} \hat{\tau}_2^{(k,s)} \dots \hat{\tau}_k^{(k,s)} \right]^\top, \tag{4.1}$$

and then apply method (3.3) for solving the corresponding system of k nonlinear equations in order to get the zeros of the polynomial $\pi_{k,s}(t)$. Repeating this procedure $n - 3$ times, for $k = 4, \dots, n$, we obtain the zeros of the polynomial $\pi_{n,s}(t)$.

As we can see, such a method of construction requires much less numerical work than the previous procedure proposed in [20]. For example, in the case $n = s = 10$, the previous algorithm requires us to solve 100 systems of nonlinear equations with ten unknowns (see (2.2)). On the other side, using the new algorithm, one has to solve only seven systems of equations with four, five, six, seven, eight, nine, and ten unknowns, respectively. Of course, the last algorithm requires additional work for constructing the zeros of the polynomials $\pi_{2,s}(t)$ and $\pi_{3,s}(t)$. (They are systems with two and three unknowns, respectively.)

Thus, the basic problem in the new algorithm is to find an appropriate formula for the starting vector (4.1), with components

$$\hat{\tau}_\nu^{(k,s)} = S_\nu(\mathbf{t}_{k-1}, \mathbf{t}_{k-2}), \quad \nu = 1, \dots, k. \tag{4.2}$$

According to numerical investigation of zero distribution, we use empirical extrapolation formulas which include zeros as displayed in Figure 3.

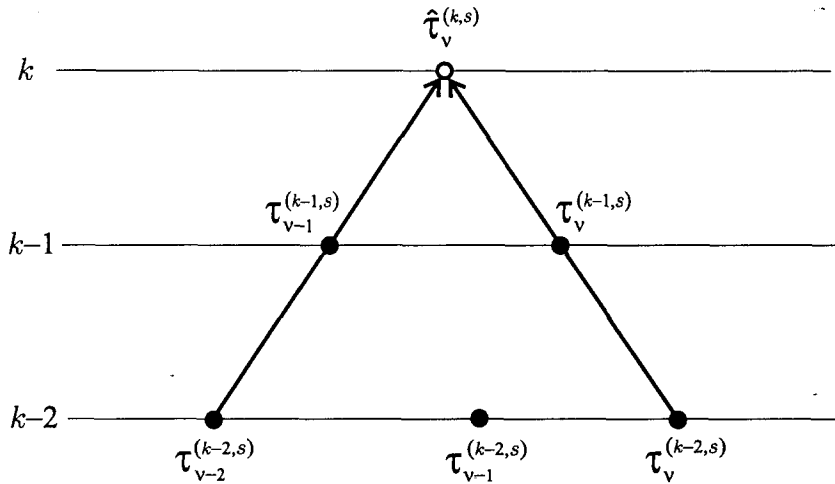


Figure 3. Extrapolation of starting values.

Typical formulas for starting values for the Jacobi measure $d\lambda(t) = (1-t)^\alpha(1+t)^\beta dt$ on $(-1, 1)$ ($\alpha, \beta > -1$) and for the Hermite measure $d\lambda(t) = e^{-t^2} dt$ on $(-\infty, +\infty)$ are

$$\hat{\tau}_\nu^{(k,s)} = \begin{cases} 2\tau_\nu^{(k-1,s)} - \tau_\nu^{(k-2,s)}, & \nu \in \{1, 2\}, \\ \tau_\nu^{(k-1,s)} + \tau_{\nu-1}^{(k-1,s)} - \frac{1}{2} (\tau_\nu^{(k-2,s)} + \tau_{\nu-2}^{(k-2,s)}), & \nu \in I_k, \\ 2\tau_{\nu-1}^{(k-1,s)} - \tau_{\nu-2}^{(k-2,s)}, & \nu \in \{k-1, k\}, \end{cases}$$

where $I_k = \{3, \dots, k-2\}$ ($k \geq 5$).

Because of the strong nonlinearity in zero distribution for the Jacobi measure (for small n), this extrapolation can give a value outside the interval $(-1, 1)$. If the value obtained with the above rule is bigger than 1 (less than -1), which can appear only for polynomials of degree four or five, one should use 1 (-1) instead of the obtained values.

In the case of the generalized Laguerre measure $d\lambda(t) = t^\alpha e^{-t} dt$ on $(0, +\infty)$ ($\alpha > -1$), we make the transformation $\tau_\nu^{(k,s)} \rightarrow \sqrt{\tau_\nu^{(k,s)}}$, so that the above formulas become

$$\hat{\tau}_\nu^{(k,s)} = \begin{cases} \left(2\sqrt{\tau_\nu^{(k-1,s)}} - \sqrt{\tau_\nu^{(k-2,s)}} \right)^2, & \nu \in \{1, 2\}, \\ \frac{1}{4} \left(2\sqrt{\tau_\nu^{(k-1,s)}} - \sqrt{\tau_\nu^{(k-2,s)}} + 2\sqrt{\tau_{\nu-1}^{(k-1,s)}} - \sqrt{\tau_{\nu-2}^{(k-2,s)}} \right)^2, & \nu \in I_k, \\ \left(2\sqrt{\tau_{\nu-1}^{(k-1,s)}} - \sqrt{\tau_{\nu-2}^{(k-2,s)}} \right)^2, & \nu \in \{k-1, k\}. \end{cases}$$

Figure 1 shows a strong nonlinearity in the zeros behavior for the Legendre polynomials of degrees two, three, and four. In our experiments, we encounter even stronger nonlinearity for the Gegenbauer measure $d\lambda(t) = (1-t^2)^\alpha dt$ on $(-1, 1)$ with the parameter α smaller than zero, but for $\alpha > 0$, this nonlinearity is smaller than in the case of the Legendre measure. This means that the Gegenbauer case with smaller parameter α needs more iterations for constructing the polynomial of degree four with respect to one with bigger α . For example, for constructing the Gegenbauer s -orthogonal polynomial with $n = 4$ and $s = 20$, we need 55 and 40 iterations if $\alpha = -9/10$ and $\alpha = 100$, respectively. Because of that, in order to avoid this strong nonlinearity for small α , it is much better to use the algorithm from [20] for $n \leq 4$ (and maybe even $n \leq 5$), and then start with the new algorithm.

A nonlinearity is also encountered for the Laguerre and Hermite case, but it is much smaller than nonlinearity presented above. There is stronger nonlinearity exhibited by the associated

Legendre polynomials (cf. [22, pp. 201–203]), in which case the algorithm breaks down if we begin the construction from polynomials of degree two and three.

The behavior of the algorithm for several classical and nonclassical measures will be considered in the next section.

5. NUMERICAL EXPERIMENTS

The algorithm was implemented in the package MATHEMATICA. All calculations were performed with 16 decimal digits mantissa (in our case, \$MachinePrecision). The same results can be obtained using FORTRAN in double precision arithmetic (with machine precision $\approx 2.22 \times 10^{-16}$).

5.1. Jacobi Measure

In this section, we consider the Jacobi measure on $(-1, 1)$ given by $d\lambda(t) = (1 - t)^\alpha(1 + t)^\beta dt$, where $\alpha, \beta > -1$.

At first, we discuss the Gegenbauer measure ($\alpha = \beta$). A distribution of zeros for $\alpha = \beta = -9/10$ is presented in Figure 4 for two values of s ($s = 1$ and $s = 10$).

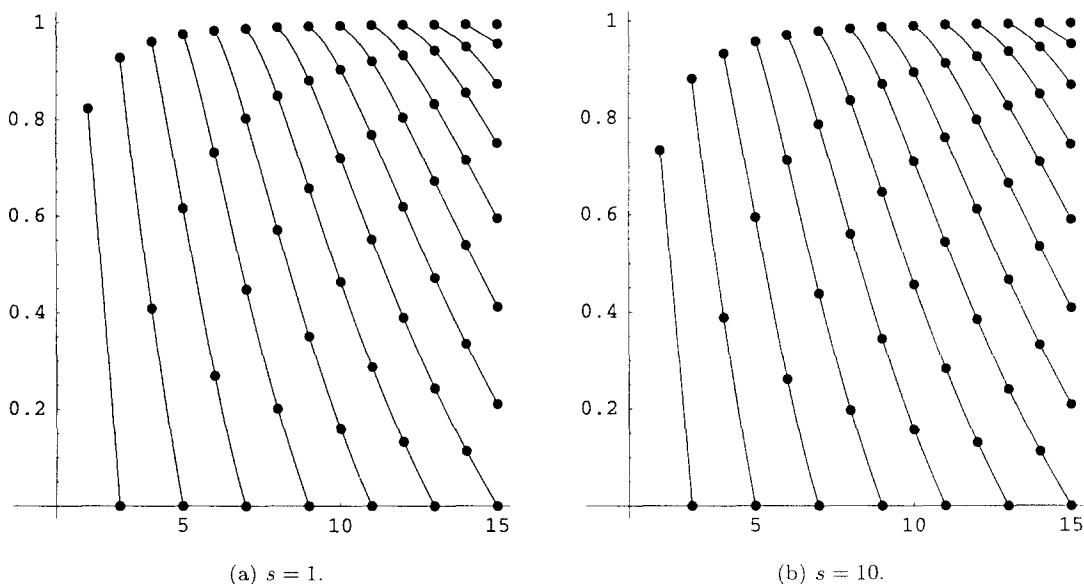


Figure 4. Nonnegative zeros of the s -orthogonal Gegenbauer polynomials with parameter $\alpha = -9/10$ for $s = 1$ (a) and $s = 10$ (b), when $n = 2(1)15$.

In Table 1, we present the zeros $\tau_\nu^{(n,s)}$ of the s -orthogonal Gegenbauer polynomials for $n = 12$ and $s = 10$, taking $\alpha = \beta = -9/10, 3/2$, and 100 . The corresponding numbers of iterations i_{12} for finding these zeros are also given in the same table. The number of iterations $i_n, n = 4(1)15$, for $s = 1$ and $s = 10$ are given in Table 2.

We can see that i_n becomes smaller as the parameter $\alpha (= \beta)$ increases. This is explained easily if we adopt that nonlinearity in zero distribution decreases when α increases. Notice also that the number of iterations for getting polynomials with odd degree decreases slower than one for even degree.

A distribution of zeros in the nonsymmetric Jacobi case with parameters $\alpha = -9/10$ and $\beta = 10$ is displayed in Figure 5 for $s = 1$ and $s = 10$.

The numerical results in this case for some selected values of n and s are presented in Table 3, including the necessary number of iterations i_4 and i_n .

Table 1. Zeros of the s -orthogonal Gegenbauer polynomials for $n = 12$ and $s = 10$ and the number of iterations i_{12} .

α	$\tau_{\nu}^{(n,s)}$	i_{12}
$-\frac{9}{10}$	$\pm 0.992587218229164, \pm 0.925814075750528$ $\pm 0.795538460358687, \pm 0.610717369841159$ $\pm 0.384024309720464, \pm 0.131001991782728$	11
$\frac{3}{2}$	$\pm 0.987558902610725, \pm 0.916149943757799$ $\pm 0.784210770279372, \pm 0.600411542500815$ $\pm 0.376902939023624, \pm 0.128466528934527$	9
100	$\pm 0.813124164758066, \pm 0.686762815789464$ $\pm 0.549006446594587, \pm 0.400464289428178$ $\pm 0.243684696049418, \pm 0.081802954927467$	8

Table 2. The number of iterations $i_n, n = 4(1)15$, in the Gegenbauer case for $s = 1$ (first row) and $s = 10$ (second row), and some selected values of α .

n	4	5	6	7	8	9	10	11	12	13	14	15
$\alpha = -\frac{9}{10}$	9	10	8	7	7	6	6	6	6	6	6	6
$\alpha = \frac{3}{2}$	9	7	7	6	6	6	6	6	6	6	6	6
$\alpha = 100$	8	6	6	6	6	6	6	6	6	6	6	6
	29	21	20	19	21	16	12	11	11	11	11	11
	28	21	19	15	16	14	11	10	9	10	10	10
	24	15	12	11	10	10	9	9	8	8	7	7

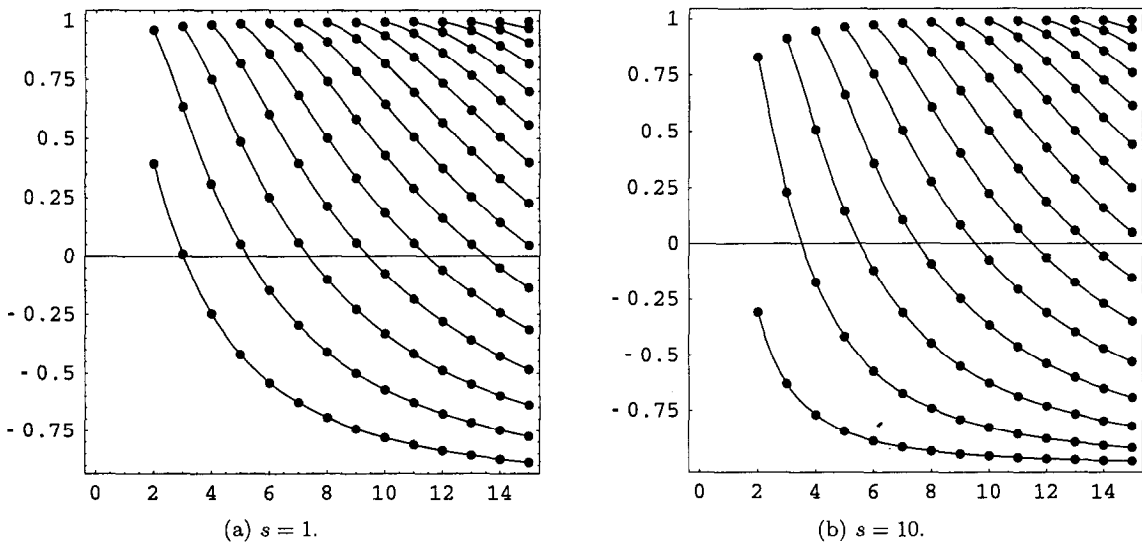


Figure 5. Distribution of zeros for the Jacobi measure with $\alpha = -9/10, \beta = 10$ for $s = 1$ (a) and $s = 10$ (b).

5.2. Generalized Gegenbauer Measure

We also investigate the case of the generalized Gegenbauer measure on $(-1, 1)$ given by $d\lambda(t) = |t|^{1+2\beta}(1-t^2)^\alpha dt, \alpha, \beta > -1$. The standard orthogonal polynomials $W_n^{(\alpha, \beta)}(t)$ with this measure was first investigated by Lascenov [23] (see also [22, pp. 155-156]). The rela-

Table 3. Zeros of s -orthogonal Jacobi polynomials with $\alpha = -9/10$, $\beta = 10$, and some selected values of n and s .

$n = 10$ $s = 10$	-0.956958840560754,	-0.828446385297409	$i_4 = 44$ $i_{10} = 17$
	-0.625710131602863,	-0.366897464420670	
	-0.075182888431344,	0.223312061944658	
	0.501858406743238,	0.735513030716415	
	0.903350566478815,	0.990308863737170	
$s = 8$ $n = 20$	-0.956789893504908,	-0.782967524872391	$i_4 = 62$ $i_8 = 28$
	-0.496609453149223,	-0.138703351806248	
	0.239375730489567,	0.583342824047379	
	0.843806416238132,	0.983338395742211	

tions between generalized monic Gegenbauer polynomials and the standard Jacobi polynomials $P_n^{(\alpha,\beta)}(t)$ are given by

$$W_{2n}^{(\alpha,\beta)}(t) = \frac{n!}{(n + \alpha + \beta + 1)_n} P_n^{(\alpha,\beta)}(2t^2 - 1), \tag{5.1}$$

$$W_{2n+1}^{(\alpha,\beta)}(t) = \frac{n!}{(n + \alpha + \beta + 2)_n} t P_n^{(\alpha,\beta+1)}(2t^2 - 1). \tag{5.2}$$

These polynomials satisfy the three-term recurrence relation (3.2), with $\alpha_j = 0$ and

$$\beta_{2j} = \frac{j(j + \alpha)}{(2j + \alpha + \beta)(2j + \alpha + \beta + 1)},$$

$$\beta_{2j-1} = \frac{(j + \beta)(j + \alpha + \beta)}{(2j + \alpha + \beta - 1)(2j + \alpha + \beta)},$$

for $j = 1, 2, \dots$, except for $\alpha + \beta = -1$ when $\beta_1 = (\beta + 1)/(\alpha + \beta + 2)$.

The distributions of zeros of s -orthogonal generalized Gegenbauer polynomials with $\alpha = -1/2$ and $\beta = -1/4$ ($d\lambda(t) = \sqrt{|t|/(1 - t^2)} dt$) and $s = 1$ and $s = 10$ are given in Figure 6.

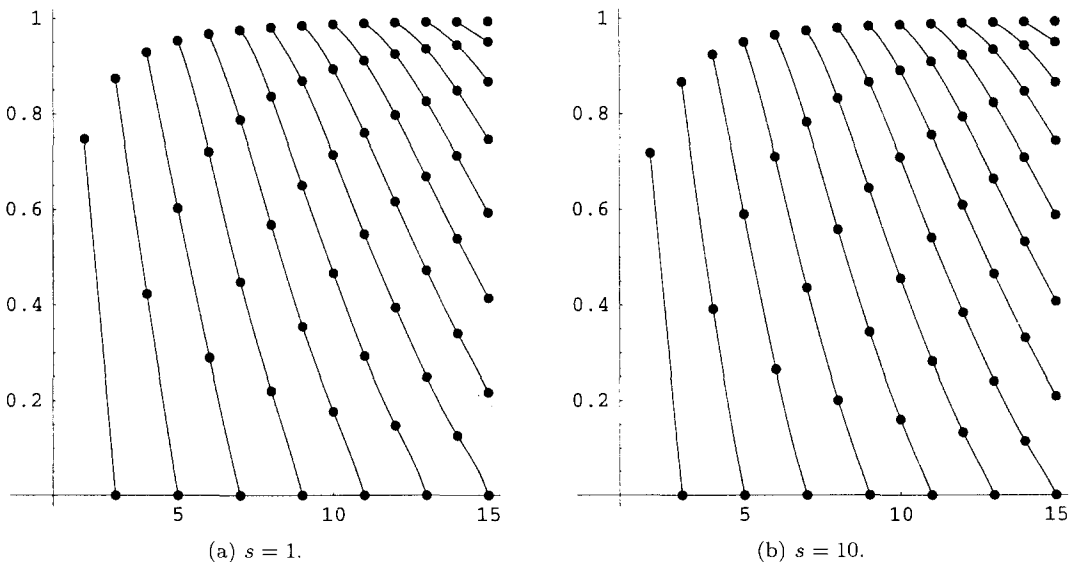


Figure 6. Nonnegative zeros of s -orthogonal generalized Gegenbauer polynomials ($\alpha = -1/2$, $\beta = -1/4$) for $s = 1$ (a) and $s = 10$ (b), when $n = 2(1)10$.

The extrapolation rule for the generalized Gegenbauer measure is the same as in the case of the Jacobi measure. The calculations can be performed when the ratio $|\beta/\alpha|$ is not so large, for

example, ≤ 8 . However, when this ratio becomes bigger, then we need another extrapolation rule like one which will be considered in Section 5.5. However, in this case, we can use an alternative way based on a connection between these s -orthogonal polynomials $W_{n,s}^{(\alpha,\beta)}(t)$ and the Jacobi s -orthogonal polynomials considered before. Such formulas for $s = 0$ reduce to (5.1) and (5.2).

PROPOSITION 5.1. *Let $P_{n,s}^{(\gamma,\delta)}(t)$ be the s -orthogonal polynomial with respect to the Jacobi measure $d\sigma(t) = (1 - t)^\gamma(1 + t)^\delta dt$ on $(-1, 1)$, where $\gamma, \delta > -1$, and let its zeros be $\tau_\nu^{(n,s)}(\gamma, \delta)$, $\nu = 1, \dots, n$.*

Then, the zero set of the s -orthogonal polynomial $W_{m,s}^{(\alpha,\beta)}(t)$ with respect to the generalized Gegenbauer measure on $(-1, 1)$; $d\lambda(t) = |t|^{1+2\beta}(1 - t^2)^\alpha dt$, $\alpha, \beta > -1$, is

$$\left\{ \pm \sqrt{\frac{1}{2} \left(1 + t_\nu^{(n,s)}(\alpha, \beta) \right)}, \nu = 1, \dots, n \right\},$$

if $m = 2n$, or

$$\left\{ 0, \pm \sqrt{\frac{1}{2} \left(1 + t_\nu^{(n,s)}(\alpha, \beta + s + 1) \right)}, \nu = 1, \dots, n \right\},$$

if $m = 2n + 1$.

PROOF. At first, it is easy to conclude that

$$W_{m,s}^{(\alpha,\beta)}(-t) = (-1)^m W_{m,s}^{(\alpha,\beta)}(t).$$

If m is odd, then $W_{m,s}^{(\alpha,\beta)}(0) = 0$.

According to the ‘‘orthogonality relation’’ (2.1), we have, for each $k = 0, 1, \dots, n - 1$,

$$\int_{-1}^1 t^{2k} W_{2n,s}^{(\alpha,\beta)}(t)^{2s+1} d\lambda(t) = \int_0^1 W_{2n,s}^{(\alpha,\beta)}(\sqrt{x})^{2s+1} x^{k+\beta} (1-x)^\alpha dx = 0,$$

i.e., $\int_{-1}^1 t^k W_{2n,s}^{(\alpha,\beta)}(\sqrt{(1+t)/2})^{2s+1} d\sigma(t) = 0$. It means that the following equality (up to a multiplicative constant)

$$W_{2n,s}^{(\alpha,\beta)}(t) \asymp P_{n,s}^{(\alpha,\beta)}(2t^2 - 1)$$

holds. In a similar way, we conclude also that

$$W_{2n+1,s}^{(\alpha,\beta)}(t) \asymp t P_{n,s}^{(\alpha,\beta+s+1)}(2t^2 - 1).$$

These equalities give the assertion of the statement. ■

Thus, the construction of polynomials $W_{m,s}^{(\alpha,\beta)}(t)$ reduces to the corresponding problem for the Jacobi measure.

5.3. Generalized Laguerre Measure

Consider now the generalized Laguerre measure on $(0, +\infty)$, defined by $d\lambda(t) = t^\alpha e^{-t} dt$, where $\alpha > -1$.

In Table 4, we give zeros of the s -orthogonal polynomials $L_{10,1}^\alpha(t)$ and $L_{10,5}^\alpha(t)$ for $\alpha = 0$ and $\alpha = 10$. The numbers in parentheses indicate decimal exponents.

The number of iterations i_n needed for constructing polynomials $L_{n,s}^\alpha(t)$, $n = 4(1)12$, for $s = 1$ and $s = 5$ are given in Table 5 for two values of the family parameter α ($\alpha = 0$ and $\alpha = 10$).

In our numerical experiments with several different measures with the bounded and unbounded supports, the best results are achieved with the generalized Laguerre measure. The reason for this fact is mentioned before in Section 2. Namely, there is practically no nonlinearity at the beginning of the construction. On the other side, the behavior of the algorithm from [20] for this measure is quite the opposite and, in some cases, it cannot be applied.

Table 4. Zeros of the s -orthogonal polynomial $L_{10,s}^\alpha(t)$ with respect to the generalized Laguerre measure.

$\alpha = 0$ $s = 1$	1.98459896485540(-1)	1.28527246416037
	3.36337825735860	6.48664600301537
	1.07436075246883(1)	1.62743035554314(1)
	2.33035216918815(1)	3.22160614407350(1)
	4.37648986737655(1)	5.99201036691075(1)
$\alpha = 0$ $s = 5$	4.49125141861381(-1)	3.50908561222774
	9.57940678730558	1.88204476515665(1)
	3.14997451789270(1)	4.80433097574563(1)
	6.91383474053974(1)	9.59673702137306(1)
	1.30860865091953(2)	1.79994158722296(2)
$\alpha = 10$ $s = 1$	2.80298131591448	5.74831335230936
	9.55062352348923	1.43049659752845(1)
	2.01246504335371(1)	2.71711961584816(1)
	3.56922857375727(1)	4.61025567445254(1)
	5.92049759623219(1)	7.70933664426522(1)
$\alpha = 10$ $s = 5$	2.34465695813680	7.46976879233792
	1.54646389122249(1)	2.65172755498364(1)
	4.09209133509488(1)	5.91261187317375(1)
	8.18464704498663(1)	1.10298218267156(2)
	1.46867352690064(2)	1.97865999176739(2)

Table 5. The number of iterations i_n , $n = 4(1)12$, in the generalized Laguerre case.

α	s	$n = 4$	$n = 5$	$6 \leq n \leq 11$	$n = 12$
0	1	8	7	6	7
	5	14	10	9	9
10	1	8	6	6	6
	5	13	10	9	11

5.4. Generalized Hermite Measure

In this section, we consider the generalized Hermite measure defined by $d\lambda(t) = |t|^{2\mu}e^{-t^2} dt$ on \mathbb{R} , where $\mu > -1/2$ (cf. [22, pp. 156–158]). The corresponding orthogonal polynomials satisfy the three-term recurrence relation (3.2), with $\alpha_j = 0$ and $\beta_{2j} = j$, $\beta_{2j+1} = j + \mu + 1/2$.

In our procedure for constructing s -orthogonal polynomials, we use the same extrapolation rule as in the case of the ordinary Hermite measure.

Table 6 displays zeros of the s -orthogonal polynomials $H_{15,1}^\mu(t)$ and $H_{15,10}^\mu(t)$ with respect to this measure, when $\mu = 0$ and $\mu = 1$.

The number of iterations i_n needed for constructing polynomials $H_{n,s}^\mu(t)$, $n = 4(1)15$, for $s = 1$ and $s = 10$ are given in Table 7 for the previous two values of the family parameter μ .

As we can see, for smaller values of s , the convergence is faster than for larger values. The number of iterations i_n is usually less than ten for $s = 1$, except maybe at the beginning of the procedure. However, when s increases, then the number of iterations becomes larger and, for a sufficiently large s , the iterative process is not convergent. The reason for this fact can be explained from the following statement.

PROPOSITION 5.2. Let $\tau_\nu^{(n,s)}(\alpha)$, $\nu = 1, \dots, n$, be zeros of the s -orthogonal polynomial $L_{n,s}^\alpha(t)$ with respect to the generalized Laguerre measure $t^\alpha e^{-t} dt$ on $(0, +\infty)$, where $\alpha > -1$.

Table 6. Zeros of the s -orthogonal polynomial $H_{15,s}^\mu(t)$ with respect to the generalized Hermite measure.

$\mu = 0$ $s = 1$	± 6.42529123114553	± 5.23047277856464
	± 4.22528087653067	± 3.31025792178217
	± 2.44735667049862	± 1.61626345818557
	$\pm 8.03798305791586(-1)$	0
$\mu = 0$ $s = 10$	$\pm 1.51934017204560(1)$	$\pm 1.23478732101507(1)$
	± 9.96744703814704	± 7.80558209124374
	± 5.76934255721114	± 3.80952472827816
	± 1.89438018486605	0
$\mu = 1$ $s = 1$	± 6.55601548945092	± 5.36821262206449
	± 4.36947846252626	± 3.46067926704917
	± 2.60360645068994	± 1.77696133674854
	$\pm 9.62679528877572(-1)$	0
$\mu = 1$ $s = 10$	$\pm 1.52498166160723(1)$	$\pm 1.24074292858041(1)$
	$\pm 1.00298988644974(1)$	± 7.87084167582895
	± 5.83725871657473	± 3.87950232294572
	± 1.96344150189706	0

Table 7. The number of iterations i_n , $n = 4(1)15$, in the generalized Hermite case.

μ	s	Values of n											
		4	5	6	7	8	9	10	11	12	13	14	15
0	1	8	6	6	6	6	6	6	6	6	6	6	6
	10	21	12	11	11	11	11	11	11	11	11	11	11
1	1	7	8	7	7	7	7	7	7	7	7	7	7
	10	20	16	9	10	17	10	17	10	18	11	20	11

Then, the set of zeros of the s -orthogonal polynomial $H_{m,s}^\mu(t)$ with respect to the generalized Hermite measure $d\lambda(t) = |t|^{2\mu} e^{-t^2} dt$ on \mathbb{R} , $\mu > -1/2$, is given by

$$\left\{ \pm \sqrt{\tau_\nu^{(n,s)}} \left(\mu - \frac{1}{2} \right), \nu = 1, \dots, n \right\},$$

if $m = 2n$, or

$$\left\{ 0, \pm \sqrt{\tau_\nu^{(n,s)}} \left(\mu + s + \frac{1}{2} \right), \nu = 1, \dots, n \right\},$$

if $m = 2n + 1$.

The proof of this result is similar to the proof of Proposition 5.1, showing that

$$H_{2n,s}^\mu(t) \asymp L_{n,s}^{\mu-1/2}(t^2) \quad \text{and} \quad H_{2n+1,s}^\mu(t) \asymp t L_{n,s}^{\mu+s+1/2}(t^2). \tag{5.3}$$

Notice from (5.3) that zeros of even and odd s -orthogonal polynomials with respect to the generalized Hermite measure belong to different families of s -orthogonal generalized Laguerre polynomials. For polynomials of odd degree, the family parameter is bigger for $s + 1$ than in the case of even degree. An influence of the family parameter can be seen from Figure 2. Namely, the larger values of the parameter α give larger values of zeros. This means that the starting values (4.2) for the iterative process are not good enough. In such cases, it is much better to use a construction with the generalized Laguerre measure, according to Proposition 5.2. Then, we separately construct polynomials of odd and even degree.

REMARK 5.1. In order to improve the convergence for the generalized Hermite measure, we performed numerous experiments with various extrapolating rules. We found that one of the best extrapolating rules is the following:

$$\hat{\tau}_\nu^{(k,s)} = \begin{cases} 2\tau_\nu^{(k-1,s)} - \tau_\nu^{(k-2,s)}, & \nu \in \{1, 2\}, \\ \frac{2}{3} \left(\tau_\nu^{(k-1,s)} + \tau_{\nu-1}^{(k-1,s)} \right) - \frac{1}{3} \left(\tau_\nu^{(k-2,s)} - \tau_{\nu-1}^{(k-2,s)} + \tau_{\nu-2}^{(k-2,s)} \right), & \nu \in I_k, \\ 2\tau_{\nu-1}^{(k-1,s)} - \tau_{\nu-2}^{(k-2,s)}, & \nu \in \{k-1, k\}, \end{cases}$$

where again $I_k = \{3, \dots, k-2\}$ ($k \geq 5$). As we can see, this extrapolation rule differs from the previous one only in one additional term $\tau_{\nu-1}^{(k-2,s)}$ used to extrapolate zeros with indexes in I_k . In Table 8, we give the number of iterations for cases already presented in Table 7.

Table 8. The number of iterations i_n , $n = 4(1)15$, in the generalized Hermite case, with a modified extrapolation rule.

μ	s	Values of n												
		4	5	6	7	8	9	10	11	12	13	14	15	
0	1	8	6	6	6	6	6	6	6	6	6	6	6	6
	10	21	12	10	8	8	8	9	9	9	10	10	10	10
1	1	7	8	5	7	5	7	5	7	6	7	6	8	8
	10	20	16	7	10	7	11	7	11	8	12	9	13	13

As we can see, this modified extrapolation rule, in this case, gives smaller values for the number of iterations than the previous one, but it is not true in a general case. For example, if we take $\mu = 10$ and $s = 1$, the number of iterations increases considerably for odd n . On the other hand, with the old extrapolation rule for a small s (here $s = 1$), the convergence is not disturbed.

Another effect which can harm calculations is related to an inaccurate construction of the Gaussian quadrature rule (3.7), which should be used for calculations in the method described in Section 3. Namely, the standard Golub-Welsch procedure for constructing Gauss-type quadratures, based on QR -algorithm [21], which is implemented in almost all numerical software (e.g., ORTHPOL [24]), can give some inaccurate weights if the family parameter μ is sufficiently large. In order to illustrate this inaccuracy, we take the simple example with $n = 4$, $s = 10$, $\mu = 15$. The obtained zeros $\tau_\nu^{(4,20)}$, $\nu = 1, 2, 3, 4$, using the standard method for constructing weights in the quadrature rule (3.7) are presented in Table 9.

These values are not even symmetric. However, if we use the following representation for the weights $A_\nu^{(L)}$ in (3.7),

$$A_\nu^{(L)} = \frac{1}{\sum_{k=0}^{L-1} \left(p_k \left(\tau_\nu^{(L)} \right) \right)^2}, \quad \nu = 1, \dots, L, \tag{5.4}$$

where $\{p_k(t)\}$ is a system of orthonormal polynomials with respect to the measure $d\lambda(t)$ on \mathbb{R} , we can calculate the accurate zeros of $H_{4,10}^{15}(t)$, which are presented in the last column of the same table. Thus, we use here complete eigenvectors, but not only their first components. Notice that, in this modification, the nodes $\tau_\nu^{(L)}$, $\nu = 1, \dots, L$, are calculated in a usual way using QR -algorithm. An analysis of this modification can be found in [25]. The last formula (5.4) was found by Shohat [26]. It was also used in calculation of weight coefficients in the period before an application of QR -procedure (cf. [27]).

Finally, we mention here that a similar kind of inaccuracy can appear with other measures for sufficiently large family parameters (generalized Laguerre measure, generalized Gegenbauer measure).

Table 9. Zeros $\tau_\nu^{(4,10)}$, $\nu = 1, 2, 3, 4$, of $H_{4,10}^{15}(t)$ obtained by the standard and modified method.

ν	Standard Method	Modified Method
1	-7.28962206...	-7.289621792645020
2	-3.66640712...	-3.666407011304882
3	-3.66640695...	-3.666407011304883
4	-7.28962175...	-7.289621792645021

Table 10. Recursion coefficients in the three-term recurrence relation (3.2) for some measures on \mathbb{R} .

Measure	$d\lambda(t)$	α_k	β_k
Abel's Measure	$\frac{t}{e^{\pi t} - e^{-\pi t}} dt$	0	$\frac{k(k+1)}{4}$
Lindelöf's Measure	$\frac{1}{2 \cosh(\pi t)} dt$	0	$\frac{k^2}{4}$
Logistic Measure	$\frac{e^{-t}}{(1 + e^{-t})^2} dt$	0	$\frac{k^4 \pi^2}{4k^2 - 1}$

5.5. Abel, Lindelöf, and Logistic Measures

We also perform experiments with respect to some other measures, supported on \mathbb{R} . For three kinds of such measures (Abel, Lindelöf, and logistic), in Table 10, we give the coefficients α_k and β_k in the three-term recurrence relation for the corresponding orthogonal polynomials.

For these measures, we use the following extrapolation rule:

$$\hat{\tau}_\nu^{(k,s)} = -\hat{\tau}_{k+1-\nu}^{(k,s)} = 2\tau_\nu^{(k-1,s)} - \tau_\nu^{(k-2,s)}, \quad \nu = 1, \dots, \left\lfloor \frac{k-1}{2} \right\rfloor$$

and

$$\begin{aligned} \hat{\tau}_{k/2}^{(k,s)} &= -\hat{\tau}_{k/2+1}^{(k,s)} = 2\sqrt{\tau_{k/2-1}^{(k-1,s)}} - \sqrt{\tau_{k/2-2}^{(k-2,s)}} && (k \text{ is even}), \\ \hat{\tau}_{(k+1)/2}^{(k,s)} &= 0 && (k \text{ is odd}). \end{aligned}$$

Zero distributions of s -orthogonal polynomials ($s = 1$) with respect to the Abel's, Lindelöf's, and logistic measure are presented in Figures 7 and 8. As we can see, these distributions are very similar. The same situation is also for $s > 1$. As an example, we give numerical results obtained for the Abel's measure, when $s = 10$ and $n = 2(1)6$ and $n = 10$ (see Table 11).

Table 11. Zeros of s -orthogonal polynomials with respect to the Abel's measure for $s = 10$.

n	$\tau_\nu^{(n,10)}$		
2	± 5.34981302878875		
3	0	$\pm 1.28798951031962(1)$	
4	± 4.32924349049201	$\pm 2.08850396601357(1)$	
5	0	$\pm 1.03361961308960(1)$	$\pm 2.95870116229020(1)$
6	± 3.88320551057493	$\pm 1.69259140377544(1)$	$\pm 3.84702162279135(1)$
10	± 3.43514608627397 $\pm 4.79585235400877(1)$	$\pm 1.38517514830389(1)$ $\pm 7.61209334780026(1)$	$\pm 2.83611830753627(1)$

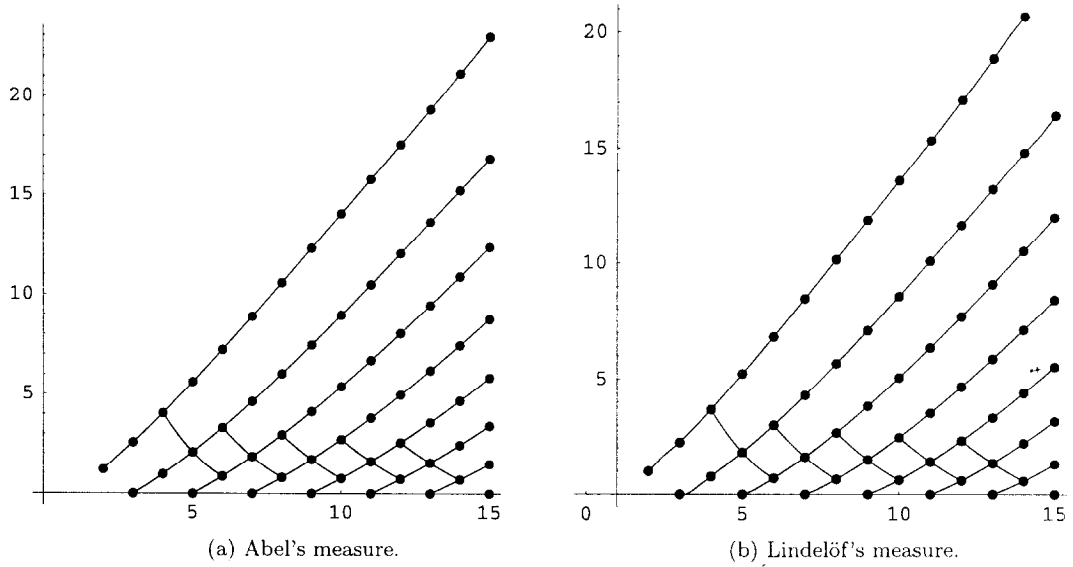


Figure 7. Nonnegative zeros of s -orthogonal polynomials for the Abel's measure (a) and for the Lindelöf's (b), when $s = 1$ and $n = 2(1)15$.

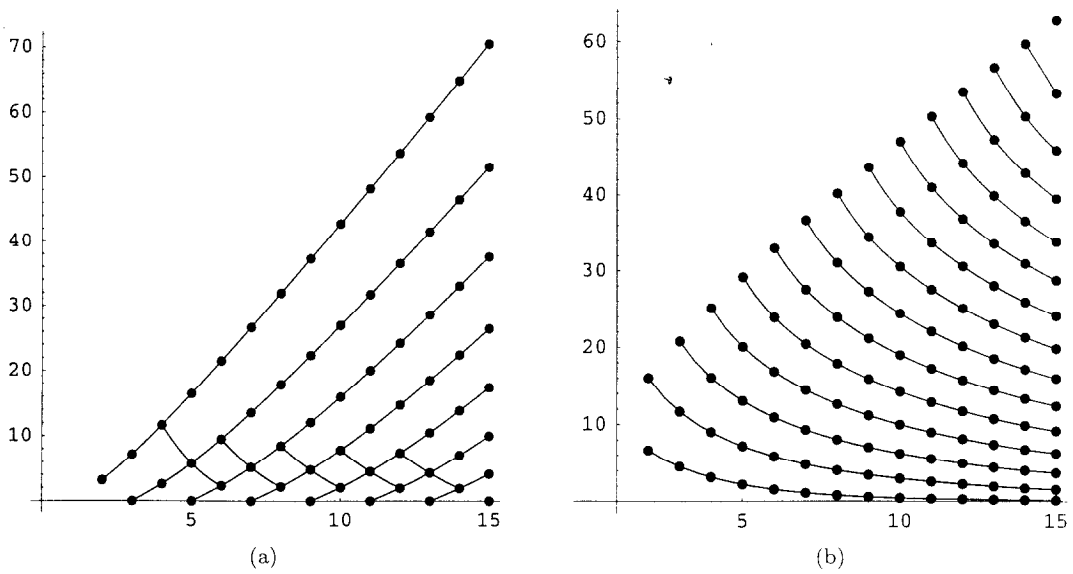


Figure 8. Nonnegative zeros of the logistic s -orthogonal polynomials (a) and zeros of s -orthogonal polynomials with respect to the Charlier measure (b), when $s = 1$ and $n = 2(1)15$.

5.6. Charlier Measure

We also investigate a discrete measure known as the Charlier measure (cf. [22, pp. 170–172]), with jumps

$$\frac{a^t e^{-a}}{t!}, \quad \text{at } t = 0, 1, 2, \dots,$$

where $a > 0$. The Charlier polynomials are orthogonal with respect to the inner product defined by

$$\langle f, g \rangle = \sum_{k=0}^{+\infty} \frac{a^k e^{-a}}{k!} f(k)g(k). \tag{5.5}$$

They satisfy the three-term recurrence relation with following coefficients $\alpha_k = a + k, \beta_k = ak$.

The extrapolation rule in this case is given by the following empirical formulas:

$$\hat{\tau}_\nu^{(k,s)} = \begin{cases} \left(2\sqrt{\tau_\nu^{(k-1,s)}} - \sqrt{\tau_\nu^{(k-2,s)}} \right)^2, & \nu \in \{1, 2\}, \\ \frac{1}{2} \left(2\sqrt{\tau_\nu^{(k-1,s)}} - \sqrt{\tau_\nu^{(k-2,s)}} \right)^2 + \tau_{\nu-1}^{(k-1,s)} - \frac{1}{2}\tau_{\nu-2}^{(k-2,s)}, & \nu \in I_k, \\ 2\tau_{\nu-1}^{(k-1,s)} - \tau_{\nu-2}^{(k-2,s)}, & \nu \in \{k-1, k\}, \end{cases}$$

where $I_k = \{3, \dots, k-2\}$ ($k \geq 5$).

In Figure 8b, a distribution of zeros for Charlier s -orthogonal polynomials is displayed for $a = 10$ and $s = 1$.

6. CALCULATION OF THE WEIGHT COEFFICIENTS

We return now to the linear task of determination of the weight coefficients $A_{i,\nu}$ and $B_{i,\nu}$ in Gauss-Stancu quadrature formula (1.1), assuming that we previously calculated Gaussian nodes τ_1, \dots, τ_n (zeros of a certain s - or σ -orthogonal polynomial). For this purpose, we can adopt a method described in [28] and [29] for Gauss-Turán and Chakalov-Popoviciu quadratures, respectively (see also [30]). Thus, let the sets of fixed and Gaussian nodes

$$F_m = \{\eta_1, \dots, \eta_m\} \quad \text{and} \quad G_n = \{\tau_1, \dots, \tau_n\}$$

be known and let $F_m \cap G_n = \emptyset$. Otherwise, we should make an adjustment as we mentioned in Section 1.

Putting

$$X_p = \{\xi_1, \dots, \xi_p\} := F_m \cup G_n \quad (p = m + n)$$

and denoting the corresponding multiplicity of the node ξ_ν by r_ν ($\nu = 1, \dots, p$), our task is to determine the coefficients $C_{i,\nu}$ (i.e., $A_{i,\nu}$ and $B_{i,\nu}$) in an interpolatory quadrature formula of the form

$$\int_{\mathbb{R}} f(t) d\lambda(t) = \sum_{\nu=1}^p \sum_{i=0}^{r_\nu-1} C_{i,\nu} f^{(i)}(\xi_\nu) + R_p(f). \tag{6.1}$$

Notice that the multiplicity of a Gaussian node must be an odd number.

As in [29], we define

$$\Omega_\nu(t) = \prod_{i \neq \nu} (t - \xi_i)^{r_i}, \quad \nu = 1, \dots, p,$$

and use the polynomials

$$f_{k,\nu}(t) = (t - \xi_\nu)^k \Omega_\nu(t) = (t - \xi_\nu)^k \prod_{i \neq \nu} (t - \xi_i)^{r_i},$$

where $0 \leq k \leq r_\nu - 1$, $1 \leq \nu \leq p$, in order to decompose the problem to p mutually independent triangular systems of linear equations with r_ν ($\nu = 1, \dots, p$) unknown coefficients, i.e.,

$$\begin{bmatrix} f_{0,\nu}(\xi_\nu) & f'_{0,\nu}(\xi_\nu) & \dots & f_{0,\nu}^{(r_\nu-1)}(\xi_\nu) \\ & f'_{1,\nu}(\xi_\nu) & \dots & f_{1,\nu}^{(r_\nu-1)}(\xi_\nu) \\ & & \ddots & \vdots \\ & & & f_{r_\nu-1,\nu}^{(r_\nu-1)}(\xi_\nu) \end{bmatrix} \begin{bmatrix} C_{0,\nu} \\ C_{1,\nu} \\ \vdots \\ C_{r_\nu-1,\nu} \end{bmatrix} = \begin{bmatrix} \mu_{0,\nu} \\ \mu_{1,\nu} \\ \vdots \\ \mu_{r_\nu-1,\nu} \end{bmatrix},$$

where

$$\mu_{k,\nu} = \int_{\mathbb{R}} f_{k,\nu}(t) d\lambda(t) = \int_{\mathbb{R}} (t - \xi_\nu)^k \prod_{i \neq \nu} (t - \xi_i)^{r_i} d\lambda(t).$$

Now, we put $a_{k,k+j} = f_{k-1,\nu}^{(k-1+j)}(\xi_\nu)$, so that the matrix of the system has elements $a_{\ell,j}$, $1 \leq \ell, j \leq r_\nu$, with $a_{\ell,j} = 0$ for $j < \ell$.

Introducing the normalization

$$\hat{a}_{k,j} = \frac{a_{k,j}}{(j-1)!a_{1,1}}, \quad 1 \leq k, j \leq r_\nu,$$

putting $b_k = (k-1)!A_{k-1,\nu}$, $1 \leq k \leq r_\nu$,

$$\hat{\mu}_{k,\nu} = \frac{\mu_{k,\nu}}{a_{1,1}} = \frac{\mu_{k,\nu}}{\prod_{i \neq \nu} (\xi_\nu - \xi_i)^{r_i}} = \int_{\mathbb{R}} (t - \xi_\nu)^k \prod_{i \neq \nu} \left(\frac{t - \xi_i}{\xi_\nu - \xi_i} \right)^{r_i} d\lambda(t),$$

and following [29], we get the following.

THEOREM 6.1. *For fixed ν , $1 \leq \nu \leq p$, the coefficients $C_{i,\nu}$ in the quadrature formula (6.1) are given by*

$$b_{r_\nu} = (r_\nu - 1)!C_{r_\nu-1,\nu} = \hat{\mu}_{r_\nu-1,\nu},$$

$$b_k = (k-1)!C_{k-1,\nu} = \hat{\mu}_{k-1,\nu} - \sum_{j=k+1}^{r_\nu} \hat{a}_{k,j}b_j, \quad k = r_\nu - 1, \dots, 1,$$

where

$$\hat{a}_{k,k} = 1, \quad \hat{a}_{k,k+j} = -\frac{1}{j} \sum_{\ell=1}^j u_\ell \hat{a}_{\ell,j},$$

and

$$u_\ell = \sum_{i \neq \nu} r_i (\xi_i - \xi_\nu)^{-\ell}, \quad \ell = 1, \dots, r_\nu - 1.$$

Thus, for fixed ν , the coefficients b_k , $1 \leq k \leq r_\nu$, i.e., the weight coefficients $C_{i,\nu}$ in (6.1), are obtained from the corresponding upper triangular system of equations $\hat{A}\vec{b} = \vec{c}$, where

$$\hat{A} = [\hat{a}_{ij}], \quad \vec{b} = [b_1 \dots b_{r_\nu}]^\top, \quad \vec{c} = [\hat{\mu}_{0,\nu} \dots \hat{\mu}_{r_\nu-1,\nu}]^\top.$$

The normalized moments $\hat{\mu}_{k,\nu}$ can be computed exactly, except for rounding errors, by using the Gauss-Christoffel formula (3.7), taking $L = p + \sum_{\nu=1}^p r_\nu$ knots.

EXAMPLE 6.1. Now we want to construct a Lobatto type quadrature rule of the form

$$\int_{-1}^1 f(t) dt \cong Q_{n,s}(f) = \sum_{\nu=1}^n \sum_{i=0}^{2s} A_{i,\nu} f^{(i)}(\tau_\nu) + B_{0,2}f(0) + B_{1,2}f'(0) + B_{0,1}f(-1) + B_{0,3}f(1),$$

with Gaussian nodes τ_1, \dots, τ_n .

Thus, in this case, we introduce three fixed nodes: $\eta_1 = -1$, $\eta_2 = 0$, $\eta_3 = 1$, with multiplicities 1, 2, 1, respectively, so that $M = 4$, $q_4(t) = (t^2 - 1)t^2$ (see (1.2)), and according to (1.4), $d\hat{\lambda}(t) = t^2(1 - t^2) dt$ is the generalized Gegenbauer measure on $(-1, 1)$, with $\alpha = 1$, $\beta = 1/2$ (see Section 5.2).

If the maximum degree of exactness is $d_{\max} = 2(s+1)n + 3$, free nodes in $Q_{n,s}(f)$ must be zeros of the s -orthogonal polynomial $W_{n,s}^{(1,1/2)}(t)$ with respect to the generalized Gegenbauer measure $d\hat{\lambda}(t)$.

Table 12. Parameters of $Q_{2,s}(f)$ for $s = 1, 2$.

	$s = 1$	$s = 2$
τ_1	-0.667724357906923	-0.675112000977284
i	$A_{i,1}$	$A_{i,1}$
0	0.668946557387391	0.728669656880520
1	0.290757109134606(-1)	0.495168812842977(-1)
2	0.827917955975223(-2)	0.140806820439479(-1)
3		0.516533600625606(-3)
4		0.422667424219621(-4)
B	0.573503803772122(-1)	0.399205534871742(-1)
B_0	0.547406124470793	0.462819579264612

Table 13. Parameters of $Q_{3,s}(f)$ for $s = 1, 2$.

	$s = 1$	$s = 2$
τ_1	-0.782465625283903	-0.801032639658859
i	$A_{i,1}$	$A_{i,1}$
0	0.466114900228077	0.482247415802680
1	0.170146372659433(-1)	0.263895403842581(-1)
2	0.263525214201978(-2)	0.401261800734473(-2)
3		0.108127113066279(-3)
4		0.451390243547896(-5)
B	0.361899495634558(-1)	0.235365436186576(-1)
A_0	0.995390300416934	0.988432081157324
A_1	0.331196251997634(-1)	0.346136792399800(-1)
A_2	0.194062137754975(-3)	0.270188945759357(-3)
A_3		0.566748161962253(-6)

Notice that, by symmetry,

$$\tau_\nu = -\tau_{n+1-\nu}, \quad A_{i,\nu} = (-1)^i A_{i,n+1-\nu}, \quad B_{0,1} = B_{0,3} = B,$$

as well as that for odd n , one of free nodes must be zero ($\tau_{(n+1)/2} = 0$). In that case, we remove the fixed node $\eta_2 = 0$ and increase the multiplicity of the Gaussian node $\tau_{(n+1)/2} = 0$ from $2s + 1$ to $2s + 3$. Therefore, we have

$$Q_{n,s}(f) = \sum_{\nu=1}^{[n/2]} \sum_{i=0}^{2s} A_{i,\nu} \left[f^{(i)}(\tau_\nu) + (-1)^i f^{(i)}(-\tau_\nu) \right] + B[f(-1) + f(1)] + L_{n,s}(f),$$

where

$$L_{n,s}(f) = \begin{cases} B_{0,2}f(0) + B_{1,2}f'(0) & (n \text{ is even}), \\ \sum_{i=0}^{2s+2} A_{i,(n+1)/2} f^{(i)}(0) & (n \text{ is odd}). \end{cases}$$

Furthermore, it is easy to prove that $B_{1,2} = 0$ and $A_{2j+1,(n+1)/2} = 0$, so that (with a simpler index notation)

$$L_{n,s}(f) = \begin{cases} B_0 f(0) & (n \text{ is even}), \\ \sum_{j=0}^{s+1} A_j f^{(2j)}(0) & (n \text{ is odd}). \end{cases}$$

The parameters of $Q_{n,s}(f)$ are presented only for $n = 2(1)5$ and $s = 1, 2$ (see Tables 12–15).

Table 14. Parameters of $Q_{4,s}(f)$ for $s = 1, 2$.

$s = 1$	τ_1	-0.864343260009839	τ_2	-0.441646700727031
	i	$A_{i,1}$	i	$A_{i,2}$
	0	0.291988548489762	0	0.514638063715358
	1	0.677444243326017(-2)	1	0.498531656314293(-2)
	2	0.648273517991189(-3)	2	0.359603976374291(-2)
	B	0.224364945126899(-1)	B_0	0.341873786564380
$s = 2$	τ_1	-0.879394021458197	τ_2	-0.428674810876148
	i	$A_{i,1}$	i	$A_{i,2}$
	0	0.295178181352631	0	0.552804147355119
	1	0.101143495853744(-1)	1	0.680687022397463(-2)
	2	0.922248277774315(-3)	2	0.555113515690070(-2)
	3	0.154530837011859(-4)	3	0.388306859303889(-4)
	4	0.383168236065884(-6)	4	0.926773668549215(-5)
	B	0.141557058476428(-1)	B_0	0.275723930889215

Table 15. Parameters of $Q_{5,s}(f)$ for $s = 1, 2$.

$s = 1$	τ_1	-0.900169737733269	τ_2	-0.574018204835000
	i	$A_{i,1}$	i	$A_{i,2}$
	0	0.217690600610764	0	0.421359837858011
	1	0.389164846928562(-2)	1	0.551679530132521(-2)
	2	0.265641103999405(-3)	2	0.191245109502987(-2)
	B	0.163654269057924(-1)	A_0	0.689168269250866
	A_1	0.107188288005793(-1)	A_2	0.280948737674689(-4)
$s = 2$	τ_1	-0.914006400993315	τ_2	-0.576411308297384
	i	$A_{i,1}$	i	$A_{i,2}$
	0	0.213409270452064	0	0.443741913748343
	1	0.544240785455850(-2)	1	0.796047097661861(-2)
	2	0.348080210407537(-3)	2	0.282629281215632(-2)
	3	0.427800489449208(-5)	3	0.267694393447469(-4)
	4	0.736267007987303(-7)	4	0.284224160106976(-5)
	B	0.100121930330481(-1)	A_0	0.665673245533091
A_1	0.103811992392277(-1)	A_2	0.350419067557081(-4)	
A_3	0.306279814773751(-7)			

In order to test the quadrature formula $Q_{n,s}(f)$, we take the function $f(t) = t/\sin t$ (see [31, Example 2.2]) such that

$$I(f) = 2.119525586696611661037623273595157\dots$$

All calculations we perform now in quadruple precision (with 34 decimal digits mantissa).

An elementary computation yields that

$$f^{(i)}(t) \sin t = tP_i(\cot t) + Q_{i-1}(\cot t),$$

where the polynomials $P_i(x)$ and $Q_i(x)$ satisfy

$$\begin{aligned} P_{i+1}(x) &= -xP_i(x) - (1+x^2)P'_i(x), \\ Q_i(x) &= -xQ_{i-1}(x) - (1+x^2)Q'_{i-1}(x) + P_i(x), \end{aligned}$$

Table 16. Relative errors in quadrature sums $Q_{n,s}(f)$.

s	$n = 2$	$n = 3$	$n = 4$	$n = 5$	$n = 6$	$n = 7$
1	2.39(-9)	3.09(-12)	1.38(-15)	1.44(-18)	7.39(-22)	6.99(-25)
2	3.99(-12)	1.67(-16)	1.90(-21)	5.84(-26)	7.75(-31)	m.p.

with $P_0(x) = 1$, $Q_{-1}(x) = 0$. The limiting values of derivatives $f^{(i)}(t)$, $i = 1(1)7$, at $t = 0$ are 0, $1/3$, 0, $7/15$, 0, $31/21$, 0, respectively.

Table 16 shows the relative errors $|(Q_{n,s}(f) - I(f))/I(f)|$ for $n = 2(1)7$ and $s = 1$ and $s = 2$ (m.p. stands for machine precision).

7. CONCLUDING REMARKS

The presented algorithm for construction of s -orthogonal polynomials with quadratic convergence has a few nice properties. We emphasize the following.

- The number of nonlinear equations to be solved is small. Ideally, if the starting values are known, our algorithm needs only $n - 3$ nonlinear equations with $4, 5, \dots, n$ variables.
- The construction of the Jacobian matrix for the system of nonlinear equations is simplified, and requests only evaluations of $2n$ integrals for a system of n variables.
- The algorithm can be applied for both bounded and unbounded supports.

As we mentioned before, the Gauss-Christoffel quadrature rule is used for calculation of integrals. The construction of these quadrature rules is not needed for every value of n . In our implementation, we construct a new quadrature rule after n is increased for 8, i.e., we always construct Gaussian rules for $n = 8, 16, 24, \dots$

Finally, for finding all weights, our method uses an upper triangular system of linear equations for the weights associated with each (Gaussian or prescribed) node.

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