

SOME CLASSES OF ORTHOGONAL POLYNOMIALS AND APPLICATIONS

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Abstract: Orthogonal polynomial systems on the real line and orthogonal systems on the unit semicircle are considered. A short account on classical and non-classical orthogonal polynomials on the real line, as well as the basic properties of polynomials on the semicircle are included. Finally, some applications in numerical integration, numerical differentiation and summation of slowly convergent series are done.

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1. INTRODUCTION AND BASIC DEFINITIONS

Orthogonal polynomials are very important in many branches of mathematics, physics and engineering. In this paper we study a few orthogonal polynomial systems and give some applications in numerical integration, numerical differentiation and summation of slowly convergent series.

Given an inner product (\cdot, \cdot) on the space of polynomials, one calls $\{\pi_k\}$ a system of (monic) orthogonal polynomials if

$$p_k(t) = t^k + \text{lower degree terms}, \quad k = 0, 1, \dots,$$

and $(p_k, p_m) = \|p_k\|^2 \delta_{km}$, $k, m \geq 0$, where δ_{km} is the Kronecker's delta. However, if

$$p_k(t) = b_k t^k + c_k t^{k-1} + \text{lower degree terms}, \quad b_k > 0,$$

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and $\|p_k\| = 1$, then $\{p_k\}$ is a system of orthonormal polynomials with respect to the inner product (\cdot, \cdot) .

The most common type of orthogonality is with respect to a given nonnegative measure $d\lambda(t)$ on the real line \mathbb{R} , with compact or infinite support, for which all moments

$$\mu_\nu = \int_{\mathbb{R}} t^\nu d\lambda(t), \quad \nu = 0, 1, \dots,$$

exist and are finite, and $\mu_0 > 0$. We mention that $\text{supp}(d\lambda)$ is the set of points of increase of $t \mapsto \lambda(t)$. If $\text{supp}(d\lambda)$ is bounded, then the smallest closed interval containing $\text{supp}(d\lambda)$ we denote by $\Delta(d\lambda)$. A typical case is when $t \mapsto \lambda(t)$ is an absolutely continuous function, and then the measure $d\lambda(t)$ can be express as $d\lambda(t) = w(t) dt$, where $w(t) = \lambda'(t)$ is a weight function, i.e., a non-negative and measurable function in Lebesgue's sense for which all moments exists and $\mu_0 = \int_{\mathbb{R}} w(t) dt > 0$.

In the general case the function λ can be written in the form $\lambda = \lambda_{ac} + \lambda_s + \lambda_j$, where λ_{ac} is absolutely continuous, λ_s is singular, and λ_j is a jump function.

Defining the inner product (f, g) by

$$(f, g) = \int_{\mathbb{R}} f(t)\overline{g(t)} d\lambda(t) \quad (1.1)$$

it can be proved that for any $d\lambda(t)$ there exists a unique system of (monic) polynomials $\{p_k(t)\}$.

A few basic properties of these orthogonal polynomials $p_k(\cdot) = p_k(\cdot; d\lambda)$ are given below:

THEOREM 1.1. *A system of monic polynomials $\{p_k\}$ orthogonal with respect to the inner product (1.1) satisfy a three-term recurrence relation of the form*

$$p_{k+1}(t) = (t - a_k)p_k(t) - b_k p_{k-1}(t), \quad k = 0, 1, 2, \dots, \quad (1.2)$$

where

$$a_k = \frac{(tp_k, p_k)}{(p_k, p_k)} \quad (k \geq 0), \quad b_k = \frac{(p_k, p_k)}{(p_{k-1}, p_{k-1})} > 0 \quad (k \geq 1).$$

The coefficient b_0 , which multiplies $p_{-1} = 0$ in three-term recurrence relation may be arbitrary. Sometimes, it is convenient to define it by $b_0 = \mu_0 = \int_{\mathbb{R}} d\lambda(t)$. Then the norm of p_k can be express in the form

$$\|p_k\| = \sqrt{(p_k, p_k)} = \sqrt{b_0 b_1 \cdots b_k}. \quad (1.3)$$

We mention that the existence of a three-term recurrence relation for orthogonal polynomials is a consequence of the property $(tf, g) = (f, tg)$ of the inner product (1.1).

THEOREM 1.2. All zeros of $p_n(t; d\lambda)$, $n \geq 1$, are real and distinct and are located in the interior of the interval $\Delta(d\lambda)$.

Let $\tau_k^{(n)}$, $k = 1, \dots, n$, denote the zeros of $p_n(t; d\lambda)$ in increasing order

$$\tau_1^{(n)} < \tau_2^{(n)} < \dots < \tau_n^{(n)}.$$

THEOREM 1.3. The zeros of $p_n(t; d\lambda)$ and $p_{n+1}(t; d\lambda)$ interlace, i.e.,

$$\tau_k^{(n+1)} < \tau_k^{(n)} < \tau_{k+1}^{(n+1)} \quad (k = 1, \dots, n; n \in \mathbb{N}).$$

Using the three-term recurrence relation (1.2) for $k = 0, 1, \dots, n-1$, we can obtain the following determinant representation of the monic polynomials

$$p_n(t) = \det(tI_n - J_n),$$

where I_n is the identity matrix of the order n and J_n is the Jacobi matrix

$$J_n = J_n(d\lambda) = \begin{bmatrix} a_0 & \sqrt{b_1} & & & \text{O} \\ \sqrt{b_1} & a_1 & \sqrt{b_2} & & \\ & \sqrt{b_2} & a_2 & \ddots & \\ & & \ddots & \ddots & \sqrt{b_{n-1}} \\ \text{O} & & & \sqrt{b_{n-1}} & a_{n-1} \end{bmatrix}.$$

Thus, the zeros $\tau_k^{(n)}$ of $p_n(t)$ are the same as the eigenvalues of the Jacobi tridiagonal matrix J_n .

A survey on characterization theorems for orthogonal polynomials on the real line was given recently by Al-Salam [3]. In next section we consider a special class of orthogonal polynomials so-called *classical orthogonal polynomials*. For some extensions of this polynomial class see Andrews and Askey [4], Askey and Wilson [5–6], and Atakishiyev and Suslov [7].

2. CLASSICAL ORTHOGONAL POLYNOMIALS

A very important class of orthogonal polynomials on an interval of orthogonality $(a, b) \in \mathbb{R}$ is constituted by so-called the *classical orthogonal polynomials*. They are distinguished by several particular properties.

Let \mathcal{P}_n be the set of all algebraic polynomials $P (\neq 0)$ of degree at most n and the inner product is given by

$$(f, g)_w = \int_a^b w(t)f(t)g(t) dt. \quad (2.1)$$

Since every interval (a, b) can be transformed by a linear transformation to one of following intervals: $(-1, 1)$, $(0, +\infty)$, $(-\infty, +\infty)$, we will restrict our consideration (without loss of generality) only to these three intervals.

DEFINITION 2.1. The orthogonal polynomials $\{Q_k\}$ on (a, b) with respect to the inner product (2.1) are called the *classical orthogonal polynomials* if their weight functions $t \mapsto w(t)$ satisfy the differential equation $(A(t)w(t))' = B(t)w(t)$, where

$$A(t) = \begin{cases} 1 - t^2, & \text{if } (a, b) = (-1, 1), \\ t, & \text{if } (a, b) = (0, +\infty), \\ 1, & \text{if } (a, b) = (-\infty, +\infty), \end{cases}$$

and $B(t)$ is a polynomial of the first degree. For such classical weights we will write $w \in CW$.

We note that if $w \in CW$, then $w \in C^1(a, b)$, and also the following property:

THEOREM 2.1. *If $w \in CW$ then for each $m = 0, 1, \dots$ we have*

$$\lim_{t \rightarrow a^+} t^m A(t)w(t) = 0 \quad \text{and} \quad \lim_{t \rightarrow b^-} t^m A(t)w(t) = 0.$$

Based on the above definition, the classical orthogonal polynomials $\{Q_k\}$ on (a, b) can be specified as the *Jacobi polynomials* $P_k^{(\alpha, \beta)}(t)$ ($\alpha, \beta > -1$) on $(-1, 1)$, the *generalized Laguerre polynomials* $L_k^s(t)$ ($s > -1$) on $(0, +\infty)$, and finally as the *Hermite polynomials* $H_k(t)$ on $(-\infty, +\infty)$. Their weight functions and the corresponding polynomials $A(t)$ and $B(t)$ are given in Table 2.1.

TABLE 2.1. Classification of the Classical Orthogonal Polynomials

| (a, b) | $w(t)$ | $A(t)$ | $B(t)$ | λ_k |
|----------------------|---------------------------|---------|--|-----------------------------|
| $(-1, 1)$ | $(1-t)^\alpha(1+t)^\beta$ | $1-t^2$ | $\beta - \alpha - (\alpha + \beta + 2)t$ | $k(k + \alpha + \beta + 1)$ |
| $(0, +\infty)$ | $t^s e^{-t}$ | t | $s + 1 - t$ | k |
| $(-\infty, +\infty)$ | e^{-t^2} | 1 | $-2t$ | $2k$ |

Special cases of the Jacobi polynomials are:

- 1° The *Legendre polynomials* $P_k(t)$ (for $\alpha = \beta = 0$);
- 2° The *Chebyshev polynomials of the first kind* $T_k(t)$ (for $\alpha = \beta = -1/2$);
- 3° The *Chebyshev polynomials of the second kind* $S_k(t)$ (for $\alpha = \beta = 1/2$);
- 4° The *Chebyshev polynomials of the third kind* $U_k(t)$ (for $\alpha = -\beta = -1/2$);
- 5° The *Chebyshev polynomials of the fourth kind* $V_k(t)$ (for $\alpha = -\beta = 1/2$);
- 6° The *Gegenbauer or ultraspherical polynomials* $C_k^\lambda(t)$ (for $\alpha = \beta = \lambda - 1/2$).

If $s = 0$, the generalized Laguerre polynomials reduces to the standard Laguerre polynomials $L_k(t)$.

There are many characterizations of the classical orthogonal polynomials. In sequel we mention the basic common properties of these polynomials (cf. [51]).

THEOREM 2.2. *The derivatives of the classical orthogonal polynomials $\{Q_k\}_{k \in \mathbb{N}_0}$ form also a sequence of the classical orthogonal polynomials.*

THEOREM 2.3. *The classical orthogonal polynomial $t \mapsto Q_k(t)$ is a particular solution of the second order linear differential equation of hypergeometric type*

$$L[y] = A(t)y'' + B(t)y' + \lambda_k y = 0, \quad (2.2)$$

where $\lambda_k = -k \left(\frac{1}{2}(k-1)A'(0) + B'(0) \right)$.

The coefficients λ_k are also displayed in Table 2.1.

The characterization of the classical orthogonal polynomials by differential equation (2.2), was proved by Lesky [40], and conjectured by Aczél [1] (see also Bochner [9]). Such a differential equation appears in many mathematical models in atomic physics, electrodynamics and acoustics. As an example we mention the well-known Schrödinger equation.

The classical orthogonal polynomials possess a Rodrigues' type formula (cf. [8] and [62–64])

$$Q_k(t) = \frac{C_k}{w(t)} \cdot \frac{d^k}{dt^k} (A(t)^k w(t)), \quad (2.3)$$

where C_k are constants different from zero. The constants C_k in (2.3) can be chosen in different way; e.g., Q_k to be monic, orthonormal, etc. (see [51] for some details).

Similarly to the well-known Landau inequality (see Landau [37]) for continuously-differentiable functions and other generalizations (see Milovanović [43]), Agarwal and Milovanović [2] stated the following characterization of the classical orthogonal polynomials:

THEOREM 2.4. *Let $\|f\|^2 = (f, f)_w$, where $w \in CW$. For all $P \in \mathcal{P}_n$ the inequality*

$$(2\lambda_n + B'(0)) \|\sqrt{A}P'\|^2 \leq \lambda_n^2 \|P\|^2 + \|AP''\|^2 \quad (2.4)$$

holds, with equality if only if $P(t) = cQ_n(t)$, where $Q_n(t)$ is the classical orthogonal polynomial on (a, b) with respect to the weight function $t \mapsto w(t)$, and c is an arbitrary real constant. λ_n , $A(t)$ and $B(t)$ are given in Table 2.1.

The equality case in (2.4) gives a characterization of the classical orthogonal polynomials. For $w(t) = e^{-t^2}$ on $(-\infty, +\infty)$, the inequality (2.4) reduces to Varma's result [65]

$$\|P'\|^2 \leq \frac{1}{2(2n-1)} \|P''\|^2 + \frac{2n^2}{2n-1} \|P\|^2.$$

Recently, Guessab and Milovanović [34] have considered a weighted L^2 analogues of the well-known Bernstein's inequality, which can be stated in the following form (cf. [51]):

$$\|\sqrt{1-t^2}P'(t)\|_\infty \leq n\|P\|_\infty \quad (P \in \mathcal{P}_n), \quad (2.5)$$

where $\|f\|_\infty = \max_{-1 \leq x \leq 1} |f(x)|$. Using the norm $\|f\|^2 = (f, f)_w$, $w \in CW$, they have considered the following problem connected with the Bernstein's inequality (2.5): Determine the best constant $C_{n,m}(w)$ ($1 \leq m \leq n$) such that the inequality

$$\|A^{m/2}P^{(m)}\|_w \leq C_{n,m}(w)\|P\|_w \quad (2.6)$$

holds for all $P \in \mathcal{P}_n$.

THEOREM 2.5. For all $P \in \mathcal{P}_n$ the inequality (2.6) holds with the best constant

$$C_{n,m}(w) = \sqrt{\lambda_{n,0}\lambda_{n,1} \cdots \lambda_{n,m-1}}, \quad (2.7)$$

where $\lambda_{n,k} = -(n-k) \left(\frac{1}{2}(n+k-1)A''(0) + B'(0)\right)$. The equality is attained in (2.7) if and only if $P(t)$ is a constant multiple of the classical polynomial $Q_n(t)$ orthogonal with respect to the weight function $w \in CW$ on (a, b) .

We list now the coefficients a_k ($k \geq 0$) and b_k ($k \geq 1$) in the three-term recurrence relation for the monic classical orthogonal polynomials $\hat{Q}_k(t)$ on (a, b) ,

$$\hat{Q}_{k+1}(t) = (t - a_k)\hat{Q}_k(t) - b_k\hat{Q}_{k-1}(t) \quad (k \geq 0), \quad (2.8)$$

where $\hat{Q}_1(t) = 0$ and $\hat{Q}_0(t) = 1$. We give also the moment $\mu_0 = \int_a^b w(t) dt$ ($w \in CW$).

1° *Jacobi case:* $\hat{P}_k^{(\alpha, \beta)}(t) = 2^k k! / ((k + \alpha + \beta + 1)_k) P_k^{(\alpha, \beta)}(t)$,

$$\begin{aligned} \mu_0 &= \frac{2^{\alpha+\beta+1} \Gamma(\alpha+1) \Gamma(\beta+1)}{\Gamma(\alpha+\beta+2)}, \\ a_k &= \frac{\beta^2 - \alpha^2}{(2k + \alpha + \beta)(2k + \alpha + \beta + 2)}, \\ b_k &= \frac{4k(k + \alpha)(k + \beta)(k + \alpha + \beta)}{(2k + \alpha + \beta)^2((2k + \alpha + \beta)^2 - 1)}. \end{aligned}$$

2° *Generalized Laguerre case:* $\hat{L}_k^s(t) = (-1)^k L_k^s(t)$,

$$\mu_0 = \Gamma(s+1), \quad a_k = 2k + s + 1, \quad b_k = k(k + s).$$

3° *Hermite case:* $\hat{H}_k(t) = 2^{-k} H_k(t)$,

$$\mu_0 = \sqrt{\pi}, \quad a_k = 0, \quad b_k = \frac{k}{2}.$$

The norm of monic orthogonal polynomials can be calculated using (1.3).

3. NON-CLASSICAL ORTHOGONAL POLYNOMIALS

As we have seen in the previous subsection the monic Chebyshev polynomials of the second kind

$$\hat{S}_k(t) = \frac{1}{2^k} \cdot \frac{\sin(k+1)\theta}{\sin \theta}, \quad t = \cos \theta,$$

have a very simple three-term recurrence relation (2.8) with $a_k = 0$ and $b_k = 1/4$. A system of orthogonal polynomials for which the recursion coefficients satisfy

$$\lim_{k \rightarrow +\infty} a_k = 0 \quad \text{and} \quad \lim_{k \rightarrow +\infty} b_k = \frac{1}{4} \quad (3.1)$$

will be said to be a perturbation of the polynomials $\hat{S}_k(t)$. Similarly, one can consider orthogonal polynomials with such coefficients that

$$\lim_{k \rightarrow +\infty} a_k = a \quad \text{and} \quad \lim_{k \rightarrow +\infty} b_k = \frac{b^2}{4} > 0,$$

where $a, b \in \mathbb{R}$. These polynomials are perturbations of $t \mapsto b^k \hat{S}_k((t-a)/b)$ and are said to belong to the class $\mathcal{N}(a, b)$, which was introduced and considered in detail by Nevai [55]¹⁾. Evidently, (3.1) holds for polynomials from the class $\mathcal{N}(0, 1)$.

There are several classes of orthogonal polynomials which are in certain sense close to the classical orthogonal polynomials. For example, when the weight $t \mapsto W(t)$ is the product of a classical weight $t \mapsto w(t)$ times a polynomial, Ronveaux [57] found the second-order differential equation for the corresponding orthogonal polynomials. Ronveaux and Thiry [59] developed a REDUCE package giving such differential equations. The following cases have been studied by Ronveaux and Marcellán [58]:

1° *Rational Case.* $W(t) = R(t)w(t)$, where R is a rational function with poles and zeros outside the support of w ;

2° *δ Dirac distribution.*

$$W(t) = w(t) + \sum_{k=1}^m \lambda_k \delta(t - t_k),$$

where the positive mass λ_k is located at t_k (t_k outside or inside the support of w).

In both cases, orthogonal polynomials are *semi-classical* (see Maroni [42]).

A nice survey about orthogonal polynomials and spectral theory was given by Everitt and Littlejohn [14].

In many applications of orthogonal polynomials it is very important to know the recursion coefficients a_k and b_k . If $d\lambda(t)$ is one of the classical measures, then a_k

¹⁾Originally, Nevai defined this class for orthonormal polynomials.

and b_k are known explicitly. Furthermore, there are certain non-classical measures when we know also these coefficients. In sequel we mention only a few of them:

1° *Generalized Gegenbauer weight* $w(t) = |t|^\mu(1-t^2)^\alpha$, $\mu, \alpha > -1$, on $[-1, 1]$. The (monic) generalized Gegenbauer polynomials $W_k^{(\alpha, \beta)}(t)$, $\beta = (\mu-1)/2$, were introduced by Lascenov [38] (see, also, Chihara [13, pp. 155–156]). These polynomials can be expressed in terms of the Jacobi polynomials,

$$W_{2k}^{(\alpha, \beta)}(t) = \frac{k!}{(k + \alpha + \beta + 1)_k} P_k^{\alpha, \beta}(2t^2 - 1),$$

$$W_{2k+1}^{(\alpha, \beta)}(t) = \frac{k!}{(k + \alpha + \beta + 2)_k} x P_k^{\alpha, \beta+1}(2t^2 - 1).$$

Notice that $W_{2k+1}^{(\alpha, \beta)}(t) = tW_{2k}^{(\alpha, \beta+1)}(t)$. Their three-term recurrence relation is

$$W_{k+1}^{(\alpha, \beta)}(t) = tW_k^{(\alpha, \beta)}(t) - b_k W_{k-1}^{(\alpha, \beta)}(t), \quad k = 0, 1, \dots,$$

$$W_{-1}^{(\alpha, \beta)}(t) = 0, \quad W_0^{(\alpha, \beta)}(t) = 1,$$

where

$$b_{2k} = \frac{k(k + \alpha)}{(2k + \alpha + \beta)(2k + \alpha + \beta + 1)}, \quad b_{2k-1} = \frac{(k + \beta)(k + \alpha + \beta)}{(2k + \alpha + \beta - 1)(2k + \alpha + \beta)},$$

for $k = 1, 2, \dots$, except when $\alpha + \beta = -1$; then $b_1 = (\beta + 1)/(\alpha + \beta + 2)$. Some applications of these polynomials in numerical quadratures and least square approximation with constraint were given in [36] and [50], respectively.

2° *The hyperbolic weight* $w(t) = 1/\cosh t$ on $(-\infty, +\infty)$. The coefficients in three-term recurrence relation are given by

$$a_k = 0, \quad b_0 = \pi, \quad b_k = \frac{\pi^2 k^2}{4} \quad (k \geq 1).$$

For details and generalizations see Chihara [13, pp. 191–193] and Carlitz [12].

3° *The logistic weight* $w(t) = e^{-t}/(1 + e^{-t})^2$ on $(-\infty, +\infty)$. Here we have

$$a_k = 0, \quad b_0 = 1, \quad b_k = \frac{\pi^2 k^4}{4k^2 - 1} \quad (k \geq 1).$$

This can be obtained from the papers of Askey and Wilson [5–6]. Namely, their last equality in Section 1 of [5] for $\gamma = 1/2$ gives the case of the logistic weight $e^{-t}/(1 + e^{-t})^2$ (i.e., $1/\cosh^2 \pi x$) on $(-\infty, +\infty)$.

4° $w(t) = t/\sinh \pi t$ on $(-\infty, +\infty)$. In [5] it was proved that polynomials

$$P_n(x) = i^n {}_3F_2 \left(\begin{matrix} -n, n + 2\alpha + 2\gamma - 1, \gamma - ix \\ \alpha + \gamma, 2\gamma \end{matrix}; 1 \right), \quad n = 0, 1, \dots,$$

are orthogonal on $(-\infty, +\infty)$ with respect to the weight

$$w(x) = |\Gamma(\alpha + ix)\Gamma(\gamma + ix)|^2.$$

For $\alpha = 1/2$ and $\gamma = 1$ this weight reduces to $w(x) = 2\pi^2 x / \sinh(2\pi x)$, and polynomials can be expressed in the form

$$P_n(x) = \frac{i^n}{n+1} \sum_{k=0}^n (-1)^k \frac{4^k (n+k+1)!}{(k+1)!(2k+1)!(n-k)!} (1-ix)_k.$$

If we denote the corresponding monic polynomials orthogonal with respect to the weight $w(t) = t / \sinh \pi t$ by $\pi_n(t)$ (changing variable $2x = t$), we can prove that

$$\pi_{n+1}(t) = t\pi_n(t) - \frac{1}{4}n(n+1)\pi_{n-1}(t), \quad n = 1, 2, \dots$$

A system of orthogonal polynomials for which the recursion coefficients are not known explicitly will be said to be *strong non-classical* orthogonal polynomials. In such cases there are a few known approaches to compute the first n coefficients a_k , b_k , $k = 0, 1, \dots, n-1$. These then allow us to compute all orthogonal polynomials of degree $\leq n$ by a straightforward application of the three-term recurrence relation (2.8).

One of approaches for numerical construction of the monic orthogonal polynomials $\{\hat{\pi}_k\}$ is the *method of moments*, or precisely, *Chebyshev* or *modified Chebyshev algorithm*.

The second method makes use of explicit representations

$$a_k = \frac{(t\hat{\pi}_k, \hat{\pi}_k)}{(\hat{\pi}_k, \hat{\pi}_k)} \quad (k \geq 0), \quad b_0 = (\hat{\pi}_0, \hat{\pi}_0), \quad b_k = \frac{(\hat{\pi}_k, \hat{\pi}_k)}{(\hat{\pi}_{k-1}, \hat{\pi}_{k-1})} \quad (k \geq 1),$$

in terms of the inner product (\cdot, \cdot) . The method is known as the *Stieltjes procedure*. Using a discretization of the inner product by some appropriate quadrature

$$(f, g) \approx (f, g)_N = \sum_{k=1}^N w_k f(x_k) g(x_k), \quad w_k > 0,$$

the corresponding method is called the *discretized Stieltjes procedure*.

For details in numerical construction of orthogonal polynomials see papers of Gautschi [18], [23–24], [27]. In Section 3 we will mention a few non-classical weights for which the recursion coefficients were constructed numerically as well as the corresponding Gaussian formulas.

4. SOME APPLICATIONS OF ORTHOGONAL POLYNOMIALS

This section is devoted to some important applications of orthogonal polynomials on the real line as Gauss-Christoffel quadrature formulas and summation of slowly convergent series.

4.1. GAUSSIAN TYPE OF QUADRATURES

One of the important uses of orthogonal polynomials is in the construction of quadrature formulas of maximum, or nearly maximum, algebraic degree of exactness for integrals involving a positive measure $d\lambda(t)$.

The n -point *Gaussian quadrature formula*

$$\int_{\mathbb{R}} f(t) d\lambda(t) = \sum_{\nu=1}^n \lambda_{\nu}^{(n)} f(\tau_{\nu}^{(n)}) + R_n(f) \quad (4.1.1)$$

has maximum algebraic degree of exactness $2n - 1$, in the sense that $R_n(f) = 0$ for all $f \in \mathcal{P}_{2n-1}$. In formula (4.1.1), $\tau_{\nu} = \tau_{\nu}^{(n)}$ are the *Gauss nodes*, and $\lambda_{\nu} = \lambda_{\nu}^{(n)}$ the *Gauss weights* or *Christoffel numbers*. This formula is also known as *Gauss-Christoffel quadrature formula*. A nice survey on that was given by Gautschi [17].

The nodes τ_{ν} are the zeros of the n -th orthogonal polynomial $\pi_n(\cdot, d\lambda)$, and the weights λ_{ν} , which are all positive, can be also expressed in terms of the same orthogonal polynomials. As we have seen in 2.1, the nodes τ_{ν} are the eigenvalues of the n -th order Jacobi matrix

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

where α_{ν} and β_{ν} are the coefficients in three-term recurrence relation for the monic orthogonal polynomials $\pi_n(\cdot, d\lambda)$. The weights λ_{ν} are given by

$$\lambda_{\nu} = \beta_0 v_{\nu,1}^2, \quad \nu = 1, \dots, n,$$

where $\beta_0 = \int_{\mathbb{R}} d\lambda(t)$ and $v_{\nu,1}$ is the first component of the normalized eigenvector \mathbf{v}_{ν} corresponding to the eigenvalue τ_{ν} (cf. Golub and Welsch [33], and Gautschi [16]),

$$J_n(d\lambda)\mathbf{v}_{\nu} = \tau_{\nu}\mathbf{v}_{\nu}, \quad \mathbf{v}_{\nu}^T \mathbf{v}_{\nu} = 1, \quad \nu = 1, \dots, n.$$

There are well-known and efficient algorithms, such as the *QR* algorithm with shifts, to compute eigenvalues and eigenvectors of symmetric tridiagonal matrices (cf. the

routine GAUSS in the package ORTHPOL given by Gautschi [27]). There are many methods for estimating the remainder term $R_n(f)$ in (4.1.1). Error bounds in the class of analytic functions were investigated by Gautschi and Varga [32].

A simple modification of the previous method can be applied to the construction of Gauss-Radau and Gauss-Lobatto quadrature formulas.

In sequel we mention a few non-classical measures $d\lambda(t) = w(t) dt$ for which recursion coefficients $\alpha_k(d\lambda)$, $\beta_k(d\lambda)$, $k = 0, 1, \dots, n-1$, have been tabulated in the literature and used in the construction of Gaussian quadratures.

1° *One-side Hermite weight* $w(t) = \exp(-t^2)$ on $[0, c]$, $0 < c \leq +\infty$. This distribution $w(t) d\lambda(t)$ is known as the *Maxwell (velocity) distribution*. The cases $c = 1$, $n = 10$ and $c = +\infty$, $n = 15$ were considered by Steen, Byrne and Gelbard [61] (see also Gautschi [24]).

2° *Logarithmic weight* $w(t) = t^\alpha \log(1/t)$, $\lambda > -1$ on $(0, 1)$. Piessens and Branders [56] considered cases when $\alpha = 0, \pm 1/2, \pm 1/3, -1/4, -1/5$ (see also Gautschi [23]).

3° *Airy weight* $w(t) = \exp(-t^3/3)$ on $(0, +\infty)$. The inhomogeneous Airy functions $\text{Hi}(x)$ and $\text{Gi}(x)$, arise in theoretical chemistry (e.g. in harmonic oscillator models for large quantum numbers) and their integral representations (see Lee [39]) are given by

$$\begin{aligned}\text{Hi}(x) &= \frac{1}{\pi} \int_0^{+\infty} w(t) e^{tx} dt, \\ \text{Gi}(x) &= -\frac{1}{\pi} \int_0^{+\infty} w(t) e^{-tx/2} \cos\left(\frac{\sqrt{3}}{2} tx + \frac{2\pi}{3}\right) dt.\end{aligned}$$

These functions can be effectively evaluated by Gaussian quadrature relative to the Airy weight $w(t)$. It needs orthogonal polynomials with respect to this weight. Gautschi [21] computed the recursion coefficients for $n = 15$ with 16 decimal digits after the decimal point (D).

3° *Reciprocal gamma function* $w(t) = 1/\Gamma(t)$ on $(0, +\infty)$. Gautschi [20] determined the recursion coefficients for $n = 40$ with 20 significant decimal digits (S). This function could be useful as a probability density function in reliability theory (see Fransén [15]).

4° *Einstein's and Fermi's weight functions* on $(0, +\infty)$,

$$w_1(t) = \varepsilon(t) = \frac{t}{e^t - 1} \quad \text{and} \quad w_2(t) = \varphi(t) = \frac{1}{e^t + 1}. \quad (4.1.2)$$

These functions arise in solid state physics. Integrals with respect to the measure $d\lambda(t) = \varepsilon(t)^r dt$, $r = 1$ and $r = 2$, are widely used in phonon statistics and lattice specific heats and occur also in the study of radiative recombination processes. Similarly, integrals with $\varphi(t)$ are encountered in the dynamics of electrons in metals.

For $w_1(t)$, $w_2(t)$, $w_3(t) = \varepsilon(t)^2$ and $w_4(t) = \varphi(t)^2$, Gautschi and Milovanović [29] determined the recursion coefficients α_k and β_k , for $n = 40$ with 25 S, and gave an application of the corresponding Gauss-Christoffel quadratures to summation of slowly convergent series.

5° The hyperbolic weights on $(0, +\infty)$,

$$w_1(t) = \frac{1}{\cosh^2 t} \quad \text{and} \quad w_2(t) = \frac{\sinh t}{\cosh^2 t}. \quad (4.1.3)$$

The recursion coefficients α_k, β_k , for $n = 40$ with 30 S, were obtained by Milovanović [47]. The discretization was based on the Gauss-Laguerre quadrature rule.

4.2. SUMMATION OF SLOWLY CONVERGENT SERIES

We consider convergent series of the type

$$T = \sum_{k=1}^{+\infty} a_k \quad \text{and} \quad S = \sum_{k=1}^{+\infty} (-1)^k a_k \quad (4.2.1)$$

and introduce the notation: $T = T^{(m-1)} + T_m^{(\infty)}$, $S = S^{(m-1)} + S_m^{(\infty)}$,

$$T_m^{(n)} = \sum_{k=m}^n a_k, \quad S_m^{(n)} = \sum_{k=m}^n (-1)^k a_k,$$

where $T^{(m-1)}$ and $S^{(m-1)}$ are the corresponding partial sums of (4.2.1).

Some methods of summation these series can be found, for example, in the books of Henrici [35], Lindelöf [41], and Mitrinović and Kečkić [54].

Recently, a few new summation/integration procedures for slowly convergent series are developed (see [29], [25–26], [47–49]). Here we give a short account of these methods.

4.2.1. Laplace transform method. Suppose that the general term of T (and S) is expressible in terms of the derivative of a Laplace transform, or in terms of the Laplace transform itself. Namely, let $a_k = F'(k)$, where

$$F(p) = \int_0^{+\infty} e^{-pt} f(t) dt, \quad \operatorname{Re} p \geq 1.$$

Then

$$\sum_{k=1}^{+\infty} F'(k) = - \sum_{k=1}^{+\infty} \int_0^{+\infty} t e^{-kt} f(t) dt = - \int_0^{+\infty} \frac{t}{e^t - 1} f(t) dt.$$

Similarly, for “alternating” series, one obtains

$$\sum_{k=1}^{+\infty} (-1)^k F'(k) = \int_0^{+\infty} \frac{t}{e^t + 1} f(t) dt$$

and

$$\sum_{k=1}^{+\infty} (-1)^k F(k) = - \int_0^{+\infty} \frac{1}{e^t + 1} f(t) dt.$$

In a joint paper with Gautschi [29] we considered the construction of Gaussian quadrature formulas on $(0, +\infty)$,

$$\int_0^{+\infty} g(t)w(t) dt = \sum_{\nu=1}^n \lambda_\nu g(\tau_\nu) + R_n(g), \quad (4.2.2)$$

with respect to the weight functions given by (4.1.2). If the series T and S are slowly convergent and the respective function f on the right of the equalities above is smooth, then low-order Gaussian quadrature (4.2.2) applied to the integrals on the right, provides a possible summation procedure. Numerical examples show fast convergence of this procedure (see [29, §4]). A problem which arises with this procedure (*Laplace transform method*) is the determination of the original function f for a given series. For some other applications see [25–26].

4.2.2. Contour Integration Over a Rectangle. Suppose now that $a_k = f(k)$, where $z \mapsto f(z)$ is a holomorphic function in the region

$$G_m = \{z \in \mathbb{C} \mid \operatorname{Re} z \geq \alpha, m-1 < \alpha < m\}, \quad m \in \mathbb{N}.$$

In [47] we derived an alternative summation/integration method for the series (4.2.1) which requires the indefinite integral F of f chosen so as to satisfy the following decay conditions:

- (C1) F is a holomorphic function in the region G_m ;
- (C2) $\lim_{|t| \rightarrow +\infty} e^{-c|t|} F(x + it/\pi) = 0$, uniformly for $x \geq \alpha$;
- (C3) $\lim_{x \rightarrow +\infty} \int_{-\infty}^{+\infty} e^{-c|t|} |F(x + it/\pi)| dt = 0$,

where $c = 2$ or $c = 1$, when we consider $T_m^{(n)}$ or $S_m^{(n)}$, respectively.

Namely, taking $\Gamma = \partial G$ and

$$G = \left\{ z \in \mathbb{C} \mid \alpha \leq \operatorname{Re} z \leq \beta, |\operatorname{Im} z| \leq \frac{\delta}{\pi} \right\},$$

where $m-1 < \alpha < m$, $n < \beta < n+1$ ($m, n \in \mathbb{Z}, m \leq n$), we obtain that

$$T_m^{(n)} = \frac{1}{2\pi i} \oint_{\Gamma} f(z) \frac{\pi}{\tan \pi z} dz \quad \text{and} \quad S_m^{(n)} = \frac{1}{2\pi i} \oint_{\Gamma} f(z) \frac{\pi}{\sin \pi z} dz.$$

After integration by parts, these formulas reduce to

$$T_m^{(n)} = \frac{1}{2\pi i} \oint_{\Gamma} \left(\frac{\pi}{\sin \pi z} \right)^2 F(z) dz \quad (4.2.3)$$

and

$$S_m^{(n)} = \frac{1}{2\pi i} \oint_{\Gamma} \left(\frac{\pi}{\sin \pi z} \right)^2 \cos \pi z F(z) dz, \quad (4.2.4)$$

where $z \mapsto F(z)$ is an integral of $z \mapsto f(z)$.

Taking $\alpha = \alpha_m = m - 1/2$, $\beta = \beta_n = n + 1/2$, and letting $\delta \rightarrow +\infty$ and $n \rightarrow +\infty$, under conditions (C1) – (C3), the integrals in (4.2.3) and (4.2.4) over Γ reduce to integrals along the line $z = \alpha_m + iy$ ($-\infty < y < +\infty$).

After some calculations, we reduce T and S to a problem of quadrature on $(0, +\infty)$ with respect to the hyperbolic weight functions given by (4.1.3). Thus,

$$T = T^{(m-1)} + \int_0^{+\infty} \Phi(\alpha_m, t/\pi) w_1(t) dt$$

and

$$S = S^{(m-1)} + \int_0^{+\infty} \Psi(\alpha_m, t/\pi) w_2(t) dt,$$

where w_1 and w_2 are defined in (4.1.3) and

$$\Phi(x, y) = -\frac{1}{2} [F(x + iy) + F(x - iy)],$$

$$\Psi(x, y) = \frac{(-1)^m}{2i} [F(x + iy) - F(x - iy)].$$

Numerical experiments shows that is enough to use only the quadrature with respect to the first weight $w_1(t) = 1/\cosh^2 t$. Namely, in the series S we can include the hyperbolic sine as a factor in the corresponding integrand so that

$$S = S^{(m-1)} + \int_0^{+\infty} \Psi(\alpha_m, t/\pi) \sinh(t) w_1(t) dt.$$

Using this approach we gave an appropriate method for calculating values of the Riemann zeta function $\zeta(z) = \sum_{k=1}^{+\infty} k^{-z}$, which can be transformed to a weighted integral on $(0, +\infty)$ of the function $t \mapsto \exp(-(z/2) \log(1 + \beta_m^2 t^2)) \cos(z \arctan(\beta_m t))$, $\beta_m = 2/((2m + 1)\pi)$, $m \in \mathbb{N}_0$, involving the hyperbolic weight $w(t) = 1/\cosh^2 t$ (see [48]).

Also some other methods for series with irrational terms were given in [49].

5. ORTHOGONALITY ON THE SEMICIRCLE

Polynomials orthogonal on the semicircle $\Gamma_0 = \{z \in \mathbb{C} \mid z = e^{i\theta}, 0 \leq \theta \leq \pi\}$ have been introduced by Gautschi and Milovanović [30–31]. The inner product is given by

$$(f, g) = \int_{\Gamma} f(z)g(z)(iz)^{-1} dz = \int_0^{\pi} f(e^{i\theta})g(e^{i\theta}) d\theta,$$

where Γ is the semicircle $\Gamma = \{z \in \mathbb{C} \mid z = e^{i\theta}, 0 \leq \theta \leq \pi\}$. This inner product is not Hermitian, but the corresponding (monic) orthogonal polynomials $\{\pi_k\}$ exist uniquely and satisfy a three-term recurrence relation of the form

$$\begin{aligned}\pi_{k+1}(z) &= (z - i\alpha_k)\pi_k(z) - \beta_k\pi_{k-1}(z), & k = 0, 1, 2, \dots, \\ \pi_{-1}(z) &= 0, \quad \pi_0(z) = 1.\end{aligned}$$

Notice that the inner product possesses the property $(zf, g) = (f, zg)$. The general case of complex polynomials orthogonal with respect to a *complex weight function* was considered by Gautschi, Landau and Milovanović [28]. A generalization of such polynomials on a circular arc was given by M.G. de Bruin [10], and further investigations were done by Milovanović and Rajković [53].

Let $w: (-1, 1) \mapsto \mathbb{R}_+$ be a weight function which can be extended to a function $w(z)$ holomorphic in the half disc $D_+ = \{z \in \mathbb{C} \mid |z| < 1, \operatorname{Im} z > 0\}$, and

$$(f, g) = \int_{\Gamma} f(z)g(z)w(z)(iz)^{-1} dz = \int_0^{\pi} f(e^{i\theta})g(e^{i\theta})w(e^{i\theta}) d\theta. \quad (5.1)$$

Together with (5.1) consider the inner product

$$[f, g] = \int_{-1}^1 f(x)\overline{g(x)}w(x) dx, \quad (5.2)$$

which is positive definite and therefore generates a unique set of real (monic) orthogonal polynomials $\{p_k\}$:

$$[p_k, p_m] = 0 \quad \text{for } k \neq m \quad \text{and} \quad [p_k, p_m] > 0 \quad \text{for } k = m \quad (k, m \in \mathbb{N}_0).$$

These polynomials, as well as the associated polynomials of the second kind,

$$q_k(z) = \int_{-1}^1 \frac{p_k(z) - p_k(x)}{z - x} w(x) dx \quad (k = 0, 1, 2, \dots),$$

are known to satisfy a three-term recurrence relation of the form

$$y_{k+1} = (z - a_k)y_k - b_k y_{k-1} \quad (k = 0, 1, 2, \dots), \quad (5.3)$$

where

$$y_{-1} = 0, \quad y_0 = 1 \quad \text{for } \{p_k\} \quad \text{and} \quad y_{-1} = -1, \quad y_0 = 0 \quad \text{for } \{q_k\}. \quad (5.4)$$

Denote by m_k and μ_k the moments associated with the inner products (5.1) and (5.2), respectively,

$$\mu_k = (z^k, 1), \quad m_k = [x^k, 1], \quad k \geq 0,$$

where, in view of (5.4), $b_0 = m_0$.

On the other hand, the inner product (5.1) is not Hermitian; the second factor g is not conjugated and the integration is not with respect to the measure $|w(e^{i\theta})| d\theta$. The existence of corresponding orthogonal polynomials, therefore, is not guaranteed. We call a system of complex polynomials $\{\pi_k\}$ *orthogonal on the semicircle* if

$$(\pi_k, \pi_m) = 0 \quad \text{for } k \neq m \quad \text{and} \quad (\pi_k, \pi_m) > 0 \quad \text{for } k = m \quad (k, m \in \mathbb{N}_0).$$

where we assume that π_k is monic of degree k .

Assuming that the weight function w is positive on $(-1, 1)$, holomorphic in D_+ and such that the integrals (5.1) and (5.2) exist for smooth f and g (possibly) as improper integrals, Gautschi, Landau and Milovanović [28] proved the following result:

THEOREM 5.1. *If*

$$\operatorname{Re}(1, 1) = \operatorname{Re} \int_0^\pi w(e^{i\theta}) d\theta \neq 0, \quad (5.5)$$

then there exists a unique system of (monic, complex) orthogonal polynomials $\{\pi_k\}$ relative to the inner product (5.1). Denoting by $\{p_k\}$ the (monic, real) orthogonal polynomials relative to the inner product (5.2), we have

$$\pi_k(z) = p_k(z) - i\theta_{k-1}p_{k-1}(z) \quad (k = 0, 1, 2, \dots), \quad (5.6)$$

where

$$\theta_{k-1} = \frac{\mu_0 p_k(0) + iq_k(0)}{i\mu_0 p_{k-1}(0) - q_{k-1}(0)} \quad (k = 0, 1, 2, \dots). \quad (5.7)$$

Alternatively,

$$\theta_k = ia_k + \frac{b_k}{\theta_{k-1}} \quad (k = 0, 1, 2, \dots); \quad \theta_{-1} = \mu_0, \quad (5.8)$$

where a_k, b_k are the recursion coefficients in (5.3) and $\mu_0 = (1, 1)$. In particular, all θ_k are real (in fact, positive) if $a_k = 0$ for all $k \geq 0$. Finally,

$$(\pi_k, \pi_k) = \theta_{k-1}[p_{k-1}, p_{k-1}] \neq 0 \quad (k = 1, 2, \dots), \quad (\pi_0, \pi_0) = \mu_0. \quad (5.9)$$

As we can see, relation (5.6), with (5.7), gives a connection between orthogonal polynomials on the semicircle and the standard polynomials orthogonal on $[-1, 1]$ with respect to the same weight function w . The norms of these polynomials are in relation (5.9).

We assume that $\operatorname{Re}(1, 1) \neq 0$, so that orthogonal polynomials $\{\pi_k\}$ exist. Since $(zf, g) = (f, zg)$, it is known that they must satisfy a three-term recurrence relation

$$\begin{aligned} \pi_{k+1}(z) &= (z - i\alpha_k)\pi_k(z) - \beta_k\pi_{k-1}(z), & k = 0, 1, 2, \dots, \\ \pi_{-1}(z) &= 0, \quad \pi_0(z) = 1. \end{aligned} \quad (5.10)$$

Using the representation (5.6), we can find a connection between the coefficients in (5.10) and the corresponding coefficients in the three-term recurrence relation (5.3) for polynomials $\{p_k\}$ (see [28]):

THEOREM 5.2. *Under the assumption (5.5), the (monic, complex) polynomials $\{\pi_k\}$ orthogonal with respect to the inner product (5.1) satisfy the recurrence relation (5.10), where the coefficients α_k, β_k are given by*

$$\alpha_k = \theta_k - \theta_{k-1} - ia_k, \quad \beta_k = \frac{\theta_{k-1}}{\theta_{k-2}} b_{k-1} = \theta_{k-1}(\theta_{k-1} - ia_{k-1}),$$

for $k \geq 1$ and $\alpha_0 = \theta_0 - ia_0$, with the θ_k defined in Theorem 5.1.

Alternatively, the coefficients α_k can be expressed in the form

$$\alpha_k = -\theta_{k-1} + \frac{b_k}{\theta_{k-1}}, \quad k \geq 1, \quad \alpha_0 = \frac{b_0}{\theta_{-1}} = \frac{m_0}{\mu_0}.$$

One interesting question is the distribution of zeros. It follows from (5.10) that the zeros of $\pi_n(z)$ are the eigenvalues of the (complex, tridiagonal) matrix

$$J_n = \begin{bmatrix} i\alpha_0 & 1 & & & \text{O} \\ \beta_1 & i\alpha_1 & 1 & & \\ & \beta_2 & i\alpha_2 & \ddots & \\ & & \ddots & \ddots & 1 \\ \text{O} & & & \beta_{n-1} & i\alpha_{n-1} \end{bmatrix}, \quad (5.11)$$

where α_k and β_k are given in Theorem 5.2.

If the weight w is symmetric, i.e.,

$$w(-z) = w(z), \quad w(0) > 0, \quad (5.12)$$

then $\mu_0 = (1, 1) = \pi w(0) > 0$, $a_k = 0$, $\theta_k > 0$, for all $k \geq 0$, and

$$\alpha_0 = \theta_0, \quad \alpha_k = \theta_k - \theta_{k-1}, \quad \beta_k = \theta_{k-1}^2, \quad k \geq 1.$$

In that case J_n can be transformed into a real nonsymmetric tridiagonal matrix

$$A_n = -iD_n^{-1}J_nD_n = \begin{bmatrix} \alpha_0 & \theta_0 & & & \text{O} \\ -\theta_0 & \alpha_1 & \theta_1 & & \\ & -\theta_1 & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \theta_{n-2} \\ \text{O} & & & -\theta_{n-2} & \alpha_{n-1} \end{bmatrix},$$

where $D_n = \text{diag}(1, i\theta_0, i^2\theta_0\theta_1, i^3\theta_0\theta_1\theta_2, \dots) \in \mathbb{C}^{n \times n}$. The eigenvalues η_ν , $\nu = 1, \dots, n$, of A_n can be calculated using the EISPACK subroutine HQR (see [60]). Then all the zeros ζ_ν , $\nu = 1, \dots, n$, of $\pi_n(z)$ are given by $\zeta_\nu = i\eta_\nu$, $\nu = 1, \dots, n$.

In [28] we proved the following result for a symmetric weight (5.12):

THEOREM 5.3. *All zeros of π_n are located symmetrically with respect to the imaginary axis and contained in $D_+ = \{z \in \mathbb{C} \mid |z| < 1, \operatorname{Im} z > 0\}$, with the possible exception of a single (simple) zero on the positive imaginary axis.*

If we define the half strip $S_+ = \{z \in \mathbb{C} \mid \operatorname{Im} z > 0, -\xi_n \leq \operatorname{Re} z \leq \xi_n\}$, where ξ_n is the largest zero of the real polynomial p_n , then we can prove that all zeros of π_n are also in S_+ (see [28] and [31]). Thus, all zeros are contained in $D_+ \cap S_+$.

For the Gegenbauer weight $w(z) = (1 - z^2)^{\lambda-1/2}$, $\lambda > -1/2$, the exceptional case from Theorem 5.3 can only arise if $n = 1$ and $-1/2 < \lambda \leq 0$. Likewise, no exceptional cases seem to occur for Jacobi weights $w(z) = (1 - z)^\alpha(1 + z)^\beta$, $\alpha, \beta > -1$, if $n \geq 2$, as was observed by several numerical computations (see [28]). However, in a general case, Gautschi [22] exhibited symmetric functions w for which $\pi_n(\cdot; w)$, for arbitrary fixed n , has a zero iy with $y \geq 1$.

Recently M. G. de Bruin [10] considered the polynomials $\{\pi_k^R\}$ orthogonal on a circular arc with respect to the complex inner product

$$(f, g) = \int_{\varphi}^{\pi-\varphi} f_1(\theta)g_1(\theta)w_1(\theta) d\theta, \quad (5.13)$$

where $\varphi \in (0, \pi/2)$, and for $f(z)$ the function $f_1(\theta)$ is defined by

$$f_1(\theta) = f(-iR + e^{i\theta}\sqrt{R^2 + 1}), \quad R = \tan \varphi.$$

Alternatively, the inner product (5.13) can be expressed in the form

$$(f, g) = \int_{\Gamma_R} f(z)g(z)w(z)(iz - R)^{-1} dz, \quad (5.14)$$

where $\Gamma_R = \{z \in \mathbb{C} \mid z = -iR + e^{i\theta}\sqrt{R^2 + 1}, \varphi \leq \theta \leq \pi - \varphi, \tan \varphi = R\}$.

Under suitable integrability conditions on the weight function w , which is positive on $(-1, 1)$ and is holomorphic in the moon-shaped region

$$M_+ = \left\{ z \in \mathbb{C} \mid |z + iR| < \sqrt{R^2 + 1}, \operatorname{Im} z > 0 \right\},$$

where $R > 0$, the polynomials $\{\pi_k^R\}$ orthogonal on the circular arc Γ_R with respect to the complex inner product (5.13) always exist and have similar properties like polynomials orthogonal on the semicircle.

For $R = 0$ the arc Γ_R reduces to the semicircle Γ , and polynomials $\{\pi_k^R\}$ to $\{\pi_k\}$. It is easy to prove that the condition

$$\operatorname{Re} \int_{\Gamma_R} w(z)(iz - R)^{-1} dz = \operatorname{Re} \int_{\varphi}^{\pi-\varphi} w_1(\theta) d\theta \neq 0$$

is automatically satisfied for $R > 0$ in contrast to the case $R = 0$ (see condition (5.5)).

Quite analogous results to Theorems 5.1–5.4 were proved by de Bruin [10]. For example, for polynomials $\{\pi_k\}$ (the upper index R is omitted) equalities (5.6) and (5.9), as well as the three-term recurrence relation (5.10) hold, where now the θ_k is given by

$$\theta_k = -R + ia_k + \frac{b_k}{\theta_{k-1}} \quad (k = 0, 1, 2, \dots); \quad \theta_{-1} = \mu_0,$$

instead of (5.8). Also, for the symmetric weight, $w(z) = w(-z)$, all zeros of π_n are contained in M_+ with the possible exception of just one simple zero situated on the positive imaginary axis. Further results in this subject were given by Milovanović and Rajković [52–53].

6. APPLICATIONS OF POLYNOMIALS ORTHOGONAL ON THE SEMICIRCLE IN NUMERICAL ANALYSIS

Several interesting properties of polynomials orthogonal on the semicircle and applications in numerical integration, especially for Gegenbauer weight, were given in [31] and [45]. Also, differentiation formulas for higher derivatives of analytic functions, using quadratures on the semicircle, were considered in [11].

6.1. GAUSSIAN QUADRATURES

In this section we consider Gauss-Christoffel quadrature formula over the semicircle $\Gamma = \{z \in \mathbb{C} \mid z = e^{i\theta}, 0 \leq \theta \leq \pi\}$,

$$\int_0^\pi f(e^{i\theta})w(e^{i\theta})d\theta = \sum_{\nu=1}^n \sigma_\nu f(\zeta_\nu) + R_n(f), \quad (6.1.1)$$

with Gegenbauer weight $w(z) = (1 - z^2)^{\lambda-1/2}$, $\lambda > -1/2$, which is exact for all algebraic polynomials of degree at most $2n - 1$.

In this case, (5.5) reduces to $\text{Re}(1, 1) = \pi \neq 0$, so that the corresponding orthogonal polynomials exist and they can be expressed in terms of monic Gegenbauer polynomials $\hat{C}_k^\lambda(z)$,

$$\pi_k(z) = \hat{C}_k^\lambda(z) - i\theta_{k-1}\hat{C}_{k-1}^\lambda(z),$$

where the sequence $\{\theta_k\}$ is given by

$$\theta_k = \frac{1}{\lambda + k} \cdot \frac{\Gamma((k+2)/2)\Gamma(\lambda + (k+1)/2)}{\Gamma((k+1)/2)\Gamma(\lambda + k/2)}, \quad k \geq 0.$$

It was shown [28, Sect. 6.3] that all zeros of $\pi_n(z)$, $n \geq 2$, are simple and contained in the upper unit half disc $D_+ = \{z \in \mathbb{C} \mid |z| < 1, \text{Im } z > 0\}$. The nodes $\zeta_\nu = \zeta_\nu^{(n)}$ in (6.1.1) are precisely the zeros of the polynomial π_n , i.e., the eigenvalues of the

Jacobi matrix J_n given by (5.11). The weights $\sigma_\nu = \sigma_\nu^{(n)}$ can be obtained by an adaptation of the procedure of Golub and Welsch [33] (see [17] and [19]).

Following [32], we gave error bounds for the Gaussian quadratures (6.1.1), applied to analytic functions, using a contour integral representation of the remainder term (see [46]).

The Gaussian quadrature (6.1.1) can be applied to calculation of the Cauchy principal value integral

$$I_\lambda(\xi; f) = \text{v.p.} \int_{-1}^1 \frac{w(t)f(t)}{t-\xi} dt,$$

where $-1 < \xi < 1$ and $w(t) = (1-t^2)^{\lambda-1/2}$, $\lambda > -1/2$. Firstly, using the linear fractional transformation $t = (x+\xi)/(x\xi+1)$ we find

$$I_\lambda(\xi; f) = w(\xi) \text{v.p.} \int_{-1}^1 w(x) \frac{g(\xi; x)}{x} dx,$$

where $g(\xi; x) = f\left(\frac{x+\xi}{x\xi+1}\right)/(x\xi+1)^{2\lambda}$.

Let f be a meromorphic function with poles p_ν , $\nu = 1, \dots, m$, in D_+ and $\psi(z) = w(z)g(\xi; z)/z$. In [45] we proved that

$$I_\lambda(\xi; f) \approx w(\xi) \text{Im} \left\{ \sum_{\nu=1}^n \sigma_\nu g(\xi; \zeta_\nu) - 2\pi \sum_{\nu=1}^m \text{Res}_{z=p_\nu} \psi(z) \right\}.$$

6.2. NUMERICAL DIFFERENTIATION

Let f be an analytic function on some domain containing the point a and a circular neighborhood of a with radius r . Using the central difference operator δ_h defined by

$$\delta_h f(a) = \frac{1}{h} \left(f\left(a + \frac{h}{2}\right) - f\left(a - \frac{h}{2}\right) \right),$$

we can find $\delta_h^m f(a) = \delta_h (\delta_h^{m-1} f(a))$, i.e.,

$$\delta_h^m f(a) = \frac{1}{h^m} \sum_{k=0}^m (-1)^k \binom{m}{k} f\left(a + \frac{m-2k}{2} h\right). \quad (6.2.1)$$

Putting $he^{i\theta}$ instead of h , where h is such that $|a + \frac{mh}{2}e^{i\theta}| < r$, and integrating (6.2.1) over the semicircle, we obtain

$$\int_0^\pi \delta_{he^{i\theta}}^m f(a) w(e^{i\theta}) d\theta = \pi f^{(m)}(a). \quad (6.2.2)$$

Applying the Gauss-Christoffel quadrature formula on the semicircle (6.1.1) to the integral on the left side in (6.2.2), we obtain the following differentiation formula to higher derivatives

$$f^{(m)}(a) \approx D_{n,h}^m f(a) = \frac{1}{\pi} \sum_{\nu=1}^n \sigma_{\nu} \delta_{h\zeta_{\nu}}^m f(a),$$

i.e.,

$$D_{n,h}^m f(a) = \frac{1}{\pi h^m} \sum_{\nu=1}^n \frac{\sigma_{\nu}}{\zeta_{\nu}^m} \sum_{k=0}^m (-1)^k \binom{m}{k} f\left(a + \frac{m-2k}{2} h \zeta_{\nu}\right). \quad (6.2.3)$$

Regarding to the truncation error we can give the following result (see [11]):

THEOREM 6.2.1. *The error of the differentiation formula (6.2.3) for analytical functions is given by*

$$R_{n,h}^m f(a) = f^{(m)}(a) - D_{n,h}^m f(a) = \frac{1}{\pi} \sum_{p=n}^{\infty} \frac{f^{(m+2p)}(a)}{(m+2p)!} S_{m+2p}^{(m)} R_n(z^{2p}) h^{2p},$$

where

$$S_j^{(m)} = \sum_{k=0}^m (-1)^k \binom{m}{k} \left(\frac{m-2k}{2}\right)^j$$

and $R_n(z^{2p})$ is defined by (6.1.1). The dominant error term is

$$\frac{S_{m+2n}^{(m)}}{\pi(m+2n)!} \left(\frac{\Gamma((n+1)/2) \Gamma(\lambda+n/2)}{\Gamma(\lambda+n)} \right)^2 f^{(m+2n)}(a) h^{2n}.$$

Some considerations for $n=2$ and $m=1$ regarding to λ are given in [45].

For real-valued analytic functions the formula (6.2.3) can be simplified. Namely, when n is even and $\operatorname{Re} \zeta_{\nu} > 0$, for $\nu = 1, 2, \dots, n/2$, one finds

$$D_{n,h}^m f(a) = \frac{2}{\pi h^m} \sum_{\nu=1}^{n/2} \operatorname{Re} \left\{ \frac{\sigma_{\nu}}{\zeta_{\nu}^m} \sum_{k=0}^m (-1)^k \binom{m}{k} f\left(a + \frac{m-2k}{2} h \zeta_{\nu}\right) \right\}. \quad (6.2.4)$$

In the simplest case when $n=2$, we have

$$\zeta_{1,2} = \frac{1}{4} (\pm\sqrt{3} + i), \quad \sigma_{1,2} = \frac{\pi}{2} \left(1 \pm i \frac{\sqrt{3}}{3}\right).$$

Then, the corresponding differentiation formula (6.2.4) reduces to

$$D_{2,h}^m f(a) = \frac{2}{\pi h^m} \operatorname{Re} \left\{ \frac{\sigma_1}{\zeta_1^m} \sum_{k=0}^m (-1)^k \binom{m}{k} f\left(a + \frac{m-2k}{2} h \zeta_1\right) \right\}.$$

Its error is $O(h^4)$.

The formula (6.2.3) for real-valued analytic functions can be improved with a little change. Namely, if we put $he^{i\alpha}$ instead of h in (6.2.2), where α is an arbitrary real parameter, and applying again Gauss-Christoffel formula (6.1.1), we obtain the following differentiation formula

$$f^{(m)}(a) \approx D_{n,h,\alpha}^m f(a) = \frac{1}{\pi} \sum_{\nu=1}^n \sigma_\nu \delta_{he^{i\alpha}\zeta_\nu}^m f(a).$$

Similar to the above investigation we find an expression for the error, depending on the real parameter α

$$R_{n,h,\alpha}^m f(a) = f^{(m)}(a) - D_{n,h,\alpha}^m f(a) = \frac{1}{\pi} \sum_{p=n}^{\infty} \frac{f^{(m+2p)}(a)}{(m+2p)!} S_{m+2p}^{(m)} R_n(z^{2p}) e^{i2p\alpha} h^{2p}.$$

Since the derivative $f^{(m)}(a)$ is real for real a and real-valued functions the parameter α can be chosen such that the dominant error term in the last expressions be purely imaginary. Then, for such functions, the dominant error term in $R_{n,h,\alpha}^m f(a)$, i.e.,

$$\frac{1}{\pi(m+2n)!} f^{(m+2n)}(a) S_{m+2n}^{(m)} R_n(z^{2n}) e^{i2n\alpha} h^{2n},$$

becomes purely imaginary. This can be achieved for $\alpha = \pi/4n$. In that case, the dominant error term for real-valued functions becomes the real part of the term in $R_{n,h,\alpha}^m f(a)$ for $p = n + 1$. So we have the following result:

THEOREM 6.2.2. *The dominant error term of the differentiation formula*

$$f^{(m)}(a) \approx \operatorname{Re} \left\{ D_{n,h,\pi/4n}^m f(a) \right\}, \quad a \in \mathbb{R},$$

for real-valued analytic functions is given by

$$-\frac{\sin(\pi/2n)}{\pi(m+2n+2)!} S_{m+2n+2}^{(m)} R_n(z^{2n+2}) f^{(m+2n+2)}(a) h^{2n+2}, \quad (6.2.5)$$

where $R_n(g)$ is defined in (6.1.1).

With $\alpha = 3\pi/4n$ we also obtain a rule of degree precision $2n + 2$. Then, in the dominant error term (6.2.5), the factor $-\sin(\pi/2n)$ should be replaced by $\sin(3\pi/2n)$.

Several numerical experiments were done in [11], [31], and [44–45].

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