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On polynomials orthogonal on the semicircle and applications *

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Abstract

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Polynomials $\{\pi_n\}$ orthogonal on the semicircle $\Gamma = \{z \in \mathbb{C}\colon z = e^{i\theta}, 0 \leqslant \theta \leqslant \pi\}$ with respect to the inner product $(f, g) = \int_\Gamma f(z)g(z)w(z)(iz)^{-1}\,dz$, where $z \mapsto w(z)$ is a complex weight function, have been introduced in 1986–1987 by Gautschi, Landau and the author. In this paper we introduce the functions of the second kind, as well as the corresponding associated polynomials, and prove some recurrence relations. For Gauss–Gegenbauer quadrature formulae over the semicircle, applied to analytic functions, we develop error bounds from contour integral representations of the remainder term and give some numerical results.

Keywords: Complex orthogonal polynomials; recurrence relations; numerical integration; error bound

1. Introduction

Using the inner product $(\cdot, \cdot)$ given by

$$(f, g) = \int_\Gamma f(z)g(z)(iz)^{-1}\,dz,$$

where Γ is the semicircle $\Gamma = \{z \in \mathbb{C}\colon z = e^{i\theta}, 0 \leqslant \theta \leqslant \pi\}$, Gautschi and Milovanović [6] introduced a class of polynomials orthogonal on the semicircle Γ. A more general case with a complex weight function was considered by Gautschi, Landau and Milovanović [5]. Namely, let $w\colon (-1, 1) \mapsto \mathbb{R}_+$ be a weight function which can be extended to a function $w(z)$ holomorphic in the half disc $D_+ = \{z \in \mathbb{C}\colon |z| < 1, \operatorname{Im} z > 0\}$, and

$$(f, g) = \int_\Gamma f(z)g(z)w(z)(iz)^{-1}\,dz, \tag{1.1}$$

that is,

$$(f, g) = \int_0^\pi f(e^{i\theta})g(e^{i\theta})w(e^{i\theta})\,d\theta. \tag{1.2}$$

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This inner product is not Hermitian, but it has the property $(zf, g) = (f, zg)$. Under the assumption

$$\operatorname{Re}(1, 1) = \operatorname{Re} \int_0^{\pi} w(e^{i\theta}) \, d\theta \neq 0, \tag{1.3}$$

the monic, complex polynomials $\{\pi_k\}$ orthogonal with respect to the inner product (1.1) exist and satisfy the three-term recurrence relation

$$\begin{aligned} &\pi_{k+1}(z) = (z - i\alpha_k)\pi_k(z) - \beta_k \pi_{k-1}(z), \quad k = 0, 1, 2, \ldots, \\ &\pi_{-1}(z) = 0, \qquad \pi_0(z) = 1. \end{aligned} \tag{1.4}$$

The coefficients α_k and β_k are given by

$$\alpha_0 = \theta_0 - i a_0, \qquad \alpha_k = \theta_k - \theta_{k-1} - i a_k, \quad \beta_k = \theta_{k-1}(\theta_{k-1} - i a_{k-1}), \qquad k \geqslant 1,$$

and

$$\theta_{-1} = (1, 1), \qquad \theta_k = i a_k + \frac{b_k}{\theta_{k-1}}, \quad k \geqslant 0, \tag{1.5}$$

where a_k and b_k are the recursion coefficients in the corresponding three-term recurrence relation for real polynomials orthogonal with respect to the measure $w(t)\,dt$ on $(-1, 1)$.

Several interesting properties of such polynomials and some applications in numerical integration were given in [6,8]. Also, differentiation formulas for higher derivatives of analytic functions, using quadratures on the semicircle, were considered in [1].

Recently, de Bruin [3] has given a generalization of the orthogonal polynomials $\{\pi_k\}$. He considered the polynomials $\{\pi_k^R\}$ orthogonal on a circular arc

$$\Gamma_R = \left\{ z \in \mathbb{C}\colon z = -iR + e^{i\theta}\sqrt{R^2+1}, \ \phi \leqslant \theta \leqslant \pi - \phi, \ \tan\phi = R \right\}$$

with respect to the complex inner product

$$(f, g) = \int_{\phi}^{\pi-\phi} f_1(\theta) g_1(\theta) w_1(\theta) \, d\theta, \tag{1.6}$$

where $\phi \in (0, \frac{1}{2}\pi)$, and for $f(z)$ the function $f_1(\theta)$ is defined by

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

For $R = 0$ the inner product (1.6) reduces to (1.2) and the arc Γ_R to the semicircle Γ.

Another type of orthogonality of these polynomials, so-called Geronimus' version of orthogonality on a contour with respect to a complex weight, was investigated in [9]. Namely for monic polynomials $\{\pi_k\}$ orthogonal on the semicircle Γ, a complex weight function $z \mapsto \chi(z)$ was found, with a singularity in $z = 0$, such that

$$\langle \pi_k, \pi_m \rangle = \frac{1}{2\pi i} \oint_C \pi_k(z) \pi_m(z) \chi(z) \, dz = \begin{cases} 0, & k \neq m, \\ h_m, & k = m, \end{cases}$$

where C is any positively oriented simple closed contour surrounding some circle $|z| = r > 1$. The analogous problem for the polynomials $\{\pi_k^R\}$ orthogonal on the circular arc Γ_R, $R > 0$, was also solved [9].

This paper is organized as follows. In Section 2 we introduce the functions of the second kind, as well as the corresponding associated polynomials, and prove some recurrence relations. In Section 3, for Gauss–Gegenbauer quadrature formulae over the semicircle, applied to analytic functions, we develop error bounds from contour integral representations of the remainder term and give some numerical results.

2. Functions of the second kind and associated polynomials

In connection with polynomials $\{\pi_k\}$ orthogonal with respect to $(\cdot, \cdot)$ on Γ, we can introduce the so-called functions of the second kind

$$\rho_k(z) = \int_\Gamma \frac{\pi_k(\zeta)}{z-\zeta} \frac{w(\zeta)}{\mathrm{i}\zeta} \,\mathrm{d}\zeta, \quad k = 0, 1, 2, \ldots .$$

It is easily seen that the functions of the second kind also satisfy the same recurrence relation as the polynomials π_k. Indeed, from the recurrence relation (1.4) for $z = \zeta$, multiplying by $w(\zeta)(\mathrm{i}\zeta)^{-1}/(z-\zeta)$ and integrating, we obtain

$$\rho_{k+1}(z) = (z - \mathrm{i}\alpha_k)\rho_k(z) - \int_\Gamma \pi_k(\zeta) \frac{w(\zeta)}{\mathrm{i}\zeta} \,\mathrm{d}\zeta - \beta_k \rho_{k-1}(z).$$

By orthogonality, the integral on the right-hand side in the above equality vanishes if $k \geqslant 1$, and equals μ_0 if $k = 0$. If we define $\rho_{-1}(z) = 1$ (and $\beta_0 = \mu_0$), we have

$$\rho_{k+1}(z) = (z - \mathrm{i}\alpha_k)\rho_k(z) - \beta_k \rho_{k-1}(z), \quad k = 0, 1, 2, \ldots .$$

The following theorem gives an asymptotic form of ρ_k.

Theorem 2.1. *For $|z|$ sufficiently large, we have*

$$\rho_n(z) = \frac{\|\pi_n\|^2}{z^{n+1}} \left(1 + \mathrm{O}\left(\frac{1}{z}\right)\right), \quad \|\pi_n\|^2 = (\pi_n, \pi_n).$$

The quantities $\rho_n(z)/\pi_n(z)$, $|z| > 1$, are important in getting error bounds for Gaussian quadrature formulas over Γ, applied to analytic functions.

Introducing the polynomials

$$q_k(z) = \int_\Gamma \frac{\pi_k(z) - \pi_k(\zeta)}{z - \zeta} \frac{w(\zeta)}{\mathrm{i}\zeta} \,\mathrm{d}\zeta, \quad k = 0, 1, 2, \ldots,$$

which are called the polynomials associated with the orthogonal polynomials π_k, we can see that

$$\rho_k(z) = \pi_k(z)\rho_0(z) - q_k(z).$$

The polynomials $\{q_k\}$ satisfy the same three-term recurrence relation

$$q_{k+1}(z) = (z - \mathrm{i}\alpha_k) q_k(z) - \beta_k q_{k-1}(z), \quad k = 0, 1, 2, \ldots, \tag{2.1}$$
$$q_0(z) = 0, \qquad q_1(z) = \mu_0.$$

If we define $q_{-1}(z) = -1$ and $\beta_0 = \mu_0$, we can note that (2.1) also holds for $k = 0$ (see [4]).

3. Error bounds for Gaussian quadrature of analytic functions

In this section we consider the Gauss–Christoffel quadrature formula over the semicircle $\Gamma=\{z\in\mathbb{C}\colon z=\mathrm{e}^{\mathrm{i}\theta},\ 0\leqslant\theta\leqslant\pi\}$:

$$\int_0^{\pi} f(\mathrm{e}^{\mathrm{i}\theta})w(\mathrm{e}^{\mathrm{i}\theta})\,\mathrm{d}\theta=\sum_{\nu=1}^{n}\sigma_\nu f(\zeta_\nu)+R_n(f), \tag{3.1}$$

with Gegenbauer weight

$$w(z)=(1-z^2)^{\lambda-1/2},\quad \lambda>-\tfrac{1}{2},$$

which is exact for all algebraic polynomials of degree at most $2n-1$.

In this case, (1.3) reduces to $\mathrm{Re}(1,1)=\pi\neq 0$, so that the corresponding orthogonal polynomials exist and they can be expressed in terms of monic Gegenbauer polynomials $\hat{C}_k^{\lambda}(z)$ (see [5, Section 6.3]):

$$\pi_k(z)=\hat{C}_k^{\lambda}(z)-\mathrm{i}\theta_{k-1}\hat{C}_{k-1}^{\lambda}(z), \tag{3.2}$$

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

$$\theta_k=\frac{1}{\lambda+k}\,\frac{\Gamma\left(\frac{1}{2}(k+2)\right)\Gamma\left(\lambda+\frac{1}{2}(k+1)\right)}{\Gamma\left(\frac{1}{2}(k+1)\right)\Gamma\left(\lambda+\frac{1}{2}k\right)},\quad k\geqslant 0.$$

It was shown [5, Section 6.3] that all zeros of $\pi_n(z)$, $n\geqslant 2$, are simple and contained in the upper unit half disc $D_+=\{z\in\mathbb{C}\colon |z|<1,\ \mathrm{Im}\ z>0\}$. The nodes $\zeta_\nu=\zeta_\nu^{(n)}$ in (3.1) are precisely the zeros of the polynomial π_n. It follows from (1.4) that they are the eigenvalues of the Jacobi matrix

$$J_n=\begin{bmatrix} \mathrm{i}\alpha_0 & 1 & & & 0\\ \beta_1 & \mathrm{i}\alpha_1 & 1 & & \\ & \beta_2 & \mathrm{i}\alpha_2 & \ddots & \\ & & \ddots & \ddots & 1\\ 0 & & & \beta_{n-1} & \mathrm{i}\alpha_{n-1}\end{bmatrix},$$

where $\alpha_0=\theta_0$, $\alpha_k=\theta_k-\theta_{k-1}$, $\beta_k=\theta_{k-1}^2$, $k\geqslant 1$. Using the same procedure as in [6], we can determine the nodes $\zeta_\nu=\zeta_\nu^{(n)}$ and the weights $\sigma_\nu=\sigma_\nu^{(n)}$.

Following [7], in this section we give error bounds for the Gaussian quadratures (3.1), applied to analytic functions, using a contour integral representation of the remainder term.

Assume that f is an analytic and regular function in a certain domain G which contains the upper unit half disc $D_+=\{z\in\mathbb{C}\colon |z|<1,\ \mathrm{Im}\ z>0\}$ in its interior. Using Cauchy's integral representation of the function f,

$$f(\zeta)=\frac{1}{2\pi\mathrm{i}}\int_C\frac{f(z)}{z-\zeta}\mathrm{d}z,$$

where C is a contour in G surrounding D_+, we can express the remainder term $R_n(f)$ in the following form:

$$R_n(f)=\frac{1}{2\pi\mathrm{i}}\int_C K_n(z)f(z)\,\mathrm{d}z,$$

where the kernel K_n is given by

$$K_n(z)=R_n\left(\frac{1}{z-\cdot}\right)=\int_\Gamma\frac{1}{z-\zeta}\frac{w(\zeta)}{\mathrm{i}\zeta}\mathrm{d}\zeta-\sum_{\nu=1}^{n}\frac{\sigma_\nu}{z-\zeta_\nu}.$$

Using the orthogonal polynomials on the semicircle Γ and their functions of the second kind, we obtain that

$$K_n(z)=\frac{\rho_n(z)}{\pi_n(z)}. \tag{3.3}$$

On the other hand, expanding $(z-\zeta)^{-1}$ in powers of ζ/z, $|z|>1$, the kernel $K_n(z)$ can be expressed also in the form

$$K_n(z)=\sum_{k=2n}^{\infty}\frac{R_n(\zeta^k)}{z^{k+1}},\quad |z|>1, \tag{3.4}$$

because $R_n(\zeta^k)=0$ for $k=0,1,\dots,2n-1$.

It is interesting to find the first term in (3.4). Starting from

$$\pi_n(z)^2=z^{2n}+q(z),\quad q\in\mathscr{P}_{2n-1},$$

we have

$$\|\pi_n\|^2=\int_0^\pi \mathrm{e}^{\mathrm{i}2n\theta}w(\mathrm{e}^{\mathrm{i}\theta})\,\mathrm{d}\theta+\int_0^\pi q(\mathrm{e}^{\mathrm{i}\theta})w(\mathrm{e}^{\mathrm{i}\theta})\,\mathrm{d}\theta,$$

wherefrom, using the quadrature (3.1),

$$\|\pi_n\|^2=\int_0^\pi \mathrm{e}^{\mathrm{i}2n\theta}w(\mathrm{e}^{\mathrm{i}\theta})\,\mathrm{d}\theta-\sum_{\nu=1}^{n}\sigma_\nu\zeta_\nu^{2n}=R_n(\zeta^{2n}),$$

because $0=\pi_n(\zeta_\nu)^2=\zeta_\nu^{2n}+q(\zeta_\nu)$, $\nu=1,\dots,n$. Since

$$\|\pi_n\|^2=\beta_0\beta_1\cdots\beta_n=\beta_0(\theta_0\cdots\theta_{n-1})^2,\quad \beta_0=(1,1)=\pi,$$

we get

$$R_n(\zeta^{2n})=\|\pi_n\|^2=\left(\frac{\Gamma(\frac{1}{2}(n+1))\Gamma(\lambda+\frac{1}{2}n)}{\Gamma(\lambda+n)}\right)^2,$$

so the first term in (3.4) equals $\|\pi_n\|^2/z^{2n+1}$.

If $l(C)$ denotes the length of the contour C, an estimate of the error R_n can be given by (cf. [2,7,10])

$$|R_n(f)|\leqslant\frac{l(C)}{2\pi}\max_{z\in C}|K_n(z)|\|f\|,$$

where $\|f\|=\max_{z\in C}|f(z)|$.

In this section we will use only a circular contour. If we take $C=C_r=\{z\in\mathbb{C}\colon |z|=r>1\}$, the last estimate becomes

$$|R_n(f)|\leqslant rK_{n0}(r)\|f\|, \tag{3.5}$$

Table 3.1
Numerical values of Ψ_0 for $\lambda = 0$

n	$r=1.1$	$r=1.5$	$r=2.0$	$r=5.0$
2	$3.39\cdot10^{-2}$	$1.15\cdot10^{-1}$	$3.49\cdot10^{-1}$	$1.25\cdot10^{0}$
5	$1.57\cdot10^{-2}$	$7.22\cdot10^{-2}$	$1.34\cdot10^{-1}$	$4.54\cdot10^{-1}$
10	$8.07\cdot10^{-3}$	$3.85\cdot10^{-2}$	$7.06\cdot10^{-2}$	$2.31\cdot10^{-1}$
20	$4.36\cdot10^{-3}$	$2.00\cdot10^{-2}$	$3.63\cdot10^{-2}$	$1.17\cdot10^{-1}$

where

$$K_{n0}(r) = \max_{-\pi \leqslant \Psi \leqslant \pi} |K_n(re^{i\Psi})| = |K_n(re^{i\Psi_0})|. \tag{3.6}$$

Using (3.2), we can prove that $\overline{K_n(-\bar{z})} = -K_n(z)$ for each z. Because of that, in order to find the maximum of $|K_n(re^{i\Psi})|$ on C_r, it is enough to consider the case $-\frac{1}{2}\pi \leqslant \Psi \leqslant \frac{1}{2}\pi$. Moreover, numerical experiments show that $|K_n(z)| \geqslant |K_n(\bar{z})|$, when $\operatorname{Im} z > 0$. Numerical values of Ψ_0 in (3.6), for $\lambda = 0$ (Chebyshev case), $r = 1.1$, 1.5, 2.0, 5.0 and $n = 2$, 5, 10, 20 are given in Table 3.1. The corresponding values of $K_{n0}(r)$ are presented in Table 3.2.

For the numerical computation of $K_n(z)$ we use (3.3). Since ρ_n is a minimal solution of the basic three-term recurrence relation, its computation can be accomplished by Gautschi's algorithm [4].

Similar results were obtained for $\lambda = \frac{1}{2}$ and $\lambda = 1$. Numerical results show that $K_{n0}(r)$ decreases when λ increases. For example, $K_{n0}(r)$ for $n = 10$ and $r = 2$ takes the following values: $2.51 \cdot 10^{-11}$, $1.14 \cdot 10^{-11}$, $5.43 \cdot 10^{-12}$, when $\lambda = 0, 0.5, 1$, respectively.

Example 3.1. Let $f(z) = e^z$ and $z \in C_r$, i.e., $z = re^{i\theta}$, $r > 1$, $0 \leqslant \theta \leqslant 2\pi$. Then,

$$|f(z)| = e^{r\cos\theta} \leqslant e^r, \quad z \in C_r.$$

Using (3.5), we get

$$|R_n(f)| \leqslant B_n(r) = rK_{n0}(r)e^r, \quad r > 1. \tag{3.7}$$

The bound on the right of (3.7) may be optimized as a function of r. Thus, we obtain the problem

$$\min_{r>1}\left\{re^r \max_{z\in C_r}|K_n(z)|\right\} = B_n(r_{\text{opt}}).$$

Table 3.2
Numerical values of $K_{n0}(r)$ for $\lambda = 0$

n	$r=1.1$	$r=1.5$	$r=2.0$	$r=5.0$
2	$2.74\cdot10^{0}$	$2.23\cdot10^{-1}$	$3.84\cdot10^{-2}$	$2.92\cdot10^{-4}$
5	$2.30\cdot10^{-1}$	$6.70\cdot10^{-4}$	$1.34\cdot10^{-5}$	$2.94\cdot10^{-10}$
10	$2.75\cdot10^{-3}$	$4.36\cdot10^{-8}$	$2.51\cdot10^{-11}$	$3.18\cdot10^{-20}$
20	$3.84\cdot10^{-7}$	$1.89\cdot10^{-16}$	$9.06\cdot10^{-23}$	$3.86\cdot10^{-40}$

Table 3.3
Optimal values of r and $B_n(r)$ and actual errors e_n

n	r_{opt}	$B_n(r_{opt})$	e_n
2	4.16	$2.0 \cdot 10^{-1}$	$3.4 \cdot 10^{-2}$
3	6.09	$1.9 \cdot 10^{-3}$	$2.8 \cdot 10^{-4}$
5	10.1	$2.8 \cdot 10^{-8}$	$3.5 \cdot 10^{-9}$
8	16.0	$9.7 \cdot 10^{-17}$	m.p.

Applying the Fibonacci minimizing procedure, we find the optimal values r_{opt} of r and corresponding optimal bounds. They are presented in Table 3.3, together with the modulus of the actual errors, for $n = 2, 3, 5, 8$. Close to machine precision which is indicated in this table as m.p. ($\approx 2.76 \cdot 10^{-17}$ on the MICROVAX 3400 using VAX FORTRAN Ver. 5.3 in D-arithmetics), the actual error may be larger than the bound.

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