



ELSEVIER

Available online at www.sciencedirect.com ScienceDirect

Journal of Computational and Applied Mathematics 202 (2007) 440–449

JOURNAL OF
COMPUTATIONAL AND
APPLIED MATHEMATICSwww.elsevier.com/locate/cam

Domain of validity of Szegő quadrature formulas[☆]

O. Njåstad^a, J.C. Santos-León^{b,*}^a*Department of Mathematical Sciences, Norwegian University of Science and Technology, NO-7491 Trondheim, Norway*^b*Department of Mathematical Analysis, La Laguna University, 38271-La Laguna, Tenerife, Canary Islands, Spain*

Received 21 February 2006

Abstract

As is well known, the n -point Szegő quadrature formula integrates correctly any Laurent polynomial in the subspace $\text{span}\{1/z^{n-1}, \dots, 1/z, 1, z, \dots, z^{n-1}\}$. In this paper we enlarge this subspace. We prove that a set of $2n$ linearly independent Laurent polynomials are integrated correctly. The obtained result is used for the construction of Szegő quadrature formulas. Illustrative examples are given.

© 2006 Elsevier B.V. All rights reserved.

MSC: 41; 65D

Keywords: Domain of validity; Orthogonal polynomials; Szegő quadrature formulas

1. Introduction

In this paper we are concerned with the study of the domain of validity and with the construction of Szegő quadrature formulas introduced by Jones et al. [5]. They are used for the approximation of integrals over the unit circle in the complex plane, that is, integrals of the form,

$$I[f] = \int_{-\pi}^{\pi} f(e^{it}) \omega(t) dt, \quad (1)$$

where $\omega(t)$ is a weight function on $t \in [-\pi, \pi]$, that is, $\omega(t) \geq 0$, $t \in [-\pi, \pi]$, $0 < \int_{-\pi}^{\pi} \omega(t) dt < \infty$.

Some properties of Szegő quadrature formulas are analogous to the ones of classical Gauss quadrature formulas for integrals on the real line. For example, nodes on the region of integration and positive coefficients. Nevertheless, unlike classical Gauss quadrature formulas, Szegő quadrature formulas are based on the zeros of para-orthogonal polynomials. We next describe the Szegő quadrature formulas.

Let p and q be integers where $p \leq q$. We denote by $A_{p,q}$ the linear space of all functions of the form $\sum_{j=p}^q c_j z^j$, $c_j \in \mathbb{C}$. The functions of $A_{p,q}$ are called Laurent polynomials. We write A for the linear space of all Laurent polynomials.

[☆] This work was supported by the Ministry of Science and Technology of Spain under contracts TIC2002-00895 and MTM2005-08571.

* Corresponding author.

E-mail address: jcsantos@ull.es (J.C. Santos-León).

Consider the inner product on $A \times A$ given by

$$\langle f, g \rangle = \int_{-\pi}^{\pi} f(e^{it}) \overline{g(e^{it})} \omega(t) dt. \tag{2}$$

Let $\{\varrho_n\}_0^\infty$ be the sequence of monic polynomials obtained by orthogonalization of $\{z^n\}_0^\infty$ with respect to the inner product (2). The sequence $\{\varrho_n\}_0^\infty$ is called the sequence of Szegő polynomials with respect to the weight function ω . It is well known, see, e.g. [6, Theorem 11.4.1] that ϱ_n has its zeros in the region $|z| < 1$. Thus, they are not adequate as nodes for a general purpose quadrature formula to approximate integrals over the unit circle. Let \mathbb{T} denotes the unit circle $\mathbb{T} = \{z \in \mathbb{C} : |z| = 1\}$.

Theorem 1 (See Jones et al. [5]). *Let $\{\varrho_n\}_0^\infty$ be the sequence of Szegő polynomials (monic orthogonal polynomials) with respect to the weight function ω . Let $\{\kappa_n\}_1^\infty$ be a sequence of complex numbers satisfying $|\kappa_n| = 1, n \geq 1$. Let the para-orthogonal polynomials be defined by $B_n(z, \kappa_n) = \varrho_n(z) + \kappa_n \varrho_n^*(z)$ where $\varrho_n^*(z) = z^n \overline{\varrho_n(1/z)}$, and $\overline{\varrho_n}$ denotes the operation of conjugate the coefficients to the polynomials ϱ_n . Then $B_n(z, \kappa_n)$ has n distinct zeros $\zeta_m^{(n)}(\kappa_n), m = 1, 2, \dots, n, n \geq 1$, located on \mathbb{T} . Let*

$$\lambda_m^{(n)}(\kappa_n) = \int_{-\pi}^{\pi} \frac{B_n(e^{it}, \kappa_n)}{(e^{it} - \zeta_m^{(n)}(\kappa_n)) B_n'(\zeta_m^{(n)}(\kappa_n), \kappa_n)} \omega(t) dt, \quad 1 \leq m \leq n, \quad n \geq 1.$$

Then

$$I[f] = \int_{-\pi}^{\pi} f(e^{it}) \omega(t) dt = Q_n[f] = \sum_{m=1}^n \lambda_m^{(n)}(\kappa_n) f(\zeta_m^{(n)}(\kappa_n)) \tag{3}$$

for all $f \in A_{-(n-1), n-1}$. It holds that $\lambda_m^{(n)}(\kappa_n) > 0, 1 \leq m \leq n, n \geq 1$, and there cannot exist an n -point quadrature formula $G[f] = \sum_{m=1}^n \lambda_m f(\alpha_m), \alpha_m \in \mathbb{T}$ which correctly integrates every function $f \in A_{-(n-1), n}$ or every function $f \in A_{-n, n-1}$.

The quadrature formula Q_n given by the two last terms of (3) is called the n -point Szegő quadrature formula with respect to the weight function ω and the parameter κ_n . We sometimes briefly call it the n -point Szegő quadrature formula.

The paper is arranged as follows. In Section 2, we will prove the main result of this paper. As is stated in Theorem 1, the n -point Szegő quadrature formula integrates correctly every Laurent polynomial in the subspace $A_{-(n-1), n-1} = \text{span}\{1/z^{n-1}, \dots, 1, z, \dots, z^{n-1}\}$. We will prove that an additional linearly independent Laurent polynomial, an appropriate linear combination of both z^{-n} and z^n , is integrated correctly. The obtained result is applied in Section 3 for the computation of the n -point Szegő quadrature formula by means of moment fitting.

2. Domain of validity of Szegő quadrature formulas

Let $\delta_n = \varrho_n(0), n = 1, 2, \dots$, be the so-called reflection coefficients. It is well known that $|\delta_n| < 1, n = 1, 2, \dots$. See, e.g. [5]. (This is an straightforward consequence of Theorem 3.1 (A) there, for positive definite linear functionals as the linear functional (1)). In the following, take into account that $\delta_n + \kappa_n \neq 0$, and $1 + \overline{\delta_n} \kappa_n \neq 0$, for $\kappa_n \in \mathbb{C}, |\kappa_n| = 1$ since $|\delta_n| < 1, n = 1, 2, \dots$.

From here on and for simplicity, we sometimes write $B_n = B_n(z) = B_n(z, \kappa_n) = \varrho_n(z) + \kappa_n \varrho_n^*(z)$ for the para-orthogonal polynomials.

It holds that

$$z^n - \frac{B_n}{1 + \overline{\delta_n} \kappa_n} \in A_{0, n-1}, \quad n \geq 1.$$

Since $I[f] = Q_n[f]$, $f \in A_{-(n-1),n-1}$ we get

$$I \left[z^n - \frac{B_n}{1 + \overline{\delta_n \kappa_n}} \right] = Q_n \left[z^n - \frac{B_n}{1 + \overline{\delta_n \kappa_n}} \right] = Q_n[z^n] - \frac{1}{1 + \overline{\delta_n \kappa_n}} Q_n[B_n].$$

The nodes $\zeta_m^{(n)}(\kappa_n)$ of the n -point Szegő quadrature formula Q_n are the roots of $B_n = B_n(z, \kappa_n)$. Then it holds

$$Q_n[B_n] = Q_n[B_n(z, \kappa_n)] = \sum_{m=1}^n \lambda_m^{(n)}(\kappa_n) B_n(\zeta_m^{(n)}(\kappa_n), \kappa_n) = 0.$$

Thus,

$$I[z^n] = Q_n[z^n] + \frac{1}{1 + \overline{\delta_n \kappa_n}} I[B_n]. \tag{4}$$

On the other hand,

$$\frac{1}{z^n} \left(1 - \frac{B_n}{\delta_n + \kappa_n} \right) \in A_{-(n-1),0}, \quad n \geq 1.$$

Since $I[f] = Q_n[f]$, $f \in A_{-(n-1),n-1}$ we get

$$\begin{aligned} I \left[\frac{1}{z^n} - \frac{B_n}{(\delta_n + \kappa_n)z^n} \right] &= Q_n \left[\frac{1}{z^n} - \frac{B_n}{(\delta_n + \kappa_n)z^n} \right] \\ &= Q_n \left[\frac{1}{z^n} \right] - \frac{1}{\delta_n + \kappa_n} Q_n \left[\frac{B_n}{z^n} \right]. \end{aligned}$$

Again, since $B_n(\zeta_m^{(n)}(\kappa_n), \kappa_n) = 0$, one gets $Q_n[B_n/z^n] = 0$. Thus

$$I \left[\frac{1}{z^n} \right] = Q_n \left[\frac{1}{z^n} \right] + \frac{1}{\delta_n + \kappa_n} I \left[\frac{B_n}{z^n} \right]. \tag{5}$$

Observe that

$$I[B_n] = \langle B_n, 1 \rangle = \langle q_n, 1 \rangle + \kappa_n \langle q_n^*, 1 \rangle = \kappa_n \langle q_n, z^n \rangle. \tag{6}$$

The last equality follows from $\langle q_n, 1 \rangle = 0$ by orthogonality, and taking into account that $\langle q_n^*, 1 \rangle = \overline{\langle q_n, z^n \rangle} = \overline{\langle q_n, q_n \rangle} = \langle q_n, q_n \rangle = \langle q_n, z^n \rangle$. Furthermore,

$$I \left[\frac{B_n}{z^n} \right] = \langle B_n, z^n \rangle = \langle q_n, z^n \rangle + \kappa_n \langle q_n^*, z^n \rangle = \langle q_n, z^n \rangle. \tag{7}$$

The last equality follows from $\langle q_n^*, z^n \rangle = \overline{\langle q_n, 1 \rangle} = 0$.

From (4)–(7), one can write

$$(1 + \overline{\delta_n \kappa_n}) I[z^n] - \kappa_n (\delta_n + \kappa_n) I \left[\frac{1}{z^n} \right] = (1 + \overline{\delta_n \kappa_n}) Q_n[z^n] - \kappa_n (\delta_n + \kappa_n) Q_n \left[\frac{1}{z^n} \right].$$

Thus,

$$I \left[(1 + \overline{\delta_n \kappa_n}) z^n - \kappa_n (\delta_n + \kappa_n) \frac{1}{z^n} \right] = Q_n \left[(1 + \overline{\delta_n \kappa_n}) z^n - \kappa_n (\delta_n + \kappa_n) \frac{1}{z^n} \right],$$

or what is the same since $|\kappa_n| = 1$, $n \geq 1$,

$$I \left[\frac{z^n}{\delta_n + \kappa_n} - \frac{1}{(\overline{\delta_n + \kappa_n}) z^n} \right] = Q_n \left[\frac{z^n}{\delta_n + \kappa_n} - \frac{1}{(\overline{\delta_n + \kappa_n}) z^n} \right].$$

This means that the n -point Szegő quadrature formula with respect to the weight function ω and the parameter κ_n integrates correctly the Laurent polynomial $z^n/(\delta_n + \kappa_n) - 1/(\overline{\delta_n + \kappa_n})z^n$. Thus one has established the following

Theorem 2. Let Q_n be the n -point Szegő quadrature formula with respect to the weight function ω and the parameter κ_n as defined in Theorem 1. Then it holds that

$$Q_n[f] = I[f] \quad \text{for } f(z) = \frac{z^n}{\delta_n + \kappa_n} - \frac{1}{(\delta_n + \kappa_n)z^n}, \quad n \geq 1.$$

If we combine Theorems 1 and 2 we get the following

Corollary 1. Let Q_n be the n -point Szegő quadrature formula with respect to the weight function ω and the parameter κ_n as defined in Theorem 1. Then for $n \geq 1$ it holds that

$$Q_n[f] = I[f] \quad \text{for } f(z) = z^j, \quad -(n-1) \leq j \leq n-1 \quad \text{and} \quad f(z) = \frac{z^n}{\delta_n + \kappa_n} - \frac{1}{(\delta_n + \kappa_n)z^n}.$$

Remark 1. Let φ_n denote a not necessarily monic Szegő polynomial. Then φ_n, φ_n^* and $B_n(z, \kappa_n)$ are of the form

$$\begin{aligned} \varphi_n(z) &= \lambda_n z^n + \dots + \lambda_n \delta_n, \\ \varphi_n^*(z) &= \overline{\lambda_n} \delta_n z^n + \dots + \overline{\lambda_n}, \\ B_n(z, \kappa_n) &= \gamma_n (\varphi_n(z) + k_n \varphi_n^*(z)) \\ &= \gamma_n (\lambda_n + \overline{\lambda_n} \delta_n k_n) z^n + \dots + \gamma_n (\lambda_n \delta_n + \overline{\lambda_n} k_n), \end{aligned}$$

where $\gamma_n = 1/\lambda_n$ and $k_n = \kappa_n \lambda_n / \overline{\lambda_n}$. Thus the para-orthogonal polynomials may also be written in the form $b_n(z, k_n) = \gamma_n (\varphi_n(z) + k_n \varphi_n^*(z))$ with $|k_n| = 1$ and $\gamma_n \neq 0$.

Now consider a para-orthogonal polynomial of the form

$$b_n(z, k_n) = \varphi_n(z) + k_n \varphi_n^*(z) = (\lambda_n + \overline{\lambda_n} \delta_n k_n) z^n + \dots + (\lambda_n \delta_n + \overline{\lambda_n} k_n).$$

In the argument leading to Theorem 2 we find that

$$\begin{aligned} I[z^n] &= Q_n[z^n] + \frac{1}{\lambda_n + \overline{\lambda_n} \delta_n k_n} I[b_n], \\ I[1/z^n] &= Q_n[1/z^n] + \frac{1}{\lambda_n \delta_n + \overline{\lambda_n} k_n} I[b_n/z^n], \\ I[b_n] &= k_n \overline{\langle \varphi_n, z^n \rangle} = k_n \overline{\langle \varphi_n, \varphi_n \rangle} / \lambda_n = k_n \langle \varphi_n, \varphi_n \rangle / \lambda_n, \\ I[b_n/z^n] &= \langle \varphi_n, z^n \rangle = \langle \varphi_n, \varphi_n \rangle / \overline{\lambda_n}. \end{aligned}$$

Hence

$$\begin{aligned} I[(\lambda_n + \overline{\lambda_n} \delta_n k_n) \lambda_n \overline{k_n} z^n - (\lambda_n \delta_n + \overline{\lambda_n} k_n) \overline{\lambda_n} / z^n] \\ = Q_n[(\lambda_n + \overline{\lambda_n} \delta_n k_n) \lambda_n \overline{k_n} z^n - (\lambda_n \delta_n + \overline{\lambda_n} k_n) \overline{\lambda_n} / z^n], \end{aligned}$$

or equivalently

$$I[z^n - \eta_n / z^n] = Q_n[z^n - \eta_n / z^n],$$

where

$$\eta_n = \frac{\lambda_n \delta_n + \overline{\lambda_n} k_n \overline{\lambda_n}}{\lambda_n \delta_n + \overline{\lambda_n} k_n} \overline{\lambda_n}.$$

We note that $b_n(0, k_n) = \lambda_n \delta_n + \overline{\lambda_n} k_n$, and thus

$$\eta_n = \frac{b_n(0, k_n) \overline{\lambda_n}}{b_n(0, k_n) \lambda_n}.$$

In particular

$$\eta_n = \frac{b_n(0, k_n)}{b_n(0, k_n)}$$

when φ_n is the monic polynomial q_n .

In the following example, we illustrate Theorem 2.

Example 1. Consider the Poisson weight function $\omega(t)$ given by

$$\omega(t) = \frac{1 - r^2}{1 - 2r \cos(t) + r^2}, \quad -\pi \leq t \leq \pi, \quad 0 \leq r < 1.$$

The moments $\mu_k = I[z^k] = \int_{-\pi}^{\pi} e^{ikt} \omega(t) dt$ are given by $\mu_k = 2\pi r^{|k|}$, $k = 0, \pm 1, \pm 2, \dots$. The corresponding monic orthogonal polynomials $q_n(z)$ are given by $q_0(z) = 1$, $q_n(z) = z^n - rz^{n-1}$, $n \geq 1$, see [8]. Hence the para-orthogonal polynomials $B_n(z)$ are given by $B_n(z) = B_n(z, \kappa_n) = q_n(z) + \kappa_n q_n^*(z) = z^n - rz^{n-1} + \kappa_n(1 - rz)$, $n \geq 1$. Observe that the reflection coefficients $\delta_n = q_n(0)$ are given by $\delta_1 = -r$, and $\delta_n = 0$, $n \geq 2$. Thus, for $n \geq 1$,

$$I \left[\frac{z^n}{\delta_n + \kappa_n} - \frac{1}{(\delta_n + \kappa_n)z^n} \right] = 2\pi r^n \left(\frac{1}{\delta_n + \kappa_n} - \frac{1}{\overline{\delta_n + \kappa_n}} \right). \tag{8}$$

On the other hand, since the nodes of the n -point Szegő quadrature Q_n are the zeros the para-orthogonal polynomial $B_n(z)$ we get $Q_n[B_n(z)] = Q_n[z^n - rz^{n-1} + \kappa_n(1 - rz)] = 0$. Thus $Q_n[z^n] = Q_n[rz^{n-1} - \kappa_n(1 - rz)]$. Taking into account that $Q_n[f] = I[f]$ for $f(z) = z^j$, $-(n - 1) \leq j \leq n - 1$, see Theorem 1, we deduce for $n \geq 2$ that

$$Q_n[z^n] = Q_n[rz^{n-1} - \kappa_n(1 - rz)] = 2\pi(r^n - \kappa_n(1 - r^2)).$$

Furthermore, from Theorem 1 and after some calculations one gets that for the Poisson weight function

$$Q_1[f] = 2\pi f \left(\frac{r - \kappa_1}{1 - \kappa_1 r} \right).$$

Thus, $Q_1[z] = 2\pi(r - \kappa_1)/(1 - \kappa_1 r)$.

Note that $Q_n[1/z^n] = \overline{Q_n[z^n]}$, $n \geq 1$, since the coefficients of the Szegő quadrature formula are positive and the nodes lie on the unit circle. Thus, for $n \geq 1$, (recall that $\delta_n = 0$, $n \geq 2$)

$$\begin{aligned} Q_n \left[\frac{z^n}{\delta_n + \kappa_n} - \frac{1}{(\delta_n + \kappa_n)z^n} \right] &= \frac{1}{\delta_n + \kappa_n} Q_n[z^n] - \frac{1}{\overline{\delta_n + \kappa_n}} \overline{Q_n[z^n]} \\ &= 2\pi r^n \left(\frac{1}{\delta_n + \kappa_n} - \frac{1}{\overline{\delta_n + \kappa_n}} \right). \end{aligned} \tag{9}$$

Thus, from (8) and (9) we deduce

$$I \left[\frac{z^n}{\delta_n + \kappa_n} - \frac{1}{(\delta_n + \kappa_n)z^n} \right] = Q_n \left[\frac{z^n}{\delta_n + \kappa_n} - \frac{1}{(\delta_n + \kappa_n)z^n} \right], \quad n \geq 1,$$

which confirms Theorem 2.

3. Application to the construction of Szegő quadrature

The n -point classical Gauss quadrature formula $Q_n[f] = \sum_{j=1}^n A_j f(x_j)$, for the approximation of integrals on the real line $I[f] = \int_a^b f(x)\omega(x) dx$, where $\omega(x)$ is a weight function on $x \in [a, b]$, depends on $2n$ parameters, the n coefficients A_j and the n nodes x_j , $j = 1, 2, \dots, n$. As is well known, classical Gauss quadrature formulas integrates correctly every algebraic polynomials of degree $\leq 2n - 1$. So, if the $2n$ parameters, the nodes and the coefficients, are considered as unknowns then they can be determined by moment fitting, that is, by solving the non-linear system $I[f] = Q_n[f]$, $f = 1, x, \dots, x^{2n-1}$ of $2n$ equations. See [2, section 2.7.2] for this algebraic approach to classical Gauss quadrature formulas.

Similarly, the n -point Szegő quadrature formula (3) for the approximation of integrals over the unit circle depends on $2n$ parameters, the n coefficients and the n nodes. So, if they are considered as unknowns and if the reflection coefficient δ_n is known, then one can compute the n -point Szegő quadrature formula with respect to a given weight function ω and parameter κ_n by moment fitting using Corollary 1, that is, by solving the non-linear and non-algebraic system of $2n$ equations with $2n$ unknowns given by

$$Q_n[f] = I[f], \quad f(z) = z^j, \quad -(n-1) \leq j \leq n-1, \quad f(z) = \frac{z^n}{\delta_n + \kappa_n} - \frac{1}{(\delta_n + \kappa_n)z^n}.$$

Example 2. Consider the Jacobi weight function $\omega(t)$ on the unit circle given by

$$\omega(t) = |e^{it} - 1|^{2\gamma_1} |e^{it} + 1|^{2\gamma_2}, \quad t \in [-\pi, \pi], \quad \gamma_1, \gamma_2 > \frac{1}{2}.$$

It is known, see [4], that the reflection coefficients are given by $\delta_n = (\gamma_1 + (-1)^n \gamma_2) / (n + \gamma_1 + \gamma_2)$.

We take as example $\gamma_1 = 1$, $\gamma_2 = 2$, and $n = 2$. Then $\delta_2 = \frac{3}{5}$.

It holds that $I[1] = 8\pi$, $I[z] = I[1/z] = 2\pi$, and $I[z^2] = I[1/z^2] = -4\pi$.

Consider the construction of the 2-point Szegő quadrature formula $Q_2[f]$,

$$I[f] = \int_{-\pi}^{\pi} f(e^{it})\omega(t) dt \doteq Q_2[f] = \sum_{m=1}^2 \lambda_m^{(2)}(\kappa_2) f(\zeta_m^{(2)}(\kappa_2))$$

with respect to the particular Jacobi weight function considered and the parameter $\kappa_2 = i$, the imaginary unity.

Let $\lambda_m = \lambda_m^{(2)}(\kappa_2)$ and $z_m = \zeta_m^{(2)}(\kappa_2)$, $m = 1, 2$. In order to determine the nodes z_1, z_2 , and the coefficients λ_1, λ_2 , we require that

$$Q_2[f] = I[f] \quad \text{for } f(z) = 1, z, \frac{1}{z}, \quad \frac{z^2}{\delta_2 + \kappa_2} - \frac{1}{(\delta_2 + \kappa_2)z^2}.$$

Then, we obtain the following system of non-linear and non-algebraic equations

$$\lambda_1 + \lambda_2 = I[1],$$

$$\lambda_1 z_1 + \lambda_2 z_2 = I[z],$$

$$\lambda_1 \frac{1}{z_1} + \lambda_2 \frac{1}{z_2} = I\left[\frac{1}{z}\right],$$

$$\lambda_1 \left(\frac{z_1^2}{\delta_2 + \kappa_2} - \frac{1}{(\delta_2 + \kappa_2)z_1^2} \right) + \lambda_2 \left(\frac{z_2^2}{\delta_2 + \kappa_2} - \frac{1}{(\delta_2 + \kappa_2)z_2^2} \right) = I\left[\frac{z^2}{\delta_2 + \kappa_2} - \frac{1}{(\delta_2 + \kappa_2)z^2} \right].$$

The command *solve* of Maple gives two solutions

$$\lambda_1 \doteq 11.780972450961724644,$$

$$\lambda_2 \doteq 13.351768777756621264,$$

$$z_1 \doteq i,$$

$$z_2 \doteq 0.47058823529411764706 - 0.88235294117647058824i,$$

and

$$\begin{aligned} \lambda_1 &\doteq 10.309383824786804833, \\ \lambda_2 &\doteq 14.823357403931541074, \\ z_1 &\doteq -0.57097054535375274026 - 0.82097054535375274026i, \\ z_2 &\doteq 0.82097054535375274026 + 0.57097054535375274026i. \end{aligned} \tag{11}$$

The solution of the system given by Eq. (10) gives the nodes and weights for the considered 2-point Szegő quadrature formula $Q_2[f]$ corresponding to the parameter $\kappa_2 = i$. Indeed, observe that the value of the para-orthogonal polynomials $B_n(z, \kappa_n) = \varrho_n(z) + \kappa_n \varrho_n^*(z) = (-1)^n (1 + \kappa_n \overline{\delta_n}) \prod_{i=1}^n (z - z_i)$, at zero, admits the expressions $\delta_n + \kappa_n$ and $(-1)^n (1 + \kappa_n \overline{\delta_n}) \prod_{i=1}^n z_i$. For the solution given by Eq. (10) both values are equal. For the solution given by Eq. (11) they are different. The solution in Eq. (11) gives the weights and the nodes of the 2-point Szegő quadrature formula corresponding to $\kappa_2 \doteq -0.88235294117647058824 - 0.47058823529411764706i$.

Observe that in the case that the reflection coefficient δ_n is not known, one can still compute the n -point Szegő quadrature formula by moment fitting, if δ_n is real and one takes $\kappa_n = 1$ or $\kappa_n = -1$. Indeed, in such a case, the function $f(z) = z^n / (\delta_n + \kappa_n) - 1 / (\overline{\delta_n} + \kappa_n z^n)$ can be replaced by $f(z) = z^n - 1 / z^n$.

Note that for a given weight function $\omega(t)$, if its moments $\int_{-\pi}^{\pi} e^{ikt} \omega(t) dt$, $k = 0, \pm 1, \pm 2, \dots$, are real then the coefficients of the orthogonal polynomials $\varrho_n(z)$ are real, so, in particular, the reflection coefficient $\delta_n = \varrho_n(0)$ is real, $n = 1, 2, \dots$.

Alternatively, we do not need to know the value of the reflection coefficients δ_n to compute the n -point Szegő quadrature formula. Indeed, one can compute the n -point Szegő quadrature formula with respect to the weight function ω and parameter κ_n ,

$$Q_n[f] = \sum_{m=1}^n \lambda_m^{(n)}(\kappa_n) f(\zeta_m^{(n)}(\kappa_n)) \doteq I[f] = \int_{-\pi}^{\pi} f(e^{it}) \omega(t) dt$$

by solving two algebraic systems of linear equations. The para-orthogonal polynomials satisfy the following orthogonality equations, see [5],

$$\langle B_n, z^k \rangle = 0, \quad k = 1, 2, \dots, n - 1, \quad n \geq 2.$$

Next, we obtain an additional orthogonality equation for the para-orthogonal polynomials. Indeed, it holds

$$I \left[B_n(z, \kappa_n) \left(\frac{1}{z^n} - \overline{\kappa_n} \right) \right] = I \left[\frac{B_n(z, \kappa_n)}{z^n} \right] - \overline{\kappa_n} I [B_n(z, \kappa_n)].$$

From (6) and (7) one can write

$$I \left[B_n(z, \kappa_n) \left(\frac{1}{z^n} - \overline{\kappa_n} \right) \right] = \langle \varrho_n, z^n \rangle (1 - \overline{\kappa_n} \kappa_n).$$

Since the expression in brackets is equal to zero ($|\kappa_n| = 1, n \geq 1$) we get

$$I \left[B_n(z, \kappa_n) \left(\frac{1}{z^n} - \overline{\kappa_n} \right) \right] = 0,$$

or what is the same

$$\langle B_n, z^n - \kappa_n \rangle = 0.$$

Thus one can establish the following

Theorem 3. *Let the para-orthogonal polynomials $B_n(z, \kappa_n)$, $\kappa_n \in \mathbb{C}$, $|\kappa_n| = 1, n \geq 1$, be defined as in Theorem 1. Then, they satisfy*

$$\langle B_n, z^k \rangle = 0, \quad k = 1, \dots, n - 1 \quad \text{and} \quad \langle B_n, z^n - \kappa_n \rangle = 0, \quad n \geq 2.$$

Hence, from Theorem 3 we get a linear system of n equations with n unknowns, the coefficients c_0, c_1, \dots, c_{n-1} of the n th monic para-orthogonal polynomial $B_n(z, \kappa_n) = c_0 + c_1z + c_2z^2 + \dots + c_{n-1}z^{n-1} + z^n$. This linear system takes the form

$$\begin{array}{cccccc}
 m_{-1}c_0 + & m_0c_1 + & \cdots + & m_{n-2}c_{n-1} + & m_{n-1} & = & 0 \\
 m_{-2}c_0 + & m_{-1}c_1 + & \cdots + & m_{n-3}c_{n-1} + & m_{n-2} & = & 0 \\
 \vdots & \vdots & \ddots & \vdots & \vdots & & \vdots \\
 m_{-(n-1)}c_0 + & m_{-(n-2)}c_1 + & \cdots + & m_0c_{n-1} + & m_1 & = & 0 \\
 d_0c_0 + & d_1c_1 + & \cdots + & d_{n-1}c_{n-1} + & d_n & = & 0
 \end{array} \tag{12}$$

where

$$m_k = \int_{-\pi}^{\pi} e^{ikt} \omega(t) dt, \quad -n \leq k \leq n \quad \text{and} \quad d_j = m_{-n+j} - m_j \overline{\kappa_n}, \quad 0 \leq j \leq n. \tag{13}$$

Recall, see Theorem 1, that the nodes $\zeta_m^{(n)}(\kappa_n)$, $1 \leq m \leq n$, of the n -point Szegő quadrature formula with respect to a weight function ω and parameter κ_n are the zeros of $B_n(z, \kappa_n)$.

Once the nodes are computed, one can compute the weights $\lambda_m^{(n)}(\kappa_n)$, $1 \leq m \leq n$, by solving the linear system

$$Q_n[z^j] = I[z^j], \quad 0 \leq j \leq n - 1. \tag{14}$$

As illustration of the computation of the Szegő quadrature formula through the resolution of the two linear systems (12) and (14) we give the next example.

Example 3. We compute again the $n = 2$ points Szegő quadrature formula

$$Q_2[f] = \sum_{m=1}^2 \lambda_m^{(2)}(\kappa_2) f(\zeta_m^{(2)}(\kappa_2)) \doteq I[f] = \int_{-\pi}^{\pi} f(e^{it}) \omega(t) dt$$

for the Jacobi weight function

$$\omega(t) = |e^{it} - 1|^2 |e^{it} + 1|^4, \quad t \in [-\pi, \pi], \tag{15}$$

considered in Example 2.

Recall from Example 2 that $m_0 = I[1] = 8\pi$, $m_1 = I[z] = 2\pi$, $m_{-1} = I[1/z] = 2\pi$, $m_2 = I[z^2] = -4\pi$, $m_{-2} = I[1/z^2] = -4\pi$, and $\kappa_2 = i$. (The value of the reflection coefficient δ_2 is not used now.)

We first determine the coefficients c_0 and c_1 of the monic para-orthogonal polynomial $B_2(z, \kappa_2) = z^2 + c_1z + c_0$ by solving the linear system (12) for this particular case, which takes the form

$$\begin{aligned}
 m_{-1}c_0 + m_0c_1 + m_1 &= 0, \\
 d_0c_0 + d_1c_1 + d_2 &= 0,
 \end{aligned}$$

where

$$d_j = m_{-2+j} + im_j, \quad 0 \leq j \leq 2.$$

The solution of this linear system is given by $c_0 = \frac{15}{17} + \frac{8}{17}i$ and $c_1 = -\frac{8}{17} - \frac{2}{17}i$.

Thus,

$$B_2(z, \kappa_2) = z^2 + c_1z + c_0 = z^2 - \left(\frac{8}{17} + \frac{2}{17}i \right) z + \frac{15}{17} + \frac{8}{17}i.$$

The nodes $z_m = \zeta_m^{(2)}(\kappa_2)$, $m = 1, 2$ are the zeros of $B_2(z, \kappa_2)$. Hence,

$$z_1 = i,$$

$$z_2 = \frac{8}{17} - \frac{15}{17}i \doteq 0.47058823529411764706 - 0.88235294117647058824i.$$

Once we have computed the nodes, we can compute the weights $\lambda_m = \lambda_m^{(2)}(\kappa_2)$, $m = 1, 2$ by solving the linear system (14) for this particular case, which takes the form

$$\lambda_1 + \lambda_2 = m_0,$$

$$z_1\lambda_1 + z_2\lambda_2 = m_1.$$

The solution is given by

$$\lambda_1 = \frac{15}{4}\pi \doteq 11.780972450961724644,$$

$$\lambda_2 = \frac{17}{4}\pi \doteq 13.351768777756621264.$$

So, we have completely determined again the 2-point Szegő quadrature formula for the particular Jacobi weight function (15) and the parameter $\kappa_2 = i$.

The computation of the para-orthogonal polynomials by means of the linear system (12) is a competitive way to compute them under certain conditions. In the following we compare with other frequently used methods for the computation of the para-orthogonal polynomials.

A well-known procedure to obtain the para-orthogonal polynomial $B_n(z, \kappa_n)$ is based on the computation of the monic orthogonal polynomial $q_n(z) = z^n + a_{n-1}^{(n)}z^{n-1} + \dots + a_1^{(n)}z + a_0^{(n)}$ by solving the linear system of equations

$$\sum_{j=0}^{n-1} a_j^{(n)} m_{-k+j} = -m_{-k+n}, \quad k = 0, 1, \dots, n - 1, \tag{16}$$

obtained from,

$$\langle q_n, z^k \rangle = 0, \quad k = 0, 1, \dots, n - 1,$$

and then compute the para-orthogonal polynomial by its definition $B_n(z, \kappa_n) = q_n(z) + \kappa_n q_n^*(z)$.

If the reflection coefficient $\delta_n = q_n(0) = a_0^{(n)}$ is known then one can skip one equation in the linear system (16). In order to retain as much as possible the valuable properties of the coefficient matrix in (16), the equation corresponding to $k = 0$ is skipped. So one obtains the linear system

$$\sum_{j=1}^{n-1} a_j^{(n)} m_{-k+j} = -m_{-k+n} - a_0^{(n)} m_{-k}, \quad k = 1, 2, \dots, n - 1. \tag{17}$$

On the other hand, if the reflection coefficient $\delta_n = q_n(0) = a_0^{(n)}$ is known then the coefficient $c_0^{(n)}$ of the monic para-orthogonal polynomial $B_n(z, \kappa_n) = q_n(z) + \kappa_n q_n^*(z) = z^n + c_{n-1}z^{n-1} + \dots + c_1z + c_0 = z^n + c_{n-1}^{(n)}z^{n-1} + \dots + c_1^{(n)}z + c_0^{(n)}$ is also known since $c_0^{(n)} = (\delta_n + \kappa_n)/(1 + \kappa_n \overline{\delta_n})$. Hence, one can skip one equation in the linear system (12). If the last equation is skipped, the system

$$\sum_{j=1}^{n-1} c_j^{(n)} m_{-k+j} = -m_{-k+n} - c_0^{(n)} m_{-k}, \quad k = 1, 2, \dots, n - 1 \tag{18}$$

is obtained.

The coefficient matrix of the linear systems (17) and (18) is the same. It is a Toeplitz and positive definite matrix. Furthermore, it is also a symmetric matrix if the moments are real. A numerical method for solving real positive definite Toeplitz systems is given in [1]. This method requires $O(n \log_2^2(n))$ arithmetic operations. See also [3,7].

Observe that with the objective of computing the para-orthogonal polynomial $B_n(z, \kappa_n)$, monic or not, the solution of the linear system (18), based on the linear system (12), uses at least an order of $O(2n)$ arithmetic operations less than the procedure composed of the solution of the linear system (17) to compute the orthogonal polynomial $q_n(z)$ and then the computation of the para-orthogonal polynomial through $q_n(z) + \kappa_n q_n^*(z)$. This is due precisely to the need of the computation of this last expression that defines the para-orthogonal polynomials. The difference in the number of arithmetic operations can be greater, of order $O(3n)$. Indeed, this holds in the particular case that δ_n is real and κ_n takes the frequently encountered value $\kappa_n = 1$ or -1 since then $c_0^{(n)} = 1$ or -1 , respectively, and hence the computation of the right-hand side of (18) needs only $O(n)$ arithmetic operations previous to the solution but the computation of the right-hand side of (17) needs $O(2n)$ arithmetic operations.

We compare next with another usual method to compute the orthogonal polynomials, and hence the para-orthogonal polynomials through $q_n(z) + \kappa_n q_n^*(z)$. It is well known that the monic orthogonal polynomials satisfy the recurrence relation, see [6, Theorem 11.4.2],

$$q_0(z) = 1, \quad q_n(z) = zq_{n-1}(z) + \delta_n q_{n-1}^*(z), \quad n = 1, 2, \dots \quad (19)$$

From this recurrence, the reflection coefficients can be computed by

$$\delta_k = -\frac{\langle zq_{k-1}, 1 \rangle}{\langle q_{k-1}^*, 1 \rangle}, \quad k = 1, 2, \dots$$

(So, computing both expressions appropriately one can generate the sequence of monic orthogonal polynomials.) Observe that under the assumption that the reflection coefficients are known then solely the recurrence (19) completely serves as a method for the computation of the orthogonal polynomials. The order of arithmetic operations needed to compute the n th orthogonal polynomial $q_n(z)$ is $O(n^2)$. Hence, also the order of arithmetic operations to compute the para-orthogonal polynomial $B_n(z, \kappa_n)$ is $O(n^2)$. This is a greater order than the method proposed above based on the solution of the linear system (18) obtained from (12) for the case of real moments. Observe that (19) computes the sequence $q_1(z), q_2(z), \dots, q_n(z)$ and then one computes $B_n(z, \kappa_n)$ and not only $B_n(z, \kappa_n)$ directly as in (18).

References

- [1] G. Ammar, W.B. Gragg, Superfast solution of real positive definite Toeplitz systems, *SIAM J. Matrix Anal. Appl.* 9 (1988) 61–76.
- [2] P.J. Davis, P. Rabinowitz, *Methods of Numerical Integration*, second ed., Academic Press, New York, 1984.
- [3] D.J. Evans, G. Okša, Parallel solution of symmetric positive definite Toeplitz systems, *Parallel Algorithms Appl.* 12 (4) (1997) 297–303.
- [4] B.L. Golinskii, On asymptotic behavior of the prediction error, *Teor. Veroyatnost. Primenen* 19 (4) (1974) 724–739.
- [5] W.B. Jones, O. Njåstad, W.J. Thron, Moment theory, orthogonal polynomials, quadrature, and continued fractions associated with the unit circle, *Bull. London Math. Soc.* 21 (1989) 113–152.
- [6] G. Szegő, *Orthogonal Polynomials*, American Mathematical Society, fourth ed., vol. 23, Colloquium Publications, 1978.
- [7] M. Van Barel, G. Heinig, P. Kravanja, A stabilized superfast solver for nonsymmetric Toeplitz systems, *SIAM J. Matrix Anal. Appl.* 23 (2) (2001) 494–510.
- [8] H. Waadeland, A Szegő quadrature formula for the Poisson formula, in: C. Brezinski, U. Kulish (Eds.), *Computations and Applied Mathematics*, vol. I, 1992 IMACS, Elsevier, North-Holland, Amsterdam, pp. 479–486.