

Szegő–Lobatto quadrature rules

Carl Jagels^{a,*}, Lothar Reichel^{b,1}

^a*Department of Mathematics and Computer Science, Hanover College, Hanover, IN 47243, USA*

^b*Department of Mathematical Sciences, Kent State University, Kent, OH 44242, USA*

Received 16 September 2005; received in revised form 11 December 2005

Dedicated to Ed Saff on the occasion of his 60th birthday

Abstract

Gauss-type quadrature rules with one or two prescribed nodes are well known and are commonly referred to as Gauss–Radau and Gauss–Lobatto quadrature rules, respectively. Efficient algorithms are available for their computation. Szegő quadrature rules are analogs of Gauss quadrature rules for the integration of periodic functions; they integrate exactly trigonometric polynomials of as high degree as possible. Szegő quadrature rules have a free parameter, which can be used to prescribe one node. This paper discusses an analog of Gauss–Lobatto rules, i.e., Szegő quadrature rules with two prescribed nodes. We refer to these rules as Szegő–Lobatto rules. Their properties as well as numerical methods for their computation are discussed.

© 2006 Elsevier B.V. All rights reserved.

Keywords: Gauss–Szegő quadrature rule; Lobatto rule; Periodic function; Szegő polynomial; Szegő quadrature rule

1. Introduction

Let dw be a non-negative measure with infinitely many points of increase on the interval $[-\pi, \pi]$ and such that all moments

$$\mu_k := \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{ikt} dw(t), \quad k = 0, \pm 1, \pm 2, \dots,$$

exist, where $i := \sqrt{-1}$. For notational convenience, we assume that dw is scaled so that $\mu_0 = 1$. The present paper is concerned with the approximation of integrals of the form

$$I(f) := \frac{1}{2\pi} \int_{-\pi}^{\pi} f(e^{it}) dw(t)$$

*Corresponding author.

E-mail addresses: jagels@hanover.edu (C. Jagels), reichel@math.kent.edu (L. Reichel).

¹Research supported in part by NSF grant DMS-0107858.

by quadrature rules

$$S^{(n+2)}(f) = \sum_{k=1}^{n+2} w_k^{(n+2)} f(\lambda_k^{(n+2)}), \quad (1)$$

with weights $w_k^{(n+2)} > 0$ and nodes $\lambda_k^{(n+2)}$ on the unit circle. Let $\mathcal{A}_{-n-1, n+1}$ denote the set of Laurent polynomials

$$L_{n+1}(z) = \sum_{k=-n-1}^{n+1} c_k z^k, \quad c_k \in \mathbb{C},$$

of degree at most $n+1$. The nodes and weights of Szegő quadrature rules are determined so that they integrate exactly Laurent polynomials of as high degree as possible. The characterizing property of $(n+2)$ -point Szegő quadrature rules is that

$$S^{(n+2)}(p) = I(p), \quad \forall p \in \mathcal{A}_{-n-1, n+1}, \quad (2)$$

see, e.g., Gragg [10], Grenander and Szegő [14, Chapter 4], and Jones et al. [17] for discussions on properties of Szegő quadrature rules. We remark that Laurent polynomials on the unit circle can be identified with trigonometric polynomials on the interval $[-\pi, \pi]$. Hence, Eq. (2) expresses that $(n+2)$ -point Szegő quadrature rules integrate all trigonometric polynomials of degree at most $n+1$ exactly. They are therefore well suited for the integration of periodic functions.

Szegő quadrature rules are sometimes referred to as Gauss–Szegő quadrature rules, because they are analogs of Gauss rules for the integration of 2π -periodic functions. Several modifications of Gauss rules are available, such as Gauss–Radau rules (in which one node is fixed at an end point of the convex hull of the support of the measure) and Gauss–Lobatto rules (in which two nodes are fixed at the end points of the convex hull of the support of the measure); see Gautschi [8,9] for recent discussions of these Gauss-type quadrature rules.

The present paper discusses modifications of Szegő rules in which one or two nodes are fixed on the unit circle. We refer to these quadrature rules as Szegő–Radau and Szegő–Lobatto rules, respectively. Szegő–Radau rules are Szegő rules with an auxiliary parameter chosen so that one of the nodes is at a desired location on the unit circle. Szegő–Lobatto rules are believed to be new.

This paper is organized as follows. Section 2 introduces Szegő polynomials and discusses the computation of Szegő and Szegő–Radau quadrature rules. Section 3 describes Szegő–Lobatto rules for general non-negative measures dw and discusses their computation. The special case when the measure is symmetric about zero is addressed in Section 4. In this case, the nodes are either real or appear in complex conjugate pairs. Szegő–Radau and Szegő–Lobatto rules for a symmetric measure with the fixed nodes in the set $\{\pm 1\}$ have recently been considered by Bultheel et al. [3]. Section 5 describes a few computed examples, and Section 6 contains concluding remarks.

We note that the development of extensions of Szegő quadrature rules and the investigation of the connection between Szegő rules and Gauss quadrature rules on the interval $[-1, 1]$ are active areas of research; see, e.g., Bultheel et al. [3,4], Cruz-Barroso et al. [5,6], and Daruis et al. [7].

2. Szegő quadrature rules

Introduce the inner product

$$(f, g) := \frac{1}{2\pi} \int_{-\pi}^{\pi} \overline{f(e^{it})} g(e^{it}) dw(t),$$

where the bar denotes complex conjugation. Polynomials orthogonal with respect to this inner product are known as Szegő polynomials. The monic Szegő polynomials satisfy recursion relations of the form

$$\phi_{j+1}(z) = z\phi_j(z) + \gamma_{j+1}\phi_j^*(z), \quad j = 0, 1, 2, \dots, \quad (3)$$

$$\phi_{j+1}^*(z) = \bar{\gamma}_{j+1}z\phi_j(z) + \phi_j^*(z), \quad j = 0, 1, 2, \dots, \quad (4)$$

with $\phi_0(z) = \phi_0^*(z) = 1$. The positivity of the measure dw implies that the recursion coefficients $\gamma_{j+1} \in \mathbb{C}$ are of magnitude strictly smaller than one, and so are the zeros of the Szegő polynomials; see, e.g., Gragg [10], Grenander and Szegő [14, Chapters 2–3], Jones et al. [17], and Saff [20] for properties of Szegő polynomials. For future reference, we note that the *reverse polynomials* $\phi_j^*(z)$ satisfy

$$\phi_j^*(z) = z^j \overline{\phi_j(1/z)}, \quad j = 0, 1, 2, \dots \quad (5)$$

Gragg [10] shows that the eigenvalues of the $(n+2) \times (n+2)$ upper Hessenberg matrix

$$H_{n+2}(\tau) := D_{n+2}^{-1/2} \begin{bmatrix} -\bar{\gamma}_0 \gamma_1 & -\bar{\gamma}_0 \gamma_2 & \cdots & -\bar{\gamma}_0 \gamma_{n+1} & -\bar{\gamma}_0 \tau \\ \sigma_1^2 & -\bar{\gamma}_1 \gamma_2 & \cdots & -\bar{\gamma}_1 \gamma_{n+1} & -\bar{\gamma}_1 \tau \\ & \sigma_2^2 & \cdots & -\bar{\gamma}_2 \gamma_{n+1} & -\bar{\gamma}_2 \tau \\ & & \ddots & \vdots & \vdots \\ 0 & & & \sigma_{n+1}^2 & -\bar{\gamma}_{n+1} \tau \end{bmatrix} D_{n+2}^{1/2} \quad (6)$$

are the zeros of the polynomial

$$\phi_{n+2}(\tau, z) := \phi_{n+2}(z) + \tau \phi_{n+2}^*(z), \quad (7)$$

where $\sigma_k := \sqrt{1 - |\gamma_k|^2}$, $\gamma_0 := 1$ and

$$D_{n+2} = \text{diag}[\delta_0, \delta_1, \delta_2, \dots, \delta_{n+1}] \in \mathbb{R}^{(n+2) \times (n+2)},$$

with $\delta_0 := 1$, $\delta_k := \delta_{k-1} \sigma_k^2$, $k = 1, 2, \dots, n+1$, and $\tau \in \mathbb{C}$ is a parameter. Jones et al. [17] refer to the sequence of polynomials $\phi_k(\tau, z)$, $k = 0, 1, 2, \dots$, as a family of para-orthogonal polynomials. For clarity, we will sometimes refer to the matrix $H_{n+2}(\tau)$ as $H_{n+2}(\gamma_1, \dots, \gamma_{n+1}, \tau)$.

It is easy to see that when $|\tau| = 1$, the zeros of $\phi_{n+2}(\tau, z)$ are the zeros of $\phi_{n+2}(z) = z\phi_{n+1}(z) + \gamma_{n+2}\phi_{n+1}^*(z)$ for $\gamma_{n+2} = \tau$. Substituting the recursion relations (3) and (4) with $\gamma_{n+2} = \tau$ into (7) yields

$$\phi_{n+2}(\tau, z) = z\phi_{n+1}(z) + \tau\phi_{n+1}^*(z) + \tau(\bar{\tau}z\phi_{n+1}(z) + \phi_{n+1}^*(z)) = 2(z\phi_{n+1}(z) + \tau\phi_{n+1}^*(z)).$$

We will use this property below.

Let the recursion coefficients $\gamma_1, \gamma_2, \dots, \gamma_{n+1}$ be fixed. The properties of the matrix (6) and its eigenvalues depend on the choice of the parameter τ . When $\tau = \gamma_{n+2}$, the eigenvalues of $H_{n+2}(\tau)$ are the zeros of $\phi_{n+2}(z)$. These could be of the highest possible multiplicity. We are interested in the case when $|\tau| = 1$. Then $H_{n+1}(\tau)$ is an unreduced unitary upper Hessenberg matrix; its eigenvalues therefore are distinct and of unit magnitude. The eigenvalues are nodes $\{\lambda_k^{(n+2)}\}_{k=1}^{n+2}$ of a Szegő rule (1) and the square of the first component of the eigenvector of unit length associated with $\lambda_k^{(n+2)}$ yields the weight $w_k^{(n+2)}$, where we recall that $\mu_0 = 1$; see Gragg [10] for details. The application of pairs of Szegő quadrature rules associated with different values of τ on the unit circle is discussed in [19].

Gragg [10] observed that the matrix (6) can be expressed as a product of elementary Givens matrices

$$H_{n+2}(\tau) = G_1(\gamma_1)G_2(\gamma_2) \cdots G_{n+1}(\gamma_{n+1})\hat{G}_{n+2}(\tau). \quad (8)$$

Here

$$G_j(\gamma_j) := \begin{bmatrix} I_{j-1} & & & \\ & -\gamma_j & \sigma_j & \\ & \sigma_j & \bar{\gamma}_j & \\ & & & I_{n-j-1} \end{bmatrix} \in \mathbb{C}^{(n+2) \times (n+2)}, \quad j = 1, 2, \dots, n+1,$$

and

$$\hat{G}_{n+2}(\tau) := \text{diag}[1, 1, \dots, 1, -\tau].$$

The representation (8) is the basis for several fast algorithms for the computation of nodes and weights of Szegő quadrature rules; see Gragg [11,12] and Stewart [21,22] for QR-algorithms and their properties, and Ammar et al. [2], Gragg and Reichel [13], and Gu et al. [15] for divide-and conquer methods.

It is easy to choose $\tau \in \mathbb{C}$ of unit magnitude so that the Szegő rule has a node at a particular point, say z_α , on the unit circle. It follows from (3) that

$$\tau := -z_\alpha \frac{\phi_{n+1}(z_\alpha)}{\phi_{n+1}^*(z_\alpha)} \quad (9)$$

yields an $(n+2)$ -point Szegő quadrature rule with a node at z_α . We obtain from (5) that

$$\phi_{n+1}^*(z_\alpha) = z_\alpha^{n+1} \overline{\phi_{n+1}(z_\alpha)}, \quad (10)$$

and therefore the parameter τ determined by (9) is, indeed, unimodular. Thus, the $(n+2)$ -point Szegő quadrature rule with τ determined by (9) is a Szegő–Radau rule with a node at z_α .

In order to determine Szegő–Lobatto rules with nodes at the distinct points z_α and z_β on the unit circle, we replace the last two recursion coefficients parameters γ_{n+1} and γ_{n+2} by $\tilde{\gamma}_{n+1}$ and $\tilde{\gamma}_{n+2}$, respectively, where $|\tilde{\gamma}_{n+2}| = 1$. Thus, $\tilde{\gamma}_{n+1}$ and $\tilde{\gamma}_{n+2}$ are to be chosen so that z_α and z_β are zeros of the polynomial

$$\tilde{\phi}_{n+2}(z) := z\tilde{\phi}_{n+1}(z) + \tilde{\gamma}_{n+2}\tilde{\phi}_{n+1}^*(z), \quad (11)$$

where

$$\tilde{\phi}_{n+1}(z) := z\phi_n(z) + \tilde{\gamma}_{n+1}\phi_n^*(z). \quad (12)$$

The determination of $\tilde{\gamma}_{n+1}$ and $\tilde{\gamma}_{n+2}$ is discussed in the following two sections. The nodes and weights of the desired Szegő–Lobatto rule are the eigenvalues and square of the first component of the normalized eigenvectors of the unitary upper Hessenberg matrix $H(\gamma_1, \dots, \gamma_n, \tilde{\gamma}_{n+1}, \tilde{\gamma}_{n+2})$.

3. Szegő–Lobatto rules

The applications of the recursion relations (3) and (4) for the Szegő polynomials to the equation $\tilde{\phi}_{n+2}(z_\alpha) = 0$, using (11) and (12), as well as (10) with $n+1$ replaced by n , yields

$$z_\alpha^2\phi_n(z_\alpha) + \tilde{\gamma}_{n+1}z_\alpha^{n+1}\overline{\phi_n(z_\alpha)} + z_\alpha\tilde{\gamma}_{n+2}\tilde{\gamma}_{n+1}\phi_n(z_\alpha) + \tilde{\gamma}_{n+2}z_\alpha^n\overline{\phi_n(z_\alpha)} = 0. \quad (13)$$

Since all zeros of $\phi_n(z)$ are strictly inside the unit circle, the constant $a := z_\alpha^{n-1}\overline{\phi_n(z_\alpha)}/\phi_n(z_\alpha)$ is well defined and of unit magnitude. Dividing (13) by $z_\alpha\phi_n(z_\alpha)$ yields

$$az_\alpha\tilde{\gamma}_{n+1} + \tilde{\gamma}_{n+2}\tilde{\gamma}_{n+1} + a\tilde{\gamma}_{n+2} = -z_\alpha. \quad (14)$$

Similarly, $\tilde{\phi}_{n+2}(z_\beta) = 0$ gives the equation

$$bz_\beta\tilde{\gamma}_{n+1} + \tilde{\gamma}_{n+2}\tilde{\gamma}_{n+1} + b\tilde{\gamma}_{n+2} = -z_\beta, \quad (15)$$

where $b := z_\beta^{n-1}\overline{\phi_n(z_\beta)}/\phi_n(z_\beta)$ is well defined and of unit magnitude. Thus, we wish to determine the recursion coefficients $\tilde{\gamma}_{n+1}$ and $\tilde{\gamma}_{n+2}$ that satisfy (14) and (15), as well as the constraints

$$|\tilde{\gamma}_{n+1}| < 1, \quad (16)$$

$$|\tilde{\gamma}_{n+2}| = 1. \quad (17)$$

Subtracting (15) from (14) yields the linear equation

$$(az_\alpha - bz_\beta)\tilde{\gamma}_{n+1} + (a - b)\tilde{\gamma}_{n+2} = -(z_\alpha - z_\beta). \quad (18)$$

Example 3.1. Let $dw(t) := dt$ be the Lebesgue measure. Then $\gamma_j = 0$ for $j \geq 1$, and $\phi_j(z) = z^j$ and $\phi_j^*(z) = 1$ for $j \geq 0$. Let $z_\alpha := e^{i\theta}$ and $z_\beta := e^{-i\theta}$ for some θ with $-\pi < \theta < \pi$. Then $a = e^{-i(n+1)\theta}$, $b = e^{i(n+1)\theta}$, and Eq. (18) reduces to

$$\sin(n\theta)\tilde{\gamma}_{n+1} + \sin((n+1)\theta)\tilde{\gamma}_{n+2} = \sin(\theta).$$

We will return to this example below.

Since $z_\alpha \neq z_\beta$, at most one of the coefficients of $\tilde{\gamma}_{n+1}$ and $\tilde{\gamma}_{n+2}$ in Eq. (18) can be zero. We first consider the cases when one of these coefficients vanishes, and then turn to the situation when they are both non-zero.

Assume that $az_\alpha = bz_\beta$, which can be expressed as

$$\frac{\phi_n(z_\alpha)}{\phi_n^*(z_\alpha)} = \frac{\phi_n(z_\beta)}{\phi_n^*(z_\beta)}.$$

This situation occurs when z_α and z_β are zeros of the para-orthogonal polynomial $\phi_n(\tau, z)$ with

$$\tau = -\frac{\phi_n(z_\alpha)}{\phi_n^*(z_\alpha)},$$

cf. (7). It follows that the nodes z_α and z_β belong to the spectrum of the matrix $H_n(\tau)$ and the n -point Szegő rule $S^{(n)}$ determined by this matrix is a Szegő–Lobatto rule with nodes at z_α and z_β .

Example 3.2. Let $n := 4$ and $\theta := \pi/4$ in Example 3.1. Then $az_\alpha = bz_\beta$ and $\tau = -z_\alpha^4 = 1$. The nodes for the 4-point Szegő rule are the zeros of the polynomial $z^4 + 1 = 0$, and include the points $z_\alpha = e^{i\pi/4}$ and $z_\beta = e^{-i\pi/4}$.

We turn to the situation when $a = b$, which is equivalent to

$$z_\alpha \frac{\phi_n(z_\alpha)}{\phi_n^*(z_\alpha)} = z_\beta \frac{\phi_n(z_\beta)}{\phi_n^*(z_\beta)}.$$

If we choose τ according to Eq. (9) with $n+1$ replaced by n , then the eigenvalues and the square of the first component of associated eigenvectors of $H_{n+1}(\tau)$ determine an $(n+1)$ -point Szegő rule with nodes at z_α and z_β . This rule therefore is a Szegő–Lobatto rule with nodes at the desired positions. It is exact for all Laurent polynomials in the set $\mathcal{A}_{-n,n}$.

Example 3.3. Consider Example 3.1 with $\theta := \pi/4$ and $n := 3$. Then $a = b$ and determining τ as described above yields $\tau = -z_\alpha^4 = 1$. We obtain a 4-point Szegő–Lobatto rule whose nodes and weights are the same as of the Szegő rule of Example 3.2. In particular, the points z_α and z_β are among the nodes.

We now turn to the generic case when both $a \neq b$ and $az_\alpha \neq bz_\beta$. Introduce the constants

$$c := -\frac{z_\alpha - z_\beta}{az_\alpha - bz_\beta}, \quad r := \left| \frac{a - b}{az_\alpha - bz_\beta} \right|. \quad (19)$$

Combining (17) and (18) shows that

$$|\tilde{\gamma}_{n+1} - c| = r, \quad (20)$$

i.e., $\tilde{\gamma}_{n+1}$ must lie on a circle with center c and radius r . We refer to this circle as C_γ . In view of the constraint (16), $\tilde{\gamma}_{n+1}$ must lie in the intersection of C_γ and the open unit disk. The following theorem shows that this intersection is non-empty. We remark that the special case when $r = 0$ in (20) already has been discussed above.

Theorem 3.1. Assume that $a \neq b$ and $az_\alpha \neq bz_\beta$. Then the intersection of the circle C_γ and the open unit disk is non-empty.

Proof. We will show that

$$\gamma := (|c| - r)e^{i\omega}, \quad \omega := \arg(c), \quad (21)$$

lies on C_γ and is of magnitude strictly smaller than one. The representation $\gamma = c - re^{i\omega}$ shows that $\gamma \in C_\gamma$. It remains to be shown that

$$||z_\alpha - z_\beta| - |a - b|| < |az_\alpha - bz_\beta|. \quad (22)$$

Let $u := z_\alpha/z_\beta$ and $v := a/b$. Then (22) can be expressed as

$$||1 - u| - |1 - v|| < |1 - uv|.$$

Applying the triangle inequality to

$$1 - uv = (1 - v) + v(1 - u),$$

and using the fact that $|v| = 1$, we immediately have

$$||1 - u| - |1 - v|| \leq |1 - uv|. \quad (23)$$

Equality can occur in (23) if one of u or v is 1. But this implies that $z_\alpha = z_\beta$ or $a = b$ both of which are excluded cases. The only other possibility for equality is if $(1 - v)$ and $v(1 - u)$ are co-linear with $z = 0$. But this will only occur when $uv = 1$ which is equivalent to $az_\alpha = bz_\beta$, an excluded case. \square

We have shown how to determine a pair of recursion coefficients $\{\tilde{\gamma}_{n+1}, \tilde{\gamma}_{n+2}\}$ that satisfies the constraints (16) and (17) as well as the Eq. (18). Such a coefficient pair also satisfies (14) and (15). This can be seen as follows. Introduce

$$\hat{\gamma} := a^{1/2}b^{1/2}\tilde{\gamma}_{n+1}, \quad \hat{c} := -\frac{z_\alpha - z_\beta}{a^{1/2}\bar{b}^{1/2}z_\alpha - \bar{a}^{1/2}b^{1/2}z_\beta}, \quad (24)$$

where we note that $\hat{c} \in \mathbb{R}$. Then (20) is equivalent to $|\hat{\gamma} - \hat{c}| = r$, i.e.,

$$|\hat{\gamma}|^2 - 2\hat{c}\operatorname{Re}(\hat{\gamma}) = r^2 - \hat{c}^2. \quad (25)$$

We turn to Eq. (14). Multiplying (14) by $a - b$ and eliminating $\tilde{\gamma}_{n+2}$ by using (18) yields

$$\frac{az_\alpha - bz_\beta}{z_\alpha - z_\beta}(|\tilde{\gamma}_{n+1}|^2 - 1) + ab\tilde{\gamma}_{n+1} + \bar{\tilde{\gamma}}_{n+1} = -(a + b), \quad (26)$$

which, using the quantities (24), can be written as

$$|\hat{\gamma}|^2 - 2\hat{c}\operatorname{Re}(\hat{\gamma}) = \hat{c}(a^{1/2}\bar{b}^{1/2} + \bar{a}^{1/2}b^{1/2}) + 1. \quad (27)$$

Both Eqs. (25) and (27) represent circles with center \hat{c} . It is easy to verify that $\hat{\gamma} = -\bar{a}^{1/2}b^{1/2}$ and $\hat{\gamma} = -a^{1/2}\bar{b}^{1/2}$ satisfy both (25) and (27), or equivalently, that $\tilde{\gamma}_{n+1} = -\bar{a}$ and $\tilde{\gamma}_{n+1} = -\bar{b}$ satisfy (20) and (26). It follows that Eqs. (20) and (26) represent the same circle.

Turning to (15), we find that multiplying this equation by $a - b$ and then applying (18) to eliminate $\tilde{\gamma}_{n+2}$ also yields (26). Thus, any $\tilde{\gamma}_{n+1}$ that satisfies (16), (18) and (20), also satisfies (26). In view of Theorem 3.1 there is a continuum of values of γ_{n+1} that satisfy these requirements. Let $\tilde{\gamma}_{n+1}$ denote one of these values. We compute an associated value of $\tilde{\gamma}_{n+2}$ by (18), i.e., we let

$$\tilde{\gamma}_{n+2} := -\frac{az_\alpha - bz_\beta}{a - b}\tilde{\gamma}_{n+1} - \frac{z_\alpha - z_\beta}{a - b}. \quad (28)$$

Example 3.4. Let $\theta := \pi/4$ and $n := 2$ in Example 3.1. Then Eq. (18) reduces to

$$\sqrt{2}\tilde{\gamma}_3 + \tilde{\gamma}_4 = 1,$$

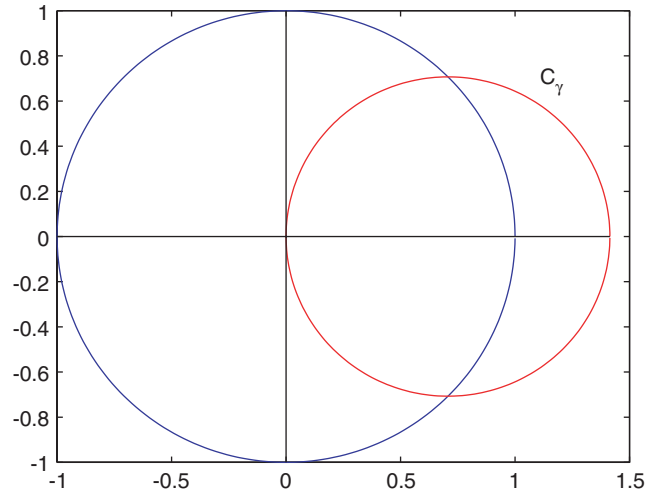


Fig. 1. The circle C_γ of Example 3.4 and the unit circle.

and $C_\gamma = \{z : |z - 1/\sqrt{2}| = 1/\sqrt{2}\}$; see Fig. 1. The value $\tilde{\gamma}_3 = 0$ corresponds to the choice (21) of Theorem 3.1 and (28) gives $\tilde{\gamma}_4 = 1$. The nodes of the associated 4-point Szegő–Lobatto rule are the roots of the equation $z^4 + 1 = 0$, or equivalently, the eigenvalues of the matrix $H_4(0, 0, 0, 1)$. In particular, the points $e^{\pm i\pi/4}$ are among the nodes.

If instead we choose $\tilde{\gamma}_3 := 1/2 - i\sqrt{1/\sqrt{2} - 1/4}$, then (28) yields $\tilde{\gamma}_4 := 1 - \sqrt{2} \tilde{\gamma}_3$. The nodes of the associated 4-point Szegő–Lobatto rule are the roots of the equation $z^4 + (\tilde{\gamma}_3 - 1)z^3 + \tilde{\gamma}_3 z + \tilde{\gamma}_4 = 0$, or equivalently, the eigenvalues of the matrix $H_4(0, 0, \tilde{\gamma}_3, \tilde{\gamma}_4)$. The points $e^{\pm i\pi/4}$ are among the nodes. The other nodes are approximately $-0.9463 - 0.3234i$ and $0.0321 + 0.9995i$.

The existence of a Szegő quadrature rule for a given set of moments and its relation to the orthogonal polynomials is demonstrated, e.g., by Grenander and Szegő [14, Chapter 4]. Given a sequence of moments $\mu_0, \mu_{\pm 1}, \mu_{\pm 2}, \dots$, with $\mu_0 = 1$ and $\mu_{-k} = \bar{\mu}_k$, we can determine a sequence of recursion coefficients $\gamma_1, \gamma_2, \gamma_3, \dots$ of magnitude strictly smaller than one of the associated Szegő polynomials. Conversely, given a sequence of recursion coefficients, we can determine a sequence of associated moments as follows. Let

$$\phi_k(z) = z^k + \sum_{j=0}^{k-1} d_{j,k} z^j, \quad d_{0,k} = \gamma_k,$$

be the k th monic Szegő polynomial determined by the recursion relations (3) and (4). Let $\mu_0 := 1$ and $d_{0,0} := 1$. Then $(\phi_k, 1) = 0$ for $k \geq 1$ yields

$$\mu_k := - \sum_{j=0}^{k-1} d_{j,k} \mu_j, \quad k = 1, 2, 3, \dots, \quad (29)$$

and we define $\mu_{-k} := \bar{\mu}_k$. The $(n+1)$ st recursion coefficient $\tilde{\gamma}_{n+1}$ associated with the $(n+2)$ -point Szegő–Lobatto rule generally differs from γ_{n+1} . It follows that this quadrature rule is a Szegő rule associated with the moments $\mu_0, \mu_{\pm 1}, \dots, \mu_{\pm n}, \tilde{\mu}_{\pm(n+1)}$, where $\tilde{\mu}_{\pm(n+1)}$ are given by (29) with $d_{0,n+1} := \tilde{\gamma}_{n+1}$. Therefore the $(n+2)$ -point Szegő–Lobatto quadrature rule integrates exactly all powers $\{z^{\pm k}\}_{k=0}^n$ with respect to the original measure $dw(t)$. We have shown the following result.

Theorem 3.2. *The $(n+2)$ -point Szegő–Lobatto quadrature rule (1) is exact for all Laurent polynomials in $\Lambda_{-n,n}$. Moreover, if $\tilde{\gamma}_{n+1} \neq \gamma_{n+1}$ then there are Laurent polynomials in $\Lambda_{-n-1,n+1} \setminus \Lambda_{-n,n}$ that the quadrature rule does not integrate exactly. If $\tilde{\gamma}_{n+1} = \gamma_{n+1}$ then the quadrature rule is exact for all Laurent polynomials in $\Lambda_{-n-1,n+1}$.*

4. Real Szegő–Lobatto rules

This section discusses the situation when the measure $dw(t)$ is symmetric about zero and the nodes z_α and z_β are complex conjugate. The symmetry of the measure implies that all recursion coefficients γ_j , $j = 1, 2, 3, \dots$, are real. It follows that the constants a and b introduced in Section 3 are complex conjugate. Throughout this section we assume that $a \neq b$ and $az_\alpha \neq bz_\beta$.

We obtain from (5) with $z = \pm 1$ that $\phi_{n+1}^*(1) = \phi_{n+1}(1)$ and $\phi_{n+1}^*(-1) = (-1)^{n+1}\phi_{n+1}(-1)$. Substitution into $\tilde{\phi}_{n+2}(z) := z\phi_{n+1}(z) + \tilde{\gamma}_{n+2}\phi_{n+1}^*(z)$ with $\tilde{\gamma}_{n+2} \in \{-1, 1\}$ shows when $\tilde{\phi}_{n+2}(z)$ vanishes at $z = 1$ or $z = -1$; see Table 1.

Hence, when the recursion coefficients γ_j are real, we can allocate nodes of the Szegő quadrature rule $S^{(n+2)}$ at ± 1 by choosing a suitable value of $\tilde{\gamma}_{n+2} \in \{-1, 1\}$ and n . For instance, n odd and $\tilde{\gamma}_{n+2} = 1$ yields an $(n+2)$ -point Szegő quadrature rule, which is exact for all Laurent polynomials in $\mathcal{A}_{-n-1, n+1}$, with a node at $z_\alpha = -1$. This quadrature rule may be considered a Szegő–Radau rule with a prescribed node at -1 . Similarly, n even and $\tilde{\gamma}_{n+2} = -1$ gives an $(n+2)$ -point Szegő rule with nodes at $z_\alpha = 1$ and $z_\beta = -1$. The latter rule may be regarded a Szegő–Lobatto rule with prescribed nodes at ± 1 . This kind of Szegő–Radau and Szegő–Lobatto rules are discussed by Bultheel et al. [3].

We remark that Example 3.4 shows a Szegő–Lobatto rule associated with a symmetric measure and $z_\beta = \bar{z}_\alpha$. The center of C_γ is seen to lie on the real axis, and $\tilde{\gamma}_{n+1}$ and $\tilde{\gamma}_{n+2}$ can be chosen to be real. The nodes of the Szegő–Lobatto rule occur in complex conjugate pairs.

Combining the approach of Section 3 with the above observations allows us to prescribe nodes at distinct complex conjugate points z_α and z_β as well as at $z = 1$ and/or $z = -1$.

Theorem 4.1. *Let $\tilde{\gamma}_{n+1}$ be determined by (21). Then $\tilde{\gamma}_{n+1}$ is real and*

$$\tilde{\gamma}_{n+2} = -\text{sign}\left(\frac{z_\alpha - z_\beta}{a - b}\right). \quad (30)$$

Proof. We note that the center c defined by (19) is real; hence $e^{i\omega}$ in (21) is real and so is $\tilde{\gamma}_{n+1}$. The constant $(z_\alpha - z_\beta)/(a - b)$ is real, and therefore so is $\tilde{\gamma}_{n+2}$ determined by (28). Thus, $\tilde{\gamma}_{n+2} \in \{-1, 1\}$. It is now straightforward to determine the sign of $\tilde{\gamma}_{n+2}$ using (28). \square

Example 4.1. Let $S^{(4)}$ be a 4-point Szegő rule with $\tilde{\gamma}_4 = -1$. According to Table 1 this rule has distinct zeros at ± 1 and at complex conjugate points, which we denote by z_α and z_β .

Now construct the 8-point Szegő–Lobatto quadrature rule with prescribed nodes at z_α and z_β . If $\tilde{\gamma}_{n+2}$ determined by (30) is -1 , then the Szegő–Lobatto rule has nodes at ± 1 ; thus, the nodes of $S^{(4)}$ are a subset of the nodes of the Szegő–Lobatto rule. If, instead, $\tilde{\gamma}_{n+2} = 1$, then the 4-point Szegő and 8-point Szegő–Lobatto quadrature rules have three nodes in common. It may be possible to use such pairs of Szegő and Szegő–Lobatto quadrature rules to estimate the quadrature error of the Szegő rule in a similar manner as pairs of Gauss and Gauss–Kronrod quadrature rules furnish an estimate of the quadrature error of the Gauss rule; see, e.g., Kahaner et al. [18, p. 154] for a computed example with a pair of Gauss and Gauss–Kronrod rules.

Table 1
Zeros of $\tilde{\phi}_{n+2}(z) = z\phi_{n+1}(z) + \tilde{\gamma}_{n+2}\phi_{n+1}^*(z)$ at $z = \pm 1$ for $\tilde{\gamma}_{n+2} \in \{-1, 1\}$

n	$\tilde{\gamma}_{n+2}$	$\tilde{\phi}_{n+2}(1)$	$\tilde{\phi}_{n+2}(-1)$
even	1	$\neq 0$	$\neq 0$
even	-1	0	0
odd	1	$\neq 0$	0
odd	-1	0	$\neq 0$

5. Numerical examples

The numerical computations in this section were performed using MATLAB. Our program requires the input of $\{\gamma_j\}_{j=1}^n$, z_α , and z_β , and determines $\tilde{\gamma}_{n+1}$ from (21), $\tilde{\gamma}_{n+2}$ from (28), as well as the nodes and weights of the $(n+2)$ -point Szegő–Lobatto rule. The latter are computed as the eigenvalues and square of the first components of normalized eigenvectors of the unitary upper Hessenberg matrix $H_{n+2}(\gamma_1, \gamma_2, \dots, \gamma_n, \tilde{\gamma}_{n+1}, \tilde{\gamma}_{n+2}) \in \mathbb{C}^{(n+2) \times (n+2)}$. We remark that the computations of the QR-algorithms [11,12,21,22] and the divide-and-conquer methods [2,13,15] can be arranged so that these quantities can be determined in only $O(n^2)$ arithmetic floating point operations. The computations are carried out with about 16 significant digits, and all computed values are displayed to four decimal places.

Example 5.1. Let $dw(t)$ be the Lebesgue measure introduced in Example 3.1. Fig. 2 shows the nodes of a 12-point Szegő–Lobatto rule with the prescribed nodes $z_\alpha := e^{-i\pi/4}$ and $z_\beta := e^{2i\pi/3}$. The nodes are the eigenvalues of the matrix $H_{12}(0, \dots, 0, \tilde{\gamma}_{11}, \tilde{\gamma}_{12})$ with $\tilde{\gamma}_{11} = 0.5426 + 0.7071i$ and $\tilde{\gamma}_{12} = -i$.

Example 5.2. Consider the symmetric measure $dw(t) := 2 \sin^2(t/2) dt$ on the interval $[-\pi, \pi]$. This measure is discussed by Bultheel et al. [3], who provide explicit expressions for the associated Szegő polynomials. The recursion coefficients are given by

$$\gamma_j := \frac{1}{1+j}, \quad j = 1, 2, 3, \dots$$

Fig. 3 shows the nodes of the 13-point Szegő–Lobatto rule with $n = 11$, $z_\alpha = e^{i\pi/12}$, $z_\beta = e^{i\pi/4}$, $\tilde{\gamma}_{12} = -0.1705 - 0.4900i$, and $\tilde{\gamma}_{13} = 0.1877 - 0.9822i$.

Example 5.3. Consider the non-symmetric measure $dw(t) = \pi / \sinh(\pi) d(e^t)$ on the interval $[-\pi, \pi]$. The associated moments are given by

$$\mu_k := \frac{(-1)^k}{1+k^2} (1+ik).$$

In order to avoid explicitly forming the Szegő polynomials, we used Schur's algorithm, see, e.g., [1,16], to compute the recursion coefficients directly from the moments. Fig. 4 shows the nodes of the 11-point Szegő–Lobatto quadrature rule (1) for $n = 9$, $z_\alpha = 1$, and $z_\beta = -1$. The computed values for $\tilde{\gamma}_{10}$ and $\tilde{\gamma}_{11}$ are $-0.2061 + 0.8308i$ and $0.9706 + 0.2408i$, respectively.

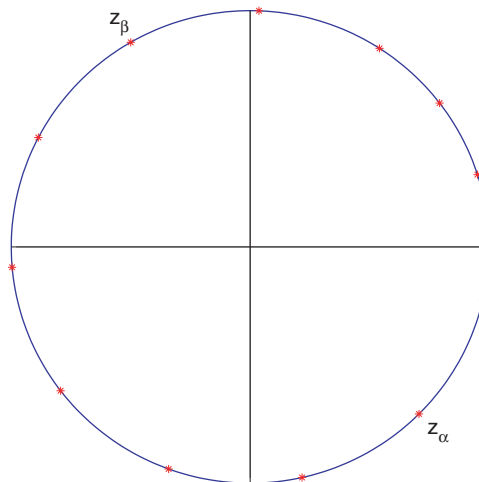


Fig. 2. Nodes of the 12-point Szegő–Lobatto rule of Example 5.1 with prescribed nodes $z_\alpha := e^{-i\pi/4}$ and $z_\beta := e^{2i\pi/3}$.

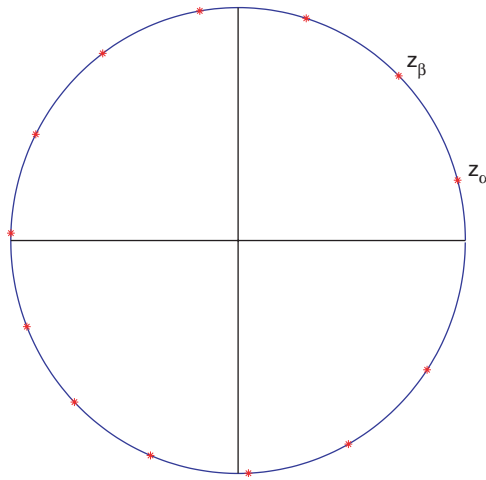


Fig. 3. Nodes of the 13-point Szegő–Lobatto rule of Example 5.2 with prescribed nodes $z_\alpha := e^{i\pi/12}$ and $z_\beta := e^{i\pi/4}$.

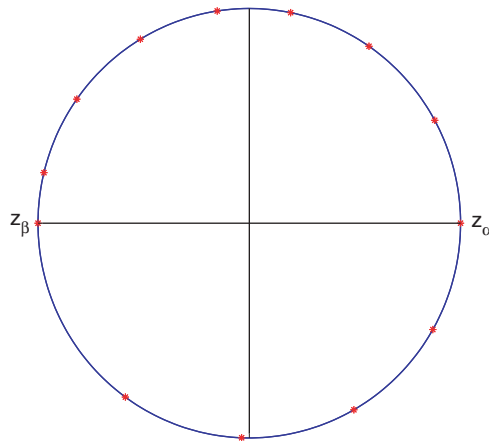


Fig. 4. Nodes of the 11-point Szegő–Lobatto rule of Example 5.3 with prescribed nodes $z_\alpha := 1$ and $z_\beta := -1$.

6. Conclusion

We have shown that Szegő–Lobatto rules exist, and that, generally, they depend on a parameter $\tilde{\gamma}_{n+1}$ which can be chosen freely on a circular arc. Thus, differently from Gauss–Lobatto quadrature rules, Szegő–Lobatto rules generally are not unique. They can be computed with software for the unitary eigenvalue problem for upper Hessenberg matrices.

Acknowledgement

We would like to thank Bill Gragg and a referee for comments.

References

- [1] G.S. Ammar, W.B. Gragg, The generalized Schur algorithm for the superfast solution of Toeplitz systems, in: J. Gilewicz, M. Pindor, W. Siemaszko (Eds.), *Rational Approximation and its Applications in Mathematics and Physics*, Lecture Notes in Mathematics, vol. 1237, Springer, Berlin, 1987, pp. 315–330.

- [2] G.S. Ammar, L. Reichel, D.C. Sorensen, Algorithm 730: an implementation of a divide and conquer algorithm for the unitary eigenproblem, *ACM Trans. Math. Software* 18 (1992) 292–307 and 20 (1994) 161.
- [3] A. Bultheel, L. Daruis, P. González-Vera, A connection between quadrature formulas on the unit circle and the interval $[-1, 1]$, *J. Comput. Appl. Math.* 132 (2001) 1–14.
- [4] A. Bultheel, L. Daruis, P. González-Vera, Positive interpolatory quadrature formulas and para-orthogonal polynomials, *J. Comput. Appl. Math.* 179 (2005) 97–119.
- [5] R. Cruz-Barroso, L. Daruis, P. González-Vera, O. Njåstad, Quadrature rules for periodic integrands. Bi-orthogonality and para-orthogonality, *Annales Mathematicae et Informaticae* 32 (2005) 5–44.
- [6] R. Cruz-Barroso, P. González-Vera, Orthogonal Laurent polynomials and quadratures on the unit circle and real half-line, *Electron. Trans. Numer. Anal.* 19 (2005) 113–134. Available at (<http://etna.mcs.kent.edu>).
- [7] L. Daruis, P. González-Vera, F. Marcellán, Gaussian quadrature formulae on the unit circle, *J. Comput. Appl. Math.* 140 (2002) 159–183.
- [8] W. Gautschi, The interplay between classical analysis and (numerical) linear algebra—a tribute to Gene Golub, *Electron. Trans. Numer. Anal.* 13 (2002) 119–147. Available at (<http://etna.mcs.kent.edu>).
- [9] W. Gautschi, *Orthogonal Polynomials: Computation and Approximation*, Oxford University Press, Oxford, 2004.
- [10] W.B. Gragg, Positive definite Toeplitz matrices, the Arnoldi process for isometric operators, and Gaussian quadrature on the unit circle, *J. Comput. Appl. Math.* 46 (1993) 183–198. This is a slight revision of a paper originally published (in Russian), in: E.S. Nicholaev (Ed.), *Numerical Methods in Linear Algebra*, Moscow University Press, Moscow, 1982, pp. 16–32.
- [11] W.B. Gragg, The QR algorithm for unitary Hessenberg matrices, *J. Comput. Appl. Math.* 16 (1986) 1–8.
- [12] W.B. Gragg, Stabilization of the UHQR algorithm, in: Z. Chen, Y. Li, C. Micchelli, Y. Xu (Eds.), *Advances in Computational Mathematics*, Lecture Notes in Pure and Applied Mathematics, vol. 202, Marcel Dekker, Hong Kong, 1999, pp. 139–154.
- [13] W.B. Gragg, L. Reichel, A divide and conquer method for the unitary and orthogonal eigenproblems, *Numer. Math.* 57 (1990) 695–718.
- [14] U. Grenander, G. Szegő, *Toeplitz Forms and Their Applications*, Chelsea, New York, NY, 1984.
- [15] M. Gu, R. Guzzo, X.-b. Chi, X.-Q. Cao, A stable divide and conquer algorithm for the unitary eigenproblem, *SIAM J. Matrix Anal. Appl.* 25 (2003) 385–404.
- [16] C. Jagels, L. Reichel, On the construction of Szegő polynomials, *J. Comput. Appl. Math.* 46 (1993) 241–254.
- [17] W.B. Jones, O. Njåstad, W.J. Thron, Moment theory and continued fractions associated with the unit circle, *Bull. London Math. Soc.* 21 (1989) 113–152.
- [18] D. Kahaner, C. Moler, S. Nash, *Numerical Methods and Software*, Prentice-Hall, Englewood Cliffs, NJ, 1989.
- [19] S.-M. Kim, L. Reichel, Anti-Szegő quadrature rules, *Math. Comp.*, accepted for publication.
- [20] E.B. Saff, Orthogonal polynomials from a complex perspective, in: P. Nevai (Ed.), *Orthogonal Polynomials: Theory and Practice*, Kluwer, Dordrecht, 1990, pp. 363–393.
- [21] M. Stewart, Stability properties of several variants of the unitary QR algorithm, in: V. Olshevsky (Ed.), *Structured Matrices in Mathematics, Computer Science, and Engineering*, vol. II, American Mathematical Society, Providence, RI, 2001, pp. 57–72.
- [22] M. Stewart, An error analysis of a unitary Hessenberg QR algorithm, *SIAM J. Matrix. Anal. Appl.*, to appear.