

## ANTI-SZEGŐ QUADRATURE RULES

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ABSTRACT. Szegő quadrature rules are discretization methods for approximating integrals of the form  $\int_{-\pi}^{\pi} f(e^{it})d\mu(t)$ . This paper presents a new class of discretization methods, which we refer to as anti-Szegő quadrature rules. Anti-Szegő rules can be used to estimate the error in Szegő quadrature rules: under suitable conditions, pairs of associated Szegő and anti-Szegő quadrature rules provide upper and lower bounds for the value of the given integral. The construction of anti-Szegő quadrature rules is almost identical to that of Szegő quadrature rules in that pairs of associated Szegő and anti-Szegő rules differ only in the choice of a parameter of unit modulus. Several examples of Szegő and anti-Szegő quadrature rule pairs are presented.

### 1. INTRODUCTION

Let  $\mu(t)$  be a distribution function, i.e., a real-valued, bounded, nondecreasing function, with infinitely many points of increase in the interval  $[-\pi, \pi]$ , and define the integral

$$(1.1) \quad I(f) := \frac{1}{2\pi} \int_{-\pi}^{\pi} f(e^{it})d\mu(t)$$

and the inner product

$$(1.2) \quad (f, g) := \frac{1}{2\pi} \int_{-\pi}^{\pi} \overline{f(e^{it})}g(e^{it})d\mu(t),$$

where  $i := \sqrt{-1}$  and the bar denotes complex conjugation. The functions  $f$  and  $g$  are assumed to be sufficiently smooth so that the integrals (1.1) and (1.2) exist. Moreover, the *moments*

$$(1.3) \quad \mu_j := \frac{1}{2\pi} \int_{-\pi}^{\pi} e^{-ijt}d\mu(t), \quad j = 0, \pm 1, \pm 2, \dots,$$

associated with  $\mu(t)$  are all assumed to exist and, for notational convenience,  $\mu(t)$  is scaled so that  $\mu_0 = 1$ . The *moment matrices* are Hermitian Toeplitz matrices

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defined by

$$M_n = \begin{bmatrix} \mu_0 & \mu_{-1} & \cdots & \mu_{-n+1} \\ \mu_1 & \mu_0 & \cdots & \mu_{-n+2} \\ \vdots & \vdots & \ddots & \vdots \\ \mu_{n-1} & \mu_{n-2} & \cdots & \mu_0 \end{bmatrix} \in \mathbb{C}^{n \times n}, \quad n = 1, 2, 3, \dots$$

Each moment matrix is positive definite, because for any nonvanishing vector  $\xi = [\xi_1, \xi_2, \dots, \xi_n]^t$ , we have

$$\bar{\xi}^t M_n \xi = (p, p) = \frac{1}{2\pi} \int_{-\pi}^{\pi} |p(e^{it})|^2 d\mu(t) > 0,$$

where  $p(z) = \xi_1 + \xi_2 z + \cdots + \xi_n z^{n-1}$ .

There is an infinite sequence of monic polynomials  $\{\psi_j\}_{j=0}^{\infty}$ , known as *Szegő polynomials*, that are orthogonal with respect to the inner product (1.2). Properties of Szegő polynomials are discussed by, e.g., Szegő [28], Grenander and Szegő [16], Freud [8], and Geronimus [9]. Of particular importance is the fact that the monic Szegő polynomials satisfy recursion relations of the form

$$(1.4) \quad \begin{aligned} \psi_0(z) &= \psi_0^*(z) = 1, \\ \psi_j(z) &= z\psi_{j-1}(z) + \gamma_j \psi_{j-1}^*(z), \quad j = 1, 2, 3, \dots, \\ \psi_j^*(z) &= \bar{\gamma}_j z \psi_{j-1}(z) + \psi_{j-1}^*(z), \end{aligned}$$

where  $\psi_j^*(z) := z^j \bar{\psi}_j(z^{-1})$ , i.e., if  $\psi_j(z) = \sum_{k=0}^j \beta_k^{(j)} z^k$ , then  $\psi_j^*(z) = \sum_{k=0}^j \bar{\beta}_{j-k}^{(j)} z^k$ . The  $\psi_j^*$  are sometimes referred to as *reversed polynomials*.

The recursion coefficients  $\gamma_j \in \mathbb{C}$  can be determined for  $j = 1, 2, 3, \dots$ , by combining (1.4) with

$$(1.5) \quad \gamma_j = -(1, z\psi_{j-1})/\delta_{j-1},$$

$$(1.6) \quad \delta_j = \delta_{j-1}(1 - |\gamma_j|^2), \quad \delta_0 = 1;$$

see, e.g., [28]. The  $\gamma_j$  in the literature are sometimes called *Schur parameters* or *reflection coefficients*. Algorithms for computing Szegő polynomials, such as the Levinson and Schur algorithms, are described in, e.g., [1, 11, 21]. Specifically, these algorithms determine the set of coefficients  $\{\gamma_j\}_{j=1}^n$  from the set of moments  $\{\mu_j\}_{j=0}^n$  for  $n = 1, 2, 3, \dots$ .

Let  $\Delta_j$  denote the determinant of  $M_j$ . It follows from the recursion formulas of the Levinson algorithm that

$$(1.7) \quad \Delta_j = \delta_{j-1} \delta_{j-2} \cdots \delta_0, \quad j = 1, 2, 3, \dots;$$

see, e.g., Ammar and Gragg [1, Sections 2.1–2.2] for a proof. The positive definiteness of the moment matrices  $M_j$  yields that all  $\delta_j$  are positive, and therefore, by (1.6),

$$|\gamma_j| < 1, \quad j = 1, 2, 3, \dots$$

Moreover, for  $n = 0, 1, 2, \dots$ ,

$$(1.8) \quad (z^m, \psi_n) = \begin{cases} 0, & m = 0, 1, 2, \dots, n-1, \\ \delta_n, & m = n, \end{cases}$$

and in particular  $(\psi_n, \psi_n) = \delta_n$ .

The following theorem given by Krein yields valuable information about the zeros of orthogonal polynomials. In this theorem, the moment matrices  $M_k$  are only assumed to be invertible for  $1 \leq k \leq n+1$  for some fixed  $n \geq 1$ . Thus, the

$M_k$  may be indefinite and the distribution function  $\mu(t)$  in (1.2) is allowed to be nonmonotonic. In this situation (1.2) is a sesquilinear form rather than an inner product. This weaker requirement on the matrices  $M_k$  suffices to guarantee the existence of a finite set of unique monic orthogonal polynomials  $\{\psi_j\}_{j=0}^n$ , where as usual  $\psi_j$  is a polynomial of degree  $j$ . We note, however, that if some moment matrix  $M_k$  is indefinite, then, in view of (1.6), there are recursion coefficients  $\gamma_j$  of magnitude larger than unity. For proofs of the theorem, see, e.g., [6, Theorem 2.1] or [22, Theorem 2].

**Theorem 1.1.** *Let  $n \geq 1$ , and assume that  $\Delta_k \neq 0$ ,  $1 \leq k \leq n+1$ . Let  $\alpha_n$  and  $\beta_n (= n - \alpha_n)$  denote, respectively, the number of permanences and sign changes in the sequence*

$$1, \Delta_1, \Delta_2, \dots, \Delta_n.$$

*Then the orthogonal polynomial  $\psi_n$  has  $\alpha_n$  or  $\beta_n$  zeros in  $|z| < 1$ , as  $\Delta_n \Delta_{n+1}$  is positive or negative, respectively. In particular,  $\psi_n$  has no zeros on the unit circle.*

Since the determinant of every moment matrix associated with the distribution function  $\mu(t)$  in (1.2) is positive, Theorem 1.1 implies that all zeros of all Szegő polynomials  $\psi_1, \psi_2, \dots$  lie in the open unit disk; see [6, Theorem 1.1] and [28, Theorem 11.4.1] for alternative proofs.

An  $n$ -point Szegő quadrature rule is of the form

$$(1.9) \quad S_{\mu, \tau}^{(n)}(f) = \sum_{m=1}^n \omega_m^{(n)} f(\lambda_m^{(n)}), \quad \omega_m^{(n)} > 0, \quad \lambda_m^{(n)} \in \Gamma,$$

where  $\Gamma$  denotes the unit circle in  $\mathbb{C}$ . The characterizing property of  $S_{\mu, \tau}^{(n)}$  is that

$$(1.10) \quad S_{\mu, \tau}^{(n)}(p) = I(p), \quad \forall p \in \Lambda_{-(n-1), n-1},$$

where the integral  $I$  is defined by (1.1) and  $\Lambda_{-(n-1), n-1}$  denotes the set of Laurent polynomials

$$(1.11) \quad L_{n-1}(z) = \sum_{k=-(n-1)}^{n-1} c_k z^k, \quad c_k \in \mathbb{C},$$

of degree at most  $n-1$ ; see, e.g., [20] for details.

The Laurent polynomial (1.11) with  $z = \exp(it)$  can be expressed as a trigonometric polynomial  $T_{n-1}(t)$  of degree at most  $n-1$ ; i.e.,

$$L_{n-1}(z) = a_0 + \sum_{k=1}^{n-1} (a_k \cos(kt) + b_k \sin(kt)) =: T_{n-1}(t), \quad z = \exp(it),$$

where  $a_j, b_j \in \mathbb{C}$ . With a slight abuse of notation, we write  $S_{\mu, \tau}^{(n)}(L_{n-1})$  as

$$(1.12) \quad S_{\mu, \tau}^{(n)}(T_{n-1}) = \sum_{m=1}^n \omega_m^{(n)} T_{n-1}(\theta_m^{(n)}), \quad \lambda_m^{(n)} = \exp(i\theta_m^{(n)}),$$

and  $I(L_{n-1})$  as

$$(1.13) \quad I(T_{n-1}) = \frac{1}{2\pi} \int_{-\pi}^{\pi} T_{n-1}(t) d\mu(t).$$

It follows from (1.10) that

$$(1.14) \quad S_{\mu, \tau}^{(n)}(T_{n-1}) = I(T_{n-1}).$$

Gragg [11] and Jones et al. [20] show that the nodes  $\lambda_m^{(n)}$  of an  $n$ -point Szegő quadrature rule are the zeros of

$$(1.15) \quad \hat{\psi}_n(z) := z\psi_{n-1}(z) + \tau\psi_{n-1}^*(z),$$

where  $\tau \in \Gamma$  is arbitrary but fixed. The corresponding weights are given by

$$(1.16) \quad \omega_m^{(n)} = I(l_m), \quad m = 1, 2, \dots, n,$$

where the  $l_m$  are Lagrange polynomials defined by

$$(1.17) \quad l_m(z) := \prod_{\substack{k=1 \\ k \neq m}}^n \frac{z - \lambda_k^{(n)}}{\lambda_m^{(n)} - \lambda_k^{(n)}}.$$

In particular, the nodes and weights depend on the parameter  $\tau$ , but (1.10) holds for all  $\tau \in \Gamma$ .

We introduce the  $n \times n$  matrices

$$\hat{H}_n(\tau) := \begin{bmatrix} -\bar{\gamma}_0\gamma_1 & -\bar{\gamma}_0\gamma_2 & \cdots & -\bar{\gamma}_0\gamma_{n-1} & -\bar{\gamma}_0\tau \\ 1 - |\gamma_1|^2 & -\bar{\gamma}_1\gamma_2 & \cdots & -\bar{\gamma}_1\gamma_{n-1} & -\bar{\gamma}_1\tau \\ 0 & 1 - |\gamma_2|^2 & \cdots & -\bar{\gamma}_2\gamma_{n-1} & -\bar{\gamma}_2\tau \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 - |\gamma_{n-1}|^2 & -\bar{\gamma}_{n-1}\tau \end{bmatrix}$$

and

$$D_n := \text{diag}[\delta_0, \delta_1, \dots, \delta_{n-1}],$$

where  $\gamma_0 := 1$  and  $\tau \in \Gamma$ . Gragg [11] showed that the zeroes of (1.15), i.e., the nodes  $\lambda_m^{(n)}$  associated with this value of  $\tau$ , are the eigenvalues of the unitary upper Hessenberg matrix

$$(1.18) \quad H_n(\tau) := D_n^{-1/2} \hat{H}_n(\tau) D_n^{1/2},$$

and the corresponding weights  $\omega_m^{(n)}$  are the magnitude squared of the first component of the eigenvectors of  $H_n(\tau)$  normalized to have unit length.

The  $n \times n$  unitary upper Hessenberg matrix (1.18) is determined by only  $n$  parameters:  $\gamma_1, \gamma_2, \dots, \gamma_{n-1}, \tau$ . Several algorithms for computing the spectral decomposition of  $H_n(\tau)$  by manipulating these parameters, rather than the matrix entries, are available and can be used to determine the Szegő quadrature rule associated with (1.18); see [2, 3, 12, 13, 14, 15, 18, 26, 27]. Some of these algorithms do not require the computation of all components of the eigenvectors in order to determine the quadrature rule. Recent discussions on Szegő quadrature rules can be found in [4, 5, 17].

Consider briefly the approximation of integrals of the form

$$(1.19) \quad I(h) := \int_a^b h(t) d\nu(t), \quad -\infty \leq a < b \leq \infty,$$

where  $\nu(t)$  is a distribution function with infinitely many points of increase in the real (finite or infinite) interval  $[a, b]$ , such that all associated moments exist and are bounded. When the integrand  $h(t)$  is a smooth real-valued function, accurate approximations of (1.19) can be computed by Gauss quadrature rules. In addition, if certain (high order) derivatives of  $h(t)$  are of constant sign in the interval  $[a, b]$ , then it is possible to determine upper and lower bounds for (1.19) by evaluating pairs of Gauss and Gauss–Radau rules; see Golub and Meurant [10] for a discussion. Laurie

[23] recently proposed that pairs of Gauss and associated anti-Gauss quadrature rules be evaluated in order to determine error estimates; the  $(n + 1)$ -point anti-Gauss rule yields an integration error of opposite sign as the  $n$ -point Gauss rule for all polynomials of degree at most  $2n + 1$ . Under suitable conditions, pairs of Gauss and anti-Gauss rules yield upper and lower bounds for the integral (1.19) even when derivatives of the integrand change sign in the interval of integration.

It is the purpose of the present paper to define new quadrature rules for approximating the integral (1.1). These rules are analogous to the anti-Gauss rules introduced by Laurie [23], and we therefore refer to them as anti-Szegő quadrature rules. Pairs of associated Szegő and anti-Szegő quadrature rules provide estimates of upper and lower bounds for the integral (1.1), and under suitable conditions on the integrand they provide upper and lower bounds. We remark that the technique advocated by Golub and Meurant [10] for computing upper and lower bounds for (1.19) generally is not applicable to integrals of the form (1.1).

Section 2 discusses the construction of a quadrature rule  $A_{\mu,\tau}^{(n)}$ , whose integration error is a negative multiple of the integration error obtained with the Szegő rule  $S_{\mu,\tau}^{(n)}$  for all Laurent polynomials of degree at most  $n$ ; i.e.,

$$(1.20) \quad I(p) - A_{\mu,\tau}^{(n)}(p) = -c(I(p) - S_{\mu,\tau}^{(n)}(p)), \quad \forall p \in \Lambda_{-n,n},$$

for some positive constant  $c$ . Note that (1.10) yields

$$(1.21) \quad I(p) - A_{\mu,\tau}^{(n)}(p) = 0, \quad \forall p \in \Lambda_{-(n-1),n-1}.$$

The relation (1.20) can also be expressed as

$$(1.22) \quad I(p) - S_{\mu,\tau}^{(n)}(p) = \frac{1}{c+1}(A_{\mu,\tau}^{(n)} - S_{\mu,\tau}^{(n)})(p), \quad \forall p \in \Lambda_{-n,n},$$

and

$$(1.23) \quad I(p) = \left(\frac{1}{c+1}\right)A_{\mu,\tau}^{(n)} + \left(\frac{c}{c+1}\right)S_{\mu,\tau}^{(n)}(p), \quad \forall p \in \Lambda_{-n,n}.$$

Equation (1.22) expresses the quadrature error of  $S_{\mu,\tau}^{(n)}(p)$  in the left-hand side as a linear combination of computable quantities in the right-hand side for  $p \in \Lambda_{-n,n}$ , and suggests that the right-hand side may yield a useful estimate of the quadrature error also for integrands not in  $\Lambda_{-n,n}$ . Analogously, equation (1.23) suggests that the right-hand side may furnish a better approximation of  $I(p)$  than  $S_{\mu,\tau}^{(n)}(p)$  also for integrands  $p$  not in  $\Lambda_{-n,n}$ ; see Section 4 for further discussions of (1.22) and (1.23).

We show that for  $c$  in a certain range, the quadrature rule  $A_{\mu,\tau}^{(n)}$  has either  $n$  or  $n + 1$  nodes on the unit circle with positive weights. Furthermore, there always exists a constant  $c$  such that the associated quadrature rule  $A_{\mu,\tau}^{(n)}$  is an  $n$ -point rule. We shall call such  $n$ -point quadrature rules *anti-Szegő quadrature rules*. The special case when  $c = 1$  in (1.20) is discussed in Section 3. Applications of and computations with anti-Szegő quadrature rules are presented in Section 4. Concluding remarks can be found in Section 5.

The construction of anti-Szegő quadrature rules is almost identical to the construction of Szegő quadrature rules. In particular, the parameter of unit length for the anti-Szegő quadrature rule is determined by the parameter  $\tau$  of unit length for the Szegő quadrature rule and by the coefficient  $c$  in (1.20). The case when  $c = 1$  therefore sheds light on the roles of the parameters  $\tau$  in Szegő rules and the corresponding parameter in anti-Szegő rules.

2. CONSTRUCTION OF  $A_{\mu,\tau}^{(n)}$ 

In this section we let  $\tau \in \Gamma$  be fixed, and we denote the nodes and the weights of  $S_{\mu,\tau}^{(n)}$  by  $\lambda_m$  and  $\omega_m$ ,  $m = 1, 2, \dots, n$ , respectively. It follows from (1.20) that

$$(2.1) \quad A_{\mu,\tau}^{(n)}(p) = (1+c)I(p) - cS_{\mu,\tau}^{(n)}(p), \quad \forall p \in \Lambda_{-n,n},$$

where  $c$  is a positive constant. Comparing (2.1) and (1.10) suggests that we consider  $A_{\mu,\tau}^{(n)}$  a Szegő quadrature rule for the linear functional

$$(2.2) \quad \tilde{I} := (1+c)I - cS_{\mu,\tau}^{(n)}.$$

Analogously to (1.2), we introduce the sesquilinear form

$$(2.3) \quad (f, g)_{\tilde{I}} := \tilde{I}(\bar{f}g).$$

We can determine the nodes and weights for the quadrature rule  $A_{\mu,\tau}^{(n)}$  by first computing the coefficients  $\{\tilde{\gamma}_j\}_{j=1}^n$  in the recursion relations

$$(2.4) \quad \begin{aligned} \phi_0(z) &= \phi_0^*(z) := 1, \\ \phi_j(z) &= z\phi_{j-1}(z) + \tilde{\gamma}_j\phi_{j-1}^*(z), \quad j = 1, 2, \dots, n, \\ \phi_j^*(z) &= \tilde{\gamma}_jz\phi_{j-1}(z) + \phi_{j-1}^*(z), \end{aligned}$$

for the monic orthogonal polynomials  $\phi_j$ ,  $j = 0, 1, \dots, n$ , with respect to the sesquilinear form (2.3). Thus, the  $\phi_j$  satisfy  $(\phi_j, \phi_k)_{\tilde{I}} = 0$  for  $j \neq k$ . Analogously to (1.5) and (1.6), we have

$$(2.5) \quad \begin{aligned} \tilde{\gamma}_j &= -(1, z\phi_{j-1})_{\tilde{I}}/\tilde{\delta}_{j-1}, \\ \tilde{\delta}_j &= \tilde{\delta}_{j-1}(1 - |\tilde{\gamma}_j|^2), \quad \tilde{\delta}_0 := 1, \end{aligned}$$

and similarly as in Section 1,

$$(2.6) \quad (z^m, \phi_j)_{\tilde{I}} = \begin{cases} 0, & m = 0, 1, 2, \dots, j-1, \\ \tilde{\delta}_j, & m = j, \end{cases}$$

for  $j = 0, 1, \dots, n$ . The following relations will be applied below:

$$\begin{aligned} S_{\mu,\tau}^{(n)}(z^j) &= I(z^j) = \mu_{-j}, \quad 0 \leq |j| \leq n-1, \\ S_{\mu,\tau}^{(n)}(z^n) &= \omega_1\lambda_1^n + \dots + \omega_n\lambda_n^n. \end{aligned}$$

The polynomial  $\hat{\psi}_n$ , given by (1.15), can be written in the form

$$(2.7) \quad \hat{\psi}_n(z) = z^n + c_{n-1}z^{n-1} + \dots + c_1z + \tau,$$

for certain coefficients  $c_j \in \mathbb{C}$ . Since the nodes  $\lambda_m$  of  $S_{\mu,\tau}^{(n)}$  are zeros of  $\hat{\psi}_n$ , it follows that  $\lambda_m^n = -c_{n-1}\lambda_m^{n-1} - \dots - c_1\lambda_m - \tau$ , and therefore

$$\begin{aligned} S_{\mu,\tau}^{(n)}(z^n) &= \omega_1(-c_{n-1}\lambda_1^{n-1} - \dots - c_1\lambda_1 - \tau) + \omega_2(-c_{n-1}\lambda_2^{n-1} - \dots - c_1\lambda_2 - \tau) \\ &\quad + \dots + \omega_n(-c_{n-1}\lambda_n^{n-1} - \dots - c_1\lambda_n - \tau) \\ &= -c_{n-1}(\omega_1\lambda_1^{n-1} + \dots + \omega_n\lambda_n^{n-1}) - \dots - c_1(\omega_1\lambda_1 + \dots + \omega_n\lambda_n) \\ &\quad - \tau(\omega_1 + \dots + \omega_n) \\ &= -c_{n-1}\mu_{-(n-1)} - c_{n-2}\mu_{-(n-2)} - \dots - c_1\mu_{-1} - \tau\mu_0. \end{aligned}$$

Hence, the moments associated with  $\tilde{I}$  can be expressed as

$$\begin{aligned} m_{-j} &:= ((1+c)I - cS_{\mu,\tau}^{(n)})(z^j) = I(z^j) = \mu_{-j}, \quad 0 \leq |j| \leq n-1, \\ m_{-n} &:= ((1+c)I - cS_{\mu,\tau}^{(n)})(z^n) \\ &= (1+c)\mu_{-n} + c(c_{n-1}\mu_{-(n-1)} + c_{n-2}\mu_{-(n-2)} + \dots + c_1\mu_{-1} + \tau\mu_0). \end{aligned}$$

From this relation of the moments  $m_{-j}$  and  $\mu_{-j}$  one can deduce, e.g., by using the recursion relations (1.4), (1.5), and (1.6), or even more straightforwardly by using the recursion relations of the Levinson or Schur algorithms, that

$$(2.8) \quad \tilde{\gamma}_j = \gamma_j, \quad \tilde{\delta}_j = \delta_j, \quad \text{and} \quad \phi_j = \psi_j, \quad j = 0, 1, 2, \dots, n-1.$$

We turn to the computation of the coefficients  $\tilde{\gamma}_n$  and  $\tilde{\delta}_n$ , and obtain

$$\begin{aligned} \tilde{\gamma}_n &:= -\frac{(1, z\phi_{n-1})_{\bar{I}}}{\tilde{\delta}_{n-1}} = -\frac{(1, z\psi_{n-1})_{\bar{I}}}{\delta_{n-1}} \\ &= -\frac{(1, \hat{\psi}_n)_{\bar{I}} - (1, \tau\psi_{n-1}^*)_{\bar{I}}}{\delta_{n-1}} \\ &= -\frac{(1, \hat{\psi}_n)_{\bar{I}}}{\delta_{n-1}} + \tau \frac{(1, \psi_{n-1}^*)_{\bar{I}}}{\delta_{n-1}}. \end{aligned}$$

Using (2.7) yields

$$\begin{aligned} \frac{(1, \hat{\psi}_n)_{\bar{I}}}{\delta_{n-1}} &= \frac{m_{-n} + c_{n-1}m_{-n+1} + \dots + c_1m_{-1} + \tau m_0}{\delta_{n-1}} \\ &= (1+c) \frac{\mu_{-n} + c_{n-1}\mu_{-n+1} + \dots + c_1\mu_{-1} + \tau\mu_0}{\delta_{n-1}} \\ &= (1+c) \frac{(1, \hat{\psi}_n)}{\delta_{n-1}} \\ &= (1+c) \frac{(1, z\psi_{n-1})}{\delta_{n-1}} + (1+c)\tau \frac{(1, \psi_{n-1}^*)}{\delta_{n-1}} \\ &= -(1+c)\gamma_n + (1+c)\tau. \end{aligned}$$

The last equality follows from the definition of  $\gamma_n$  and the fact that

$$(1, \psi_{n-1}^*) = (\psi_{n-1}, z^{n-1}) = \delta_{n-1},$$

cf. (1.8). Since  $\psi_{n-1}^*$  is a polynomial of degree at most  $n-1$ , we have

$$(1, \psi_{n-1}^*)_{\bar{I}} = (1, \psi_{n-1}^*),$$

and therefore

$$(2.9) \quad \tilde{\gamma}_n = (1+c)\gamma_n - c\tau, \quad \tilde{\delta}_n = \delta_{n-1}(1 - |\tilde{\gamma}_n|^2).$$

In particular,  $\phi_n(z) = z\psi_{n-1}(z) + \tilde{\gamma}_n\psi_{n-1}^*(z)$ .

### 3. ANTI-SZEGŐ QUADRATURE RULES

Introduce the moment matrices

$$\tilde{M}_l = [m_{j-k}]_{j,k=0}^{l-1}, \quad l = 1, 2, \dots, n+1,$$

associated with the linear functional  $\tilde{I}$  and let  $\tilde{\Delta}_l$  denote the determinant of  $\tilde{M}_l$ . Analogously to (1.7),

$$\tilde{\Delta}_j = \tilde{\delta}_{j-1}\tilde{\delta}_{j-2}\cdots\tilde{\delta}_0, \quad j = 1, 2, \dots, n+1.$$

It follows from (2.8) that  $\tilde{\delta}_j > 0$  and  $|\tilde{\gamma}_j| < 1$  for  $1 \leq j < n$ , and therefore  $\tilde{\Delta}_j > 0$  for  $1 \leq j \leq n$ . Thus,  $\tilde{\Delta}_{n+1} > 0$  is equivalent to  $\tilde{\delta}_n > 0$ , and in view of (2.5) the

latter inequality is equivalent to  $|\tilde{\gamma}_n| < 1$ . Moreover,  $\tilde{\Delta}_{n+1} = 0$  is equivalent to  $|\tilde{\gamma}_n| = 1$  and  $\tilde{\delta}_n = 0$ . If

$$\tilde{\Delta}_l > 0, \text{ for } 1 \leq l \leq n, \text{ and } \tilde{\Delta}_{n+1} = 0,$$

then, following Jones et al. [20], we say that  $\tilde{I}$  is *positive  $n$ -definite*, and we refer to  $\{\phi_j\}_{j=0}^n$  as a *sequence of Szegő polynomials with respect to the positive  $n$ -definite linear functional  $\tilde{I}$* . In this situation, the sesquilinear form  $(\cdot, \cdot)_{\tilde{I}}$  is an inner product on  $\Lambda_{-(n-1), n-1}$ , and it follows from (2.6) that

$$(3.1) \quad (z^m, \phi_n)_{\tilde{I}} = 0, \quad m = 0, 1, \dots, n.$$

In the following lemma  $\tilde{I}$  denotes an arbitrary positive  $n$ -definite linear functional. In particular, the result holds for the linear functional defined by (2.2) when the associated recursion coefficient  $\tilde{\gamma}_n$ , given by (2.9), is of unit modulus.

**Lemma 3.1.** (Jones et al. [20, Theorem 9.2]) *Let  $\{\phi_j\}_{j=1}^n$  be a finite sequence of monic Szegő polynomials with respect to a positive  $n$ -definite linear functional  $\tilde{I}$ . Then the  $n$  zeros of  $\phi_n$ , denoted by  $\tilde{\lambda}_1^{(n)}, \tilde{\lambda}_2^{(n)}, \dots, \tilde{\lambda}_n^{(n)}$ , are all simple and lie on the unit circle. Moreover, there are positive real numbers  $\tilde{\omega}_1^{(n)}, \tilde{\omega}_2^{(n)}, \dots, \tilde{\omega}_n^{(n)}$ , which we refer to as weights, such that*

$$(3.2) \quad \tilde{I}(L_n) = \sum_{m=1}^n \tilde{\omega}_m^{(n)} L_n(\tilde{\lambda}_m^{(n)}), \quad \forall L_n \in \Lambda_{-n, n},$$

*i.e., the right-hand side is a quadrature rule for  $\tilde{I}$ , and it is exact for all  $L_n \in \Lambda_{-n, n}$ .*

We note that the property of the zeros  $\tilde{\lambda}_j^{(n)}$ ,  $j = 1, 2, \dots, n$ , to all be of unit modulus under the conditions of the above lemma follows from Theorem 1.1.

Assume that the linear functional  $\tilde{I}$ , defined by (2.2), is positive  $n$ -definite; i.e., the associated  $n$ th recursion coefficient, given by (2.9), satisfies  $|\tilde{\gamma}_n| = 1$ . Then the  $n$ -point Szegő quadrature rule (3.2) for approximating  $\tilde{I}$  is exact for a larger class of Laurent polynomials than the  $n$ -point Szegő rule (1.9) for approximating the integral (1.1) (cf. (1.10)). The following theorem shows the importance of the recursion coefficient  $\tilde{\gamma}_n$ .

**Theorem 3.2.** *Let the linear functional  $\tilde{I}$  be given by (2.2) and let  $\tilde{\gamma}_n$ , defined by (2.9), denote the  $n$ th recursion coefficient for the monic orthogonal polynomials associated with  $\tilde{I}$ . Then the quadrature rule  $A_{\mu, \tau}^{(n)}$  has the following properties. If  $|\tilde{\gamma}_n| < 1$ , then  $A_{\mu, \tau}^{(n)}$  is an  $(n+1)$ -point Szegő quadrature rule with respect to  $\tilde{I}$ . The rule depends on a parameter  $\rho \in \Gamma$ . If instead  $|\tilde{\gamma}_n| = 1$ , then  $A_{\mu, \tau}^{(n)}$  is an  $n$ -point Szegő quadrature rule with respect to the positive  $n$ -definite linear functional  $\tilde{I}$  with positive weights and nodes on  $\Gamma$ . In either case, the quadrature rule  $A_{\mu, \tau}^{(n)}$  is exact for all  $p \in \Lambda_{-n, n}$ .*

*Proof.* We first consider the case when  $|\tilde{\gamma}_n| < 1$ . Then  $\tilde{\Delta}_l > 0$  for  $l = 1, 2, \dots, n+1$ , and it follows that  $\{\phi_j\}_{j=0}^n$  is the finite sequence of monic Szegő polynomials with respect to  $\tilde{I}$ . In particular, there are  $(n+1)$ -point Szegő quadrature rules determined by the recursion coefficients  $\gamma_1, \dots, \gamma_{n-1}, \tilde{\gamma}_n$  and by an arbitrary parameter  $\rho \in \Gamma$ . These rules are exact for all  $p \in \Lambda_{-n, n}$ . Let  $A_{\mu, \tau}^{(n)}$  denote any one of these quadrature



rules. The following unitary upper Hessenberg matrix determines the weights and nodes of  $A_{\mu,\tau}^{(n)}$ :

$$\tilde{H}_{n+1}(\rho) := \tilde{D}_{n+1}^{-1/2} \begin{bmatrix} -\tilde{\gamma}_0\gamma_1 & -\tilde{\gamma}_0\gamma_2 & \cdots & -\tilde{\gamma}_0\tilde{\gamma}_n & -\tilde{\gamma}_0\rho \\ 1 - |\gamma_1|^2 & -\tilde{\gamma}_1\gamma_2 & \cdots & -\tilde{\gamma}_1\tilde{\gamma}_n & -\tilde{\gamma}_1\rho \\ 0 & 1 - |\gamma_2|^2 & \cdots & -\tilde{\gamma}_2\tilde{\gamma}_n & -\tilde{\gamma}_2\rho \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1 - |\tilde{\gamma}_n|^2 & -\tilde{\gamma}_n\rho \end{bmatrix} \tilde{D}_{n+1}^{1/2},$$

where  $\tilde{D}_{n+1} := \text{diag}[\tilde{\delta}_0, \tilde{\delta}_1, \dots, \tilde{\delta}_{n-1}, \tilde{\delta}_n]$  and  $\gamma_0 := 1$ ; cf. the discussion in Section 1 related to the matrix  $H_n(\tau)$  defined by (1.18). The weights are positive and the nodes lie on the unit circle. Note that the matrices  $\tilde{H}_{n+1}(\rho)$  and  $H_n(\tau)$  have the same  $(n-1) \times (n-1)$  leading principal submatrix.

We turn to the case when  $|\tilde{\gamma}_n| = 1$ . Now  $\tilde{I}$  is a positive  $n$ -definite linear functional, and Lemma 3.1 shows the existence of an  $n$ -point quadrature rule whose nodes are the zeros of  $\phi_n$  and whose weights are positive. We denote this rule by  $A_{\mu,\tau}^{(n)}$ , and note that, in view of Lemma 3.1,  $A_{\mu,\tau}^{(n)}$  is exact for all  $p \in \Lambda_{-n,n}$ . Since the  $n$ th coefficient  $\tilde{\gamma}_n$  is of unit modulus, the associated  $n \times n$  upper Hessenberg matrix  $H_n(\tilde{\gamma}_n)$ , defined by (1.18) with  $\tau := \tilde{\gamma}_n$  is unitary. In particular, the nodes determined by  $H_n(\tilde{\gamma}_n)$  lie on the unit circle and the corresponding weights are positive.  $\square$

We remark that if  $|\tilde{\gamma}_n| > 1$ , then  $\tilde{\Delta}_{n+1} < 0$ , and by Theorem 1.1 all zeros of  $\phi_n$  are outside the unit circle. Further properties of polynomials orthogonal with respect to an indefinite sesquilinear form are discussed by Landau [22].

We turn to the choice of coefficient  $c > 0$  in (1.20) and (2.2). It is convenient to write the expression (2.9) for  $\tilde{\gamma}_n$  in the form

$$(3.3) \quad \tilde{\gamma}_n = \gamma_n + c(\gamma_n - \tau).$$

**Corollary 3.3.** *For every  $\tau \in \Gamma$ , there is a unique positive constant  $c$ , given by*

$$(3.4) \quad c = \frac{1 - |\gamma_n|^2}{1 + |\gamma_n|^2 - 2 \text{Re}(\gamma_n \bar{\tau})},$$

such that  $\tilde{\gamma}_n$  defined by (3.3) is of unit modulus. The associated quadrature rule  $A_{\mu,\tau}^{(n)}$  is an  $n$ -point rule with positive weights and nodes on the unit circle.

*Proof.* Consider the function

$$F(x) = |\gamma_n + x(\gamma_n - \tau)|^2, \quad x \in \mathbb{R},$$

and recall that  $|\gamma_n| < 1$ . Clearly,  $\lim_{x \rightarrow 0} F(x) = |\gamma_n|^2$  and  $\lim_{x \rightarrow \infty} F(x) = \infty$ . By continuity of  $F$ , there is a constant  $c > 0$ , such that  $F(c) = 1$ . The unicity of this constant follows from the fact that  $F(x)$  is a parabola, and straightforward computation yields the value (3.4). Finally, the existence of the quadrature rule  $A_{\mu,\tau}^{(n)}$  with the specified properties is a consequence of Theorem 3.2.  $\square$

We refer to the  $n$ -point quadrature rule  $A_{\mu,\tau}^{(n)}$  determined in Corollary 3.3 as an anti-Szegő quadrature rule associated with the  $n$ -point Szegő rule  $S_{\mu,\tau}^{(n)}$ . Both rules  $A_{\mu,\tau}^{(n)}$  and  $S_{\mu,\tau}^{(n)}$  depend on the parameter  $\tau$  of unit modulus.

**Example 3.1.** Consider  $n$ -point quadrature rules associated with the measure  $d\mu(t) = dt$ . The Szegő polynomials are  $\psi_j(z) = z^j$ ,  $j = 0, 1, 2, \dots$ . In particular, all recursion coefficients  $\gamma_j$  vanish. Therefore, by (3.3),  $\tilde{\gamma}_n = -c\tau$ , and, by (3.4),  $c = 1$ . It follows that  $\tilde{\gamma}_n = -\tau$ . For any  $\tau \in \Gamma$ , the  $n$ -point Szegő and anti-Szegő quadrature rules are determined by the  $n \times n$  unitary upper Hessenberg matrices  $H_n(\tau)$  and  $H_n(-\tau)$ , respectively (cf. (1.18)). The nodes for the  $n$ -point Szegő rule are the zeros of  $\hat{\psi}_n(z) = z^n + \tau$  (cf. (1.15)), and the nodes for the associated anti-Szegő rule are the zeros of  $\hat{\phi}_n(z) = z^n - \tau$ . Thus, the nodes and weights for the  $n$ -point Szegő rule are given by

$$(3.5) \quad \lambda_m^{(n)} = \exp(i(\theta + 2m\pi)/n), \quad \omega_m^{(n)} = \frac{1}{n}, \quad m = 1, 2, \dots, n,$$

where  $-\tau = \exp(i\theta)$ , and the nodes and weights for the associated anti-Szegő rule are

$$(3.6) \quad \tilde{\lambda}_m^{(n)} = \exp(i(\theta + (2m + 1)\pi)/n), \quad \tilde{\omega}_m^{(n)} = \frac{1}{n}, \quad m = 1, 2, \dots, n.$$

**Example 3.2.** The monic Szegő polynomials associated with the measure  $d\mu(t) = 2\sin^2(t/2)dt$  are given by

$$\psi_j(z) = \frac{1}{j+1} \frac{1 - (j+2)z^{j+1} + (j+1)z^{j+2}}{(1-z)^2}, \quad j = 0, 1, 2, \dots,$$

with recursion coefficients  $\gamma_j = \psi_j(0) = 1/(j+1)$ ; see Bultheel et al. [4]. Let  $\tau \in \Gamma$  and consider  $n$ -point Szegő and anti-Szegő rules. Equations (3.3) and (3.4) yield

$$\tilde{\gamma}_n = \frac{c+1}{n+1} - c\tau, \quad c = \frac{n^2 + 2n}{n^2 + 2n + 2 - 2(n+1)\operatorname{Re}(\bar{\tau})}.$$

For instance,  $\tau = 1$  gives  $c = 1 + 2/n$  and  $\tilde{\gamma}_n = -1$ , and the desired Szegő and anti-Szegő quadrature rules are determined by the  $n \times n$  unitary Hessenberg matrices  $H_n(1)$  and  $H_n(-1)$ , respectively (cf. (1.18)). Similarly,  $\tau = -1$  yields  $c = n/(n+2)$  and  $\tilde{\gamma}_n = 1$ . The associated  $n$ -point Szegő and anti-Szegő rules are determined by the matrices  $H_n(-1)$  and  $H_n(1)$ , respectively.

The parameter  $\tau$  can be chosen arbitrarily on  $\Gamma$ . The choice

$$(3.7) \quad \tau := \begin{cases} \frac{\gamma_n}{|\gamma_n|}, & \text{if } \gamma_n \neq 0, \\ 1, & \text{if } \gamma_n = 0, \end{cases}$$

has received attention because the unitary upper Hessenberg matrix  $H_n(\tau)$  obtained for this value of  $\tau$  is a closest unitary matrix, in any unitarily invariant norm, to the upper Hessenberg matrix  $H_n(\gamma_n)$ ; see, e.g., [25] for a proof. The following theorem discusses Szegő and anti-Szegő quadrature rules obtained for  $\tau$  given by (3.7).

**Theorem 3.4.** *Let the parameter  $\tau$  be defined by (3.7). Then the pair of matrices  $H_n(\tau)$  and  $H_n(-\tau)$  determine the  $n$ -point Szegő and associated anti-Szegő quadrature rules, respectively.*

*Proof.* Let  $\gamma_n = 0$ . Then  $\tau = 1$  and, by (3.4),  $c = 1$ . It follows from (3.3) that  $\tilde{\gamma}_n = -1$ . Therefore, the pair of matrices  $H_n(1)$  and  $H_n(-1)$  determine the  $n$ -point Szegő and associated anti-Szegő quadrature rules.

We turn to the case  $\gamma_n \neq 0$ . Equations (3.4) and (3.7) yield

$$c = \frac{1 + |\gamma_n|}{1 - |\gamma_n|},$$

and it follows from (3.3) that

$$\tilde{\gamma}_n = -\frac{\gamma_n}{|\gamma_n|} = -\tau.$$

Thus, the pair of matrices  $H_n(\gamma_n/|\gamma_n|)$  and  $H_n(-\gamma_n/|\gamma_n|)$  determine associated  $n$ -point Szegő and anti-Szegő quadrature rules.  $\square$

In Laurie's discussion of anti-Gauss quadrature rules [23], the coefficient  $c$  in his analogue of equation (1.20) is set to one. In the remainder of this section we consider the case when  $c = 1$  in (1.20). Then the integration errors achieved with the Szegő rule  $S_{\mu,\tau}^{(n)}$  and anti-Szegő rule  $A_{\mu,\tau}^{(n)}$  are of opposite sign and of the same modulus for all Laurent polynomials in  $\Lambda_{-n,n}$ . The following theorem is concerned with the expression (3.3) for  $\tilde{\gamma}_n$  when  $c = 1$ , and shows how to choose the auxiliary parameter  $\tau$  in (1.18) so that  $|\tilde{\gamma}_n| = 1$ .

**Theorem 3.5.** *Let  $\tau \in \Gamma$  satisfy  $|2\gamma_n - \tau| = 1$ , and define  $\tilde{\gamma}_n = 2\gamma_n - \tau$ . Then  $S_{\mu,\tau}^{(n)}$  and  $A_{\mu,\tau}^{(n)}$  form a pair of  $n$ -point Szegő and anti-Szegő quadrature rules.*

*Proof.* We remark that the choice of  $\tilde{\gamma}_n$  corresponds to  $c = 1$  in (2.9). Since  $|\gamma_n| < 1$ , the set  $W := \{w \in \Gamma : |2\gamma_n - w| = 1\}$  is not empty. In particular,  $\gamma_n \neq 0$  yields  $W = \{\frac{\gamma_n}{|\gamma_n|} \exp(\pm i\theta)\}$  with  $\cos(\theta) = |\gamma_n|$ . If  $\gamma_n = 0$ , then  $W = \Gamma$ . The result now follows from Theorem 3.2.  $\square$

*Remark.* By Corollary 3.3 there is a unique positive constant  $c$  associated with each parameter  $\tau \in \Gamma$ . The different possible values of  $\tau$  in Theorem 3.5 correspond to  $c = 1$  in (3.3). Thus, different values of  $\tau$  may yield the same constant  $c$ .

**Example 3.3.** Consider the same measure as in Example 3.2. We have  $\gamma_n = 1/(n+1)$  and would like to determine  $\tau \in \Gamma$ , so that  $|\frac{2}{n+1} - \tau| = 1$ . This yields

$$\tau = \frac{1}{n+1} \pm i\sqrt{1 - \left(\frac{1}{n+1}\right)^2}, \quad \tilde{\gamma}_n \frac{1}{n+1} \mp i\sqrt{1 - \left(\frac{1}{n+1}\right)^2} = \bar{\tau}.$$

Thus, the nodes and weights of the  $n$ -point Szegő and associated anti-Szegő quadrature rules are determined by  $H_n(\tau)$  and  $H_n(\bar{\tau})$ , respectively.

#### 4. APPLICATIONS OF ANTI-SZEGŐ QUADRATURE RULES

An important application of Szegő and anti-Szegő quadrature rules is the approximation of integrals with periodic integrands. Let  $T$  be a  $2\pi$ -periodic function. Analogously to (1.12) and (1.13), we define

$$(4.1) \quad S_{\mu,\tau}^{(n)}(T) = \sum_{m=1}^n \omega_m^{(n)} T(\theta_m^{(n)}), \quad \lambda_m^{(n)} = \exp(i\theta_m^{(n)}),$$

$$(4.2) \quad A_{\mu,\tau}^{(n)}(T) = \sum_{m=1}^n \tilde{\omega}_m^{(n)} T(\tilde{\theta}_m^{(n)}), \quad \tilde{\lambda}_m^{(n)} = \exp(i\tilde{\theta}_m^{(n)}),$$

$$(4.3) \quad I(T) = \frac{1}{2\pi} \int_{-\pi}^{\pi} T(t) d\mu(t).$$

We may assume that  $T(t)$  is real-valued; otherwise, we integrate the real and imaginary parts separately.

There is a sequence of orthogonal trigonometric polynomials  $P_{0,0}, P_{1,0}, P_{1,1}, P_{2,1}, P_{2,2}, \dots$  with respect to the inner product

$$(T, U) := \frac{1}{2\pi} \int_{-\pi}^{\pi} T(t)U(t)d\mu(t).$$

Here  $P_{r,s}$  denotes a trigonometric polynomial of degree  $r$ ; i.e.,

$$\begin{aligned} P_{0,0}(t) &= 1, \\ P_{k,k-1}(t) &= \sin(kt) + \sum_{j=0}^{k-1} (\tilde{s}_j \sin(jt) + \tilde{c}_j \cos(jt)), \\ P_{k,k}(t) &= \cos(kt) + s_k \sin(kt) + \sum_{j=0}^{k-1} (\hat{s}_j \sin(jt) + \hat{c}_j \cos(jt)) \end{aligned}$$

for certain coefficients  $\tilde{s}_j, \tilde{c}_j, s_j, \hat{s}_j$ , and  $\hat{c}_j$ ; see, e.g., [7, 24] for details.

Assume that  $T(t)$  can be expressed as

$$T(t) = \sum_{j=0}^{\infty} (\alpha_j P_{j,j-1}(t) + \beta_j P_{j,j}(t)),$$

where the coefficients  $\alpha_j, \beta_j \in \mathbb{R}$  converge sufficiently rapidly to zero to allow term-wise integration and  $P_{0,-1}(t) := 0$ . The orthogonality of the  $P_{r,s}$  yields  $I(P_{0,0}) = 1$  and  $I(P_{r,s}) = 0$  for all  $r, s > 0$ . It follows that  $I(T) = \beta_0$ . We obtain from (1.14) that  $S_{\mu,\tau}^{(n)}(P_{0,0}) = 1$  and  $S_{\mu,\tau}^{(n)}(P_{r,s}) = 0$  for  $0 < r, s < n$ . Analogous results hold for the anti-Szegő rule  $A_{\mu,\tau}^{(n)}$ . Combining these properties shows that

$$(4.4) \quad \begin{aligned} S_{\mu,\tau}^{(n)}(T) &= I(T) + \alpha_n S_{\mu,\tau}^{(n)}(P_{n,n-1}) + \beta_n S_{\mu,\tau}^{(n)}(P_{n,n}) \\ &\quad + \sum_{j=n+1}^{\infty} \{ \alpha_j S_{\mu,\tau}^{(n)}(P_{j,j-1}) + \beta_j S_{\mu,\tau}^{(n)}(P_{j,j}) \} \end{aligned}$$

$$(4.5) \quad \begin{aligned} A_{\mu,\tau}^{(n)}(T) &= \sum_{j=0}^n \{ (1+c)I - cS_{\mu,\tau}^{(n)} \} (\alpha_j P_{j,j-1} + \beta_j P_{j,j}) \\ &\quad + \sum_{j=n+1}^{\infty} A_{\mu,\tau}^{(n)}(\alpha_j P_{j,j-1} + \beta_j P_{j,j}) \\ &= I(T) - c\alpha_n S_{\mu,\tau}^{(n)}(P_{n,n-1}) - c\beta_n S_{\mu,\tau}^{(n)}(P_{n,n}) \\ &\quad + \sum_{j=n+1}^{\infty} \{ \alpha_j A_{\mu,\tau}^{(n)}(P_{j,j-1}) + \beta_j A_{\mu,\tau}^{(n)}(P_{j,j}) \}. \end{aligned}$$

Assume that the coefficients  $\alpha_j$  and  $\beta_j$  converge so rapidly to zero with increasing index that the leading terms in (4.4) and (4.5) dominate the integration errors, i.e.,

$$(4.6) \quad E^{(n)}(T) := (I - S_{\mu,\tau}^{(n)})(T) \approx -\alpha_n S_{\mu,\tau}^{(n)}(P_{n,n-1}) - \beta_n S_{\mu,\tau}^{(n)}(P_{n,n}),$$

$$(4.7) \quad \tilde{E}^{(n)}(T) := (I - A_{\mu,\tau}^{(n)})(T) \approx c\alpha_n S_{\mu,\tau}^{(n)}(P_{n,n-1}) + c\beta_n S_{\mu,\tau}^{(n)}(P_{n,n}),$$

where  $\approx$  stands for ‘‘approximately equal to’’. In this situation, the errors  $E^{(n)}(T)$  and  $\tilde{E}^{(n)}(T)$  are of opposite sign; i.e., the computed approximations  $S_{\mu,\tau}^{(n)}(T)$  and

TABLE 4.1. This is a description of Example 4.1. Error  $E^{(n)}(T)$  and error estimate  $\hat{E}^{(n)}(T)$  for the  $n$ -point Szegő rule, error  $\tilde{E}^{(n)}(T)$  for the  $n$ -point anti-Szegő rule, and error  $\mathcal{E}^{(n)}(T)$  for the associated average rule for the integrand  $T(t) := \ln(1 + \cos(t) + \sin^2(t/2))$  and three values of  $n$ .  $I(T) = 0.37645281291920$ .

	$n = 4$	$n = 5$	$n = 6$
$E^{(n)}(T)$	$4.3 \cdot 10^{-4}$	$-5.9 \cdot 10^{-5}$	$8.5 \cdot 10^{-6}$
$\hat{E}^{(n)}(T)$	$4.3 \cdot 10^{-4}$	$-5.9 \cdot 10^{-5}$	$8.5 \cdot 10^{-6}$
$\tilde{E}^{(n)}(T)$	$-4.3 \cdot 10^{-4}$	$5.9 \cdot 10^{-5}$	$-8.5 \cdot 10^{-6}$
$\mathcal{E}^{(n)}(T)$	$1.9 \cdot 10^{-7}$	$4.4 \cdot 10^{-9}$	$1.1 \cdot 10^{-10}$

$A_{\mu,\tau}^{(n)}(T)$  bracket  $I(T)$ . Note that the expressions (4.6) and (4.7) are consistent with (1.20); i.e., they show that

$$\tilde{E}^{(n)}(T_n) = -cE^{(n)}(T_n)$$

for all trigonometric polynomials  $T_n$  of degree at most  $n$ .

Consider the estimate

$$(4.8) \quad \hat{E}^{(n)} := \frac{1}{c+1}(A_{\mu,\tau}^{(n)} - S_{\mu,\tau}^{(n)})$$

of the integration error  $E^{(n)}$  (cf. (1.22)). It follows from (4.6) and (4.7) that

$$\hat{E}^{(n)}(T) = \frac{1}{c+1}\{E^{(n)}(T) - \tilde{E}^{(n)}(T)\} \approx -\alpha_n S_{\mu,\tau}^{(n)}(P_{n,n-1}) - \beta_n S_{\mu,\tau}^{(n)}(P_{n,n}).$$

In particular,  $\hat{E}^{(n)}(T_n) = E^{(n)}(T_n)$  for every trigonometric polynomial  $T_n$  of degree at most  $n$ .

Equation (1.23) suggests that the quadrature rule

$$(4.9) \quad \mathcal{L}^{(n)} := \left(\frac{1}{c+1}\right)A_{\mu,\tau}^{(n)} + \left(\frac{c}{c+1}\right)S_{\mu,\tau}^{(n)}$$

be considered. We refer to this rule as the *average rule*. It satisfies

$$\begin{aligned} \mathcal{L}^{(n)}(T) &= I(T) + \frac{1}{1+c} \sum_{j=n+1}^{\infty} \{\alpha_j A_{\mu,\tau}^{(n)}(P_{j,j-1}) + \beta_j A_{\mu,\tau}^{(n)}(P_{j,j})\} \\ &\quad + \frac{c}{1+c} \sum_{j=n+1}^{\infty} \{\alpha_j S_{\mu,\tau}^{(n)}(P_{j,j-1}) + \beta_j S_{\mu,\tau}^{(n)}(P_{j,j})\} \\ &= I(T) + \sum_{j=n+1}^{\infty} \{\alpha_j \mathcal{L}^{(n)}(P_{j,j-1}) + \beta_j \mathcal{L}^{(n)}(P_{j,j})\}. \end{aligned}$$

Thus,  $\mathcal{L}^{(n)}(T_n) = I(T_n)$  for all trigonometric polynomials  $T_n$  of degree at most  $n$ . The following computed example illustrates that the average rule  $\mathcal{L}^{(n)}$  may yield higher accuracy than the associated Szegő and anti-Szegő quadrature rules. We tabulate the integration error

$$\mathcal{E}^{(n)}(T) := (I - \mathcal{L}^{(n)})(T).$$

**Example 4.1.** We illustrate the performance of Szegő and anti-Szegő quadrature rules associated with the measure  $d\mu(t) = dt$  considered in Example 3.1. In particular, the constant  $c$  in (4.8) and (4.9) is unity. For  $2\pi$ -periodic integrands, the Szegő quadrature rule (4.1) determined by the nodes and weights (3.5) with  $\theta = 0$  is the trapezoidal rule, and the anti-Szegő quadrature rule (4.2) defined by the nodes and weights (3.6) with  $\theta = 0$  is the midpoint rule. We would like to determine approximations of the integral (4.3) with the integrand  $T(t) := \ln(1 + \cos(t) + \sin^2(t/2))$  using these and the average quadrature rules. The value of the integral can be shown to be

$$I(T) = \ln\left(\frac{3}{4} + \frac{1}{2}\sqrt{2}\right) \approx 0.37645281291920.$$

The integration errors  $E^{(n)}(T)$  for the trapezoidal rule and  $\tilde{E}^{(n)}(T)$  for the midpoint rule are displayed in Table 4.1. They can be seen to be of opposite sign for fixed values of  $n$ . The table also shows  $\hat{E}^{(n)}(T)$  to be an accurate approximation of  $E^{(n)}(T)$ .

In this example  $\mathcal{L}^{(n)} = S_{\mu,\tau}^{(2n)}$ . It is known that the trapezoidal rule converges rapidly for analytic periodic integrands with an increasing number of nodes; see, e.g., Henrici [19, Section 11.11]. Formula (4.9) therefore suggests that the errors in  $S_{\mu,\tau}^{(n)}(T)$  and  $A_{\mu,\tau}^{(n)}(T)$  are of about the same modulus but of opposite sign. Table 4.1 shows this indeed to be the case.

**Example 4.2.** Let the measure be defined by the Poisson kernel

$$d\mu(t) = \frac{1 - r^2}{1 - 2r \cos(t) + r^2} dt,$$

where  $0 < r < 1$ . The associated orthonormal Szegő polynomials are given by  $\psi_0(z) = 1$  and

$$\psi_n(z) = \frac{z^n - rz^{n-1}}{\sqrt{1 - r^2}}, \quad n = 1, 2, \dots ;$$

see, e.g., [17]. In particular,  $\gamma_1 = -r$ ,  $\delta_1 = 1 - r^2$ , and  $\gamma_n = 0$  for  $n > 1$ . Hence,  $c = 1$  and  $\tilde{\gamma}_n = -\tau$  for  $n > 1$ .

Consider the approximation of the integral (4.3) for  $T(t) := \frac{1}{2} \log(5 + 4 \cos(t))$ . Table 4.2 shows the performance of Szegő and anti-Szegő rules, as well as of the average rule (4.9), for  $r = 1/2$  and  $\tau = 1$ . The errors (4.6) and (4.7) can be seen to be of about the same magnitude and of opposite sign. Note that  $S_{\mu,\tau}^{(n)}(T)$  is larger

TABLE 4.2. This is a description of Example 4.2. Error  $E^{(n)}(T)$  and error estimate  $\hat{E}^{(n)}(T)$  for the  $n$ -point Szegő rule, error  $\tilde{E}^{(n)}(T)$  for the  $n$ -point anti-Szegő rule, and error  $\mathcal{E}^{(n)}(T)$  for the associated average rule for the integrand  $T(t) := \frac{1}{2} \log(5 + 4 \cos(t))$  for three values of  $n$ .  $I(T) = 0.91629073187416$ .

	$n = 9$	$n = 12$	$n = 18$
$E^{(n)}(T)$	$1.1 \cdot 10^{-4}$	$-1.0 \cdot 10^{-5}$	$-1.0 \cdot 10^{-7}$
$\hat{E}^{(n)}(T)$	$1.1 \cdot 10^{-4}$	$-1.0 \cdot 10^{-5}$	$-1.0 \cdot 10^{-7}$
$\tilde{E}^{(n)}(T)$	$-1.1 \cdot 10^{-4}$	$1.0 \cdot 10^{-5}$	$1.0 \cdot 10^{-7}$
$\mathcal{E}^{(n)}(T)$	$1.7 \cdot 10^{-7}$	$2.0 \cdot 10^{-9}$	$3.3 \cdot 10^{-13}$

than  $A_{\mu,\tau}^{(n)}(T)$  for  $n = 12$  and  $18$ , but smaller than  $A_{\mu,\tau}^{(n)}(T)$  for  $n = 9$ . Moreover,  $\hat{E}^{(n)}(T)$  furnishes an accurate estimate of the error (4.6). The average rule  $\mathcal{L}^{(n)}(T)$  is seen to give better approximations of  $I(T)$  than  $S_{\mu,\tau}^{(n)}(T)$  and  $A_{\mu,\tau}^{(n)}(T)$  for the same values of  $n$ .

We conclude with some comments on the computation of the exact value of  $I(T)$ . For functions  $u(z)$  which are harmonic in the unit disk, we have

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} u(e^{it}) \frac{1-r^2}{1-2r\cos(\theta-t)+r^2} dt = u(re^{i\theta}).$$

Since  $T(t) = \log|e^{it} + 2|$ , we define  $u(z) = \log|z + 2|$ . Then, for  $r = 1/2$ , we obtain that  $I(T) = u(\frac{1}{2}e^{i0}) = u(1/2) = \log(5/2) = 0.91629073187416$ .

## 5. CONCLUSIONS

This paper presents and analyzes anti-Szegő rules, a new type of quadrature rule for Laurent and trigonometric polynomials. When used together with Szegő rules, they furnish error estimates for the latter. Moreover, they can be used to define the average rule (4.9) which often yields higher accuracy than the corresponding Szegő and anti-Szegő rules.

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## REFERENCES

1. G. S. Ammar and W. B. Gragg, *Generalized Schur Algorithm for the superfast solution of Toeplitz systems*, In J. Gilewicz, M. Pindor, and W. Siemaszko, eds., *Rational Approximation and its Application in Mathematics and Physics*, Lecture Notes in Mathematics #1237, pages 315–330, Springer, Berlin, 1987. MR0886705 (88c:65032)
2. G. S. Ammar, W. B. Gragg, and L. Reichel, *On the eigenproblem for orthogonal matrices*, In *Proceedings of the 25th IEEE Conference on Decision and Control*, pages 1963–1966, IEEE, Piscataway, 1986.
3. G. S. Ammar, L. Reichel, and D. C. Sorensen, *Algorithm 730: An implementation of a divide and conquer algorithm for the unitary eigenproblem*, *ACM Trans. Math. Software*, 18:292–307, 1992, and 20:161, 1994.
4. A. Bultheel, L. Daruis, and P. González-Vera, *A connection between quadrature formulas on the unit circle and the interval  $[-1, 1]$* , *J. Comput. Appl. Math.*, 132:1–14, 2001. MR1834799 (2002c:65042)
5. L. Daruis, P. González-Vera, and O. Njåstad, *Szegő quadrature formulas for certain Jacobi-type weight functions*, *Math. Comp.*, 71:683–701, 2002. MR1885621 (2002k:41043)
6. R. L. Ellis and I. Gohberg, *Orthogonal Systems and Convolution Operators*. *Operator Theory: Advances and Applications*, vol. 140. Birkhäuser, Basel, 2003. MR1942683 (2004b:42055)
7. H. Faßbender, *A note on Newbery's algorithm for discrete least-squares approximation by trigonometric polynomials*, *Electron. Trans. Numer. Anal.*, 4:64–74, 1996. MR1401445 (97k:65034)
8. G. Freud, *Orthogonal Polynomials*, Pergamon Press, New York, 1971.
9. L. Y. Geronimus, *Orthogonal Polynomials*, Consultants Bureau, New York, 1961. MR0133643 (24:A3469)
10. G. H. Golub and G. Meurant, *Matrices, moments and quadrature*, In D. F. Griffiths and G. A. Watson, eds, *Numerical Analysis 1993*, pages 105–156. Longman, Essex, 1994. MR1267758 (95b:65042)
11. W. B. Gragg, *Positive definite Toeplitz matrices, the Arnoldi process for isometric operators, and Gaussian quadrature on the unit circle*(in Russian), In E. S. Nicholaev, ed., *Numerical Methods in Linear Algebra*, pages 16–32, Moscow University Press, Moscow, 1982. Published

- in English in slightly modified form in *J. Comput. Appl. Math.*, 46:183–198, 1993. MR1222480 (94e:65046)
12. W. B. Gragg, *The QR algorithm for unitary Hessenberg matrices*, *J. Comput. Appl. Math.*, 16:1–8, 1986.
  13. W. B. Gragg, *Stabilization of the UHQR algorithm*, In Z. Chen, Y. Li, C. Micchelli, and Y. Xu, eds, *Advances in Computational Mathematics, Lecture Notes in Pure and Applied Mathematics*, vol. 202, pages 139–154. Marcel Dekker, Hong Kong, 1999. MR1661531
  14. W. B. Gragg and L. Reichel, *A divide and conquer method for the unitary eigenproblem*, In M. T. Heath, ed., *Hypercube Multiprocessors 1987*, pages 639–647, SIAM, Philadelphia, 1987. MR1014280
  15. W. B. Gragg and L. Reichel, *A divide and conquer method for the unitary and orthogonal eigenproblems*, *Numer. Math.*, 57:695–718, 1990. MR1065519 (91h:65052)
  16. U. Grenander and G. Szegő, *Toeplitz Forms and Their Application*, Chelsea, New York, 1984. MR0890515 (88b:42031)
  17. P. González-Vera, J.C. Santos-León, and O. Njåstad, *Some results about numerical quadrature on the unit circle*, *Adv. Comput. Math.*, 5:297–328, 1996. MR1414284 (98f:41028)
  18. M. Gu, R. Guzzo, X.-b. Chi, and X.-Q. Cao, *A stable divide and conquer algorithm for the unitary eigenproblem*, *SIAM J. Matrix Anal. Appl.*, 25:385–404, 2003. MR2047425 (2005d:65056)
  19. P. Henrici, *Applied and Computational Complex Analysis*, vol. 2. Wiley, New York, 1977. MR0453984 (56:12235)
  20. W. B. Jones, O. Njåstad, and W. J. Thron, *Moment theory, orthogonal polynomials, quadrature and continued fractions associated with the unit circle*, *Bull. London Math. Soc.*, 21:113–152, 1989. MR0976057 (90e:42027)
  21. T. Kailath, *Linear estimation for stationary and near-stationary processes*, In T. Kailath, ed., *Modern Signal Processing*, pages 59–128. Hemisphere Publ., Washington, DC, 1985.
  22. H. J. Landau, *Polynomials orthogonal in an indefinite metric*, In I. Gohberg, ed., *Orthogonal Matrix-Valued Polynomials and Applications, Operator Theory: Advances and Applications*, vol. 34, pages 203–214, Birkhäuser, Basel, 1988. MR1021064
  23. D. P. Laurie, *Anti-Gaussian quadrature formulas*, *Math. Comp.*, 65: 739–747, 1996. MR1333318 (96m:65026)
  24. A. C. R. Newbery, *Trigonometric interpolation and curve-fitting*, *Math. Comp.*, 24: 869–876, 1970. MR0279966 (43:5687)
  25. L. Reichel and G. S. Ammar, *Fast approximation of dominant harmonics by solving an orthogonal eigenvalue problem*, In J. G. McWhirter, ed., *Mathematics in Signal Processing II*, pages 575–591, Clarendon Press, Oxford, 1990.
  26. M. Stewart, *Stability properties of several variants of the unitary QR algorithm*, In V. Olshevsky, ed., *Structured Matrices in Mathematics, Computer Science, and Engineering II*, pages 57–72, Amer. Math. Soc., Providence, 2001. MR1855505 (2002f:65055)
  27. M. Stewart, *An error analysis of a unitary Hessenberg QR algorithm*, *SIAM J. Matrix. Anal. Appl.*, to appear.
  28. G. Szegő, *Orthogonal Polynomials*, 4th ed., Amer. Math. Soc., Providence, 1975. MR0372517 (51:8724)

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