Generalized averaged Szegő quadrature rules

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Abstract

Szegő quadrature rules are commonly applied to integrate periodic functions on the unit circle in the complex plane. However, often it is difficult to determine the quadrature error. Recently, Spalević introduced generalized averaged Gauss quadrature rules for estimating the quadrature error obtained when applying Gauss quadrature over an interval on the real axis. We describe analogous quadrature rules for the unit circle that often yield higher accuracy than Szegő rules using the same moment information and may be used to estimate the error in Szegő quadrature rules.

Keywords: Szegő quadrature, error estimation, periodic functions, generalized averaged Gauss quadrature

1. Introduction

We are concerned with quadrature rules for integrals of the form

$$\mathcal{I}(f) := \frac{1}{2\pi}\int_{-\pi}^{\pi} f(e^{i\theta})\mathrm{d}\mu(\theta), \tag{1.1}$$

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Dedicated to Bill Gragg on the occasion of his 80th birthday.

where the measure $\mu(\theta)$ is nondecreasing and has infinitely many points of increase, and is such that all *moments*

$$\mu_j \coloneqq \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-ij\theta}\,\mathrm{d}\mu(\theta), \quad j = 0, \pm 1, \pm 2, \dots\ , \tag{1.2}$$

exist and are finite. For notational convenience, we let μ be scaled so that $\mu_0 = 1$. The integrand f is assumed to be continuous on the interval $[-\pi, \pi]$.

Introduce for polynomials g and h the inner product

$$(g, h) \coloneqq \frac{1}{2\pi}\int_{-\pi}^{\pi} \overline{g(e^{i\theta})} h(e^{i\theta}) \mathrm{d}\mu(\theta), \tag{1.3}$$

where $i := \sqrt{-1}$ and the bar denotes complex conjugation. There is an infinite sequence of monic orthogonal polynomials $\{\psi_j\}_{j=0}^{\infty}$ with respect to this inner product. The ψ_j are known as *Szegő polynomials* and satisfy the following recursion relations

$$\begin{aligned}
\psi_0(z) &= \psi_0^*(z) = 1, && (1.4)\\
\psi_j(z) &= z\psi_{j-1}(z) + \gamma_j \psi_{j-1}^*(z), \qquad j = 1, 2, 3, \dots\ , && (1.5)\\
\psi_j^*(z) &= \bar{\gamma}_j z \psi_{j-1}(z) + \psi_{j-1}^*(z), && (1.6)
\end{aligned}$$

where $\psi_j^*(z) := z^j \bar{\psi}_j(z^{-1})$. Thus, 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 ψ_j^* are sometimes referred to as *reversed polynomials*. We have $\psi_j^*(0) = 1$ for all $j \geq 0$ and, therefore, by (1.5), the recursion coefficients satisfy $\gamma_j = \psi_j(0)$, $j = 1, 2, 3, \dots$. They are known as *Schur parameters* or *reflection coefficients* and satisfy $|\gamma_j| < 1$ for all j. The recursion coefficients can be computed by combining (1.4)-(1.6) with

$$\begin{aligned}
&\gamma_j = -(1, z\psi_{j-1})/\delta_{j-1},\\
&\delta_j = \delta_{j-1}(1 - |\gamma_j|^2),
\end{aligned} \qquad j = 1, 2, 3, \dots\ , \tag{1.7}$$

where $\delta_0 = 1$. Many properties of Szegő polynomials are described in, e.g., [22, 26].

We are interested in approximating the integral (1.1) by quadrature rules of the form

$$S_\tau^{(n)}(f) = \sum_{k=1}^{n} \omega_k^{(n)} f(\lambda_k^{(n)}), \quad \omega_k^{(n)} > 0, \quad \lambda_k^{(n)} \in \Gamma, \tag{1.8}$$

where $\Gamma := \{z \in \mathbb{C} : |z| = 1\}$ denotes the unit circle in the complex plane. The $\lambda_k^{(n)}$ are nodes and the $\omega_k^{(n)}$ weights of the quadrature rule. The nodes depend on the parameter τ. This will be discussed below.

Let $\Lambda_{-(n-1),n-1}$ denote the set of Laurent polynomials

$$L_{n-1}(z) = \sum_{k=-(n-1)}^{n-1} c_k z^k, \quad c_k \in \mathbb{C}, \tag{1.9}$$

of order at most $n-1$. The quadrature rule (1.8) is said to be a *Szegő quadrature rule* if

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

where the integral $\mathcal{I}$ is defined by (1.1). This requirement defines the n-point Szegő rule uniquely up to the location of one node, say $\lambda_1^{(n)}$, which can be chosen arbitrarily on the unit circle; see, e.g., [9, 15]. There are no quadrature rules of the form (1.8) that are exact for all Laurent polynomials of order n. The parameter τ will be used to fix the node $\lambda_1^{(n)}$; see Section 2.

Laurent polynomials (1.9) with $z = \exp(i\theta)$, $\theta \in \mathbb{R}$, are trigonometric polynomials in θ. For instance,

$$L_{n-1}(\exp(i\theta)) = a_0 + \sum_{k=1}^{n-1}(a_k \cos(k\theta) + b_k \sin(k\theta)),$$

for appropriate coefficients $a_k, b_k \in \mathbb{C}$. Szegő quadrature rules are quadrature rules for trigonometric polynomials of maximal order. This makes them attractive to use for the integration of periodic functions.

Example 1.1. In the special case when $\mathrm{d}\mu(t) = \mathrm{d}t$, the moments are given by $\mu_0 = 1$ and $\mu_j = 0$ for $j \geq 1$. All recursion coefficients γ_j vanish and, therefore, $\psi_j(z) = z^j$ for $j = 0, 1, 2, \ldots$. The Szegő rule (1.8) has equidistant nodes $\lambda_k^{(n)} \in \Gamma$ on the unit circle and weights $\omega_k^{(n)} = 1/n$ for $1 \leq k \leq n$. This follows from Proposition 2.1 below. The node $\lambda_1^{(n)} \in \Gamma$ can be chosen arbitrarily. Thus, the Szegő rule is a trapezoidal rule. It is well known that the trapezoidal rule gives high accuracy when applied to the integration of smooth periodic functions. Assume that the integrand f is analytic in the annulus $\{z \in \mathbb{C} : 1/\rho \leq |z| \leq \rho\}$ for some $\rho > 1$. Then

$$|S_\tau^{(n)}(f) - \mathcal{I}(f)| \leq C\rho^{-n}, \tag{1.11}$$

where the constant C can be chosen independently of n; see Henrici [13] or Trefethen and Weideman [27] for details. □

It is the purpose of the present paper to present new quadrature rules for the approximation of integrals of the form (1.1). They are analogues for

integration on the unit circle of the generalized averaged Gauss rules proposed by Spalević [23, 24]. The new rules use the same moment information as the Szegő rule (1.8) but can yield higher accuracy, because they use more nodes. They also can be used to estimate the quadrature error

$$\mathcal{E}_n(f) := \mathcal{I}(f) - S_\tau^{(n)}(f)$$

in Szegő rules (1.8). Estimation of the size of this error is helpful in determining how large n should be chosen in order to obtain an approximation of desired accuracy.

This paper is organized as follows. Section 2 reviews an approach proposed by Gragg [9] for computing the nodes and weights of an n-node Szegő quadrature rule (1.8) from the recursion coefficients. The latter can be determined from the moments (1.2) by the Levinson or Schur algorithms; see, e.g., [9, 14, 17] for details on these algorithms. Sections 3 and 4 describe two analogues of the averaged Gauss rules proposed by Spalević [23, 24] for integration on (part of) the real axis. The new quadrature rules have $2n$ nodes on the unit circle; the set of quadrature nodes of the rules in Section 3 generally do not contain the nodes of the Szegő rule (1.8) as a subset, while the rules described in Section 4 do. Anti-Szegő quadrature rules, described in [18], furnish another approach to estimate the error in Szegő rules (1.8). They are analogues of the anti-Gauss rules introduced by Laurie [19] for estimating the error in Gauss quadrature rules. We outline anti-Szegő rules in Section 5. Computed examples that illustrate the performance of the generalized averaged quadrature rules and compare them to anti-Szegő rules are presented in Section 6. Concluding remarks can be found in Section 7.

2. Computation of Szegő quadrature rules

Gragg [9] and Jones et al. [16] show that the nodes $\lambda_m^{(n)}$ of an n-point Szegő quadrature rule (1.8) are the zeros of the para-orthogonal polynomial

$$B_n(z;\tau) := \psi_n(z) + \tau\psi_n^*(z), \tag{2.1}$$

where $\tau \in \Gamma$ is an arbitrary but fixed parameter. The weights can be expressed as

$$\omega_k^{(n)} = \mathcal{I}(\ell_k), \quad k = 1, 2, \ldots, n,$$

where the ℓ_k are Lagrange polynomials determined by the nodes,

$$\ell_k(z) := \prod_{\substack{j=1 \\ j\neq k}}^{n} \frac{z - \lambda_j^{(n)}}{\lambda_k^{(n)} - \lambda_j^{(n)}}.$$

Introduce the upper Hessenberg matrix

$$\widetilde{H}_n(\tau) \coloneqq \begin{bmatrix} -\bar{\gamma}_0\gamma_1 & -\bar{\gamma}_0\gamma_2 & \cdots & -\bar{\gamma}_0\gamma_{n-1} & -\bar{\gamma}_0\tau \\ 1-|\gamma_1|^2 & -\bar{\gamma}_1\gamma_2 & \cdots & -\bar{\gamma}_1\gamma_{n-1} & -\bar{\gamma}_1\tau \\ 0 & 1-|\gamma_2|^2 & \cdots & -\bar{\gamma}_2\gamma_{n-1} & -\bar{\gamma}_2\tau \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \cdots & 1-|\gamma_{n-1}|^2 & -\bar{\gamma}_{n-1}\tau \end{bmatrix} \in \mathbb{C}^{n\times n}, \quad (2.2)$$

where $\gamma_0 \coloneqq 1$ and $\tau \in \Gamma$, and define the diagonal matrix

$$D_n \coloneqq \operatorname{diag}[\delta_0, \delta_1, \ldots, \delta_{n-1}].$$

Gragg [9] considered the matrix

$$H_n(\tau) \coloneqq D_n^{-1/2}\widetilde{H}_n(\tau)D_n^{1/2}, \quad (2.3)$$

which is similar to $\widetilde{H}_n(\tau)$. The following results are due to Gragg [9].

Proposition 2.1. *The matrix* (2.3) *is unitary, its eigenvalues are the zeros of the para-orthogonal polynomial* (2.1) *and therefore are the nodes* $\lambda_k^{(n)}$, $k = 1, 2, \ldots, n$, *of the Szegő rule* (1.8), *and the magnitude squared of the first component of the unit eigenvectors of* $H_n(\tau)$ *are the weights* $\omega_k^{(n)}$, $k = 1, 2, \ldots, n$, *of the Szegő rule.*

The matrix (2.3) is determined by the parameters $\gamma_1, \gamma_2, \ldots, \gamma_{n-1}, \tau$, where $\gamma_1, \gamma_2, \ldots, \gamma_{n-1}$ can be computed with the Levinson or Schur algorithms from the moments $\{\mu_j\}_{j=0}^{n-1}$; see, e.g., [9, 14, 17].

Example 2.1. Consider the case when $\mathrm{d}\mu(t) = \mathrm{d}t$. As pointed out in Example 1.1, all recursion coefficients γ_j vanish. Therefore $\delta_j = 1$ for all j and it follows that the matrices (2.2) and (2.3) are identical with all entries zero except for the subdiagonal entries 1 and the $(1, n)$-entry $-\tau$. When $\tau = -1$, we have that (2.2) is the cyclic downshift matrix with eigenvalues $\lambda_k^{(n)} = \exp(2\pi i(k-1)/n)$, $k = 1, 2, \ldots, n$. These are the nodes of the Szegő rule; the weights are $1/n$. Changing $\tau \in \Gamma$ rotates the nodes on the unit circle. For instance, $\tau = 1$ yields a Hessenberg matrix (2.2) with eigenvalues $\lambda_k^{(n)} = \exp(2\pi i(k-1/2)/n)$, $k = 1, 2, \ldots, n$. □

Several fast algorithms for computing the nodes and weights of the Szegő rule (1.8) from $\gamma_1, \gamma_2, \ldots, \gamma_{n-1}, \tau$, without explicitly forming the matrix (2.3), are discussed in [2, 3, 5, 10, 11, 12, 25].

3. Generalized averaged Szegő rules I

The nodes and weights of an n-point Gauss quadrature rule are the eigenvalues and square of the first components of suitably normalized eigenvectors of a symmetric tridiagonal matrix T_n, respectively; see, e.g., Gautschi [8]. Spalević [23] proposed that the last diagonal entry of T_n be replaced by the matrix S_{n-1} obtained by flipping the leading principal $(n-1)\times(n-1)$ submatrix of T_n upside-down and right-left. This yields a symmetric tridiagonal matrix of order $2n-2$ that defines a new quadrature rule that Spalević refers to as a generalized averaged Gauss rule. Properties and applications are described in [21, 23, 24]. This section describes an extension of the rules (1.8). This extension is inspired by the work of Spalević [23, 24]. We refer to the extended quadrature rules obtained as generalized averaged Szegő rules. A different extension will be considered in the next section.

We define the generalized averaged Szegő quadrature rule

$$\widehat{S}_\tau^{(2n-2)}(f)=\sum_{k=1}^{2n-2}\widehat{\omega}_k^{(2n-2)}f(\widehat{\lambda}_k^{(2n-2)}),\quad \widehat{\omega}_k^{(2n-2)}>0,\quad \widehat{\lambda}_k^{(2n-2)}\in\Gamma, \tag{3.1}$$

by using the recursion coefficients $\gamma_1,\gamma_2,\ldots,\gamma_{n-1}$ that determine the Szegő rule (1.8) first forwards and then backwards. Thus, introduce the recursion coefficients

$$\begin{array}{rcll}\widehat{\gamma}_j &=& \gamma_j, & j=1,2,\ldots,n-1,\\ \widehat{\gamma}_j &=& \gamma_{2n-2-j}, & j=n,n+1,\ldots,2n-3,\end{array} \tag{3.2}$$

as well as the auxiliary coefficients

$$\widehat{\delta}_j=\widehat{\delta}_{j-1}(1-|\widehat{\gamma}_j|^2),\qquad j=1,2,\ldots,2n-3,$$

with $\widehat{\delta}_0=1$. The recursion coefficients $\{\widehat{\gamma}_j\}_{j=1}^{2n-3}$ and the parameter $\tau\in\Gamma$ define the matrix $\widehat{H}_{2n-2}$ similarly as the matrix (2.2) is determined by $\gamma_1,\gamma_2,\ldots,\gamma_{n-1}$ and τ. Expressing $\widehat{H}_{2n-2}$ in terms of the latter recursion

coefficients, we obtain the $(2n-2)\times(2n-2)$ upper Hessenberg matrix

$$\widehat{H}_{2n-2}(\tau) \coloneqq \begin{bmatrix} -\bar{\gamma}_0\gamma_1 & -\bar{\gamma}_0\gamma_2 & \cdots & -\bar{\gamma}_0\gamma_{n-1} & -\bar{\gamma}_0\gamma_{n-2} & \cdots & -\bar{\gamma}_0\gamma_1 & -\bar{\gamma}_0\tau \\ 1-|\gamma_1|^2 & -\bar{\gamma}_1\gamma_2 & \cdots & -\bar{\gamma}_1\gamma_{n-1} & -\bar{\gamma}_1\gamma_{n-2} & \cdots & -\bar{\gamma}_1\gamma_1 & -\bar{\gamma}_1\tau \\ 0 & 1-|\gamma_2|^2 & \cdots & -\bar{\gamma}_2\gamma_{n-1} & -\bar{\gamma}_2\gamma_{n-2} & \cdots & -\bar{\gamma}_2\gamma_1 & -\bar{\gamma}_2\tau \\ \vdots & 0 & \ddots & \vdots & -\bar{\gamma}_3\gamma_{n-2} & \cdots & -\bar{\gamma}_3\gamma_1 & -\bar{\gamma}_3\tau \\ & \vdots & 0 & & \vdots & & \vdots & \vdots \\ & & \vdots & 0 & & & & \\ & & & \vdots & & & -\bar{\gamma}_3\gamma_1 & -\bar{\gamma}_3\tau \\ & & & & \ddots & \ddots & -\bar{\gamma}_2\gamma_1 & -\bar{\gamma}_2\tau \\ 0 & & \cdots & & & 0 & 1-|\gamma_1|^2 & -\bar{\gamma}_1\tau \end{bmatrix}$$

with $\gamma_0 = 1$. Introduce

$$\widehat{D}_{2n-2} = \operatorname{diag}[\widehat{\delta}_0, \widehat{\delta}_1, \ldots, \widehat{\delta}_{2n-3}].$$

Similarly as in Section 2, the upper Hessenberg matrix

$$\breve{H}_{2n-2}(\tau) \coloneqq \widehat{D}_{2n-2}^{-1/2}\widehat{H}_{2n-2}(\tau)\widehat{D}_{2n-2}^{1/2} \tag{3.3}$$

is unitary. Its eigenvalues $\widehat{\lambda}_k^{(2n-2)}$, $k = 1, 2, \ldots, 2n-2$, are the nodes of the quadrature rule (3.1) and the magnitude squared of the first component of associated unit eigenvectors are the weights $\widehat{\omega}_k^{(2n-2)}$.

Proposition 3.1. *The generalized averaged Szegő quadrature rule* (3.1) *with the nodes and weights determined as described above is exact for all Laurent polynomial in* $\Lambda_{-n+1,n-1}$.

Proof. The result follows because the first recursion coefficients $\widehat{\gamma}_j$, $j = 1, 2, \ldots, n-1$, that define (3.1) agree with the recursion coefficients γ_j, $j = 1, 2, \ldots, n-1$, that determine (1.8), and the latter rule is exact for all Laurent polynomials in $\Lambda_{-n+1,n-1}$. The exactness of the latter rule follows from the fact that the Levinson or Schur algorithms determine the recursion coefficients γ_j, $j = 1, 2, \ldots, n-1$, so that the quadrature rule (1.8) integrates the moments μ_j, $j = 0, \pm 1, \ldots, \pm(n-1)$ exactly. □

The generalized averaged Szegő rule may be more accurate than indicated by the above proposition. We illustrate this with an example.

Example 3.1. Let the recursion coefficients $\gamma_0, \gamma_1, \ldots, \gamma_{n-1}$ be the same as in Example 2.1. Then the coefficients (3.2) associated with the generalized averaged Szegő rule (3.1) are given by $\widehat{\gamma}_0 = 1$ and $\widehat{\gamma}_j = 0$ for $1 \leq j \leq 2n-3$.

All entries of the associated upper Hessenberg matrix (3.3) vanish, except for the subdiagonal entries 1 and the last entry in the first row $-\tau$. It follows that the nodes of the rule (3.1) are equidistant and the weights are $\omega_k^{(2n-2)} = 1/(2n-2)$. Hence, the generalized averaged Szegő rule (3.1) is a trapezoidal rule with $2n-2$ equidistant nodes. It is exact for all Laurent polynomials in $\Lambda_{-2n+2,2n-2}$. Under the same conditions on the integrand f as in Example 1.1, we have the error bound

$$|S_\tau^{(2n-2)}(f) - \mathcal{I}(f)| \leq C\rho^{-(2n-2)}.$$

The constant C above and in (1.11) can be chosen to be the same. When $\rho > 1$ is not very close to one, this bound is much smaller than the bound (1.11). □

4. Generalized averaged Szegő rules II

The previous section presents a rule based on the spectral decomposition of a Hessenberg matrix that is structurally analogous to the tridiagonal matrix used by Spalević in [23, 24]. This section illustrates that an ordering of the Schur parameters exists in the generalized averaged Szegő rule that duplicates two of the properties of Spalević's generalized averaged Gauss rules, namely:

1. The spectra of the leading and trailing principal $(n-1) \times (n-1)$ tridiagonal submatrices of the augmented matrix are identical.
2. The spectrum of the leading $(n-1) \times (n-1)$ submatrix is a subset of the spectrum of the $(2n-2) \times (2n-2)$ augmented matrix.

The proofs and derivations in this section are based on the observation that a $k \times k$ unitary upper Hessenberg matrix H can be expressed as a product of k elementary unitary matrices

$$H(\tau) = G_1(\gamma_1)G_2(\gamma_2)\dots G_{k-1}(\gamma_{k-1})\tilde{G}_k(\tau).$$

Here $G_j(\gamma_j)$ denotes the $k \times k$ unitary Givens matrix

$$G_j(\gamma_j) := \begin{bmatrix} I_{j-1} & & & \\ & -\gamma_j & \sigma_j & \\ & \sigma_j & \overline{\gamma}_j & \\ & & & I_{k-j-1} \end{bmatrix} \tag{4.1}$$

for some $\gamma_j \in \mathbb{C}$ strictly inside the unit circle and $\sigma_j := (1 - |\gamma_j|^2)^{1/2}$. I_l is the $l \times l$ identity matrix. If γ_j is real-valued, then the matrix $G_j(\gamma_j)$ is

a Givens reflector in the $(j, j+1)$-plane. The parameter $\tau \in \mathbb{C}$ lies on the unit circle and determines the unitary matrix

$$\tilde{G}_k(\tau) := \mathrm{diag}[1, 1, \ldots, 1, -\tau];$$

see, for example, [11]. The matrix (3.3) can then be expressed in the form

$$\breve{H}_{2n-2}(\tau) = G_1(\gamma_1) \ldots G_{n-1}(\gamma_{n-1}) G_n(\gamma_{n-2}) \ldots G_{2n-3}(\gamma_1) \tilde{G}_{2n-2}(\tau).$$

More generally, we construct an augmented unitary Hessenberg matrix H_{2n-2}, from the $n-1$ Schur parameters $\gamma_1, \gamma_2, \ldots, \gamma_{n-1}$ as follows. Define the $(2n-2) \times (2n-2)$ matrices

$$H_1'(\tau_1) = G_1(\gamma_1) G_2(\gamma_2) \ldots G_{n-2}(\gamma_{n-2}) \tilde{G}_{n-1}(\tau_1)$$

and

$$H_2'(\tau_2) = G_n(\alpha_n(\gamma_{p_1})) G_{n+1}(\alpha_{n+1}(\gamma_{p_2})) \ldots G_{2n-3}(\alpha_{2n-3}(\gamma_{p_{n-2}})) \tilde{G}_{2n-2}(\tau_2),$$

where the p_j are permutations of $\{1, 2, \ldots, n-2\}$ and the α_j are functions of the Schur parameters that satisfy $|\alpha_j(\gamma_{p_{j-n+1}})| < 1$. Here $G_j(\gamma_j)$ denotes the $(2n-2) \times (2n-2)$ Givens matrix defined by (4.1) with $k = 2n-2$ and $|\tau_1| = |\tau_2| = 1$. The augmented matrix can now be expressed as

$$H_{2n-2}(\tau_1, \tau_2) = H_1'(\tau_1) G_{n-1}(\gamma_{n-1}) H_2'(\tau_2) \tag{4.2}$$

Observe that the matrix (3.3) is of the form $H_{2n-2}(-1, \tau)$ with $\alpha_{n+j-1}(\gamma_{p_j}) = \gamma_{n-j-1}$, $j = 1, 2, \ldots, n-2$. The statement of Proposition 3.1 with $\tau_1 = -1$ remains valid for the generalized averaged Szegő quadrature rule with the nodes and weights determined by the spectral decomposition of (4.2).

We now show that, given a real-valued γ_{n-1}, there is a matrix $H_2'(\tau_2)$ for which the two properties of the Spalević scheme are satisfied. To this end we use a technique found in [11]. Observe that the matrices H_1' and H_2' can be expressed in the form

$$H_1' = \begin{bmatrix} H_1 & \\ & I_{n-1} \end{bmatrix}, \qquad H_2' = \begin{bmatrix} I_{n-1} & \\ & H_2 \end{bmatrix}, \tag{4.3}$$

where H_1 and H_2 are the leading and trailing $(n-1) \times (n-1)$ principal submatrices of H_1' and H_2', respectively. The spectral decomposition of H_1 yields the nodes and weights of an $(n-1)$-node Szegő quadrature rule. Suppose that in addition we are given a real-valued $\gamma_{n-1} \in (-1, 1)$. Since

γ_{n-1} is real-valued, $G_{n-1}(\gamma_{n-1})$ as defined in (4.2) can be expressed as a rank-one update of the identity matrix,

$$G_{n-1}(\gamma_{n-1}) = I_{2n-2} - 2\boldsymbol{w}\boldsymbol{w}^T,$$

where $\boldsymbol{w} = [\boldsymbol{w}_1^T \boldsymbol{w}_2^T]^T$, $\boldsymbol{w}_1 = a\boldsymbol{e}_{n-1}$, and $\boldsymbol{w}_2 = b\boldsymbol{e}_1$ with $a = \sqrt{(1+\gamma_{n-1})/2}$, $b = \sqrt{(1-\gamma_{n-1})/2}$.

The augmented matrix (4.2) with $\tau_1 = -1$ can now be expressed as

$$\begin{aligned} H_{2n-2}(-1,\tau_2) &= H_1' G_{n-1}(\gamma_{n-1}) H_2' \\ &= \begin{bmatrix} H_1 & \\ & I_{n-1} \end{bmatrix} (I_{2n-2} - 2\boldsymbol{w}\boldsymbol{w}^T) \begin{bmatrix} I_{n-1} & \\ & H_2 \end{bmatrix} \\ &= \begin{bmatrix} H_1 & \\ & H_2 \end{bmatrix} - 2 \begin{bmatrix} H_1 & \\ & I_{n-1} \end{bmatrix} \boldsymbol{w}\boldsymbol{w}^T \begin{bmatrix} I_{n-1} & \\ & H_2 \end{bmatrix}. \end{aligned} \tag{4.4}$$

Theorem 4.1. *Assign $\tau_1 = \tau_2 = -1$ in (4.2) and let*

$$\alpha_{n+j-1}(\gamma_{p_j}) = -\overline{\gamma}_{n-j-1}.$$

Then the following conditions are satisfied.

i. H_1 and H_2 have identical spectra.

ii. The spectrum of H_1 is a subset of the spectrum of $H_{2n-2}(-1,-1)$.

Proof. The assignment of $\alpha_{n+j-1}(\gamma_{p_j}) = -\overline{\gamma}_{n-j-1}$ is equivalent to

$$H_2' = P H_1'^T P,$$

where $P = [\boldsymbol{e}_{n-1}\ \boldsymbol{e}_{n-2}\ \ldots\ \boldsymbol{e}_2\ \boldsymbol{e}_1]$ is the reversal matrix and $\boldsymbol{e}_j$ denotes the jth axis vector; thus $\boldsymbol{e}_j = [0,\ldots,0,1,0,\ldots,0]^T$. It follows that the spectra of H_1 and H_2 as defined in (4.3) are identical. To see *ii.*, let λ be an eigenvalue of H_1 and H_2. Further, let $\boldsymbol{x}$ and $\boldsymbol{y}$ satisfy $H_1\boldsymbol{x} = \lambda\boldsymbol{x}$ and $H_2\boldsymbol{y} = \lambda\boldsymbol{y}$. Require $\boldsymbol{x}$ and $\boldsymbol{y}$ to be scaled so that $\boldsymbol{e}_n^T\boldsymbol{x} = b\lambda$ and $\boldsymbol{e}_1^T\boldsymbol{y} = -a$, and let $\boldsymbol{v} = [\boldsymbol{x}^T \boldsymbol{y}^T]^T$. Then by (4.4),

$$H_{2n-2}\boldsymbol{v} = \begin{bmatrix} H_1\boldsymbol{x} \\ H_2\boldsymbol{y} \end{bmatrix} - 2(a\boldsymbol{e}_{n-1}^T\boldsymbol{x} + b\boldsymbol{e}_1^T H_2\boldsymbol{y}) \begin{bmatrix} aH_1\boldsymbol{e}_{n-1} \\ b\boldsymbol{e}_1 \end{bmatrix},$$

but by the conditions imposed on $\boldsymbol{x}$ and $\boldsymbol{y}$, we have

$$\begin{aligned} (a\boldsymbol{e}_{n-1}^T\boldsymbol{x} + b\boldsymbol{e}_1^T H_2\boldsymbol{y}) &= ab\lambda + b\boldsymbol{e}_1^T\lambda\boldsymbol{y} \\ &= ab\lambda - ab\lambda \\ &= 0. \end{aligned}$$

Hence,

$$H_{2n-2}\boldsymbol{v} = \begin{bmatrix} \lambda\boldsymbol{x} \\ \lambda\boldsymbol{y} \end{bmatrix} = \lambda\boldsymbol{v}.$$

□

We present in Section 6 numerical experiments with generalized averaged Szegő quadrature rules

$$\widetilde{S}^{(2n-2)}(f) = \sum_{k=1}^{2n-2} \widetilde{\omega}_k^{(2n-2)} f(\widetilde{\lambda}_k^{(2n-2)}), \quad \widetilde{\omega}_k^{(2n-2)} > 0, \quad \widetilde{\lambda}_k^{(2n-2)} \in \Gamma, \quad (4.5)$$

that satisfy the conditions of Theorem 4.1. Our interest in these quadrature rules stems from that they share property *ii* of the Szegő–Kronrod extension of the Szegő rule defined by the matrix H_1 in Theorem 4.1. However, the quadrature rules (4.5) are much easier to compute than the Szegő–Kronrod extensions; see [6, 7] for properties of the latter.

5. Anti-Szegő quadrature rules

The n-node anti-Szegő rules are of the form

$$A_\tau^{(n)}(f) = \sum_{k=1}^{n} \tilde{\omega}_k^{(n)} f(\tilde{\lambda}_k^{(n)}), \quad \tilde{\omega}_k^{(n)} > 0, \quad \tilde{\lambda}_k^{(n)} \in \Gamma. \quad (5.1)$$

They are characterized by the property that the quadrature error for Laurent polynomials of order at most n is a specified negative multiple of the quadrature error obtained with the n-node Szegő rule (1.8). Thus, for some chosen constant $c > 0$,

$$\mathcal{I}(p) - A_\tau^{(n)}(p) = -c(\mathcal{I}(p) - S_\tau^{(n)}(p)), \quad \forall p \in \Lambda_{-n,n}. \quad (5.2)$$

It follows from (1.10) that

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

However, $A_\tau^{(n)}(p) \neq \mathcal{I}(p)$ for some $p \in \Lambda_{-n,n} \backslash \Lambda_{-(n-1),n-1}$. Solving (5.2) for $\mathcal{I}(p)$ yields

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

which suggests the definition of the averaged Szegő rule

$$M_\tau^{(n)}(f) = \left(\frac{1}{c+1}\right) A_\tau^{(n)}(f) + \left(\frac{c}{c+1}\right) S_\tau^{(n)}(f); \tag{5.3}$$

see [18] for details on anti-Szegő and the above averaged rules. We will illustrate the performance of the averaged rule (5.3) in Section 6.

Since the averaged rule (5.3) is exact for $f \in \Lambda_{-n,n}$, while the n-node Szegő and anti-Szegő rules (1.8) and (5.1) are not, we can expect the averaged anti-Szegő rule to yield higher accuracy for many integrands f. This can be verified by computations; see [18] for examples.

The construction of the anti-Szegő rule (5.1) requires that the Schur parameter γ_n be known; see [18]. This construction is particularly simple when the auxiliary parameter $\tau \in \Gamma$ is chosen to be

$$\tau := \begin{cases} \frac{\gamma_n}{|\gamma_n|}, & \text{if } \gamma_n \neq 0, \\ 1, & \text{if } \gamma_n = 0. \end{cases} \tag{5.4}$$

For this choice of τ, the unitary upper Hessenberg matrix $H_n(\tau)$ is a closest unitary matrix, in any unitarily invariant norm, to the upper Hessenberg matrix $H_n(\gamma_n)$; see, e.g., [20] for a proof. We have

$$c_n = \begin{cases} \frac{1+|\gamma_n|}{1-|\gamma_n|}, & 0 < |\gamma_n| < 1, \\ 1, & \gamma_n = 0. \end{cases} \tag{5.5}$$

6. Numerical experiments

Szegő quadrature rules are well suited for the integration of periodic functions. Let $T(\theta)$ be a 2π-periodic function. We illustrate the performance of the quadrature rules discussed in the previous sections when applied to approximate integrals

$$\mathcal{I}(T) = \frac{1}{2\pi} \int_{-\pi}^{\pi} T(t) \mathrm{d}\mu(t). \tag{6.1}$$

With a slight abuse of notation, we express the Szegő rule (1.8) as

$$S_\tau^{(n)}(T) = \sum_{k=1}^{n} \omega_k^{(n)} T(\theta_k^{(n)}), \quad \theta_m^{(n)} = \mathtt{arg}(\lambda_k^{(n)}).$$

The other quadrature rules are applied in a similar fashion. All computations are carried out in MATLAB with about 15 significant decimal digits.

Example 6.1. Define the measure $\mathrm{d}\mu(t) = 2\sin^2(t/2)\mathrm{d}t$. The associated monic Szegö polynomials are given by

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

and have recursion coefficients $\gamma_j = \psi_j(0) = 1/(j+1)$; see [4].

Let $\tau = 1$. The nodes and weights of the n-node Szegő rule are determined by the unitary upper Hessenberg matrix $H_n(1) \in \mathbb{C}^{n\times n}$ given by (2.3), and the nodes and weights of the $(2n-2)$-node generalized averaged Szegő rule (3.1) are determined by the unitary upper Hessenberg matrix $\breve{H}_{2n-2}(1)$ defined by (3.3). Both the n-node Szegő and the $(2n-2)$-node generalized averaged Szegő rules require only the recursion coefficients $\gamma_1, \gamma_2, \dots, \gamma_{n-1}$. We also determine the n-node anti-Szegő rule (5.1), defined by $H_n(-1)$, and the rule (5.3) obtained by averaging the n-node Szegő and anti-Szegő rules. The latter rule requires that the recursion coefficient γ_n be known because it is used to determine the coefficient c_n in (5.2), defined by (5.5). We have for the present example $c_n = 1 + 2/n$.

We compute approximations of the integral (6.1) with the integrand

$$T(t) \coloneqq \frac{1}{2}\log(5 + 4\cos(t)). \tag{6.2}$$

The value of the integral can be shown to be $\mathcal{I}(T) \approx 0.44314718055995$.

Table 6.1: Example 6.1: Errors for several quadrature rules applied to the approximation of the integral (6.1) with integrand (6.2).

Rule	$n = 12$	$n = 15$	$n = 18$
$S_1^{(n)}(T)$	-2.2×10^{-5}	2.2×10^{-6}	-2.3×10^{-7}
$A_1^{(n)}(T)$	2.3×10^{-5}	-2.3×10^{-6}	2.4×10^{-7}
$M_1^{(n)}(T)$	-1.1×10^{-6}	9.0×10^{-8}	-7.9×10^{-9}
$\widehat{S}_1^{(2n-2)}(T)$	-1.5×10^{-7}	9.2×10^{-9}	-6.7×10^{-10}
$\widetilde{S}^{(2n-2)}(T)$	2.6×10^{-6}	-2.0×10^{-7}	1.8×10^{-8}

Table 6.1 displays the error for the quadrature rules discussed in this paper. The Szegő and associated anti-Szegő rules are seen to give quadrature errors of opposite sign. Therefore the quadrature error for $M_1^{(n)}(T)$ is smaller than the error for $S_1^{(n)}(T)$ and $A_1^{(n)}(T)$. The computation of the rule $M_1^{(n)}(T)$ requires the coefficient (5.5), whose computation requires knowledge of γ_n. The generalized averaged rule $\widehat{S}_1^{(2n-2)}(T)$ can be seen to yield

the highest accuracy for all choices of n. This rule does not require the evaluation of γ_n.

Table 6.2: Example 6.1: Estimate of absolute error in the approximation furnished by $S_1^{(n)}(T)$.

Difference	$n = 12$	$n = 15$	$n = 18$
$\lvert S_1^{(n)}(T) - M_1^{(n)}(T)\rvert$	2.1×10^{-5}	2.1×10^{-6}	2.2×10^{-7}
$\lvert S_1^{(n)}(T) - S_1^{(n+1)}(T)\rvert$	3.2×10^{-5}	3.2×10^{-6}	3.4×10^{-7}
$\lvert S_1^{(n)}(T) - \widehat{S}_1^{(2n-2)}(T)\rvert$	2.2×10^{-5}	2.2×10^{-6}	2.3×10^{-7}
$\lvert S_1^{(n)}(T) - \widetilde{S}^{(2n-2)}(T)\rvert$	2.4×10^{-5}	2.4×10^{-6}	2.5×10^{-7}

It is important to be able to estimate the quadrature error in a computed approximation of an integral. However. the computation of reliable error estimates can be difficult. Table 6.2 shows differences between values obtained with the different quadrature rules. These differences can be used as error estimates. The table shows the rule $\widehat{S}_1^{(2n-2)}(T)$ to give the most accurate error estimate. The estimate is more accurate than those obtained with the rules $M_1^{(n)}(T)$ and $S_1^{(n+1)}(T)$, both of which require knowledge of the recursion coefficient γ_n. Tables 6.1 and 6.2 suggest that we use $\widehat{S}_1^{(2n-2)}(T)$ as an approximation of the integral (6.1) and use the difference $|S_1^{(n)}(T) - \widehat{S}_1^{(2n-2)}(T)|$ as an estimate of the magnitude of the quadrature error. □

Table 6.3: Example 6.2: Errors for several quadrature rules applied to the approximation of the integral (6.1) with integrand (6.2).

Rule	$n = 12$	$n = 15$	$n = 18$
$S_1^{(n)}(T)$	-3.0×10^{-6}	-2.9×10^{-7}	-2.9×10^{-8}
$A_1^{(n)}(T)$	4.5×10^{-6}	4.1×10^{-7}	4.0×10^{-8}
$M_1^{(n)}(T)$	4.9×10^{-7}	3.8×10^{-8}	3.3×10^{-9}
$\widehat{S}_1^{(2n-2)}(T)$	-1.8×10^{-7}	-1.1×10^{-8}	-7.7×10^{-10}
$\widetilde{S}^{(2n-2)}(T)$	1.2×10^{-6}	8.8×10^{-8}	7.3×10^{-9}

Example 6.2. The integrand in the integral (6.1) is the same as in the previous example, but the measure is $\mathrm{d}\mu(t) = 2\cos^2(t/2)\mathrm{d}t$. The monic Szegő polynomials associated with this measure are given by

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

Table 6.4: Example 6.2: Estimate of absolute error in the approximation furnished by $S_1^{(n)}(T)$.

Difference	$n = 12$	$n = 15$	$n = 18$
$\lvert S_1^{(n)}(T) - M_1^{(n)}(T)\rvert$	3.5×10^{-6}	3.3×10^{-7}	3.3×10^{-8}
$\lvert S_1^{(n)}(T) - S_1^{(n+1)}(T)\rvert$	5.0×10^{-6}	4.7×10^{-7}	4.8×10^{-8}
$\lvert S_1^{(n)}(T) - \widehat{S}_1^{(2n-2)}(T)\rvert$	2.8×10^{-6}	2.8×10^{-7}	2.9×10^{-8}
$\lvert S_1^{(n)}(T) - \widetilde{S}^{(2n-2)}(T)\rvert$	4.1×10^{-6}	3.8×10^{-7}	3.7×10^{-8}

and have recursion coefficients $\gamma_j = (-1)^j/(j+1)$; see [4].

The value of the integral (6.1) is $\mathcal{I}(T) \approx 0.94314718055995$. Table 6.3 is analogous to Table 6.1 and lists the errors in the quadrature rules. The absolute value of the differences between the n-node Szegő rule and other rules are shown in Table 6.4. These differences can be used as estimates of the quadrature error for $S_1^{(n)}(T)$. The generalized averaged Szegő quadrature rules can be seen to yield the highest accuracy as well as accurate estimates of the error in $S_1^{(n)}(T)$. □

Example 6.3. Consider the non-symmetric measure

$$\mathrm{d}\mu(t) = \frac{\pi}{\sinh(\pi)}\mathrm{d}(e^t)$$

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, 14], to compute the complex-valued recursion coefficients directly from the moments.

Using $T(t)$ as defined by (6.2), $\mathcal{I}(T) \approx 0.41271658497332$. The error and error estimates for this example are displayed in Tables 6.5 and 6.6. The generalized averaged Szegő quadrature rules can be seen to yield the highest accuracy as well as accurate estimates of the error in $S_1^{(n)}(T)$. □

7. Conclusion

This paper describes new quadrature rules for the approximation of integrals of periodic functions. The rules are extensions of standard Szegő quadrature rules that are analogous to the generalized averaged Gauss rules

Table 6.5: Example 6.3: Errors for several quadrature rules applied to the approximation of the integral (6.1) with integrand (6.2).

Rule	$n = 12$	$n = 15$	$n = 18$
$S_1^{(n)}(T)$	-5.1×10^{-6}	-5.5×10^{-7}	-5.4×10^{-8}
$A_1^{(n)}(T)$	8.2×10^{-6}	7.9×10^{-7}	7.2×10^{-8}
$M_1^{(n)}(T)$	9.8×10^{-7}	7.4×10^{-8}	5.5×10^{-9}
$\widehat{S}_1^{(2n-2)}(T)$	1.9×10^{-7}	-1.4×10^{-8}	-2.3×10^{-9}
$\widetilde{S}^{(2n-2)}(T)$	1.0×10^{-6}	2.5×10^{-8}	-1.0×10^{-9}

Table 6.6: Example 6.3: Estimate of absolute error in the approximation furnished by $S_1^{(n)}(T)$.

Difference	$n = 12$	$n = 15$	$n = 18$
$\lvert S_1^{(n)}(T) - M_1^{(n)}(T)\rvert$	6.1×10^{-6}	6.3×10^{-7}	5.9×10^{-8}
$\lvert S_1^{(n)}(T) - S_1^{(n+1)}(T)\rvert$	8.7×10^{-6}	9.2×10^{-7}	8.7×10^{-8}
$\lvert S_1^{(n)}(T) - \widehat{S}_1^{(2n-2)}(T)\rvert$	5.3×10^{-6}	5.4×10^{-7}	5.1×10^{-8}
$\lvert S_1^{(n)}(T) - \widetilde{S}^{(2n-2)}(T)\rvert$	6.1×10^{-6}	5.8×10^{-7}	5.3×10^{-8}

for the integration of real-valued, not necessarily periodic, functions introduced by Spalević. Computed examples show the extended rules to give higher accuracy than Szegő quadrature rules defined by the same number of recursion coefficients. This can be of significance when the recursion coefficients are not explicitly known, but have to be computed from the moments and the latter are expensive or difficult to evaluate. Application of the generalized averaged Szegő rules to the estimation of the quadrature error in Szegő rules is illustrated.

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