

Decompositions of optimal averaged Gauss quadrature rules

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Abstract

Optimal averaged Gauss quadrature rules provide estimates for the quadrature error in Gauss rules, as well as estimates for the error incurred when approximating matrix functionals of the form $u^T f(A)v$ with a large matrix $A \in \mathbb{R}^{N \times N}$ by low-rank approximations that are obtained by applying a few steps of the symmetric or nonsymmetric Lanczos processes to A ; here $u, v \in \mathbb{R}^N$ are vectors. The latter process is used when the measure associated with the Gauss quadrature rule has support in the complex plane. The symmetric Lanczos process yields a real tridiagonal matrix, whose entries determine the recursion coefficients of the monic orthogonal polynomials associated with the measure, while the nonsymmetric Lanczos process determines a nonsymmetric tridiagonal matrix, whose entries are recursion coefficients for a pair of sets of bi-orthogonal polynomials. Recently, it has been shown, by applying the results of Peherstorfer, that optimal averaged Gauss quadrature rules, which are associated with a nonnegative measure with support on the real axis, can be expressed as a weighted sum of two quadrature rules. This decomposition allows faster evaluation of optimal averaged Gauss quadrature rules than the previously available representation. The present paper provides a new self-contained proof of this decomposition that is based on linear algebra techniques. Moreover, these techniques are generalized to determine a decomposition of the optimal averaged quadrature rules that are associated with the tridiagonal matrices determined by the nonsymmetric Lanczos process. Also, the splitting of complex symmetric tridiagonal matrices is discussed. The new splittings allow faster evaluation of optimal averaged Gauss quadrature rules than the previously available representations. Computational aspects are discussed.

Keywords: Gauss quadrature, averaged Gauss quadrature, optimal averaged Gauss quadrature

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1. Introduction

Let dw be a nonnegative measure on (part of) the real axis with infinitely many points of support and such that all moments $\mu_k = \int t^k dw(t)$, $k = 0, 1, \dots$, are well defined. For notational simplicity, we will assume that $\mu_0 = 1$. The first part of this paper is concerned with the approximation of integrals of the form

$$\mathcal{I}(f) = \int f(t)dw(t), \quad (1)$$

with a suitable integrand f , by a k -node Gauss quadrature rule

$$\mathcal{G}_k(f) = \sum_{j=1}^k f(t_j)w_j, \quad (2)$$

where the t_j are the nodes and the w_j are the weights of the quadrature rule. Gauss rules are closely associated with monic orthogonal polynomials $\{p_j\}_{j=0}^{\infty}$ determined by the inner product

$$\langle f, g \rangle = \int f(t)g(t)dw(t).$$

Thus, the polynomials p_j have leading coefficient one and satisfy

$$\langle p_i, p_j \rangle = \begin{cases} > 0, & i = j, \\ 0, & i \neq j. \end{cases}$$

It is well known that the polynomials p_j satisfy a three-term recurrence relation of the form

$$p_{j+1}(t) = (t - \alpha_j)p_j(t) - \beta_j p_{j-1}(t), \quad j = 0, 1, \dots,$$

with $p_{-1}(t) \equiv 0$, $p_0(t) \equiv 1$, and the coefficients α_j and β_j are given by

$$\begin{aligned} \alpha_j &= \frac{\langle tp_j, p_j \rangle}{\langle p_j, p_j \rangle}, \quad j = 0, 1, \dots, \\ \beta_j &= \frac{\langle p_j, p_j \rangle}{\langle p_{j-1}, p_{j-1} \rangle} > 0, \quad j = 1, 2, \dots, \end{aligned}$$

with $\beta_0 = 1$. The polynomial p_k has k distinct real zeros, all of which are in the convex hull of the support of dw . The nodes t_1, \dots, t_k of the Gauss rule (2) are the zeros of p_k and all the weights w_1, \dots, w_k are positive; see, e.g., [7, 20] for proofs.

Among all interpolatory quadrature rules with k nodes for approximating integral (1), the Gauss rule (2) has maximal degree of precision $2k - 1$, i.e.,

$$\mathcal{G}_k(p) = \mathcal{I}(p), \quad \forall p \in \mathbb{P}_{2k-1},$$

where \mathbb{P}_{2k-1} denotes the set of all polynomials of degree at most $2k - 1$; see [7, 20]. This makes Gauss quadrature rules well suited for the approximation of many integrals of the form (1).

The Gauss rule (2) can be associated with the symmetric tridiagonal matrix

$$T_k = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & O \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \ddots & \ddots & \ddots & \\ & & \sqrt{\beta_{k-2}} & \alpha_{k-2} & \sqrt{\beta_{k-1}} \\ O & & \sqrt{\beta_{k-1}} & \alpha_{k-1} & \end{bmatrix} \in \mathbb{R}^{k \times k}. \quad (3)$$

The nodes t_1, \dots, t_k of the Gauss rule (2) are the eigenvalues of the matrix (3), and the weights w_1, \dots, w_k are the square of the first components of normalized eigenvectors. The nodes and weights of the Gauss quadrature rule (2) can be computed efficiently in only $\mathcal{O}(k^2)$ arithmetic floating point operations by applying the Golub-Welsch algorithm [9] to the matrix T_k . The representation

$$\mathcal{G}_k(f) = e_1^T f(T_k) e_1 \quad (4)$$

of rule (2) can be seen to be valid by substituting the spectral factorization

$$T_k = U_k \Lambda_k U_k^T \quad (5)$$

into (4). Here $U_k \in \mathbb{R}^{k \times k}$ is an orthogonal matrix and $\Lambda_k = \text{diag}[t_1, t_2, \dots, t_k] \in \mathbb{R}^{k \times k}$. The representation (4) exploits the fact that $\mu_0 = 1$. Throughout this paper, $e_j = [0, \dots, 0, 1, 0, \dots, 0]^T$ denotes the j th axis vector and the superscript T stands for transposition.

It is important to be able to estimate the magnitude of the quadrature error,

$$\mathcal{E}_k(f) = |\mathcal{I}(f) - \mathcal{G}_k(f)|, \quad (6)$$

because this makes it possible to determine a suitable number of nodes k of the Gauss rule (2) when approximating the integral (1) to achieve a desired accuracy. Too few nodes do not yield an accurate enough approximation, while the use of unnecessarily many nodes requires the evaluation of the integrand f at needlessly many nodes.

A classical approach to estimate the error (6) is to evaluate the $(2k+1)$ -node Gauss-Kronrod rule \mathcal{K}_{2k+1} that is associated with \mathcal{G}_k and use

$$|\mathcal{K}_{2k+1}(f) - \mathcal{G}_k(f)|$$

as an estimate of (6). The rule \mathcal{K}_{2k+1} shares the k nodes of \mathcal{G}_k ; the remaining $k+1$ nodes and the weights are chosen so that \mathcal{K}_{2k+1} is of degree of precision at least $3k+1$. However, a difficulty when seeking to evaluate Gauss-Kronrod rules is that nodes that are not nodes of the Gauss rule (2) are not guaranteed to live in the convex hull of the support of the measure dw ; in fact, they are

not guaranteed to be real. This may limit the applicability of Gauss-Kronrod quadrature rules to integrands that can be defined in a sufficiently large domain in the complex plane that contains the support of the measure dw and all nodes of the Gauss-Kronrod rule; it also complicates the computation of the Gauss-Kronrod rules. We refer to Notaris [12] for a nice fairly recent survey of Gauss-Kronrod rules and to Ammar et al. [1], Calvetti et al. [3], and Laurie [11] for computational aspects.

These difficulties prompted the development of averaged Gauss rules, which can be used instead of Gauss-Kronrod rules, to estimate the error in Gauss rules. The first averaged Gauss rule was proposed by Laurie [10], who suggested that the average of the Gauss rule (2) and an associated so-called $(k+1)$ -node anti-Gauss rule be evaluated. We will refer to this averaged rule as $\widehat{\mathcal{G}}_{2k+1}^L$. The magnitude of the quadrature error (6) can be estimated by

$$|\widehat{\mathcal{G}}_{2k+1}^L(f) - \mathcal{G}_k(f)|. \quad (7)$$

Similarly as the Gauss-Kronrod rule \mathcal{K}_{2k+1} , the rule $\widehat{\mathcal{G}}_{2k+1}^L$ has $2k+1$ nodes, k of which are nodes of the Gauss rule (2). The rule $\widehat{\mathcal{G}}_{2k+1}^L$ is easy to compute by using the Golub-Welsch algorithm [9]; its nodes are guaranteed to be real and it has degree of precision at least $2k+1$. Moreover, computed examples reported in [16] indicate that the quadrature error achieved with these averaged rules may be smaller than suggested by their degree of precision. Therefore, the estimate (7) often is a useful approximation of the quadrature error (6).

Ehrich [5] considered k -node Gauss-Hermite and Gauss-Laguerre quadrature rules, and in this context re-weighted the averaged rule of Laurie to obtain a new $(2k+1)$ -node quadrature rule, with k of the nodes being nodes of the Gauss rule \mathcal{G}_k and with degree of precision at least $2k+2$. This degree of precision is the largest possible for all re-weighted averaged rules with $2k+1$ nodes. These rules therefore often are referred to as optimal averaged Gauss rules.

By applying results by Peherstorfer [13] on positive quadrature formulas, Spalević [19] derived a new representation of optimal averaged Gauss quadrature rules. This representation is valid not only for Gauss-Hermite and Gauss-Laguerre quadrature rules, but for all nonnegative measures dw with support on the real axis, for which there are Gauss rules. Specifically, Spalević [19] determined a real symmetric tridiagonal matrix $\widehat{T}_{2k+1} \in \mathbb{R}^{(2k+1) \times (2k+1)}$, defined below, such that

$$\widehat{\mathcal{G}}_{2k+1}^S(f) = e_1^T f(\widehat{T}_{2k+1}) e_1 \quad (8)$$

represents the optimal averaged Gauss quadrature rule associated with the Gauss rule (2). It has real nodes and degree of precision at least $2k+2$. Further, computed examples reported in [16] indicate that the quadrature error for many measures and integrands may be smaller than what is suggested by the degree of precision. Therefore, it is attractive to use

$$|\widehat{\mathcal{G}}_{2k+1}^S(f) - \mathcal{G}_k(f)| \quad (9)$$

as an estimate for the magnitude of the quadrature error (6).

Let $J_k \in \mathbb{R}^{k \times k}$ denote the skew-identity of order k , i.e., J_k has ones on the anti-diagonal and zeros elsewhere. The matrix in (8) is given by

$$\widehat{T}_{2k+1} = \begin{bmatrix} T_k & \sqrt{\beta_k} e_k & O_k \\ \sqrt{\beta_k} e_k^T & \alpha_k & \sqrt{\beta_{k+1}} e_1^T \\ O_k & \sqrt{\beta_{k+1}} e_1 & J_k T_k J_k \end{bmatrix} \in \mathbb{R}^{(2k+1) \times (2k+1)}, \quad (10)$$

where $O_k \in \mathbb{R}^{k \times k}$ denotes the zero matrix. The nodes of this quadrature formula can be computed by applying the Golub-Welsch algorithm to the matrix \widehat{T}_{2k+1} ; however, faster methods are available; see below. Moreover, when β_{k+1} in (10) is replaced by β_k , the analogue of the quadrature rule (8) so obtained is the averaged formula $\widehat{\mathcal{G}}_{2k+1}^L$ introduced by Laurie [10]; see [19] for details.

The fact that the averaged Gauss rule $\widehat{\mathcal{G}}_{2k+1}^L$ can be written as the average of the Gauss rule (2) and an associated $(k+1)$ -node anti-Gauss rule, see [10], raises the question whether the optimal averaged Gauss rule $\widehat{\mathcal{G}}_{2k+1}^S$ can be expressed as a weighted sum of the Gauss rule (2) and a $(k+1)$ -node quadrature rule. A positive answer has recently been provided in [15]. The derivation of this decomposition is based on results by Peherstorfer [13] and holds for Gauss rules determined by a nonnegative measure with support on the real axis. We remark that this representation reduces the computational effort required to determine the nodes and weights of the rule $\widehat{\mathcal{G}}_{2k+1}^S$; see [15] for details.

It is the purposes of the present paper to provide a new proof of the decomposition shown in [15], and to extend the result to measures with support in the complex plane. Section 2 provides a new self-contained proof of the result in [15] that uses linear algebra techniques. An advantage of the new proof is that it can be generalized to apply to measures dw with support in the complex plane. This is done in Section 3. Specifically, we are interested in computing approximations of matrix functionals of the form

$$\mathcal{I}(f) = u^T f(A)v, \quad (11)$$

where $A \in \mathbb{R}^{N \times N}$ is a large nonsymmetric matrix and the vectors $u, v \in \mathbb{R}^N$ satisfy $u^T v = 1$. Application of k steps the nonsymmetric Lanczos process to A with initial vectors u and v generically yields a nonsymmetric tridiagonal matrix $T_k \in \mathbb{R}^{k \times k}$; see, e.g., Saad [18] for a discussion of the nonsymmetric Lanczos process. The expression

$$\mathcal{G}_k(f) = e_1^T f(T_k) e_1 \quad (12)$$

may be considered a k -node Gauss quadrature rule for the approximation of (11); see [6]. This Gauss rule is determined by a measure that may have support in the complex plane; see Section 3 for more details. One can determine an optimal averaged $(2k+1)$ -node quadrature rule analogous to (8) for estimating the error in (12); see Section 3 or [17]. We show in Section 3 that the latter quadrature rule can be expressed as a weighted sum of two quadrature rules with k and $k+1$; the k -node rule is (12). Section 3 also discusses the situation when T_k is a non-Hermitian complex symmetric matrix determined by the Chebyshev algorithm applied to a sequence of real moments μ_j , $j = 0, 1, \dots$. This situation

has recently been considered by Djukić et al. [4] in an investigation of Padé-type approximants. Finally, Section 4 provides a computed examples with timings, and Section 5 contains concluding remarks.

2. Decomposition of optimal averaged quadrature rules associated with a real nonnegative measure on the real axis

Consider the spectral factorization (5) of the matrix (3) and define the orthogonal block diagonal matrix

$$\widehat{U}_{2k+1} = \begin{bmatrix} U_k & & O_k \\ & 1 & \\ O_k & & J_k U_k \end{bmatrix} \in \mathbb{R}^{(2k+1) \times (2k+1)},$$

where “1” denotes the scalar one, U_k is the eigenvector matrix in (5), and J_k stands for the skew-identity of order k , i.e., J_k has ones on the anti-diagonal and zeros elsewhere. Then, letting $u = U_k^T e_k$, we obtain

$$\widehat{U}_{2k+1}^T \widehat{T}_{2k+1} \widehat{U}_{2k+1} = \begin{bmatrix} \Lambda_k & u\sqrt{\beta_k} & O_k \\ \sqrt{\beta_k}u^T & \alpha_k & \sqrt{\beta_{k+1}}u^T \\ O_k & u\sqrt{\beta_{k+1}} & \Lambda_k \end{bmatrix}.$$

This matrix is the sum of a diagonal matrix and a “cross”. It is convenient to permute the rows and columns symmetrically so that the “cross” is moved to the last row and column. Thus, define the permutation matrix

$$\widehat{P}_{2k+1} = [e_1, e_2, \dots, e_k, e_{k+2}, e_{k+3}, \dots, e_{2k+1}, e_{k+1}] \in \mathbb{R}^{(2k+1) \times (2k+1)}. \quad (13)$$

Then

$$\widehat{P}_{2k+1}^T \widehat{U}_{2k+1}^T \widehat{T}_{2k+1} \widehat{U}_{2k+1} \widehat{P}_{2k+1} = \begin{bmatrix} \Lambda_k & & O_k & u\sqrt{\beta_k} \\ O_k & & \Lambda_k & u\sqrt{\beta_{k+1}} \\ u^T\sqrt{\beta_k} & & u^T\sqrt{\beta_{k+1}} & \alpha_k \end{bmatrix}.$$

We now can annihilate the vector $u\sqrt{\beta_k}$ by orthogonal similarity transformation. In the context of divide-and-conquer methods for the symmetric tridiagonal eigenproblem, this annihilation is referred to as deflation; see, e.g., Borges and Gragg [2].

Define the block Givens rotation

$$\widehat{G}_{2k+1} = \begin{bmatrix} cI_k & sI_k & & \\ -sI_k & cI_k & & \\ & & & 1 \end{bmatrix} \in \mathbb{R}^{(2k+1) \times (2k+1)},$$

where $I_k \in \mathbb{R}^{k \times k}$ denotes the identity matrix and

$$c = \frac{\sqrt{\beta_{k+1}}}{\sqrt{\beta_k + \beta_{k+1}}}, \quad s = \frac{\sqrt{\beta_k}}{\sqrt{\beta_k + \beta_{k+1}}}. \quad (14)$$

Then

$$\widehat{G}_{2k+1}^T \widehat{P}_{2k+1}^T \widehat{U}_{2k+1}^T \widehat{T}_{2k+1} \widehat{U}_{2k+1} \widehat{P}_{2k+1} \widehat{G}_{2k+1} = \begin{bmatrix} \Lambda_k & O_k & 0_k \\ O_k & \Lambda_k & u\sqrt{\widetilde{\beta}_k} \\ 0_k^T & u^T \sqrt{\widetilde{\beta}_k} & \alpha_k \end{bmatrix}.$$

Here $0_k \in \mathbb{R}^k$ denotes the zero vector and $\widetilde{\beta}_k = \beta_k + \beta_{k+1}$. This shows that the eigenproblem for the matrix \widehat{T}_{2k+1} splits into two eigenproblems: the eigenproblems for T_k and for the trailing $(k+1) \times (k+1)$ submatrix

$$\widetilde{M}_{k+1} = \begin{bmatrix} \Lambda_k & u\sqrt{\widetilde{\beta}_k} \\ u^T \sqrt{\widetilde{\beta}_k} & \alpha_k \end{bmatrix}.$$

Define the symmetric tridiagonal matrix

$$\widetilde{T}_{k+1} = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & & O \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & & \\ & \ddots & \ddots & \ddots & & \\ & & \sqrt{\beta_{k-2}} & \alpha_{k-2} & \sqrt{\beta_{k-1}} & \\ & & & \sqrt{\beta_{k-1}} & \alpha_{k-1} & \sqrt{\widetilde{\beta}_k} \\ O & & & & \sqrt{\widetilde{\beta}_k} & \alpha_k \end{bmatrix} \in \mathbb{R}^{(k+1) \times (k+1)}. \quad (15)$$

We remark that if β_{k+1} is replaced by β_k in (10), then $\widetilde{\beta}_k$ in (15) is $2\beta_k$ and the matrix defines the $(k+1)$ -node anti-Gauss rule associated with the Gauss rule (2); see Laurie [10] for a discussion of anti-Gauss rules.

Introduce the spectral factorization

$$\widetilde{T}_{k+1} = \widetilde{W}_{k+1} \widetilde{\Lambda}_{k+1} \widetilde{W}_{k+1}^T, \quad (16)$$

where the matrix $\widetilde{W}_{k+1} \in \mathbb{R}^{(k+1) \times (k+1)}$ is orthogonal and the diagonal entries of $\widetilde{\Lambda}_{k+1} = \text{diag}[\widetilde{\lambda}_1, \dots, \widetilde{\lambda}_{k+1}] \in \mathbb{R}^{(k+1) \times (k+1)}$ are eigenvalues of \widetilde{T}_{k+1} . Define the orthogonal block matrix:

$$\widetilde{U}_{k+1} = \begin{bmatrix} U_k & \\ & 1 \end{bmatrix} \in \mathbb{R}^{(k+1) \times (k+1)}.$$

Since

$$\widetilde{U}_{k+1}^T \widetilde{T}_{k+1} \widetilde{U}_{k+1} = \widetilde{M}_{k+1},$$

it follows that

$$\widetilde{M}_{k+1} = \widetilde{U}_{k+1}^T \widetilde{W}_{k+1} \widetilde{\Lambda}_{k+1} \widetilde{W}_{k+1}^T \widetilde{U}_{k+1}.$$

This shows that the eigenvector matrix for \widehat{T}_{2k+1} can be expressed as

$$\widehat{U}_{2k+1} \widehat{P}_{2k+1} \widehat{G}_{2k+1} \begin{bmatrix} I_k & O_{k,k+1} \\ O_{k+1,k} & \widetilde{U}_{k+1}^T \end{bmatrix} \begin{bmatrix} I_k & O_{k,k+1} \\ O_{k+1,k} & \widetilde{W}_{k+1} \end{bmatrix},$$

where $O_{i,j} \in \mathbb{R}^{i \times j}$ denotes the zero matrix.

Substituting the spectral factorization of the matrix \widehat{T}_{2k+1} into (8) yields a quadrature rule whose nodes are the eigenvalues of this matrix and whose weights are the square of the components of the first row of the eigenvector matrix. We first observe that

$$e_1^T \widehat{U}_{2k+1} \widehat{P}_{2k+1} \widehat{G}_{2k+1} = [ce_1^T U_k, se_1^T U_k, 0],$$

where c and s are defined by (14). Therefore,

$$e_1^T \widehat{U}_{2k+1} \widehat{P}_{2k+1} \widehat{G}_{2k+1} \begin{bmatrix} I_k & O_{k,k+1} \\ O_{k+1,k} & \widetilde{U}_{k+1}^T \end{bmatrix} = [ce_1^T U_k, se_1^T, 0]$$

and, finally,

$$\begin{aligned} & e_1^T \widehat{U}_{2k+1} \widehat{P}_{2k+1} \widehat{G}_{2k+1} \begin{bmatrix} I_k & O_{k,k+1} \\ O_{k+1,k} & \widetilde{U}_{k+1}^T \end{bmatrix} \begin{bmatrix} I_k & O_{k,k+1} \\ O_{k+1,k} & \widetilde{W}_{k+1} \end{bmatrix} \\ &= [ce_1^T U_k, se_1^T \widetilde{W}_{k+1}]. \end{aligned}$$

We have shown the following result.

Theorem 1. *Let the quadrature rule $\widetilde{\mathcal{G}}_{k+1}$ be defined by the symmetric tridiagonal matrix (15), i.e.,*

$$\widetilde{\mathcal{G}}_{k+1}(f) = e_1^T f(\widetilde{T}_{k+1})e_1. \quad (17)$$

Then the optimal averaged quadrature rule (8) can be represented as

$$\widehat{\mathcal{G}}_{2k+1}^S = \frac{\beta_{k+1}}{\beta_k + \beta_{k+1}} \mathcal{G}_k + \frac{\beta_k}{\beta_k + \beta_{k+1}} \widetilde{\mathcal{G}}_{k+1}. \quad (18)$$

Thus, the rule $\widehat{\mathcal{G}}_{2k+1}^S$ is a weighted average of the rules \mathcal{G}_k and $\widetilde{\mathcal{G}}_{k+1}$.

Proof. The weights of the Gauss rule (2) are the square of the entries of first row of the eigenvector matrix U_k in the spectral factorization (5) of T_k . Similarly, the weights of the Gauss rule (17) are the square of the entries of first row of the eigenvector matrix W_{k+1} in the spectral factorization (16). \square

The splitting (18) has been shown in [15] in a different manner by applying results of Peherstorfer [13]. When β_{k+1} is replaced by β_k in (10) and (18), then the latter formula yields a representation of the averaged rule $\widehat{\mathcal{G}}_{2k+1}^L$ used by Laurie [10].

3. Decomposition of optimal averaged quadrature rules associated with a measure with support in the complex plane

Let $A \in \mathbb{R}^{N \times N}$ be a large nonsymmetric matrix with spectral factorization

$$A = SAS^{-1}, \quad (19)$$

where the matrix $S \in \mathbb{C}^{N \times N}$ is nonsingular and $\Lambda = \text{diag}[\lambda_1, \dots, \lambda_N] \in \mathbb{C}^{N \times N}$. The entries λ_j are eigenvalues of A ; they are either real or occur in complex conjugate pairs. We are interested in computing inexpensive approximations of expressions of the form (11) with $u, v \in \mathbb{R}^N$ such that $u^T v = 1$. The nonsymmetric Lanczos algorithm provides a way to determine such approximations.

Substituting the spectral factorization (19) into (11) gives

$$\mathcal{I}(f) = u^T f(A)v = u^T S f(\Lambda) S^{-1} v = \sum_{j=1}^N f(\lambda_j) \mu_j \mu'_j, \quad (20)$$

where $[\mu_1, \dots, \mu_N] = u^T S$ and $[\mu'_1, \dots, \mu'_N] = S^{-1} v$. The right-hand side of (20) can formally be written as an integral

$$\mathcal{I}(f) = \int f(t) d\mu_{A,u,v}(t) \quad (21)$$

with the measure

$$d\mu_{A,u,v}(t) = \sum_{j=1}^N \delta(t - \lambda_j) \mu_j \mu'_j,$$

where δ denotes the Dirac δ -function. This measure depends on the matrix A and the vectors u and v ; the support is on the real axis or at complex conjugate points in the complex plane.

Application of $k+1$ steps of the nonsymmetric Lanczos process to the matrix A with initial vectors u and v gives the Lanczos decompositions

$$\begin{aligned} AV_{k+1} &= V_{k+1} T_{k+1} + \beta_{k+1} v_{k+2} e_{k+1}^T, \\ A^T U_{k+1} &= U_{k+1} T_{k+1}^T + \gamma_{k+1} u_{k+2} e_{k+1}^T, \end{aligned} \quad (22)$$

where the columns of the matrices $U_{k+1} \in \mathbb{R}^{N \times (k+1)}$ and $V_{k+1} \in \mathbb{R}^{N \times (k+1)}$ are bi-orthogonal, i.e., $U_{k+1}^T V_{k+1} = I_{k+1}$. Moreover, $U_{k+1}^T v_{k+2} = 0$, $V_{k+1}^T u_{k+2} = 0$, and $u_{k+2}^T v_{k+2} = 1$. The matrix

$$T_{k+1} = \begin{bmatrix} \alpha_0 & \gamma_1 & & & & \\ \beta_1 & \alpha_1 & \gamma_2 & & & \\ & \ddots & \ddots & \ddots & & \\ & & \beta_{k-1} & \alpha_{k-1} & \gamma_k & \\ & & & \beta_k & \alpha_k & \end{bmatrix} \in \mathbb{R}^{(k+1) \times (k+1)}.$$

is tridiagonal and generally nonsymmetric; see Saad [18, Algorithm 7.1] for details on the nonsymmetric Lanczos process. If the matrix A is nonsymmetric and the vectors u, v are such that the above matrix is symmetric, then we can apply the formulas of Section 2. Moreover,

$$\gamma_i = \beta_i \quad \text{or} \quad \gamma_i = -\beta_i \quad \text{for all} \quad 1 \leq i \leq k.$$

Throughout this section, we assume that $k \ll N$ is small enough so that the Lanczos process does not break down and therefore the Lanczos decompositions

(22) exist. This is the generic situation. We remark that the nonsymmetric Lanczos process can be associated with two families of monic bi-orthogonal polynomials, which are related to the columns of the matrices U_k and V_k ; see [6] for further details on this.

Let the matrix $T_k \in \mathbb{R}^{k \times k}$ consist of the k first rows and columns of T_{k+1} . Then

$$\mathcal{G}_k(f) = e_1^T f(T_k) e_1 \quad (23)$$

may be considered a Gauss rule with respect to the integral (21), since

$$\mathcal{G}_k(f) = \mathcal{I}(f), \quad \forall f \in \mathbb{P}_{2k-1};$$

see [6] for a proof.

Introduce the real nonsymmetric tridiagonal matrix

$$\widehat{T}_{2k+1} = \begin{bmatrix} T_k & \gamma_k e_k & O_k \\ \beta_k e_k^T & \alpha_k & \gamma_{k+1} e_1^T \\ O_k & \beta_{k+1} e_1 & J_k T_k J_k \end{bmatrix} \in \mathbb{R}^{(2k+1) \times (2k+1)} \quad (24)$$

and define the associated quadrature rule

$$\widehat{\mathcal{G}}_{2k+1}(f) = e_1^T f(\widehat{T}_{2k+1}) e_1. \quad (25)$$

Expressions of this form can be computed by evaluating the function f at the fairly small matrix \widehat{T}_{2k+1} or by first calculating the spectral factorization

$$\widehat{T}_{2k+1} = \widehat{W}_{2k+1} \widehat{\Lambda}_{2k+1} \widehat{W}_{2k+1}^{-1}, \quad (26)$$

which we assume to exist. This is the generic situation; the rare situation when \widehat{T}_{2k+1} does not have a spectral factorization is discussed by Pozza et al. [14].

Thus, the matrix $\widehat{W}_{2k+1} \in \mathbb{C}^{(2k+1) \times (2k+1)}$ is assumed to be nonsingular and the nontrivial entries of $\widehat{\Lambda}_{2k+1} = \text{diag}[\widehat{\lambda}_1, \dots, \widehat{\lambda}_{2k+1}] \in \mathbb{C}^{(2k+1) \times (2k+1)}$ are eigenvalues of \widehat{T}_{2k+1} . Substituting the spectral factorization (26) into (25) gives

$$\widehat{\mathcal{G}}_{2k+1}(f) = e_1^T \widehat{W}_{2k+1} f(\widehat{\Lambda}_{2k+1}) \widehat{W}_{2k+1}^{-1} e_1, \quad (27)$$

which shows that only the eigenvalues of $\widehat{\Lambda}_{2k+1}$, the first row of the eigenvector matrix \widehat{W}_{2k+1} , and the first column of the inverse of the eigenvector matrix are required to compute (25). We will return to this observation below.

The magnitude of the error in the Gauss rule (23),

$$|\mathcal{I}(f) - \mathcal{G}_k(f)|,$$

can be estimated by evaluating

$$|\widehat{\mathcal{G}}_{2k+1}(f) - \mathcal{G}_k(f)|.$$

Computed examples reported in [17] illustrate that this estimate of the quadrature error generally is quite accurate.

It is the aim of this section to show that the expression (25) can be decomposed into a weighted sum of simpler quadrature rules, similarly to the decomposition of Theorem 1. Consider the spectral factorization

$$T_k = S_k \Lambda_k S_k^{-1},$$

which we assume to exist. Thus, the matrix $S_k \in \mathbb{C}^{k \times k}$ is nonsingular and $\Lambda_k \in \mathbb{C}^{k \times k}$ is diagonal; its nontrivial entries are eigenvalues of T_k . Define the block matrix

$$\widehat{S}_{2k+1} = \begin{bmatrix} S_k & O_k \\ O_k & J_k S_k \end{bmatrix} \in \mathbb{C}^{(2k+1) \times (2k+1)}.$$

Then

$$\widehat{S}_{2k+1}^{-1} \widehat{T}_{2k+1} \widehat{S}_{2k+1} = \begin{bmatrix} \Lambda_k & w\gamma_k & O_k \\ u^T \beta_k & \alpha_k & u^T \gamma_{k+1} \\ O_k & w\beta_{k+1} & \Lambda_k \end{bmatrix},$$

where $u = S_k^T e_k$ and $w = S_k^{-1} e_k$. This matrix is the sum of a diagonal matrix and a ‘‘cross’’. Similarly as in Section 2, we move the cross to the last row and column by applying the permutation (13),

$$\widehat{P}_{2k+1}^T \widehat{S}_{2k+1}^{-1} \widehat{T}_{2k+1} \widehat{S}_{2k+1} \widehat{P}_{2k+1} = \begin{bmatrix} \Lambda_k & O_k & w\gamma_k \\ O_k & \Lambda_k & w\beta_{k+1} \\ u^T \beta_k & u^T \gamma_{k+1} & \alpha_k \end{bmatrix}.$$

We will apply a similarity transformation to annihilate the vectors $u^T \beta_k$ and $w\gamma_k$ in the last row and column of the above matrix. For simplicity, first consider the matrix

$$B = \begin{bmatrix} \lambda & 0 & \gamma_k \\ 0 & \lambda & \beta_{k+1} \\ \beta_k & \gamma_{k+1} & \alpha_k \end{bmatrix} \in \mathbb{C}^{3 \times 3},$$

and determine a nonsingular matrix

$$H = \begin{bmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{bmatrix} \in \mathbb{R}^{2 \times 2} \quad (28)$$

such that

$$\begin{bmatrix} H^{-1} & 0_2 \\ 0_2^T & 1 \end{bmatrix} B \begin{bmatrix} H & 0_2 \\ 0_2^T & 1 \end{bmatrix} = \begin{bmatrix} \lambda & 0 & 0 \\ 0 & \lambda & * \\ 0 & * & \alpha_k \end{bmatrix},$$

where the entries marked by $*$ generally are nonvanishing and $0_2 = [0, 0]^T \in \mathbb{R}^2$. This imposes the requirements

$$H^{-1} \begin{bmatrix} \gamma_k \\ \beta_{k+1} \end{bmatrix} = \begin{bmatrix} 0 \\ * \end{bmatrix},$$

or equivalently,

$$\begin{bmatrix} \gamma_k \\ \beta_{k+1} \end{bmatrix} = H \begin{bmatrix} 0 \\ * \end{bmatrix},$$

and

$$\begin{bmatrix} \beta_k & \gamma_{k+1} \end{bmatrix} H = \begin{bmatrix} 0 & * \end{bmatrix}.$$

We may choose

$$\begin{aligned} h_{11} &= \frac{\gamma_{k+1}}{\sqrt{\beta_k^2 + \gamma_{k+1}^2}}, & h_{21} &= -\frac{\beta_k}{\sqrt{\beta_k^2 + \gamma_{k+1}^2}}, \\ h_{12} &= \frac{\gamma_k}{\sqrt{\beta_{k+1}^2 + \gamma_k^2}}, & h_{22} &= \frac{\beta_{k+1}}{\sqrt{\beta_{k+1}^2 + \gamma_k^2}}. \end{aligned}$$

Note that if $\beta_k = \gamma_k$ and $\beta_{k+1} = \gamma_{k+1}$, which happens when the matrix T_{k+2} is symmetric, then H is orthogonal.

Expanding the matrix H to the block matrix

$$\widehat{H}_{2k+1} = \begin{bmatrix} h_{11}I_k & h_{12}I_k & & \\ h_{21}I_k & h_{22}I_k & & \\ & & & 1 \end{bmatrix} \in \mathbb{R}^{(2k+1) \times (2k+1)} \quad (29)$$

gives

$$\widehat{H}_{2k+1}^{-1} \widehat{P}_{2k+1}^T \widehat{S}_{2k+1}^{-1} \widehat{T}_{2k+1} \widehat{S}_{2k+1} \widehat{P}_{2k+1} \widehat{H}_{2k+1} = \begin{bmatrix} \Lambda_k & O_k & 0_k \\ O_k & \Lambda_k & w\check{\gamma}_k \\ 0_k^T & u^T \check{\beta}_k & \alpha_k \end{bmatrix},$$

where

$$\check{\beta}_k = \frac{\beta_k \gamma_k + \beta_{k+1} \gamma_{k+1}}{\sqrt{\beta_{k+1}^2 + \gamma_k^2}}, \quad \check{\gamma}_k = \sqrt{\beta_{k+1}^2 + \gamma_k^2}.$$

This shows that the eigenproblem for \widehat{T}_{2k+1} splits into eigenproblems for T_k and for the trailing principal submatrix

$$\check{M}_{k+1} = \begin{bmatrix} \Lambda_k & w\check{\gamma}_k \\ u^T \check{\beta}_k & \alpha_k \end{bmatrix} \in \mathbb{C}^{(k+1) \times (k+1)}.$$

Define the nonsymmetric tridiagonal matrix

$$\check{T}_{k+1} = \begin{bmatrix} \alpha_0 & \gamma_1 & & & & & & & 0 \\ \beta_1 & \alpha_1 & \gamma_2 & & & & & & \\ & \ddots & \ddots & \ddots & & & & & \\ & & & \beta_{k-2} & \alpha_{k-2} & \gamma_{k-1} & & & \\ & & & & \beta_{k-1} & \alpha_{k-1} & \check{\gamma}_k & & \\ 0 & & & & & \check{\beta}_k & \alpha_k & & \end{bmatrix} \in \mathbb{R}^{(k+1) \times (k+1)} \quad (30)$$

with spectral factorization

$$\check{T}_{k+1} = \check{W}_{k+1} \check{\Lambda}_{k+1} \check{W}_{k+1}^{-1},$$

where the matrix $\check{W}_{k+1} \in \mathbb{C}^{(k+1) \times (k+1)}$ is nonsingular and the diagonal entries of $\check{\Lambda}_{k+1} = \text{diag}[\check{\lambda}_1, \dots, \check{\lambda}_{k+1}] \in \mathbb{C}^{(k+1) \times (k+1)}$ are eigenvalues. Define the block matrix

$$\check{S}_{k+1} = \begin{bmatrix} S_k & \\ & 1 \end{bmatrix} \in \mathbb{C}^{(k+1) \times (k+1)}.$$

Then

$$\check{S}_{k+1}^{-1} \check{T}_{k+1} \check{S}_{k+1} = \check{M}_{k+1},$$

and it follows that

$$\check{M}_{k+1} = \check{S}_{k+1}^{-1} \check{W}_{k+1} \check{\Lambda}_{k+1} \check{W}_{k+1}^{-1} \check{S}_{k+1}.$$

This shows that the eigenvector matrix for the matrix \widehat{T}_{2k+1} , defined by (24), can be expressed as

$$\widehat{W}_{2k+1} = \widehat{S}_{2k+1} \widehat{P}_{2k+1} \widehat{H}_{2k+1} \begin{bmatrix} I_k & O_{k,k+1} \\ O_{k+1,k} & \check{S}_{k+1}^{-1} \end{bmatrix} \begin{bmatrix} I_k & O_{k,k+1} \\ O_{k+1,k} & \check{W}_{k+1} \end{bmatrix}.$$

The expression (27) shows that to evaluate the functional (25) it suffices to know the eigenvalues of the matrix \widehat{T}_{2k+1} , the elements of the first row of the eigenvector matrix \widehat{W}_{2k+1} , and the elements of the first column of \widehat{W}_{2k+1}^{-1} . Observe that

$$e_1^T \widehat{S}_{2k+1} \widehat{P}_{2k+1} \widehat{H}_{2k+1} = [h_{11} e_1^T S_k, h_{12} e_1^T S_k, 0],$$

from which we obtain

$$\begin{aligned} e_1^T \widehat{W}_{2k+1} &= e^T \widehat{S}_{2k+1} \widehat{P}_{2k+1} \widehat{H}_{2k+1} \begin{bmatrix} I_k & O_{k,k+1} \\ O_{k+1,k} & \check{S}_{k+1}^{-1} \end{bmatrix} \begin{bmatrix} I_k & O_{k,k+1} \\ O_{k+1,k} & \check{W}_{k+1} \end{bmatrix} \\ &= [h_{11} e_1^T S_k, h_{12} e_1^T \check{W}_{k+1}]. \end{aligned} \quad (31)$$

We turn to the entries of the vector $\widehat{W}_{2k+1}^{-1} e_1$. Let

$$H^{-1} = \begin{bmatrix} h'_{11} & h'_{12} \\ h'_{21} & h'_{22} \end{bmatrix} \in \mathbb{R}^{2 \times 2}$$

denote the inverse of the matrix (28). Then the inverse of the matrix (29) is given by the block matrix

$$\widehat{H}_{2k+1}^{-1} = \begin{bmatrix} h'_{11} I_k & h'_{12} I_k & \\ h'_{21} I_k & h'_{22} I_k & \\ & & 1 \end{bmatrix} \in \mathbb{R}^{(2k+1) \times (2k+1)},$$

and it follows that

$$\widehat{H}_{2k+1}^{-1} P_{2k+1}^T \widehat{S}_{2k+1}^{-1} e_1 = \begin{bmatrix} h'_{11} S_k^{-1} e_1 \\ h'_{21} S_k^{-1} e_1 \\ 0 \end{bmatrix}.$$

Hence,

$$\widehat{W}_{2k+1}^{-1} e_1 = \begin{bmatrix} I_k & O_{k,k+1} \\ O_{k+1,k} & \check{W}_{k+1}^{-1} \end{bmatrix} \begin{bmatrix} I_k & O_{k,k+1} \\ O_{k+1,k} & \check{S}_{k+1} \end{bmatrix} \begin{bmatrix} h'_{11} S_k^{-1} e_1 \\ h'_{21} S_k^{-1} e_1 \\ 0 \end{bmatrix}$$

and, finally,

$$\widehat{W}_{2k+1}^{-1} e_1 = \begin{bmatrix} h'_{11} S_k^{-1} e_1 \\ h'_{21} \check{W}_{k+1}^{-1} e_1 \end{bmatrix}. \quad (32)$$

We have shown the following result.

Theorem 2. *The quadrature rule (25) can be expressed as a weighted sum of the rules (23) and*

$$\check{\mathcal{G}}_{k+1}(f) = e_1^T f(\check{T}_{k+1}) e_1. \quad (33)$$

Specifically,

$$\widehat{\mathcal{G}}_{2k+1} = h_{11} h'_{11} \mathcal{G}_k + h_{12} h'_{21} \check{\mathcal{G}}_{k+1}. \quad (34)$$

In particular, the nodes of the rule \mathcal{G}_k are nodes of $\widehat{\mathcal{G}}_{2k+1}$.

Proof. Let $u \circ v = [u_1 v_1, \dots, u_\ell v_\ell]$ denote the Hadamard product of the ℓ -vectors u and v . Then the quadrature rules (23), (33), and (25) can be expressed as

$$\begin{aligned} \mathcal{G}_k(f) &= \sum_{j=1}^k f(\lambda_j) (e_1^T S_k \circ S_k^{-1} e_1)_j, \\ \check{\mathcal{G}}_{k+1}(f) &= \sum_{j=1}^{k+1} f(\check{\lambda}_j) (e_1^T \check{W}_{k+1} \circ \check{W}_{k+1}^{-1} e_1)_j, \\ \widehat{\mathcal{G}}_{2k+1}(f) &= \sum_{j=1}^{2k+1} f(\widehat{\lambda}_j) (e_1^T \widehat{W}_{2k+1} \circ \widehat{W}_{2k+1}^{-1} e_1)_j. \end{aligned}$$

The theorem now follows from (31) and (32). \square

We conclude this section by considering some special cases. Application of $k+1$ steps of the nonsymmetric Lanczos process to a nonsymmetric matrix $A \in \mathbb{R}^{N \times N}$ with initial vectors $u, v \in \mathbb{R}^N$ such that $u^T v = 1$ generically gives the Lanczos decompositions (22) with a generally nonsymmetric tridiagonal matrix $T_{k+1} \in \mathbb{R}^{(k+1) \times (k+1)}$ in which the off-diagonal entries satisfy

$$\beta_j = \gamma_j \quad \text{or} \quad \beta_j = -\gamma_j, \quad j = 1, 2, \dots, k+1.$$

It follows that the matrix (28) can be chosen to be a Givens rotation when

$$\text{sign}(\beta_k \beta_{k+1}) = \text{sign}(\gamma_k \gamma_{k+1}),$$

and then the weights in (34) can be replaced by weights c and s similarly as in Theorem 1. We recall that c and s are defined in (14).

Given moments or modified moments, the Chebyshev algorithm or modified Chebyshev algorithm determines a complex symmetric tridiagonal matrix whose entries are recurrence coefficients for orthogonal polynomials associated with a bilinear form determined by a measure that defines the moments; see. e.g., [7] for details. We assume here that the Chebyshev or modified Chebyshev algorithms do not break down. This is the generic situation. An application of the Chebyshev algorithm to the computation of certain Padé-type approximants is described in [4]. The off-diagonal entries of the complex symmetric matrix $T_{k+1} \in \mathbb{C}^{(k+1) \times (k+1)}$ determined in this manner satisfy

$$\beta_j > 0 \quad \text{or} \quad i\beta_j < 0, \quad j = 1, 2, \dots, k+1,$$

where $i = \sqrt{-1}$. The matrix (28) can be chosen as a Givens rotation when

$$\beta_k \beta_{k+1} \in \mathbb{R} \quad \text{and} \quad \gamma_k \gamma_{k+1} \in \mathbb{R},$$

and the weights in (34) then can be replaced by weights c and s similarly as in Theorem 1.

We finally consider the application of the non-Hermitian Lanczos algorithm to a large matrix $A \in \mathbb{C}^{N \times N}$ with initial vectors $u, v \in \mathbb{C}^N$, such that $u^H v = 1$, where the superscript H denotes transposition and complex conjugation. If the matrix A is complex symmetric and $\bar{u} = v$, where the bar denotes complex conjugation, then the decompositions (22) with T replaced by H simplify to only one decomposition.

4. A computed example

The performance of the optimal averaged Gauss quadrature rules has already been illustrated in [16, 17] and timings for the representation (18) are presented in [15]. We therefore only show some timings that demonstrate that the evaluation of (34) can be carried out faster than the evaluation of (25). All computations are carried out using Matlab version R2021a on a MacBook Pro laptop computer with an M1 processor and 8GB of RAM. The computations are performed with about 15 significant decimal digits.

We evaluate Gauss and optimal averaged Gauss rules associated with non-symmetric tridiagonal matrices by computing the spectral factorization of these matrices. For instance, the optimal averaged Gauss rule (25) is evaluated by first computing the spectral factorization (26) and then evaluating (27). This approach of evaluating (25) works well if the eigenvector matrix \widehat{W}_{2k+1} is not very ill-conditioned. The computation of the spectral factorization (26) by the QR algorithm requires about $21\frac{2}{3}(2k+1)^3 + O(k^2)$ arithmetic floating point

operations (flops); see, e.g., [8, p. 376 and p. 391]. This flop count takes into account that the matrix \widehat{T}_{2k+1} is of upper Hessenberg form. The evaluation of (25) also requires the evaluation of $\widehat{W}_{2k+1}^{-1}e_1$, which can be carried out by solving a linear system of equations with the matrix \widehat{W}_{2k+1} by computing its LU factorization. This requires $2(2k+1)^3/3 + O(k^2)$ flops; see, e.g., [8, p. 116]. We do not count the computational effort required to evaluate the integrand f in (25), because this is independent of the representation of the quadrature rule (25) being used. Thus, the flop count for the evaluation of (25) is $178\frac{2}{3}k^3 + O(k^2)$.

We turn to the evaluation of the representation (34) of (25). Similarly as above, the evaluation of each integral in the representation (34) demands $22\frac{1}{3}k^3 + O(k^2)$ flops resulting in a total flop count of $44\frac{2}{3}k^3 + O(k^2)$. This flop count is much smaller than the count for the evaluation of (25). This also is the flop count for evaluating (9) when the quadrature rules are defined by (23) and (25), and the representation (34) is used.

When, instead, using the representation (27), the evaluation of (9) requires $178\frac{2}{3}k^3 + 22\frac{1}{3}k^3 + O(k^2) = 201k^3 + O(k^2)$ flops, because the Gauss rule (23) also has to be evaluated. We remark that for certain integrands with special properties, it may be possible to evaluate of the representations (25) and (34) with a lower flop counts by calculating the integrals without using the spectral factorizations of the tridiagonal matrices. We will not dwell on these special situations.

Flop counts provide a measure of computational complexity. However, timings of algorithms do not only include arithmetic work, but also the time required to access and move data. Therefore, timings of algorithms generally are not proportional to flop counts. Table 1 shows the ratio of the timings for the evaluation of the quadrature rules (12) and (25), and the evaluation of the representation (34). The timings are for the dominating computational effort discussed above. If the timings would be proportional to the flop count, then the ratio should be about 4.5.

Timings of the same computations carried out at different times typically differ. Table 1 therefore reports mean values over 1000 runs. The table shows that the representation (34) can be evaluated faster than the formulas (12) and (25). The reported timings illustrate that when the number of nodes k in (12) is small, the time required for data access and data movement dominates the time needed for arithmetic operations.

5. Conclusion

Section 2 of this paper presents a new derivation of the representation (18) of the rule (8). This derivation has the advantage of carrying over, *mutatis mutandis*, to the situation when the tridiagonal matrix \widehat{T}_{2k+1} is nonsymmetric. Section 3 presents the derivation. The advantages of using the new derived formulas is that they can be evaluated faster than available formulas. This is illustrated by timings reported in Section 4, where we show that the new representation (34) can be evaluated faster than the representation (25).

Table 1: Ratios of average CPU times for computing the Gauss rule (12) and the generalized averaged Gauss rule using the representation (25), and for computing the generalized averaged Gauss rule using the representation (34), which yields the Gauss rule (12) without additional work, for several values of k . The table shows averages over 1000 runs.

k	$\frac{\text{time for computing the rules (12) and (25)}}{\text{time for computing the rule (34)}}$
1000	3.3
100	2.5
50	2.4
25	2.6
12	1.9
6	1.7

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