The extended symmetric block Lanczos method for matrix-valued Gauss-type quadrature rules

In Memory of Luc Wuytack

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Abstract

This paper describes methods based on the extended symmetric block Lanczos process for computing element-wise estimates of upper and lower bounds for matrix functions of the form $V^T f(A)V$, where the matrix $A \in \mathbb{R}^{n\times n}$ is large, symmetric, and nonsingular, $V \in \mathbb{R}^{n\times s}$ is a block vector with $1 \le s \ll n$ orthonormal columns, and f is a function that is defined on the convex hull of the spectrum of A. Pairs of block Gauss–Laurent and block anti-Gauss–Laurent quadrature rules are defined and applied to determine the desired estimates. The methods presented generalize methods discussed by Fenu et al. [8], which use (standard) block Krylov subspaces, to allow the application of extended block Krylov subspaces. The latter spaces are the union of a (standard) block Krylov subspace determined by positive powers of A and a block Krylov subspace defined by negative powers of A. Computed examples illustrate the effectiveness of the proposed method.

Keywords: Extended block Krylov subspace, matrix function, Laurent polynomial, Gauss quadrature, anti-Gauss quadrature.

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1. Introduction

We are concerned with the approximation of expressions of the form

$$\mathbb{I}(f) := V^T f(A)V, \tag{1}$$

where $A \in \mathbb{R}^{n\times n}$ is a large symmetric nonsingular matrix and $V \in \mathbb{R}^{n\times s}$ is a "block vector" with $1 \le s \ll n$ orthonormal columns. The function f is assumed to be continuous on the convex hull of the spectrum of A. Then the matrix function $f(A)$ can be defined by the spectral factorization of A; see below. Here and throughout this paper the superscript ^{T} denotes transposition. The need to evaluate expressions of the form (1) arises in various applications including machine learning ($f(t) = \log(t)$) [11], quantum chromodynamics ($f(t) = t^{1/2}$) [13], and electronic structure computation [3, 5, 22].

When the matrix A is of small to moderate size, the expression (1) can be evaluated by first computing the spectral factorization

$$A = U\Lambda U^T, \qquad \Lambda = \mathrm{diag}[\lambda_1, \lambda_2, \ldots, \lambda_n], \tag{2}$$

where $\lambda_1 \le \lambda_2 \le \ldots \le \lambda_n$ denote the eigenvalues of A, and the matrix $U \in \mathbb{R}^{n\times n}$ is orthogonal; its columns are eigenvectors of A. Then

$$f(A) = Uf(\Lambda)U^T, \qquad f(\Lambda) = \mathrm{diag}[f(\lambda_1), f(\lambda_2), \ldots, f(\lambda_n)],$$

and the expression (1) easily can be calculated by using this factorization.

We are interested in computing inexpensive approximations of (1) when A is too large to make the evaluation of the spectral factorization (2) feasible or attractive. In the following, we will use (2) to describe properties of the methods discussed, but the application of these methods does not require the evaluation of the spectral factorization.

Golub and Meurant [9] observed that the expression (1) can be written as a Stieltjes-type integral with a matrix-valued measure. This suggests that (1) can be approximated by a quadrature rule. We have

$$\mathbb{I}(f) = V^T f(A)V = \widehat{V} f(\Lambda)\widehat{V}^T = \sum_{i=1}^{n} f(\lambda_i)\widehat{V}_i\widehat{V}_i^T = \int f(\lambda)d\alpha(\lambda), \tag{3}$$

where $\widehat{V} = [\widehat{V}_1, \ldots, \widehat{V}_n] = V^T U \in \mathbb{R}^{s \times n}$ and $\alpha : \mathbb{R} \longrightarrow \mathbb{R}^{s\times s}$ is a piece-wise constant matrix-valued function with a jump of size $\widehat{V}_i \widehat{V}_i^T$ at the eigenvalue λ_i of A; $d\alpha(\lambda)$ is the associated measure. Application of a few, say $1 \leq m \ll n/s$, steps of the symmetric block Lanczos process to A with initial block vector V generically gives the block Lanczos decomposition [8, 9]

$$A\mathbb{V}_m = \mathbb{V}_m \mathbb{T}_m + G_m \widetilde{E}_m^T. \tag{4}$$

Here the matrix $\mathbb{V}_m = [V_1, V_2, \ldots, V_m] \in \mathbb{R}^{n \times ms}$ consists of orthonormal block vectors $V_j \in \mathbb{R}^{n\times s}$, i.e.,

$$V_i^T V_j = \begin{cases} I_s & i = j, \\ O_s & i \neq j, \end{cases}$$

where $I_s \in \mathbb{R}^{s\times s}$ denotes the identity matrix and $O_s \in \mathbb{R}^{s\times s}$ the zero matrix. Moreover, $V_1 = V$ and the block vectors $V_1, V_2, \ldots, V_m$ span the block Krylov subspace

$$\mathcal{K}_m(A, V) := \text{range}\{V, AV, \ldots, A^{m-1}V\} \subset \mathbb{R}^{n\times s}. \tag{5}$$

Further, the block vector $G_m \in \mathbb{R}^{n\times s}$ in (4) satisfies $\mathbb{V}_m^T G_m = O \in \mathbb{R}^{ms\times s}$, and $\widetilde{E}_m = [O_s, \ldots, O_s, I_s]^T \in \mathbb{R}^{ms\times s}$. We assume for notational simplicity that n/s is an integer. The matrix $\mathbb{T}_m \in \mathbb{R}^{ms\times ms}$ is symmetric and block tridiagonal with blocks of order s; see, e.g., [8, 9] for details. It is shown by Golub and Meurant [9] as well as by Fenu et al. [8] that the matrix $\mathbb{T}_m$ defines a block Gauss quadrature rule,

$$\mathbb{G}_m(f) = \widetilde{E}_1^T f(\mathbb{T}_m) \widetilde{E}_1,$$

with ms nodes (the eigenvalues of $\mathbb{T}_m$) associated with the measure $d\alpha(\lambda)$. Here $\widetilde{E}_1 = [I_s, O_s, \ldots, O_s]^T \in \mathbb{R}^{ms\times s}$. This quadrature rule satisfies

$$\mathbb{G}_m(f) = \mathbb{I}(f), \qquad \forall f \in \mathbb{P}_{2m-1},$$

where $\mathbb{P}_{2m-1}$ denotes the set of all polynomials of degree at most $2m-1$; see [8, 9] for proofs. Block Gauss quadrature rules are fairly inexpensive to compute; the dominating computational cost for large problems is the evaluation of m matrix-block-vector products with the matrix A.

It is important to be able to determine how accurately a block Gauss quadrature rule approximates (1), because this makes it possible to choose an appropriate number of steps, m, of the block Lanczos process. Fenu et al. [8] describe how estimates of the element-wise error can be determined quite inexpensively by evaluating a block anti-Gauss quadrature rule associated with the block Gauss rule used. These block anti-Gauss rules generalize the anti-Gauss rules proposed by Laurie [19], who considered the situation when the measure $d\alpha$ is real-valued and nonnegative. Further extensions of Laurie's anti-Gauss rules have recently been described in [1].

If the function f cannot be approximated accurately by a polynomial of low to moderate degree, then block Gauss quadrature rules with moderately many nodes will not furnish accurate approximations of the expression (1). This situation occurs, for instance, when the function f or one of its low-order derivatives has a singularity at or close to some eigenvalue of A. Then it may be beneficial to approximate f by a rational function with a pole at or close to a singularity of f or of one of its derivatives. In fact, Druskin and Knizhnerman [6] showed that it also may be beneficial to approximate entire functions f by rational functions with a pole in the finite complex plane, compared with polynomial approximation. The analysis of Druskin and Knizhnerman [6] suggests that the expression $f(A)V$ be approximated by an element in an extended block Krylov subspace of the form

$$\mathcal{K}_m^e(A,V) := \text{range}\{V, A^{-1}V, AV, A^{-2}V, \ldots, A^{m-1}V, A^{-m}V\} \subset \mathbb{R}^{n\times s}, \qquad (6)$$

where the matrix A is assumed to be nonsingular; see also [4, 12, 16, 17, 18, 20] for discussions on properties and applications of extended Krylov subspace methods and some generalizations.

A block Gauss–Laurent quadrature rule, which is based on a Krylov subspace of the form (6), may yield a more accurate approximation of (1) than a (standard) block Gauss quadrature rule, which is based on a standard Krylov subspace of the form (5), with the same number of nodes. This is illustrated by computed examples in Section 5. The present paper therefore develops block

Gauss–Laurent and block anti-Gauss–Laurent quadrature rules. This work extends results by Fenu et al. [8] for (standard) block Gauss and block anti-Gauss rules to analogous Gauss–Laurent-type quadrature rules.

The remainder of this paper is organized as follows. Section 2 introduces the extended block Lanczos process for generating a basis of orthonormal block vectors for the extended block Krylov subspace (6). This process generalizes the extended Krylov process (with block size one) described in [16]. We express a basis for the extended block Krylov subspace with the aid of orthogonal $s \times s$ matrix Laurent polynomials, analogously as in [14, 16]. Section 3 is concerned with the computation of block Gauss–Laurent quadrature rules associated with the subspace (6). Block anti-Gauss–Laurent quadrature are described in Section 4, and numerical experiments are presented in Section 5 to illustrate the quality of the computed approximations. Concluding remarks can be found in Section 6.

2. The extended symmetric block Lanczos process

We describe the extended block Lanczos process for generating an orthonormal basis $\{V_j\}_{j=1}^{2m}$ of block vectors $V_j \in \mathbb{R}^{n\times s}$ for the extended block Krylov subspace (6). This block Lanczos process is a special case of block rational Krylov subspace methods, which recently have received considerable attention; see, e.g., [7, 10, 15, 20]. The derivation of the proposed method uses short recursion relations which are based on recursion formulas that are satisfied by orthogonal matrix Laurent polynomials. The derivation of this paper generalizes the derivation of the extended symmetric Lanczos process for vectors (with block size one) described in [16]. Related but different recursion formulas form the basis for the extended global Lanczos method presented in [4]. The present paper discusses extended Krylov subspaces, for which the highest positive and negative powers of the matrix A are about the same; cf. (6). The derivation can be extended to the situation when the highest positive and negative powers differ significantly. This case is addressed in [17] when the block size is one. In the interest of brevity, we do not discuss this situation in the present paper.

Assume that the block vector $V \in \mathbb{R}^{n\times s}$ has orthonormal columns. Then we initialize the computations with the extended symmetric block Lanczos process by

$$V_1 = V, \quad \widehat{V}_2 = A^{-1}V_1 - V_1\Gamma_{1,2}, \quad \widehat{V}_2 = V_2\Gamma_{2,2}, \tag{7}$$

where $\Gamma_{1,2} = V_1^T A^{-1} V_1 \in \mathbb{R}^{s\times s}$ and $\Gamma_{2,2} \in \mathbb{R}^{s\times s}$ is the upper triangular matrix in the skinny QR factorization of $\widehat{V}_2$; the matrix $V_2 \in \mathbb{R}^{n\times s}$ has orthonormal columns. We will show that the extended symmetric block Lanczos process satisfies recursion relations of the form

$$\begin{array}{rcl} \widetilde{V}_{2j+1} & = & AV_{2j-1} - \sum\limits_{i=2j-3}^{2j} V_i H_{i,2j-1}, \\ \widetilde{V}_{2j+2} & = & A^{-1}V_{2j} - \sum\limits_{i=2j-2}^{2j+1} V_i H_{i,2j}, \end{array} \qquad j = 1, 2, \ldots, m, \tag{8}$$

where terms with an index $i < 1$ are ignored. Computing the skinny QR factorizations of the matrices $\widetilde{V}_{2j+1}$ and $\widetilde{V}_{2j+2}$, we obtain

$$\widetilde{V}_{2j+1} = V_{2j+1}H_{2j+1,2j-1} \quad \text{and} \quad \widetilde{V}_{2j+2} = V_{2j+2}H_{2j+2,2j},$$

where the matrices $V_{2j+1}, V_{2j+2} \in \mathbb{R}^{n\times s}$ have orthonormal columns and the matrices $H_{2j+1,2j-1}, H_{2j+2,2j} \in \mathbb{R}^{s\times s}$ are upper triangular. The remaining matrices $H_{i,j} \in \mathbb{R}^{s\times s}$ in (8) are determined so that the block vectors $\widetilde{V}_{2j+1}$ and $\widetilde{V}_{2j+2}$ are orthogonal to all already available block vectors $\widetilde{V}_i$. This leads to the expressions

$$H_{i,2j-1} = V_i^T A V_{2j-1}, \quad H_{i,2j} = V_i^T A^{-1} V_{2j}. \tag{9}$$

The following proposition provides recursion formulas that can be used to compute the matrices $H_{i,j} \in \mathbb{R}^{s\times s}$.

Proposition 1. *The matrices* $\Gamma_{i,j}, H_{i,j} \in \mathbb{R}^{s\times s}$ *defined by* (7) *and* (9) *can be computed as follows:*

$$H_{1,2} = \Gamma_{2,2}^T,$$
$$H_{2,1} = (\Gamma_{2,2}^{-1})^T (I_s - \Gamma_{1,2} H_{1,1}),$$
$$H_{2,3} = -(\Gamma_{2,2}^{-1})^T \Gamma_{1,2} H_{1,3},$$

and for $j = 2, 3, \ldots, m$, we have

$$
\begin{aligned}
H_{2j-3,2j-1} &= H_{2j-1,2j-3}^T, \\
H_{2j-2,2j-1} &= -(H_{2j-2,2j-4}^{-1})^T H_{2j-3,2j-4}^T H_{2j-3,2j-1}, \\
H_{2j,2j-1} &= -(H_{2j,2j-2}^{-1})^T \sum_{i=2j-3}^{2j-1} H_{i,2j-2}^T H_{i,2j-1}, \\
H_{2j-2,2j} &= H_{2j,2j-2}^T, \\
H_{2j-1,2j} &= -(H_{2j-1,2j-3}^{-1})^T H_{2j-2,2j-3}^T H_{2j-2,2j}, \\
H_{2j+1,2j} &= -(H_{2j+1,2j-1}^{-1})^T \sum_{i=2j-2}^{2j} H_{i,2j-1}^T H_{i,2j}.
\end{aligned}
$$

In actual computations, we do not form inverses of matrices, but instead solve systems of equations. These systems are assumed to be uniquely solvable.

Proof. The relations (7) and (9), and using the orthonormality of the block vectors $\{V_i\}_{i=1}^{2m+2}$, give

$$H_{1,2} = V_1^T A^{-1} V_2 = [V_2^T A^{-1} V_1]^T = [V_2^T (V_1 \Gamma_{1,2} + V_2 \Gamma_{2,2})]^T = \Gamma_{2,2}^T.$$

We obtain from (7) that

$$AV_2 \Gamma_{2,2} = V_1 - AV_1 \Gamma_{1,2},$$

and it follows that

$$
\begin{aligned}
H_{2,1} &= [V_1^T A V_2]^T = [V_1^T (V_1 - AV_1 \Gamma_{1,2}) \Gamma_{2,2}^{-1}]^T = [(I_s - H_{1,1} \Gamma_{1,2}) \Gamma_{2,2}^{-1}]^T \\
&= (\Gamma_{2,2}^{-1})^T (I_s - \Gamma_{1,2} H_{1,1})
\end{aligned}
$$

and

$$
\begin{aligned}
H_{2,3} &= [V_3^T A V_2]^T = [V_3^T (V_1 - AV_1 \Gamma_{1,2}) \Gamma_{2,2}^{-1}]^T = [-H_{3,1} \Gamma_{1,2} \Gamma_{2,2}^{-1}]^T \\
&= -(\Gamma_{2,2}^{-1})^T \Gamma_{1,2} H_{1,3}.
\end{aligned}
$$

We also have

$$H_{2j-3,2j-1} = V_{2j-3}^T A V_{2j-1} = [V_{2j-1}^T A V_{2j-3}]^T = H_{2j-1,2j-3}^T.$$

The matrices $H_{2j-2,2j-1}$ and $H_{2j,2j-1}$ are obtained from the expressions for AV_{2j+2}. Multiplying the second equation in (8) by A from the left-hand side gives

$$AV_{2j+2}H_{2j+2,2j} = V_{2j} - \sum_{i=2j-2}^{2j+1} AV_i H_{i,2j},$$

and assuming that the matrix $H_{2j+2,2j}$ is invertible, we get

$$AV_{2j+2} = V_{2j}H_{2j+2,2j}^{-1} - \sum_{i=2j-2}^{2j+1} AV_i H_{i,2j} H_{2j+2,2j}^{-1}. \tag{10}$$

It follows that

$$H_{2j-2,2j-1} = V_{2j-2}^T AV_{2j-1} = [V_{2j-1}^T AV_{2j-2}]^T.$$

Using (10), we obtain

$$\begin{aligned}
H_{2j-2,2j-1} &= \left[V_{2j-1}^T \left[V_{2j-4} - \sum_{i=2j-6}^{2j-3} AV_i H_{i,2j-4}\right] H_{2j-2,2j-4}^{-1}\right]^T \\
&= -\left[\sum_{i=2j-6}^{2j-3} V_{2j-1}^T AV_i H_{i,2j-4} H_{2j-2,2j-4}^{-1}\right]^T \\
&= -\left[\sum_{i=2j-6}^{2j-3} H_{i,2j-1}^T H_{i,2j-4} H_{2j-2,2j-4}^{-1}\right]^T.
\end{aligned}$$

Since $H_{i,2j-1} = O_s$ for $i = 1, 2, \ldots, 2j-4$, we have

$$\begin{aligned}
H_{2j-2,2j-1} &= -[H_{2j-3,2j-1}^T H_{2j-3,2j-4} H_{2j-2,2j-4}^{-1}]^T \\
&= -(H_{2j-2,2j-4}^{-1})^T H_{2j-3,2j-4}^T H_{2j-3,2j-1}.
\end{aligned}$$

For the matrix $H_{2j,2j-1}$, we have

$$H_{2j,2j-1} = V_{2j}^T AV_{2j-1} = [V_{2j-1}^T AV_{2j}]^T.$$

Applying an analogue of (10) to the expression AV_{2j}, and similar manipulations as above, yield

$$H_{2j,2j-1} = -(H_{2j,2j-2}^{-1})^T \sum_{i=2j-3}^{2j-1} H_{i,2j-2}^T H_{i,2j-1},$$

as well as

$$H_{2j-2,2j} = V_{2j-2}^T A^{-1} V_{2j} = [V_{2j}^T A^{-1} V_{2j-2}]^T = H_{2j,2j-2}^T.$$

The matrices $H_{2j-1,2j}$ and $H_{2j+1,2j}$ are obtained from the expressions for $A^{-1}V_{2j+1}$ as follows. Multiplying the first equation in (8) by A^{-1} from the left, and assuming that the matrix $H_{2j+1,2j-1}$ is invertible, we obtain

$$A^{-1}V_{2j+1} = \left[V_{2j-1} - \sum_{i=2j-3}^{2j} A^{-1}V_i H_{i,2j-1}\right] H_{2j+1,2j-1}^{-1}. \tag{11}$$

The matrix $H_{2j-1,2j}$ is defined by

$$H_{2j-1,2j} = V_{2j-1}^T A^{-1} V_{2j} = [V_{2j}^T A^{-1} V_{2j-1}]^T.$$

Using (11) yields

$$\begin{aligned} H_{2j-1,2j} &= \left[V_{2j}^T \left[V_{2j-3} - \sum_{i=2j-5}^{2j-2} A^{-1}V_i H_{i,2j-3}\right] H_{2j-1,2j-3}^{-1}\right]^T \\ &= -\left[\sum_{i=2j-5}^{2j-2} V_{2j}^T A^{-1} V_i H_{i,2j-3} H_{2j-1,2j-3}^{-1}\right]^T \\ &= -\left[\sum_{i=2j-5}^{2j-2} H_{i,2j}^T H_{i,2j-3} H_{2j-1,2j-3}^{-1}\right]^T. \end{aligned}$$

In view of that $H_{i,2j} = O_s$ for $i = 1, 2, \ldots, 2j-1$, we obtain

$$H_{2j-1,2j} = -(H_{2j-1,2j-3}^{-1})^T H_{2j-2,2j-3}^T H_{2j-2,2j}.$$

For the matrix $H_{2j+1,2j}$, we have

$$H_{2j+1,2j} = V_{2j+1}^T A V_{2j} = [V_{2j}^T A V_{2j+1}]^T.$$

The expression (11) and similar manipulations as above give

$$H_{2j+1,2j} = -(H_{2j+1,2j-1}^{-1})^T \sum_{i=2j-2}^{2j} H_{i,2j-1}^T H_{i,2j}.$$

This completes the proof. $\square$

We next discuss some useful properties of extended block Krylov subspaces. Here and below we will tacitly assume that the number of steps of the extended symmetric block Lanczos process is small enough to avoid breakdown, i.e., that all required inverses in Proposition 1 exist. This is the generic situation; breakdown is very rare.

Application of $1 \leq m \ll n/s$ steps of the extended symmetric block Lanczos process to the matrix A with initial block vector V with orthonormal columns yields the decomposition

$$\begin{aligned} A\mathbb{V}_{2m} &= \mathbb{V}_{2m+1}\widetilde{\mathbb{T}}_{2m}, \\ &= \mathbb{V}_{2m}\mathbb{T}_{2m} + V_{2m+1}\left[T_{2m+1,2m-1},\ T_{2m+1,2m}\right]E_m^T, \end{aligned} \tag{12}$$

where the matrix $E_m = [e_{2s(m-1)+1}, \ldots, e_{2ms}] \in \mathbb{R}^{2ms \times 2s}$ is made up of the last $2s$ columns of the identity matrix $I_{2ms} \in \mathbb{R}^{2ms \times 2ms}$ and

$$\mathbb{T}_{2m} = \mathbb{V}_{2m}^T A \mathbb{V}_{2m} \in \mathbb{R}^{2ms \times 2ms}, \quad \widetilde{\mathbb{T}}_{2m} = \mathbb{V}_{2m+1}^T A \mathbb{V}_{2m} \in \mathbb{R}^{(2m+1)s \times 2ms} \tag{13}$$

are block pentadiagonal matrices with $s \times s$ blocks of the form $T_{i,j} = V_i^T A V_j$, $i, j = 1, 2, \ldots$. The matrices

$$\mathbb{V}_{2m} = [V_1, V_2, \ldots, V_{2m}] \in \mathbb{R}^{n \times 2ms}, \ \ \mathbb{V}_{2m+1} = [V_1, V_2, \ldots, V_{2m+1}] \in \mathbb{R}^{n \times (2m+1)s},$$

are made up of orthonormal block vectors $V_j \in \mathbb{R}^{n \times s}$.

The block entries of $\mathbb{T}_{2m}$ and $\widetilde{\mathbb{T}}_{2m}$ can be expressed in terms of recursion coefficients for the extended block symmetric Lanczos process as shown below. This makes them easy to compute.

Proposition 2. *Let the matrices $\Gamma_{i,j}$ and $H_{i,j}$ be defined by* (7) *and* (9)*. Then the nontrivial entries of the matrices $\mathbb{T}_{2m} = [T_{i,j}]$ and $\widetilde{\mathbb{T}}_{2m} = [T_{i,j}]$ in* (13) *can be expressed as*

$$\begin{aligned} T_{i,2j-1} &= H_{i,2j-1} \quad \textit{for} \quad i = 2j-3, \ldots, 2j+1, \quad j = 1, 2, \ldots, m, \\ T_{1,2} &= T_{2,1}^T, \\ T_{2,2} &= -T_{2,1}\Gamma_{1,2}\Gamma_{2,2}^{-1}, \\ T_{3,2} &= -T_{3,1}\Gamma_{1,2}\Gamma_{2,2}^{-1}. \end{aligned}$$

Moreover, for $j = 1, 2, \ldots, m-1$, we have

$$T_{2j+1,2j+2} = T^T_{2j+2,2j+1},$$
$$T_{2j+2,2j+2} = -T_{2j+2,2j+1} H_{2j+1,2j} H^{-1}_{2j+2,2j},$$
$$T_{2j+3,2j+2} = -T_{2j+3,2j+1} H_{2j+1,2j} H^{-1}_{2j+2,2j}.$$

Proof. We have $T_{i,j} = V_i^T A V_j$ for all i and j. The definition of $H_{i,2j-1}$ in (9) yields $T_{i,2j-1} = H_{i,2j-1}$. Using (7), we obtain

$$V_1 \Gamma_{1,2} + V_2 \Gamma_{2,2} = A^{-1} V_1.$$

Multiplying this equation by A from the left gives

$$AV_1 \Gamma_{1,2} + AV_2 \Gamma_{2,2} = V_1,$$

from which we obtain

$$AV_2 = \left[V_1 - AV_1 \Gamma_{1,2} \right] \Gamma^{-1}_{2,2}.$$

It follows that

$$T_{1,2} = V_1^T A V_2 = [V_2^T A V_1]^T = T^T_{2,1},$$
$$T_{2,2} = V_2^T A V_2 = -T_{2,1} \Gamma_{1,2} \Gamma^{-1}_{2,2},$$
$$T_{3,2} = V_3^T A V_2 - T_{3,1} \Gamma_{1,2} \Gamma^{-1}_{2,2}.$$

For $i = 4, 5, \ldots, 2m+1$, we get

$$T_{i,2} = V_i^T A V_2 = -T_{i,1} \Gamma_{1,2} \Gamma^{-1}_{2,2} = O_s.$$

The following formulas are obtained from the expressions of AV_{2j+2} for $j = 1, 2, \ldots, m-1$. Multiplying the second equation in (8) by A from the left gives

$$AV_{2j+2} = \left[V_{2j} - \sum_{i=1}^{2j+1} AV_i H_{i,2j} \right] H^{-1}_{2j+2,2j}.$$

We obtain from (8) that the $s \times s$ matrices

$$T_{2j+1,1}, \ldots, T_{2j+1,2j-2}, \quad T_{2j+2,1}, \ldots, T_{2j+2,2j}, \quad \text{and} \quad T_{2j+3,1}, \ldots, T_{2j+3,2j}$$

vanish. Hence,

$$
\begin{aligned}
T_{2j+1,2j+2} &= V_{2j+1}^T A V_{2j+2} = [V_{2j+2}^T A V_{2j+1}]^T = T_{2j+2,2j+1}^T, \\
T_{2j+2,2j+2} &= V_{2j+2}^T A V_{2j+2} = -\left[\sum_{i=1}^{2j+1} T_{2j+2,i} H_{i,2j}\right] H_{2j+2,2j}^{-1} \\
&= -T_{2j+2,2j+1} H_{2j+1,2j} H_{2j+2,2j}^{-1}, \\
T_{2j+3,2j+2} &= V_{2j+3}^T A V_{2j+2} = -\sum_{i=1}^{2j+1} T_{2j+3,i} H_{i,2j} H_{2j+2,2j}^{-1} \\
&= -T_{2j+3,2j+1} H_{2j+1,2j} H_{2j+2,2j}^{-1}.
\end{aligned}
$$

This completes the proof. □

It follows from the recursion formulas (7) and (8) that the orthonormal block vector basis $\{V_j\}_{j=1}^{2m+1}$ can be expressed in the form

$$
V_{2j} = \sum_{k=-j}^{j-1} A^k V C_k^{(2j-1)} \quad \text{and} \quad V_{2j+1} = \sum_{k=-j}^{j} A^k V C_k^{(2j)},
$$

where $C_k^{(2j-1)}, C_k^{(2j)} \in \mathbb{R}^{s\times s}$. Introduce for $\lambda \in \mathbb{R}$ the matrix-valued Laurent polynomials

$$
R_{2j-1}(\lambda) := \sum_{k=-j}^{j-1} \lambda^k C_k^{(2j-1)} \quad \text{and} \quad R_{2j}(\lambda) := \sum_{k=-j}^{j} \lambda^k C_k^{(2j)}, \tag{14}
$$

and define

$$
R_{2j-1}(A) \circ V = \sum_{k=-j}^{j-1} A^k V C_k^{(2j-1)} \quad \text{and} \quad R_{2j}(A) \circ V = \sum_{k=-j}^{j} A^k V C_k^{(2j)}. \tag{15}
$$

Then

$$
\begin{aligned}
V_{2j} &= R_{2j-1}(A) \circ V, \qquad j = 1, 2, \ldots, m, \\
V_{2j+1} &= R_{2j}(A) \circ V, \qquad j = 0, 1, \ldots, m.
\end{aligned} \tag{16}
$$

By construction, the Laurent polynomials (15) are orthonormal with respect to the bilinear form

$$
\begin{aligned}
\langle P, Q\rangle &= (P(A)\circ V)^T (Q(A)\circ V) = \textstyle\sum_{i=1}^n P^T(\lambda_i)\widehat{V}_i \widehat{V}_i^T Q(\lambda_i) \\
&= \textstyle\int P^T(\lambda) d\alpha(\lambda) Q(\lambda),
\end{aligned} \tag{17}
$$

where P and Q are real $(s\times s)$-matrix-valued functions and $\alpha : \mathbb{R} \longrightarrow \mathbb{R}^{s\times s}$ is a piece-wise constant matrix-valued function with jumps at the eigenvalues

λ_i of A, and with $\widehat{V} = [\widehat{V}_1, \widehat{V}_2, \ldots, \widehat{V}_n] \in \mathbb{R}^{s\times n}$ defined in (2). Substituting $V_i = R_{i-1}(A) \circ V$ into (8) shows that the Laurent polynomials satisfy a pair of five-term recurrence relations of the form

$$\begin{aligned} R_{2j}(\lambda)H_{2j+1,2j-1} &= \lambda R_{2j-2}(\lambda) - \textstyle\sum_{i=2j-3}^{2j} R_{i-1}(\lambda)H_{i,2j-1}, \\ R_{2j+1}(\lambda)H_{2j+2,2j} &= \lambda^{-1} R_{2j-1}(\lambda) - \textstyle\sum_{i=2j-2}^{2j+1} R_{i-1}(\lambda)H_{i,2j}, \end{aligned}$$

for $j = 1, 2, \ldots, m$, where

$$R_0(\lambda) = I_s, \quad R_1(\lambda) = (\lambda^{-1} I_s - \Gamma_{1,2})\Gamma_{2,2}^{-1}, \quad R_{-2}(\lambda) = R_{-1}(\lambda) = O_s.$$

3. Block Gauss–Laurent quadrature rules

Application of m steps of the extended symmetric block Lanczos process to A with initial block vector V gives the approximation

$$\mathbb{G}_{2m}^{e}(f) := E_1^T f(\mathbb{T}_{2m}) E_1, \tag{18}$$

of the Stieltjes integral (3), where the block vector $E_1 \in \mathbb{R}^{2ms\times s}$ is made up of the first s columns of the identity matrix I_{2ms}. Introduce the spectral factorization $\mathbb{T}_{2m} = Y_{2m}\Theta_{2m}Y_{2m}^T$ with

$$\begin{aligned} Y_{2m} &:= [y_1^{(m)}, y_2^{(m)}, \ldots, y_{2ms}^{(m)}] \in \mathbb{R}^{2ms\times 2ms}, \\ \Theta_{2m} &:= \mathrm{diag}[\theta_1^{(m)}, \theta_2^{(m)}, \ldots, \theta_{2ms}^{(m)}] \in \mathbb{R}^{2ms\times 2ms}. \end{aligned} \tag{19}$$

The columns of the orthogonal matrix Y_{2m} are eigenvectors and the diagonal entries of the matrix Θ_{2m} are eigenvalues of $\mathbb{T}_{2m}$. We order the eigenvalues according to $\theta_1^{(m)} \leq \theta_2^{(m)} \leq \ldots \leq \theta_{2ms}^{(m)}$. The quadrature rule (18) can be written as

$$\mathbb{G}_{2m}^{e}(f) = \sum_{i=1}^{2ms} f(\theta_i^{(m)}) u_i^{(m)} (u_i^{(m)})^T,$$

where the vector $u_i^{(m)} \in \mathbb{R}^s$ is made up of the first s elements of $y_i^{(m)}$ for $1 \leq i \leq 2ms$. This shows that (18) is an $2ms$-node quadrature formula.

Theorem 1. *Consider the block vector of Laurent polynomial,*

$$\overrightarrow{R}_{2m}(\lambda) := [R_0(\lambda), R_1(\lambda), \ldots, R_{2m-1}(\lambda)] \in \mathbb{R}^{s\times 2ms},$$

where the Laurent polynomials $R_0, R_1, \ldots, R_{2m-1}$ are determined by (16)*. The $2ms$ eigenvalues of $\mathbb{T}_{2m}$ are the zeros of* $\det(R_{2m}(\lambda))$*. Moreover, the unit right eigenvector $y_i^{(m)}$ of $\mathbb{T}_{2m}$ corresponding to the eigenvalue $\theta_i^{(m)}$ is given by $y_i^{(m)} = \overrightarrow{R}_{2m}^T(\theta_i^{(m)})u_i^{(m)}$, and $R_{2m}^T(\theta_i^{(m)})u_i^{(m)} = 0$.*

Proof. The recurrence relation (12) together with (16) give

$$\lambda \overrightarrow{R}_{2m}(\lambda) = \overrightarrow{R}_{2m}(\lambda)\mathbb{T}_{2m} + R_{2m}(\lambda)[T_{2m+1,2m-1}, T_{2m+1,2m}]E_m^T. \tag{20}$$

Let θ be a zero of $\det(R_{2m}(\lambda))$. Then the rows of $R_{2m}(\theta)$ are linearly dependent. It follows that there is a vector $u \in \mathbb{R}^s \backslash \{0\}$ such that

$$u^T R_{2m}(\theta) = 0.$$

Hence,

$$\theta u^T \overrightarrow{R}_{2m}(\theta) = u^T \overrightarrow{R}_{2m}(\theta)\mathbb{T}_{2m}. \tag{21}$$

Therefore θ is an eigenvalue of $\mathbb{T}_{2m}$.

This shows that $\theta \to \det(R_{2m}(\theta))$ has $2ms$ zeros, because the determinant of $R_{2m}(\theta)\theta^m$ is a polynomial of degree $2ms$ in θ. This implies that all eigenvalues $\theta_i^{(m)}$ are zeros of $\det(R_{2m}(\theta))$. It follows from equation (21) that the vector $\overrightarrow{R}_{2m}^T(\theta_i^{(m)})u_i^{(m)}$ is a right eigenvector of $\mathbb{T}_{2m}$ associated with the eigenvalue $\theta_i^{(m)}$. Substituting (21) into (20) yields

$$(u_i^{(m)})^T R_{2m}(\theta_i^{(m)})[T_{2m+1,2m-1}, T_{2m+1,2m}]E_m^T = O_s.$$

Using the fact that the $s \times s$ matrices $T_{2m+1,2m-1}$ and $T_{2m+1,2m}$ are nonsingular, we obtain $R_{2m}^T(\theta_i^{(m)})u_i^{(m)} = 0$. This completes the proof. $\square$

We next show that the quadrature rule (18) for the approximation of (1) is exact for all Laurent polynomials in

$$\Delta_{-2m,2m-1} := \mathrm{span}\{x^{-2m}, \ldots, x^{2m-1}\}.$$

The demonstration of this property requires some auxiliary results about the matrices $\mathbb{T}_{2m}$ and

$$\mathbb{S}_{2m} := \mathbb{V}_{2m}^T A^{-1} \mathbb{V}_{2m}. \tag{22}$$

Proposition 3. *The matrix* $\mathbb{S}_{2m}$ *defined by* (22) *satisfies the following relations*

$$A^{-1}\mathbb{V}_{2m} = \mathbb{V}_{2m}\mathbb{S}_{2m} + [V_{2m+1}, V_{2m+2}]\gamma_{m+1}E_m^T, \tag{23}$$

where

$$\gamma_{m+1} = \begin{bmatrix} V_{2m+1}^T \\ V_{2m+2}^T \end{bmatrix} A^{-1}[V_{2m-1}, V_{2m}] \in \mathbb{R}^{2s\times 2s}.$$

Proof. According to the recursion formulas (8), we have $A^{-1}\mathbb{V}_{2m} \in \mathcal{K}_{m+1}^e(A, V)$. Therefore there is a matrix $S_{2m} \in \mathbb{R}^{(2m+2)s\times 2ms}$ such that

$$A^{-1}\mathbb{V}_{2m} = \mathbb{V}_{2m+2}S_{2m}, \text{ where } \mathbb{V}_{2m+2} = [\mathbb{V}_{2m}, V_{2m+1}, V_{2m+2}] \in \mathbb{R}^{n\times(2m+2)s}.$$

This implies that

$$S_{2m} = \mathbb{V}_{2m+2}^T A^{-1}\mathbb{V}_{2m} = \begin{bmatrix} \mathbb{S}_{2m} \\ \gamma_{m+1}E_m^T \end{bmatrix}.$$

Hence,

$$A^{-1}\mathbb{V}_{2m} = \mathbb{V}_{2m+2}\begin{bmatrix} \mathbb{S}_{2m} \\ \gamma_{m+1}E_m^T \end{bmatrix} = \mathbb{V}_{2m}\mathbb{S}_{2m} + [V_{2m+1}, V_{2m+2}]\gamma_{m+1}E_m^T.$$

□

Proposition 4. *The matrix* $\mathbb{S}_{2m} = [S_{i,j}] \in \mathbb{R}^{2ms\times 2ms}$ *defined by* (22) *is symmetric block pentadiagonal with blocks* $S_{i,j} \in \mathbb{R}^{s\times s}$*. For all* $j = 1, 2, \ldots, m$*, we have*

$$\begin{aligned} S_{i,2j-1} &= O_s \quad \textit{for} \quad i < 2j-1 \quad \textit{or} \quad i > 2j, \\ S_{i,2j} &= O_s \quad \textit{for} \quad i < 2j-2 \quad \textit{or} \quad i > 2j+2. \end{aligned}$$

Proof. The result can be shown similarly as Proposition 2. □

Lemma 1. *Let the matrix* $A \in \mathbb{R}^{n\times n}$ *be nonsingular and symmetric, and let the matrices* $\mathbb{T}_{2m}$*,* $\mathbb{S}_{2m}$*, and* $E_1 \in \mathbb{R}^{2ms\times s}$ *be defined by* (13)*,* (22)*, and* (18)*, respectively. Then*

$$A^jV = \mathbb{V}_{2m}\mathbb{T}_{2m}^jE_1, \quad j = 0, 1, \ldots, m-1, \tag{24}$$

$$A^{-j}V = \mathbb{V}_{2m}\mathbb{T}_{2m}^{-j}E_1, \quad j = 0, 1, \ldots, m. \tag{25}$$

Proof. We first show (24). Assume that $m > 1$. Multiplying the second equation of (12) by E_1 from the right and using the fact that $E_m^T E_1 = O_{2s\times s}$, we obtain

$$AV = A\mathbb{V}_{2m}E_1 + \mathbb{V}_{2m}\mathbb{T}_{2m}E_1.$$

Due to the zero structure of $\mathbb{T}_{2m}$, the last term vanishes. Now consider

$$A^jV = \mathbb{V}_{2m}\mathbb{T}_{2m}^jE_1,$$

for some $2 \leq j \leq m-1$. Then

$$A^jV = A \cdot A^{j-1}V = A\mathbb{V}_{2m}\mathbb{T}_{2m}^{j-1}E_1.$$

Using the decomposition (12), we obtain

$$\begin{aligned} A^jV &= [\mathbb{V}_{2m}\mathbb{T}_{2m} + V_{2m+1}[T_{2m+1,2m-1}, T_{2m+1,2m}]E_m^T]\mathbb{T}_{2m}^{j-1}E_1 \\ &= \mathbb{V}_{2m}\mathbb{T}_{2m}^jE_1 + V_{2m+1}[T_{2m+1,2m-1}, T_{2m+1,2m}]E_m^T\mathbb{T}_{2m}^{j-1}E_1. \end{aligned}$$

This gives $E_m^T\mathbb{T}_{2m}^{j-1}E_1 = O_{2s\times s}$ since only the first $(2j-1)s$ entries the block vector $\mathbb{T}_{2m}^{j-1}E_1$ may be nonvanishing. Thus,

$$A^jV = \mathbb{V}_{2m}\mathbb{T}_{2m}^jE_1, \quad j = 0, 1, \ldots, m-1.$$

This shows (24).

We turn to (25). Due to the zero structure of $\mathbb{S}_{2m}$, we obtain by using the same techniques as above that

$$A^{-j}V = \mathbb{V}_{2m}\mathbb{S}_{2m}^jE_1, \quad j = 0, 1, \ldots, m.$$

Equation (25) is now shown by demonstrating that

$$\mathbb{S}_{2m}^jE_1 = \mathbb{T}_{2m}^{-j}E_1, \quad j = 1, 2, \ldots, m.$$

We first show that

$$\mathbb{T}_{2m}^j\mathbb{S}_{2m}^j = \mathbb{T}_{2m}^{j-1}\mathbb{S}_{2m}^{j-1} - \mathbb{T}_{2m}^{j-1}\mu_{m+1}\gamma_{m+1}E_m^T\mathbb{S}_{2m}^{j-1}, \quad j = 1, 2, \ldots, m,$$

with $\mu_{m+1} = \mathbb{V}_{2m}^TA[V_{2m+1}, V_{2m+2}]$, and where γ_{m+1} is defined by (23). Using (12) and (23), we obtain

$$I_{2ms} = \mathbb{T}_{2m}\mathbb{S}_{2m} + \mu_{m+1}\gamma_{m+1}E_m^T.$$

Let $2 \leq j \leq m$ and assume that

$$\mathbb{T}_{2m}^{k}\mathbb{S}_{2m}^{k} = \mathbb{T}_{2m}^{k-1}\mathbb{S}_{2m}^{k-1} - \mathbb{T}_{2m}^{k-1}\mu_{m+1}\gamma_{m+1}E_m^T\mathbb{S}_{2m}^{k-1}, \quad k = 1, \ldots, j-1.$$

Then

$$\begin{aligned}\mathbb{T}_{2m}^{j}\mathbb{S}_{2m}^{j} &= \mathbb{T}_{2m}\mathbb{T}_{2m}^{j-1}\mathbb{S}_{2m}^{j-1}\mathbb{S}_{2m} \\ &= \mathbb{T}_{2m}^{j-1}\mathbb{S}_{2m}^{j-1} - \mathbb{T}_{2m}^{j-1}\mu_{m+1}\gamma_{m+1}E_m^T\mathbb{S}_{2m}^{j-1}.\end{aligned}$$

Multiplying this equation by E_1 from the right gives

$$\mathbb{T}_{2m}^{j}\mathbb{S}_{2m}^{j}E_1 - \mathbb{T}_{2m}^{j-1}\mathbb{S}_{2m}^{j-1}E_1 - \mathbb{T}_{2m}^{j-1}\mu_{m+1}\gamma_{m+1}E_m^T\mathbb{S}_{2m}^{j-1}E_1.$$

Due to the zero structure of $\mathbb{S}_{2m}$, we get $E_m^T\mathbb{S}_{2m}^{j-1}E_1 = O_{2s\times s}$ for $j = 1, 2, \ldots, m$. This implies that

$$\mathbb{T}_{2m}^{j}\mathbb{S}_{2m}^{j}E_1 - \mathbb{T}_{2m}^{j-1}\mathbb{S}_{2m}^{j-1}E_1 = E_1, \quad j = 1, 2, \ldots, m.$$

Since $\mathbb{T}_{2m}$ is nonsingular, we obtain

$$\mathbb{S}_{2m}^{j}E_1 = \mathbb{T}_{2m}^{-j}E_1, \quad j = 1, 2, \ldots, m.$$

This shows (25). □

Theorem 2. *Let A be a symmetric nonsingular matrix. Carry out m steps of the extended symmetric block Lanczos process applied to A with initial block vector $V \in \mathbb{R}^{n\times s}$ with orthonormal columns, and assume that no breakdown occurs. Then the expression* (18) *is a $2ms$-node block Gauss–Laurent quadrature rule associated with the measure $d\alpha$ in* (3)*, i.e.,*

$$\mathbb{G}_{2m}^{e}(f) = \mathbb{I}(f), \quad \forall f \in \Delta_{-2m,2m-1}, \tag{26}$$

where $\Delta_{-2m,2m-1} = \mathrm{span}\{x^{-2m}, \ldots, x^{2m-1}\}$.

Proof. Let $p \in \Delta_{-2m,2m-1}$. Then $p(x) = \sum_{i=-2m}^{2m-1} c_i x^i$ for certain coefficients c_i. By linearity it suffices to show that

$$V^TA^jV = E_1^T\mathbb{T}_{2m}^{j}E_1, \quad j = 0, 1, \ldots, 2m-1, \tag{27}$$

$$V^TA^{-j}V = E_1^T\mathbb{T}_{2m}^{-j}E_1, \quad j = 0, 1, \ldots, 2m. \tag{28}$$

Let $j = j_1 + j_2$ with $0 \leq j_1, j_2 < m$. Then

$$\begin{aligned} V^T A^j V &= V^T A^{j_1} A^{j_2} V = [A^{j_1} V]^T [A^{j_2} V] = [\mathbb{V}_{2m} \mathbb{T}_{2m}^{j_1} E_1]^T [\mathbb{V}_{2m} \mathbb{T}_{2m}^{j_2} E_1] \\ &= E_1^T \mathbb{T}_{2m}^{j_1} \mathbb{V}_{2m}^T \mathbb{V}_{2m} \mathbb{T}_{2m}^{j_2} E_1 = E_1^T \mathbb{T}_{2m}^{j} E_1. \end{aligned}$$

For the power $2m-1$, we have

$$\begin{aligned} V^T A^{2m-1} V &= [A^{m-1} V]^T A [A^{m-1} V] = [\mathbb{V}_{2m} \mathbb{T}_{2m}^{m-1} E_1]^T A [\mathbb{V}_{2m} \mathbb{T}_{2m}^{m-1} E_1] \\ &= E_1^T \mathbb{T}_{2m}^{m-1} (\mathbb{V}_{2m}^T A \mathbb{V}_{2m}) \mathbb{T}_{2m}^{m-1} E_1 = E_1^T \mathbb{T}_{2m}^{2m-1} E_1. \end{aligned}$$

This shows (27). The same techniques can be used to show (28). This establishes (26). □

The extended symmetric block Lanczos method can be used not only to approximate expressions of the form (1), but also to approximate the bilinear form (17) of real $(s \times s)$-matrix-valued functions P and Q. Having carried out m steps of the extended block Lanczos method, we can evaluate the reduced bilinear form

$$\begin{aligned} \langle P, Q \rangle_{2m} &:= (P(\mathbb{T}_{2m}) \circ E_1)^T (Q(\mathbb{T}_{2m}) \circ E_1) \\ &= \sum_{i=1}^{2ms} P^T(\theta_i^{(m)}) u_i^{(m)} (u_i^{(m)})^T Q(\theta_i^{(m)}), \end{aligned} \tag{29}$$

with $\mathbb{T}_{2m}$, $\theta_1^{(m)}, \theta_2^{(m)}, \ldots, \theta_{2ms}^{(m)}$, and $u_1^{(m)}, u_2^{(m)}, \ldots, u_{2ms}^{(m)}$ defined by (18) and (19).

Lemma 2. *Let f be the function defined in* (1)*, and let $\langle \cdot, \cdot \rangle$, $\langle \cdot, \cdot \rangle_{2m}$ be the bilinear forms defined by* (17) *and* (29)*, respectively. Let $R(\lambda) = f(\lambda) I_s$ and recall that $R_0(\lambda) \equiv I_s$. Then*

$$\langle R, R_0 \rangle = \mathbb{I}(f), \tag{30}$$

$$\langle R, R_0 \rangle_{2m} = \mathbb{G}_{2m}^e(f), \tag{31}$$

$$\langle P, Q \rangle = \langle P, Q \rangle_{2m}, \tag{32}$$

where $P, Q \in \mathbb{R}^{s \times s}$ are Laurent polynomials with $s \times s$ matrix coefficients such that

$$P(\lambda) = \sum_{k=-2i}^{2i-1} \lambda^k C_k, \quad Q(\lambda) = \sum_{k=-2j}^{2j} \lambda^k D_k, \quad i + j \leq m.$$

Proof. We have

$$\langle R, R_0 \rangle = (R(A) \circ V)^T (R_0(A) \circ V) = (f(A)V)^T V = V^T f(A^T) V = \mathbb{I}(f).$$

This shows (30). In a similar way, we obtain (31),

$$\begin{aligned}\langle R, R_0 \rangle_{2m} &= (R(\mathbb{T}_{2m}) \circ E_1)^T (R_0(\mathbb{T}_{2m}) \circ E_1) \\ &= (f(\mathbb{T}_{2m}) E_1)^T E_1 = E_1^T f(\mathbb{T}_{2m}^T) E_1 = \mathbb{G}_{2m}^e(f).\end{aligned}$$

Finally, equation (17) gives

$$\begin{aligned}\langle P, Q \rangle &= (P(A) \circ V)^T (Q(A) \circ V) \\ &= (\sum_{k=-2i}^{2i-1} A^k V C_k)^T (\sum_{l=-2j}^{2j} A^l V D_l) \\ &= \sum_{k=-2i}^{2i-1} \sum_{l=-2j}^{2j} C_k^T V^T A^{k+l} V D_l.\end{aligned}$$

Application of (26) yields

$$\begin{aligned}\langle P, Q \rangle &= \sum_{k=-2i}^{2i-1} \sum_{l=-2j}^{2j} C_k^T E_1^T \mathbb{T}_{2m}^{k+l} E_1, \quad \text{since } -2m \leq k+l \leq 2m-1, \\ &= (P(\mathbb{T}_{2m}) \circ E_1)^T (Q(\mathbb{T}_{2m}) \circ E_1) \\ &= \langle P, Q \rangle_{2m}.\end{aligned}$$

This completes the proof. □

4. Block anti-Gauss–Laurent quadrature rules

Laurie [19] introduced anti-Gauss rules for the estimation of the quadrature error of Gauss rules applied to the integration of a real-valued function on a real interval. This section describes an extension that can be applied to estimate the quadrature error of the block Gauss–Laurent rules of Section 3. We introduce the $(2m+1)s$-node block anti-Gauss–Laurent quadrature rule, denoted by $\mathbb{A}_{2m+1}^e$, associated with the $2ms$-node block Gauss–Laurent rule (18). It is characterized by

$$(\mathbb{I} - \mathbb{A}_{2m+1}^e)(f) = -(\mathbb{I} - \mathbb{G}_{2m}^e)(f), \quad \forall f \in \Delta_{-2m,2m+1},$$

where $\Delta_{-2m,2m+1} = \text{span}\{x^{-2m}, \dots, x^{2m+1}\}$. This is equivalent to

$$\mathbb{A}^e_{2m+1}(f) = (2\mathbb{I} - \mathbb{G}^e_{2m})(f), \quad \forall f \in \Delta_{-2m,2m+1}.$$

Therefore, $\mathbb{A}^e_{2m+1}$ may be considered a $(2m+1)s$-node block Gauss–Laurent quadrature rule with respect to the bilinear form $\langle\cdot,\cdot\rangle_{2m+1}$ given by

$$\langle P, Q\rangle_{2m+1} := 2\langle P, Q\rangle - \langle P, Q\rangle_{2m}, \tag{33}$$

where P and Q are Laurent polynomials with $s \times s$ matrix coefficients such that

$$P(\lambda) = \sum_{k=-2i}^{2i+1} \lambda^k C_k, \quad Q(\lambda) = \sum_{k=-2j}^{2j} \lambda^k D_k, \quad i + j \leq m,$$

and $\langle\cdot,\cdot\rangle$ and $\langle\cdot,\cdot\rangle_{2m}$ are defined by (17) and (29), respectively.

We will introduce Laurent polynomials $\widetilde{R}_{2j}$ and $\widetilde{R}_{2j+1}$, for $j = 0, 1, \dots$, with $s \times s$ matrix coefficients, that are orthonormal with respect to the bilinear form (33) for all j sufficiently small. These Laurent polynomials satisfy a pair of five-term recurrence relations of the form

$$\begin{aligned} \widetilde{R}_{2j}(\lambda)\widetilde{H}_{2j+1,2j-1} &= \lambda\widetilde{R}_{2j-2}(\lambda) - \textstyle\sum_{i=2j-3}^{2j} \widetilde{R}_{i-1}(\lambda)\widetilde{H}_{i,2j-1}, \\ \widetilde{R}_{2j+1}(\lambda)\widetilde{H}_{2j+2,2j} &= \lambda^{-1}\widetilde{R}_{2j-1}(\lambda) - \textstyle\sum_{i=2j-2}^{2j+1} \widetilde{R}_{i-1}(\lambda)\widetilde{H}_{i,2j}, \end{aligned} \qquad j = 1, 2, \dots,$$

where

$$\widetilde{R}_0(\lambda) = I_s, \quad \widetilde{R}_1(\lambda) = (\lambda^{-1} I_s - \widetilde{\Gamma}_{1,2})\widetilde{\Gamma}_{2,2}^{-1}, \quad \widetilde{R}_{-1}(\lambda) = \widetilde{R}_{-2}(\lambda) = O_s,$$

with

$$\widetilde{H}_{i,2j-1} = \langle \lambda \widetilde{R}_{2j-2}, \widetilde{R}_{i-1}\rangle_{2m+1}, \quad \widetilde{H}_{i,2j} = \langle \lambda^{-1}\widetilde{R}_{2j-1}, \widetilde{R}_{i-1}\rangle_{2m+1}. \tag{34}$$

The matrices $\widetilde{H}_{2j+1,2j-1}, \widetilde{H}_{2j+2,2j} \in \mathbb{R}^{s\times s}$ are determined so that $\langle \widetilde{R}_{2j}, \widetilde{R}_{2j}\rangle_{2m+1} = I_s$ and $\langle \widetilde{R}_{2j+1}, \widetilde{R}_{2j+1}\rangle_{2m+1} = I_s$.

Due to (26) and (32), block anti-Gauss–Laurent quadrature rules yield the same result as block Gauss–Laurent quadrature rules for all Laurent polynomials in $\Delta_{-2m,2m-1}$, i.e., if P, Q are Laurent polynomials with $s\times s$ matrix coefficients,

$$P(\lambda) = \sum_{k=-2i}^{2i-1} \lambda^k C_k, \quad Q(\lambda) = \sum_{k=-2j}^{2j} \lambda^k D_k, \quad i + j \leq m,$$

then we have

$$\langle P, Q\rangle_{2m+1} = \langle P, Q\rangle. \tag{35}$$

Using this property in (34) gives

$$\begin{aligned}
\widetilde{H}_{i,j} &= H_{i,j}, \quad i,j = 1,2,\ldots,2m-1,\\
\widetilde{H}_{2m,i} &= H_{2m,i}, \quad i \in \{2m-2, 2m-1\},\\
\widetilde{H}_{i,2m} &= H_{i,2m}, \quad i \in \{2m-2, 2m-1\}.
\end{aligned}$$

This shows that $\widetilde{R}_j(\lambda) = R_j(\lambda)$ for $j = 0,1,\ldots,2m-1$. In addition, we have

$$\begin{aligned}
\widetilde{R}_{2m}(\lambda)\widetilde{H}_{2m+1,2m-1} &= \lambda\widetilde{R}_{2m-2}(\lambda) - \sum_{i=2m-3}^{2m}\widetilde{R}_{i-1}(\lambda)\widetilde{H}_{i,2m-1}\\
&= \lambda R_{2m-2}(\lambda) - \sum_{i=2m-3}^{2m} R_{i-1}(\lambda)H_{i,2m-1}\\
&= R_{2m}(\lambda)H_{2m+1,2m-1}.
\end{aligned} \tag{36}$$

Moreover,

$$\langle\lambda\widetilde{R}_{2m-1}, \widetilde{R}_{2m}\rangle_{2m} = (H_{2m+1,2m-1}\widetilde{H}^{-1}_{2m+1,2m-1})^T\langle\lambda R_{2m-1}, R_{2m}\rangle_{2m}.$$

It follows from Theorem 1 that

$$R^T_{2m}(\theta_i^{(m)})u_i^{(m)} = 0, \quad i = 1,2,\ldots,2ms.$$

We obtain $\langle\lambda\widetilde{R}_{2m-1}\widetilde{R}_{2m}\rangle_{2m} = O_s$. Furthermore,

$$\begin{aligned}
\widetilde{H}_{2m+1,2m-1} = \langle\lambda\widetilde{R}_{2m-2}, \widetilde{R}_{2m}\rangle_{2m+1} &= 2\langle\lambda\widetilde{R}_{2m-2}, \widetilde{R}_{2m}\rangle - \langle\lambda\widetilde{R}_{2m-2}, \widetilde{R}_{2m}\rangle_{2m}\\
&= 2(H_{2m+1,2m-1}\widetilde{H}^{-1}_{2m+1,2m-1})^T\langle\lambda R_{2m-2}, R_{2m}\rangle\\
&= 2(H_{2m+1,2m-1}\widetilde{H}^{-1}_{2m+1,2m-1})^T H_{2m+1,2m-1}.
\end{aligned}$$

Applying the properties $\langle\widetilde{R}_{2m}, \widetilde{R}_{2m}\rangle_{2m+1} = \langle R_{2m}, R_{2m}\rangle = I_s$, and using (36) as well as the fact that $\langle R_{2m}, R_{2m}\rangle_{2m+1} = 2I_s$, we obtain

$$\widetilde{H}^T_{2m+1,2m-1}\widetilde{H}_{2m+1,2m-1} = 2H^T_{2m+1,2m-1}H_{2m+1,2m-1}.$$

The upper triangular matrices $\widetilde{H}_{2m+1,2m-1}, H_{2m+1,2m-1} \in \mathbb{R}^{s\times s}$ are assumed to be nonsingular and can be chosen according to

$$\widetilde{H}_{2m+1,2m-1} = \sqrt{2}H_{2m+1,2m-1}.$$

Substituting this expression into (36) yields

$$\widetilde{R}_{2m}(\lambda) = \frac{1}{\sqrt{2}} R_{2m}(\lambda).$$

Consider the matrix $\mathbb{T}^a_{2m+1} = [\widetilde{T}_{i,j}] \in \mathbb{R}^{(2m+1)s\times(2m+1)s}$, which is symmetric and block pentadiagonal with $s \times s$ blocks $\widetilde{T}_{i,j}$, associated with the block $(2m+1)s$-point anti-Gauss–Laurent rule

$$\mathbb{A}^e_{2m+1}(f) = \mathbf{E}_1^T f(\mathbb{T}^a_{2m+1})\mathbf{E}_1, \tag{37}$$

where $\mathbf{E}_1 \in \mathbb{R}^{(2m+1)s\times s}$ is made up of the first s columns of the identity matrix $I_{(2m+1)s}$, and $\widetilde{T}_{i,j} = \langle \lambda \widetilde{R}_{i-1}, \widetilde{R}_{j-1}\rangle_{2m+1}$ for $i, j = 1, 2, \ldots, 2m+1$. Using the property (35), we find that

$$\widetilde{T}_{i,j} = T_{i,j} \quad \text{for} \quad i, j = 1, 2, \ldots, 2m,$$

where $T_{i,j} = \langle \lambda R_{i-1}, R_{j-1}\rangle$. In view of Theorem 1, we obtain

$$\langle \lambda R_{2m}, R_{2m-2}\rangle_{2m} = \langle \lambda R_{2m}, R_{2m-1}\rangle_{2m} = \langle \lambda R_{2m}, R_{2m}\rangle_{2m} = O_s.$$

Therefore,

$$\begin{aligned}
\widetilde{T}_{2m+1,2m-1} &= \langle \lambda \widetilde{R}_{2m}, \widetilde{R}_{2m-2}\rangle_{2m+1} = \frac{1}{\sqrt{2}} \langle \lambda R_{2m}, R_{2m-2}\rangle_{2m+1} \\
&= \frac{1}{\sqrt{2}} [2\langle \lambda R_{2m}, R_{2m-2}\rangle - \langle \lambda R_{2m}, R_{2m-2}\rangle_{2m}] \\
&= \sqrt{2}\, T_{2m+1,2m-1}, \\
\widetilde{T}_{2m+1,2m} &= \langle \lambda \widetilde{R}_{2m}, \widetilde{R}_{2m-1}\rangle_{2m+1} = \frac{1}{\sqrt{2}} \langle \lambda R_{2m}, R_{2m-1}\rangle_{2m+1} \\
&= \frac{1}{\sqrt{2}} [2\langle \lambda R_{2m}, R_{2m-1}\rangle - \langle \lambda R_{2m}, R_{2m-1}\rangle_{2m}] \\
&= \sqrt{2}\, T_{2m+1,2m}, \\
\widetilde{T}_{2m+1,2m+1} &= \langle \lambda \widetilde{R}_{2m}, \widetilde{R}_{2m}\rangle_{2m+1} = \frac{1}{2} \langle \lambda R_{2m}, R_{2m}\rangle_{2m+1} \\
&= \frac{1}{2} [2\langle \lambda R_{2m}, R_{2m}\rangle - \langle \lambda R_{2m}, R_{2m}\rangle_{2m}] \\
&= T_{2m+1,2m+1}.
\end{aligned}$$

In conclusion, the symmetric block pentadiagonal matrix $\mathbb{T}^a_{2m+1}$ with $s \times s$ blocks associated with the $(2m+1)s$-node block anti-Gauss–Laurent rule (37) can be obtained from the matrix $\mathbb{T}_{2m+1} = \mathbb{V}^T_{2m+1} A \mathbb{V}_{2m+1}$ associated with the $(2m+1)s$-node block Gauss–Laurent rule by multiplying the entries of the blocks $T_{2m+1,2m-1}$ and $T_{2m+1,2m}$ by $\sqrt{2}$, i.e.,

$$\mathbb{T}^a_{2m+1} = \begin{bmatrix} \mathbb{T}_{2m} & \Psi_{2m} \\ \Psi^T_{2m} & T_{2m+1,2m+1} \end{bmatrix},$$

where $\Psi_{2m} = [O_s, \ldots, O_s, \sqrt{2} T_{2m+1,2m-1}, \sqrt{2} T_{2m+1,2m}]^T \in \mathbb{R}^{2ms \times s}$.

Introduce the spectral factorization $\mathbb{T}^a_{2m+1} = Y_{2m+1} \Theta_{2m+1} Y^T_{2m+1}$, where

$$\begin{aligned} Y_{2m+1} &:= [\widetilde{y}^{(m)}_1, \ldots, \widetilde{y}^{(m)}_{(2m+1)s}] \in \mathbb{R}^{(2m+1)s \times (2m+1)s}, \\ \Theta_{2m+1} &:= \operatorname{diag}[\widetilde{\theta}^{(m)}_1, \ldots, \widetilde{\theta}^{(m)}_{(2m+1)s}] \in \mathbb{R}^{(2m+1)s \times (2m+1)s}. \end{aligned}$$

The approximation (37) can be written as

$$\mathbb{A}^e_{2m+1}(f) = \sum_{i=1}^{(2m+1)s} f(\widetilde{\theta}^{(m)}_i) \widetilde{u}^{(m)}_i (\widetilde{u}^{(m)}_i)^T,$$

where the vector $\widetilde{u}^{(m)}_i \in \mathbb{R}^s$ is made up of the first s elements of $\widetilde{y}^{(m)}_i$, $1 \leq i \leq (2m+1)s$. The reduced inner product associated with the $(2m+1)s$-node block anti-Gauss–Laurent rule can be expressed as follows

$$\langle P, Q \rangle_{2m+1} := \sum_{i=1}^{(2m+1)s} P^T(\widetilde{\theta}^{(m)}_i) \widetilde{u}^{(m)}_i (\widetilde{u}^{(m)}_i)^T Q(\widetilde{\theta}^{(m)}_i), \quad P, Q \in \mathbb{R}^{n \times s}.$$

Using (30) and (31) gives

$$\langle R, R_0 \rangle_{2m+1} = 2\langle R, R_0 \rangle - \langle R, R_0 \rangle_{2m} = 2\mathbb{I}(f) - \mathbb{G}^e_{2m}(f) = \mathbb{A}^e_{2m+1}(f), \quad (38)$$

where $R(\lambda) = f(\lambda) I_s$, and $R_0(\lambda) \equiv I_s$.

We now provide some results that show that pairs of a $2ms$-node block Gauss–Laurent rule (18) and a $(2m+1)s$-node block anti-Gauss–Laurent rule (37) may give element-wise upper and lower bounds for $\mathbb{I}(f)$ when the integrand f is analytic in a sufficiently large region in the complex plan that contains the convex hull of the spectrum of A. Assume that there are $M+1$ orthonormal matrix-valued Laurent polynomials $\{R_0, \ldots, R_M\}$ defined by (14) with $M \gg 4m+2$, and consider the expansion

$$g(\lambda) = \sum_{j=0}^{M} R_j(\lambda) C_j, \quad \lambda \in \sigma(A),$$

where $\sigma(A)$ denotes the spectrum of A, and the C_j are $s \times s$ matrices. By the orthonormality of $\{R_j\}_{j\geq 0}$, it holds that $\langle R_0, R_0\rangle = I_s$ and $\langle R_j, R_0\rangle = O_s$ $\forall j \geq 1$, since $R_0(\lambda) \equiv I_s$. This means that $\langle g, R_0\rangle = C_0^T$. On the other hand, we have

$$\langle g, R_0\rangle_{2m} = \sum_{j=0}^{M} C_j^T \langle R_j, R_0\rangle_{2m} = \sum_{j=0}^{4m-1} C_j^T \langle R_j, R_0\rangle_{2m} + \sum_{j=4m}^{M} C_j^T \langle R_j, R_0\rangle_{2m}.$$

It follows from (32) that

$$\langle R_j, R_0\rangle_{2m} = \langle R_j, R_0\rangle = O_s, \quad j = 1, 2, \ldots, 4m-1.$$

Hence,

$$\begin{aligned}
\langle g, R_0\rangle_{2m} \quad &= \quad \langle g, R_0\rangle + C_{4m}^T \langle R_{4m}, R_0\rangle_{2m} + C_{4m+1}^T \langle R_{4m+1}, R_0\rangle_{2m} \\
&\quad + \sum_{j=4m+2}^{M} C_j^T \langle R_j, R_0\rangle_{2m}.
\end{aligned}$$

Using (33) and the same techniques as above, we get

$$\begin{aligned}
\langle g, R_0\rangle_{2m+1} &= \sum_{j=0}^{M} C_j^T \langle R_j, R_0\rangle_{2m+1} \\
&= \sum_{j=0}^{4m-1} C_j^T \langle R_j, R_0\rangle_{2m+1} + \sum_{j=4m}^{M} C_j^T \langle R_j, R_0\rangle_{2m+1} \\
&= \langle g, R_0\rangle + C_{4m}^T \langle R_{4m}, R_0\rangle_{2m+1} \\
&\quad + C_{4m+1}^T \langle R_{4m+1}, R_0\rangle_{2m+1} + \sum_{j=4m+2}^{M} C_j^T \langle R_j, R_0\rangle_{2m+1} \\
&= \langle g, R_0\rangle - C_{4m}^T \langle R_{4m}, R_0\rangle_{2m} - C_{4m+1}^T \langle R_{4m+1}, R_0\rangle_{2m} \\
&\quad + \sum_{j=4m+2}^{M} C_j^T \langle R_j, R_0\rangle_{2m+1}.
\end{aligned}$$

When the coefficient matrices C_j decay in norm sufficiently rapidly with increasing index j, the approximations

$$\langle g, R_0\rangle_{2m} - \langle g, R_0\rangle \approx C_{4m}^T\langle R_{4m}, R_0\rangle_{2m} + C_{4m+1}^T\langle R_{4m+1}, R_0\rangle_{2m},$$
$$\langle g, R_0\rangle_{2m+1} - \langle g, R_0\rangle \approx -C_{4m}^T\langle R_{4m}, R_0\rangle_{2m} - C_{4m+1}^T\langle R_{4m+1}, R_0\rangle_{2m},$$

are quite accurate. This implies that $\langle g, R_0\rangle_{2m}$ and $\langle g, R_0\rangle_{2m+1}$ bracket $\langle g, R_0\rangle$ element-wise. This situation often occurs when f is analytic in a sufficiently large region in the complex plane that contains the convex hull of the spectrum of A. In particular, let $g(\lambda) = f(\lambda)V$, where f corresponds to the function in (1). Then an application of equations (30), (31), and (38), suggests that the block Gauss–Laurent and block anti-Gauss–Laurent quadrature rules $\mathbb{G}_{2m}^e(f)$ and $\mathbb{A}_{2m+1}^e(f)$, respectively, bracket $\mathbb{I}(f)$ element-wise, i.e., $[\mathbb{G}_{2m}^e(f)]_{i,j}$ and $[\mathbb{A}_{2m+1}^e(f)]_{i,j}$ bracket $[\mathbb{I}(f)]_{i,j}$ for all $1 \leq i, j \leq s$.

Algorithm 1 describes how an approximation of $V^T f(A)V$ and an error estimate can be computed by a pair of block Gauss–Laurent and block anti-Gauss–Laurent quadrature rules.

5. Numerical experiments

This section reports some numerical examples that illustrate the performance of pairs of block Gauss–Laurent and block anti-Gauss–Laurent quadrature rules (BGLQ) when applied to the approximation of expressions of the form (1). These quadratures are implemented by Algorithm 1. We compare the approximation errors obtained with these rules to the approximation errors achieved by (standard) block Gauss and block anti-Gauss quadrature rules (BGQ) with the same number of nodes. The latter rules are based on the symmetric block Lanczos process and are described in [8]. All experiments were coded in MATLAB R2015a on a computer with an Intel Core i-3 processor and 3.89 GB of RAM. The computations were carried out with about 15 significant decimal digits. In all experiments, except when explicitly stated otherwise, the initial block vector $V \in \mathbb{R}^{n\times s}$ is generated by first determining an $n \times s$ block vector with uniformly

Algorithm 1 Approximation of $V^T f(A)V$ by pairs of block Gauss–Laurent and block anti-Gauss–Laurent quadrature rules for a symmetric matrix A.

Input: Symmetric nonsingular matrix A, initial orthonormal block V, function f.

1. Choose tolerance $\epsilon > 0$ and the maximum number of steps $m_{\max}$.
2. $\Gamma_{1,2} = V_1^T A^{-1} V_1$; $\widetilde{V}_2 = A^{-1}V_1 - V_1\Gamma_{1,2}$;
3. Compute the (skinny) QR factorization of $\widetilde{V}_2$, i.e., $\widetilde{V}_2 = V_2\Gamma_{2,2}$;
4. $\widetilde{V}_3 = AV_1$; $H_{1,1} = V_1^T\widetilde{V}_3$;
5. for $j = 1 : m_{\max}$
   (a) $\widetilde{V}_{2j+2} = A^{-1}V_{2j}$; $h_{2j,2j} = V_{2j}^T\widetilde{V}_{2j+2}$;
   (b) Compute $H_{i,2j-1}$ and $H_{i,2j}$ from recursion relations of Proposition 1.
   (c) $\widetilde{V}_{2j+1} = \widetilde{V}_{2j+1} - \sum\limits_{i=2j-3}^{2j} V_i H_{i,2j-1}$;
   (d) if $j = 1$
   $T_{1:2,1} = H_{1:2,1}$; $T_{1,2} = T_{2,1}^T$; $T_{2,2} = -T_{2,1}\Gamma_{1,2}\Gamma_{2,2}^{-1}$;
   else
   $T_{2j-3:2j,2j-1} = H_{2j-3:2j,2j-1}$; $T_{2j-1,2j} = T_{2j,2j-1}^T$;
   $T_{2j,2j} = -T_{2j,2j-1}H_{2j-1,2j-2}H_{2j,2j-2}^{-1}$;
   end
   (e) $\mathbb{G}_{2j}^e(f) = E_1^T f(\mathbb{T}_{2j})E_1$;
   (f) Compute the (skinny) QR factorization of $\widetilde{V}_{2j+1}$, i.e., $\widetilde{V}_{2j+1} = V_{2j+1}H_{2j+1,2j-1}$;
   (g) $\widetilde{V}_{2j+2} = \widetilde{V}_{2j+2} - \sum_{i=2j-2}^{2j+1} V_i H_{i,2j}$;
   (h) if $j = 1$, $\quad T_{3,1} = H_{3,1}$; $T_{3,2} = -T_{3,1}\Gamma_{1,2}\Gamma_{2,2}^{-1}$;
   else
   $T_{2j+1,2j-1} = H_{2j+1,2j-1}$; $T_{2j+1,2j} = -T_{2j+1,2j-1}H_{2j-1,2j-2}H_{2j,2j-2}^{-1}$;
   end
   (i) $\Psi_{2j} = \sqrt{2}\,[O_s, \ldots, O_s, T_{2j+1,2j-1}, T_{2j+1,2j}]^T$;
   (j) $\widetilde{V}_{2j+3} = AV_{2j+1}$; $H_{2j+1,2j+1} = V_{2j+1}^T\widetilde{V}_{2j+3}$;
   (k) Compute $\mathbb{T}_{2j+1}^a = \begin{bmatrix} \mathbb{T}_{2j} & \Psi_{2j} \\ \Psi_{2j}^T & H_{2j+1,2j+1} \end{bmatrix}$ and $\mathbb{A}_{2j+1}^e(f) = E_1^T f(\mathbb{T}_{2j+1}^a)E_1$;
   (l) if $\|\mathbb{G}_{2j}^e(f) - \mathbb{A}_{2j+1}^e(f)\|_{\max}/\|\mathbb{G}_{2j}^e(f) + \mathbb{A}_{2j+1}^e(f)\|_{\max} < \epsilon$
   $U_{\text{app}}(f) = [\mathbb{G}_{2j}^e(f) + \mathbb{A}_{2j+1}^e(f)]/2$; Break;
   end
   (m) Compute the (skinny) QR factorization of $\widetilde{V}_{2j+2}$, i.e., $\widetilde{V}_{2j+2} = V_{2j+2}H_{2j+2,2j}$;
   (n) end

Output: Approximation $U_{\text{app}}(f)$ of $V^T f(A)V$.

distributed random entries in the interval $[0,1]$, and then orthonormalizing the columns. The number of steps, m, of Algorithm 1 is chosen to be the smallest possible so that

$$\mathrm{RelErr}_{2m}(f) := \frac{\|\mathbb{G}^e_{2m}(f) - \mathbb{A}^e_{2m+1}(f)\|_{\max}}{\|\mathbb{G}^e_{2m}(f) + \mathbb{A}^e_{2m+1}(f)\|_{\max}} \leq \epsilon \tag{39}$$

for a user-specified tolerance $\epsilon > 0$, or when m exceeds the maximum allowed number of steps $m_{\max}$. We use for $C \in \mathbb{R}^{s\times s}$ the norm $\|C\|_{\max} := \max_{1\leq i,j\leq s} |C_{i,j}|$. Assume that $\mathbb{G}^e_{2m}(f)$ satisfies (39). Then we approximate (1) by the average block Gauss–Laurent quadrature rule

$$U_{\mathrm{app}}(f) = (\mathbb{G}^e_{2m}(f) + \mathbb{A}^e_{2m+1}(f))/2.$$

In all examples, we let $\epsilon = 2\cdot 10^{-7}$ and $m_{\max} = 100$. The BGQ method [8] is terminated analogously.

Algorithm 1 requires the solution of systems of equations. This is done by computing the Cholesky factorization of A when possible; otherwise we compute an LU factorization. Faster factorization methods can be used when the structure of A allows this.

The tables report for several functions f, matrices A, and block vectors V the required CPU time (Time) in seconds, the relative error (RelErr) achieved with the BGLQ and BGQ methods, and the number of iterations (Iter), with Iter:=$2m$ for the BGLQ method and Iter:=m for the BGQ method. The block size of V is set to $s = 5$ or $s = 10$. The plots in the figures display the evolution of the relative errors as a function of the number of iterations by the BGLQ (blue) and BGQ (red) methods.

Example 1. Let $A = [a_{i,j}] \in \mathbb{R}^{1000\times 1000}$ be the symmetric positive definite Toeplitz matrix with entries $a_{i,j} = 1/(1+|i-j|)$. The initial block vector is chosen to be $V = E_1$. The approximation errors and timings for the BGLQ and BGQ methods are listed in Table 1. The table shows both the BGLQ and BGQ methods to determine approximations of about the same quality, but the BGLQ method requires fewer steps to satisfy the stopping criterion (39) and demands less CPU time. The count of arithmetic floating point operations, and

Table 1: Example 1: Approximation of $V^T f(A)V$ for several functions, $A \in \mathbb{R}^{n\times n}$, $V \in \mathbb{R}^{n\times s}$, $n = 1000$, $s = 5, 10$.

$f(x)$	BGLQ			BGQ		
	Time (s)	RelErr	Iter. $(2m)$	Time (s)	RelErr	Iter. (m)
$s = 5$						
$\exp(-x)/x$	$6.3 \cdot 10^{-2}$	$4.00 \cdot 10^{-8}$	4	$1.3 \cdot 10^{-1}$	$1.33 \cdot 10^{-7}$	9
$x^{-1/2}$	$3.8 \cdot 10^{-2}$	$3.68 \cdot 10^{-9}$	4	$1.5 \cdot 10^{-1}$	$4.37 \cdot 10^{-8}$	9
$x^{1/2}$	$3.2 \cdot 10^{-2}$	$4.81 \cdot 10^{-8}$	4	$1.3 \cdot 10^{-1}$	$5.28 \cdot 10^{-8}$	9
$\log(x)$	$4.5 \cdot 10^{-2}$	$2.40 \cdot 10^{-9}$	4	$4.1 \cdot 10^{-1}$	$3.76 \cdot 10^{-8}$	8
$\exp(-\sqrt{x})$	$5.4 \cdot 10^{-2}$	$1.45 \cdot 10^{-7}$	4	$1.4 \cdot 10^{-1}$	$1.09 \cdot 10^{-7}$	8
$s = 10$						
$\exp(-x)/x$	$9.2 \cdot 10^{-2}$	$1.24 \cdot 10^{-7}$	4	$3.2 \cdot 10^{-1}$	$1.56 \cdot 10^{-7}$	8
$x^{-1/2}$	$6.7 \cdot 10^{-2}$	$3.84 \cdot 10^{-8}$	4	$7.5 \cdot 10^{-1}$	$6.21 \cdot 10^{-8}$	8
$x^{1/2}$	$5.8 \cdot 10^{-2}$	$4.36 \cdot 10^{-8}$	4	$6.2 \cdot 10^{-1}$	$7.81 \cdot 10^{-8}$	8
$\log(x)$	$6.9 \cdot 10^{-2}$	$5.21 \cdot 10^{-8}$	4	$8.3 \cdot 10^{-1}$	$5.16 \cdot 10^{-8}$	8
$\exp(-\sqrt{x})$	$8.1 \cdot 10^{-2}$	$4.79 \cdot 10^{-8}$	4	$4.8 \cdot 10^{-1}$	$1.23 \cdot 10^{-7}$	8

therefore possibly also the CPU time, for the BGLQ method can be reduced by using a factorization method that exploits the structure of A, such as the method described by Ammar and Gragg [2]. We remark that increasing the block size s changes the function (1) and, generally, results in a larger CPU time and sometimes a larger approximation error. Also, note that the function $\exp(-x)/x$ has a simple pole at the origin. This function therefore can be approximated well by Laurent polynomials with denominator degree one and high numerator degree. However, this kind of Laurent polynomials do not satisfy the recursion relations of the present paper.

Example 2. Let the matrix $A \in \mathbb{R}^{n\times n}$ with $n = 10000$ be block diagonal with 2×2 blocks of the form

$$\begin{bmatrix} a_i & c \\ c & a_i \end{bmatrix},$$

with $c = 1/2$ and $a_i = (2i-1)/(n+1)$ for $i = 1, \dots, n/2$ [21]. Results for several functions f are reported in Table 2. The table shows the BGQ method not to be able to satisfy the stopping criterion (39) within 100 iterations. Figure 1 displays

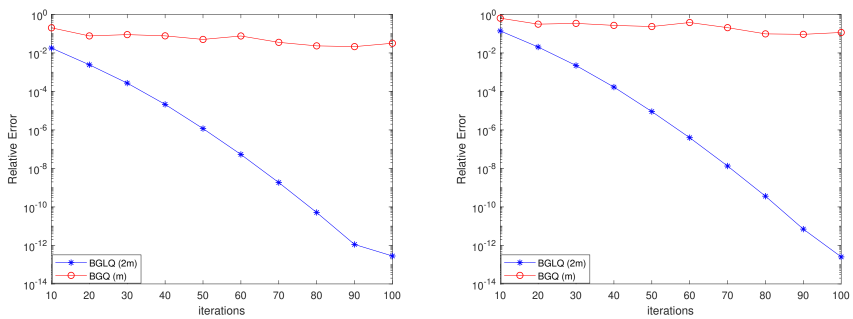
Table 2: Example 2: Approximation of $V^T f(A)V$ for several functions, $A \in \mathbb{R}^{n\times n}$, $V \in \mathbb{R}^{n\times s}$, $n = 10000$, $s = 5, 10$.

$f(x)$	BGLQ			BGQ		
	Time (s)	RelErr	Iter. ($2m$)	Time (s)	RelErr	Iter. (m)
$s = 5$						
$\exp(-x)/x$	$2.3 \cdot 10^{-1}$	$1.16 \cdot 10^{-9}$	8	$3.8 \cdot 10^{1}$	0.02	100
$x^{-1/2}$	$1.1 \cdot 10^{1}$	$1.86 \cdot 10^{-7}$	78	$6.6 \cdot 10^{1}$	0.10	100
$x^{1/2}$	$9.1 \cdot 10^{0}$	$1.77 \cdot 10^{-7}$	70	$6.7 \cdot 10^{1}$	0.02	100
$\log(x)$	$9.9 \cdot 10^{0}$	$1.86 \cdot 10^{-7}$	78	$1.2 \cdot 10^{2}$	0.02	100
$\exp(-\sqrt{x})$	$1.0 \cdot 10^{1}$	$1.91 \cdot 10^{-7}$	72	$8.3 \cdot 10^{1}$	0.02	100
$s = 10$						
$\exp(-x)/x$	$3.4 \cdot 10^{-1}$	$1.08 \cdot 10^{-7}$	6	$5.5 \cdot 10^{1}$	0.03	100
$x^{-1/2}$	$2.2 \cdot 10^{1}$	$1.09 \cdot 10^{-7}$	64	$3.1 \cdot 10^{2}$	0.08	100
$x^{1/2}$	$1.6 \cdot 10^{1}$	$1.14 \cdot 10^{-7}$	58	$2.7 \cdot 10^{2}$	0.02	100
$\log(x)$	$2.4 \cdot 10^{1}$	$1.17 \cdot 10^{-7}$	64	$3.5 \cdot 10^{2}$	0.23	100
$\exp(-\sqrt{x})$	$1.9 \cdot 10^{1}$	$1.23 \cdot 10^{-7}$	60	$2.1 \cdot 10^{2}$	0.04	100

the relative approximation error as a function of the number of iterations carried out.

Example 3. The matrix of this example is obtained from the discretization of the self-adjoint differential operator $L(u) := -\frac{1}{10}u_{xx} - 100u_{yy}$ on the unit square $[0, 1] \times [0, 1]$ with Dirichlet homogeneous boundary conditions. Discretization is carried on a uniform grid using the standard 3-point symmetric finite difference approximation in each coordinate direction. The number of inner grid points in each direction is $n_0 = 100$. This yields a symmetric positive definite matrix $A \in \mathbb{R}^{n\times n}$ of order $n = n_0^2$. The block vector is chosen to be $V = E_1$. The computed results are presented in Table 3. Approximations determined by the BGLQ method are of higher accuracy than approximations obtained by the BGQ method, because for many functions f the latter method is not able to satisfy the stopping criterion (39) within $n_{\max} = 100$ iterations. Figure 2 displays the convergence history.

Example 4. We consider the matrix $A = n^2\,\mathrm{tridiag}(-1, 2, -1)$ for $n = 10000$ [16]. Table 4 reports the performance of the BGQ and BGLQ methods. The



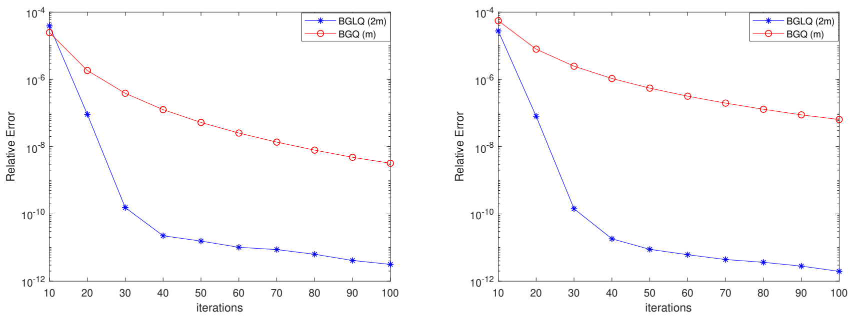
(a) $f(x) = x^{1/2}$.

(b) $f(x) = \log(x)$.

Figure 1: Example 2. Comparison of the evolution of relative errors. The block size of V is $s = 10$.

Table 3: Example 3: Approximation of $V^T f(A)V$ for several functions, $A \in \mathbb{R}^{n\times n}$, $V \in \mathbb{R}^{n\times s}$, $n = 10000$, $s = 5, 10$.

$f(x)$	BGLQ			BGQ		
	Time (s)	RelErr	Iter. $(2m)$	Time (s)	RelErr	Iter. (m)
$s = 5$						
$x^{-1/2}$	$4.2 \cdot 10^{-1}$	$1.12 \cdot 10^{-7}$	24	$3.7 \cdot 10^{1}$	$2.26 \cdot 10^{-5}$	100
$x^{1/2}$	$2.6 \cdot 10^{-1}$	$9.12 \cdot 10^{-8}$	20	$1.6 \cdot 10^{0}$	$1.84 \cdot 10^{-7}$	36
$\log(x)$	$2.8 \cdot 10^{-1}$	$8.01 \cdot 10^{-8}$	20	$1.5 \cdot 10^{1}$	$1.96 \cdot 10^{-7}$	65
$s = 10$						
$x^{-1/2}$	$1.9 \cdot 10^{0}$	$1.07 \cdot 10^{-7}$	24	$1.6 \cdot 10^{2}$	$3.88 \cdot 10^{-5}$	100
$x^{1/2}$	$6.5 \cdot 10^{-1}$	$9.12 \cdot 10^{-8}$	20	$6.1 \cdot 10^{0}$	$1.90 \cdot 10^{-7}$	36
$\log(x)$	$7.1 \cdot 10^{-1}$	$8.01 \cdot 10^{-8}$	20	$6.8 \cdot 10^{1}$	$1.97 \cdot 10^{-7}$	70



(a) $f(x) = x^{1/2}$.

(b) $f(x) = \log(x)$.

Figure 2: Example 3. Comparison of the evolution of relative errors. The block size of V is $s = 10$.

results are similar to those of Example 2, i.e., the BGLQ method yields significantly smaller approximation errors than the BGQ method. Figure 3 displays the convergence as a function of the number of iterations for two of the functions.

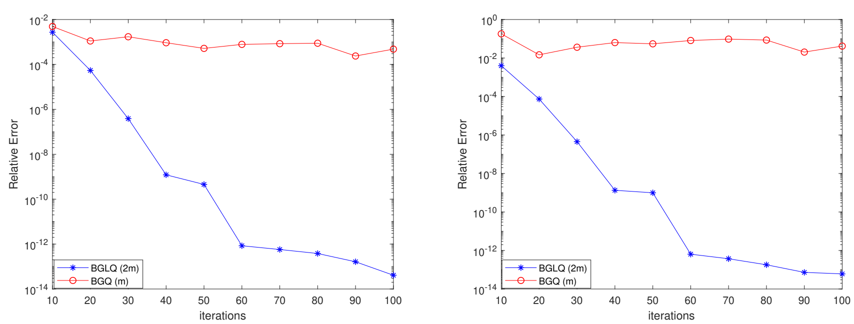
6. Conclusion and extensions

This paper presents block Gauss–Laurent-type quadrature rules for the inexpensive approximation of matrix functions of the form (1). These rules are computed with the extended block symmetric Lanczos method. Applications of these rules to the determination of estimates of upper and lower bounds for the entries of expressions of the form (1) are described. The numerical examples show the block Gauss–Laurent-type quadrature rules to require fewer steps and less CPU time, than (standard) block Gauss-type quadrature rules, to deliver approximations of the same or higher accuracy.

The work in this paper can be extended in several ways. For instance, we have omitted discussion of breakdown of the recursions due to that the block columns are not of full rank. This situation can be handled by deflation. Another topic that deserves attention is the situation when the numerator and denominator degrees of the Laurent polynomials are significantly different. This situation is discussed in [17] when the block size is one.

Table 4: Example 4: Approximation of $V^T f(A)V$ for several functions, $A \in \mathbb{R}^{n\times n}$, $V \in \mathbb{R}^{n\times s}$, $n = 10000$, $s = 5, 10$.

$f(x)$	BGLQ			BGQ		
	Time (s)	RelErr	Iter. $(2m)$	Time (s)	RelErr	Iter. $(2m)$
$s = 5$						
$x^{-1/2}$	$1.2 \cdot 10^0$	$1.25 \cdot 10^{-7}$	30	$5.5 \cdot 10^1$	$3.61 \cdot 10^{-1}$	100
$x^{1/2}$	$2.1 \cdot 10^0$	$1.12 \cdot 10^{-7}$	40	$5.5 \cdot 10^1$	$6.33 \cdot 10^{-4}$	100
$\log(x)$	$3.0 \cdot 10^0$	$1.03 \cdot 10^{-7}$	40	$1.1 \cdot 10^2$	$1.28 \cdot 10^{-1}$	100
$s = 10$						
$x^{-1/2}$	$1.6 \cdot 10^0$	$1.01 \cdot 10^{-7}$	24	$2.7 \cdot 10^2$	$2.36 \cdot 10^{-2}$	100
$x^{1/2}$	$5.0 \cdot 10^0$	$1.13 \cdot 10^{-7}$	32	$2.6 \cdot 10^2$	$7.28 \cdot 10^{-5}$	100
$\log(x)$	$5.1 \cdot 10^0$	$1.65 \cdot 10^{-7}$	32	$4.3 \cdot 10^2$	$1.52 \cdot 10^{-2}$	100



(a) $f(x) = x^{1/2}$.

(b) $f(x) = \log(x)$.

Figure 3: Example 4. Comparison of the evolution of relative errors. The block size of V is $s = 10$.

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