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Gauss–Laurent-type quadrature rules for the approximation of functionals of a nonsymmetric matrix

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Abstract This paper is concerned with the approximation of matrix functionals of the form $\boldsymbol{w}^T f(A)\boldsymbol{v}$, where $A \in \mathbb{R}^{n\times n}$ is a large nonsymmetric matrix, $\boldsymbol{w}, \boldsymbol{v} \in \mathbb{R}^n$, and f is a function such that $f(A)$ is well defined. We derive Gauss–Laurent quadrature rules for the approximation of these functionals, and also develop associated anti-Gauss–Laurent quadrature rules that allow us to estimate the quadrature error of the Gauss–Laurent rule. Computed examples illustrate the performance of the quadrature rules described.

Keywords matrix function evaluation, extended Krylov subspace, orthogonal Laurent polynomial, Gauss–Laurent quadrature, anti-Gauss–Laurent quadrature

1 Introduction

We are concerned with the approximation of matrix functionals of the form

$$F(A) := \boldsymbol{w}^T f(A)\boldsymbol{v} \tag{1}$$

by quadrature rules. Here $\boldsymbol{v}, \boldsymbol{w} \in \mathbb{R}^n$ with $\boldsymbol{v}^T\boldsymbol{w} = 1$, the superscript ^{T} denotes transposition, and $A \in \mathbb{R}^{n\times n}$ is a large nonsingular matrix, which may be nonsymmetric.

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Assume for the moment that the matrix A has the spectral factorization

$$A = S\Lambda S^{-1}, \tag{2}$$

where $S \in \mathbb{C}^{n\times n}$ is nonsingular and $\Lambda = \mathrm{diag}[\lambda_1, \lambda_2, \ldots, \lambda_n] \in \mathbb{C}^{n\times n}$. We remark that the computation of the quadrature rules does not require this factorization, but it simplifies their derivation. Substituting (1) into (1) gives

$$F(A) = \boldsymbol{w}^T S f(\Lambda) S^{-1} \boldsymbol{v} = \sum_{j=1}^{n} f(\lambda_j)\nu_j \nu'_j, \tag{3}$$

where $[\nu_1, \nu_2, \ldots, \nu_n] := \boldsymbol{w}^T S$ and $[\nu'_1, \nu'_2, \ldots, \nu'_n] := (S^{-1}\boldsymbol{v})^T$. The right-hand side of (1) can be expressed as a Stieltjes integral

$$\mathcal{I}f := \int f(z) dw(z), \tag{4}$$

where dw is a complex-valued measure with support at the eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$ in the complex plane. It follows from $\boldsymbol{w}^T\boldsymbol{v} = 1$ that $\int dw(z) = 1$. A discussion on the situation when A does not have n linearly independent eigenvectors is provided by Pozza et al. [23,24].

It is the purpose of the present paper to derive Gauss–Laurent-type quadrature rules for the approximation of the integral (1) or, equivalently, of the functional (1). These rules are exact for certain Laurent polynomials, which are polynomials in z and $1/z$. Gauss–Laurent quadrature rules for the approximation of (1) can be computed by applying a few steps of the nonsymmetric rational Lanczos process to the matrix A with initial vectors $\boldsymbol{v}$ and $\boldsymbol{w}$. Associated anti-Gauss-Laurent rules also are developed. The latter rules allow us to compute estimates for the quadrature error in Gauss–Laurent rules. Specifically, pairs of Gauss–Laurent and associated anti-Gauss–Laurent quadrature rules allow the computation of estimates of upper and lower bounds for the quadrature error in Gauss–Laurent rules. With this we mean that a pair of a Gauss–Laurent rule and an associated anti-Gauss–Laurent rule for many integrands f, matrices A, and vectors $\boldsymbol{v}$ and $\boldsymbol{w}$, provide upper and lower bounds for the integral (1), and therefore for the functional (1). However, they do not provide upper and lower bounds for all integrands and it is difficult to assess a priori if the computed quantities are upper and lower bounds. We therefore refer to the computed quantities as estimates of upper and lower bounds.

Anti-Gauss rules for the estimation of the error in (standard) Gauss quadrature rules for the approximation of integrals with a nonnegative measure with support on (part of) the real axis were proposed in a seminal paper by Laurie [19]. An extension to the estimation of functionals of the form (1) by Gauss-type quadrature rules is described in [5]. Further extensions and modifications of Gauss and anti-Gauss rules are described in [1,2,7,26]. However, none of these extensions and modifications are concerned with Gauss–Laurent and anti-Gauss–Laurent quadrature rules. The reason for our interest in Gauss–Laurent-type quadrature rules is that they may provide much higher accuracy than Gauss rules with the same number of nodes if the integrand has a singularity close to the support of the measure that determines the quadrature rules. Applications of Gauss–Laurent quadrature rules to the approximation of functionals (1) with a symmetric matrix A are described in [4, 13]. However, Gauss–Laurent quadrature rules and associated anti-Gauss–Laurent quadrature rules for the approximation of functionals (1) with a nonsymmetric matrix A have not been developed until now. We remark that the present paper, as well as the references mentioned in this paragraph, generalize and modify an approach described by Golub and Meurant [10] for computing upper and lower bounds for functionals (1) with a symmetric matrix $A \in \mathbb{R}^{n\times n}$ and an integrand f with derivatives that do not change sign on the convex hull of the spectrum of A.

This paper is organized as follows. Section 2 reviews the approach described in [7] for approximating the functional (1) by first carrying out a few steps of the nonsymmetric Lanczos process to the matrix A with initial vectors $\boldsymbol{v}$ and $\boldsymbol{w}$, and then using the computed quantities to define a Gauss quadrature rule for the approximation of (1). Associated Krylov subspaces are defined. These spaces are determined by the matrix A, its transpose, and the vectors $\boldsymbol{v}$ and $\boldsymbol{w}$. Section 3 introduces extended Krylov subspaces, i.e., Krylov subspaces that are determined by the matrix A, its transpose, their inverses, as well as by the vectors $\boldsymbol{v}$ and $\boldsymbol{w}$. We remark that recursion formulas for extended Krylov subspaces that are determined by a symmetric matrix are discussed by Mach et al. [20] and recursion formulas for rational Krylov subspaces that are determined by a symmetric matrix A and inverses of shifted matrices, $(A-\sigma_j I)^{-1}$, for suitable scalars σ_j, are considered by Mach et al. [21]. Applications and recursion formulas for rational Krylov subspaces of the latter kind also can be found in [14, 27]. Recently, Van Buggenhout et al. [29] discussed the recursion relations for biorthogonal bases for rational Krylov subspaces determined by A, A^T, as well as by inverses of shifted matrices $(A-\sigma_j I)^{-1}$ and $(A^T-\sigma'_j I)^{-1}$ for suitable scalars σ_j and σ'_j. Section 3 presents an alternate derivation of these recursion formulas for the case when $\sigma_j = \sigma'_j = 0$ for all j. Our derivation extends the approach described in [16] to nonsymmetric matrices. Section 4 discusses the application of the recursions of Section 3 to the computation of Gauss–Laurent and anti-Gauss–Laurent quadrature rules. The former rules are Gauss-type quadrature rules that are exact for specified positive and negative powers of z.

A nice introduction to rational Gauss rules is provided by Gautschi [9, Section 3.1.4]. More recent discussion of rational Gauss rules can be found in [6, 25]. Applications of rational Gauss quadrature to model reduction are described by Barkouki et al. [3] and Gallivan et al. [8].

2 Gauss quadrature rules

This section describes the application of the nonsymmetric Lanczos process to the nonsymmetric matrix $A \in \mathbb{R}^{n\times n}$ to compute Gauss quadrature rules for the approximation of the functional (1). Further details and extensions can be found in [2, 5, 7]. Let the vectors $\boldsymbol{v}, \boldsymbol{w} \in \mathbb{R}^n$ satisfy $\boldsymbol{w}^T\boldsymbol{v} = 1$. Then application of $1 \le m \ll n$ steps of the nonsymmetric Lanczos process to A with initial vectors $\boldsymbol{v}$ and $\boldsymbol{w}$ gives the Lanczos decompositions

$$\begin{aligned} AV_m &= V_m T_m + t_{m+1,m}\boldsymbol{v}_{m+1}\boldsymbol{e}_m^T, \\ A^T W_m &= W_m T_m^T + t_{m,m+1}\boldsymbol{w}_{m+1}\boldsymbol{e}_m^T, \end{aligned} \tag{5}$$

where the matrices $V_m = [\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_m] \in \mathbb{R}^{n\times m}$ and $W_m = [\boldsymbol{w}_1, \boldsymbol{w}_2, \ldots, \boldsymbol{w}_m] \in \mathbb{R}^{n\times m}$ with $\boldsymbol{v}_1 := \boldsymbol{v}$ and $\boldsymbol{w}_1 := \boldsymbol{w}$ satisfy

$$W_m^T V_m = I_m, \tag{6}$$

and the columns of V_m and W_m form bases for the Krylov subspaces

$$\begin{aligned} \mathbb{K}^m(A, \boldsymbol{v}) &= \mathrm{span}\{\boldsymbol{v}, A\boldsymbol{v}, \dots, A^{m-1}\boldsymbol{v}\}, \\ \mathbb{K}^m(A^T, \boldsymbol{w}) &= \mathrm{span}\{\boldsymbol{w}, A^T\boldsymbol{w}, \dots, (A^T)^{m-1}\boldsymbol{w}\}. \end{aligned} \tag{7}$$

Moreover, the vectors $\boldsymbol{v}_{m+1}, \boldsymbol{w}_{m+1} \in \mathbb{R}^n$ satisfy $V_m^T \boldsymbol{w}_{m+1} = \boldsymbol{0}$, $W_m^T \boldsymbol{v}_{m+1} = \boldsymbol{0}$, and $\boldsymbol{w}_{m+1}^T \boldsymbol{v}_{m+1} = 1$, and the matrix $T_m = W_m^T A V_m$ is nonsymmetric and tridiagonal. Here and below $\boldsymbol{e}_j = [0, \dots, 0, 1, 0, \dots, 0]^T$ denotes the j^{th} axis vector and $I_m \in \mathbb{R}^{m \times m}$ stands for the identity matrix. We assume that m is chosen small enough so that the decompositions (2) with the stated properties exist.

It follows from the recursion relations (2) that the jth columns of V_m and W_m can be expressed as

$$\boldsymbol{v}_j = p_{j-1}(A)\boldsymbol{v}, \quad \boldsymbol{w}_j = q_{j-1}(A^T)\boldsymbol{w}, \qquad j = 1, 2, \dots, m, \tag{8}$$

where p_{j-1} and q_{j-1} are polynomials of degree $j-1$.

Introduce the bilinear form

$$(q, p) := (q(A^T)\boldsymbol{w})^T (p(A)\boldsymbol{v}) = \boldsymbol{w}^T S q(\Lambda) p(\Lambda) S^{-1} \boldsymbol{v} = \int q(z)p(z)dw(z), \tag{9}$$

where dw is the measure in (1). It follows from (2) that the families of polynomials $\{p_0, p_1, p_2, \dots\}$ and $\{q_0, q_1, q_2, \dots\}$ defined by (2) are biorthogonal with respect to the bilinear form (2). We have

$$(q_{k-1}, p_{j-1}) = (q_{k-1}(A^T)\boldsymbol{w})^T (p_{j-1}(A)\boldsymbol{v}) = \boldsymbol{w}_k^T \boldsymbol{v}_j = \begin{cases} 1 & k = j, \\ 0 & k \neq j, \end{cases}$$

where the last equality follows from (2). Using the biorthogonality, we can show that

$$\mathcal{G}_m(f) := \boldsymbol{e}_1^T f(T_m) \boldsymbol{e}_1 \tag{10}$$

is a Gauss quadrature rule for the approximation of (1), i.e.,

$$\mathcal{G}_m(f) = \boldsymbol{w}^T f(A) \boldsymbol{v} \qquad \forall f \in \mathbb{P}_{2m-1},$$

where $\mathbb{P}_{2m-1}$ denotes the set of all polynomials of degree at most $2m-1$; see, e.g., [2,5,7] for proofs.

Assume for the moment that the matrix T_m has m distinct eigenvalues. Then substituting the spectral factorization of T_m into (2) shows that $\mathcal{G}_m(f)$ is a quadrature rule with m nodes, which may be complex-valued. The situation when T_m does not have a spectral factorization with m linearly independent eigenvectors is discussed by Pozza et al. [23,24].

The application of a Gauss rule (2) to approximate the functional (1) is appropriate when the function f can be approximated well by a polynomial of small to moderate degree. However, if this is not the case, then Gauss rules (2) with a moderate number of nodes, m, may yield poor approximations of the functional (1). It sometimes is possible to circumvent this difficulty by using rational Gauss rules. The following section discusses rational Gauss rules with one pole in the finite complex plane for the approximation of (1).

3 Recursion relations for extended Krylov subspaces

When the function f in (1) has a singularity close to the support of the measure dw in (1), rational Gauss quadrature rules with a pole at or close to the singularity may yield approximations of (1) of higher accuracy than a Gauss rule (2) with the same number of nodes. This is illustrated in Section 5.

We will assume that the singularity of f close to the support of the measure is at the origin. Rational Gauss rules that are exact for as many positive and negative powers of z as possible are commonly referred to as Gauss–Laurent quadrature rules. Similarly as Gauss rules are related to the Krylov subspaces (2), Gauss–Laurent quadrature rules are related to extended Krylov subspaces

$$\begin{aligned} \mathbb{K}^{\ell,m}(A,\boldsymbol{v}) &= \operatorname{span}\{A^{-\ell+1}\boldsymbol{v},\dots,A^{-1}\boldsymbol{v},\boldsymbol{v},A\boldsymbol{v},\dots,A^{m-1}\boldsymbol{v}\}, \\ \mathbb{K}^{\ell,m}(A^T,\boldsymbol{w}) &= \operatorname{span}\{(A^T)^{-\ell+1}\boldsymbol{w},\dots,(A^T)^{-1}\boldsymbol{w},\boldsymbol{w},A^T\boldsymbol{w},\dots,(A^T)^{m-1}\boldsymbol{w}\}. \end{aligned} \tag{11}$$

Generically, the subspaces $\mathbb{K}^{\ell,m}(A,\boldsymbol{v})$ and $\mathbb{K}^{\ell,m}(A^T,\boldsymbol{w})$ are of dimension $m+\ell-1$; if $\ell=1$, then the spaces (3) simplify to the standard Krylov subspaces (2).

The computation of Gauss–Laurent quadrature rules for the approximation of (1) in the case when the matrix A is symmetric is discussed in [4,13,16], and several other applications of extended Krylov subspaces are described by Heyouni, Jbilou, Knizhnerman, and Simoncini [12,18]. Our contribution differs from these works in that we use the pair of extended Krylov subspaces (3) and develop short recursion relations for biorthogonal bases. A different approach to the derivation of such recursion relations has recently been proposed by Van Buggenout et al. [29].

The remainder of this section discusses the generation of biorthogonal bases for pairs of nested Krylov subspaces

$$\begin{aligned} \mathbb{K}^{1,i+1}(A,\boldsymbol{v}) \subset \mathbb{K}^{2,2i+1}(A,\boldsymbol{v}) \subset \dots \subset \mathbb{K}^{m,mi+1}(A,\boldsymbol{v}) \subset \mathbb{R}^n, \\ \mathbb{K}^{1,i+1}(A^T,\boldsymbol{w}) \subset \mathbb{K}^{2,2i+1}(A^T,\boldsymbol{w}) \subset \dots \subset \mathbb{K}^{m,mi+1}(A^T,\boldsymbol{w}) \subset \mathbb{R}^n, \end{aligned} \tag{12}$$

where i is a positive integer. These recursions generalize those reported in [16] for a symmetric matrix A. Schweitzer [28] recently described recursion relations for the situation when $i=1$. Each increase in the denominator degree requires the solution of linear systems of equations with the matrices A and A^T, while each increase in the numerator degree demands the evaluation of matrix-vector products with the matrices A or A^T, which typically is cheaper than the solution of systems of equations. This makes it possible to compute rational Gauss–Laurent rules corresponding to $i>1$ faster than Gauss–Laurent rules with the same number of nodes corresponding to $i=1$. Illustrative examples are presented in Section 5. Computed examples for the situation when A is symmetric can be found in [15,16].

3.1 Recursion relations for extended Krylov subspaces

In this subsection, we will use biorthogonal sequences of Laurent polynomials to generate bases for the extended Krylov subspaces (3) corresponding to the orderings

$$\begin{gathered} \boldsymbol{v},A\boldsymbol{v},\dots,A^i\boldsymbol{v},A^{-1}\boldsymbol{v},A^{i+1}\boldsymbol{v},\dots,A^{2i}\boldsymbol{v},A^{-2}\boldsymbol{v},A^{2i+1}\boldsymbol{v},\dots\ , \\ \boldsymbol{w},A^T\boldsymbol{w},\dots,(A^T)^i\boldsymbol{w},(A^T)^{-1}\boldsymbol{w},(A^T)^{i+1}\boldsymbol{w},\dots,(A^T)^{2i}\boldsymbol{w},(A^T)^{-2}\boldsymbol{w},(A^T)^{2i+1}\boldsymbol{w},\dots\ , \end{gathered}$$

where the last powers of A and A^T are required to be positive.

Introduce the space of Laurent polynomials

$$\mathcal{L}_{m,im} := \text{span}\{z^{-m}, z^{-m+1}, \dots, 1, \dots, z^{im-1}, z^{im}\} \qquad z \in \mathbb{R}\backslash\{0\}.$$

There are two sequences of monic biorthogonal Laurent polynomials

$$\begin{aligned} &\phi_0, \phi_1, \dots \phi_i, \phi_{-1}, \phi_{i+1}, \dots, \phi_{2i}, \phi_{-2}, \phi_{2i+1}, \dots, \phi_{-m+1}, \dots, \phi_{im}, \\ &\psi_0, \psi_1, \dots \psi_i, \psi_{-1}, \psi_{i+1}, \dots, \psi_{2i}, \psi_{-2}, \psi_{2i+1}, \dots, \psi_{-m+1}, \dots, \psi_{im}, \end{aligned} \tag{13}$$

of the forms

$$\phi_j(z) := \begin{cases} z^j + \displaystyle\sum_{\ell=-\lfloor (j-1)/i \rfloor}^{j-1} c_{j,\ell} z^\ell, & j = 1, 2, 3, \dots\ , \\ z^j + \displaystyle\sum_{\ell=j+1}^{-ij} c_{j,\ell} z^\ell, & j = -1, -2, -3, \dots\ , \end{cases}$$

and

$$\psi_k(z) := \begin{cases} z^k + \displaystyle\sum_{\ell=-\lfloor (k-1)/i \rfloor}^{k-1} d_{k,\ell} z^\ell, & k = 1, 2, 3, \dots\ , \\ z^k + \displaystyle\sum_{\ell=k+1}^{-ik} d_{k,\ell} z^\ell, & k = -1, -2, -3, \dots\ , \end{cases}$$

with $\phi_0(z) = \psi_0(z) = 1$. Thus,

$$(\phi_j, \psi_k) = 0, \qquad j \neq k,$$

where the bilinear form is given by (2). We assume here that i and m are small enough so that the Laurent polynomials (3.1) indeed form biorthogonal bases for the space $\mathcal{L}_{m,im}$.

The vectors

$$\boldsymbol{v}_j = \phi_j(A)\boldsymbol{v}, \qquad j = -m+1, -m+2, \dots, im, \tag{14}$$

and

$$\boldsymbol{w}_j = \psi_j(A^T)\boldsymbol{w}, \qquad j = -m+1, -m+2, \dots, im, \tag{15}$$

form biorthogonal bases for the extended Krylov subspaces $\mathbb{K}^{m,im+1}(A, \boldsymbol{v})$ and $\mathbb{K}^{m,im+1}(A^T, \boldsymbol{w})$, respectively, with $\boldsymbol{v}_0 = \boldsymbol{v}$ and $\boldsymbol{w}_0 = \boldsymbol{w}$. Hence, the determination of biorthogonal bases for these extended Krylov subspaces is equivalent to the generation of biorthogonal bases for the space $\mathcal{L}_{m-1,im}$ of Laurent polynomials.

Define for the nonsingular matrix $M \in \mathbb{R}^{n \times n}$ the bilinear form

$$[\boldsymbol{x}, \boldsymbol{y}]_M = \boldsymbol{x}^T M \boldsymbol{y}, \qquad \boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n,$$

which is needed in the following proposition. The proposition specifies some conditions that are required to compute the trailing and leading coefficients of $\{\phi_{im}, \psi_{im}\}$ and $\{\phi_{-m}, \psi_{-m}\}$.

Proposition 1 *Let the matrix A be such that*

$$[\boldsymbol{w}_{im}, \boldsymbol{v}_{im}]_{A^{-1}} \neq 0, \qquad [\boldsymbol{w}_{-m}, \boldsymbol{v}_{-m}]_{A} \neq 0.$$

Then the trailing coefficients $c_{im,-m+1}$, $d_{im,-m+1}$ of ϕ_{im}, ψ_{im}, respectively, and the leading coefficients $c_{-m,im}$, $d_{-m,im}$ of ϕ_{-m}, ψ_{-m}, respectively, are nonvanishing.

Proof We first show that the coefficient $c_{im,-m+1}$ is nonzero. Consider the Laurent polynomials $z^{-1}\phi_{im}$ and ψ_{im}. By the properties of the inner product (2), we obtain

$$(z^{-1}\phi_{im}, \psi_{im}) = [\boldsymbol{w}_{im}, \boldsymbol{v}_{im}]_{A^{-1}} \neq 0.$$

On the other hand,

$$(z^{-1}\phi_{im}, \psi_{im}) = (c_{im,-m+1}z^{-m} + \varphi, \psi_{im}),$$

where $\varphi \in \mathcal{L}_{m-1,im-1}$. Hence,

$$(z^{-1}\phi_{im}, \psi_{im}) = c_{im,-m+1}(z^{-m}, \psi_{im}).$$

It follows that $c_{im,-m+1} \neq 0$. In the same manner, we can show that $d_{im,-m+1} \neq 0$.

We now apply this argument again to show that $c_{-m,im}$ is a nonvanishing. Consider the Laurent polynomials $z\phi_{-m}$ and ψ_{-m}. Using the definition of the bilinear form (2), we have

$$(z\phi_{-m}, \psi_{-m}) = [\boldsymbol{w}_{-m}, \boldsymbol{v}_{-m}]_{A} \neq 0.$$

Further,

$$(z\phi_{-m}, \psi_{-m}) = (c_{-m,im}z^{im+1} + \varphi, \psi_{-m}),$$

where $\varphi \in \mathcal{L}_{m-1,im}$. Hence,

$$(z\phi_{-m}, \psi_{-m}) = c_{-m,im}(z^{im+1}, \psi_{-m}),$$

and therefore $c_{-m,im} \neq 0$. Analogously, we can show that $d_{-m,im} \neq 0$. $\square$

Suppose that biorthogonal bases of Laurent polynomials

$$\{\phi_0, \phi_1, \ldots, \phi_i, \phi_{-1}, \phi_{i+1}, \ldots, \phi_{2i}, \phi_{-2}, \phi_{2i+1}, \ldots, \phi_{im}\}$$
$$\{\psi_0, \psi_1, \ldots, \psi_i, \psi_{-1}, \psi_{i+1}, \ldots, \psi_{2i}, \psi_{-2}, \psi_{2i+1}, \ldots, \psi_{im}\}$$

for $\mathcal{L}_{m-1,im}$ are available. The next subsections describe how to extend these bases to biorthogonal bases for the space $\mathcal{L}_{m,i(m+1)}$.

3.2 Computation of ϕ_{-m} and ψ_{-m}

The evaluations of ϕ_{-m} and ψ_{-m} correspond to determining biorthogonal bases for $\mathcal{L}_{m,im+j}$ for $j=0$. Consider the Laurent polynomials

$$c_{im,-m+1}\phi_{-m}(z)-z^{-1}\phi_{im}(z), \quad d_{im,-m+1}\psi_{-m}(z)-z^{-1}\psi_{im}(z)\in\mathcal{L}_{m-1,im}. \quad (16)$$

By Proposition 1 the coefficients $c_{im,-m+1}$ and $d_{im,-m+1}$ of ϕ_{im} and ψ_{im}, respectively, are nonvanishing. Therefore,

$$c_{im,-m+1}\phi_{-m}(z)-z^{-1}\phi_{im}(z)=-\sum_{k=-m+1}^{im}a_{im,k}\phi_k(z),$$
$$d_{im,-m+1}\psi_{-m}(z)-z^{-1}\psi_{im}(z)=-\sum_{k=-m+1}^{im}b_{im,k}\psi_k(z),$$

with the Fourier coefficients given by

$$a_{im,k}=\frac{(z^{-1}\phi_{im},\psi_k)}{(\phi_k,\psi_k)}, \quad b_{im,k}=\frac{(z^{-1}\psi_{im},\phi_k)}{(\phi_k,\psi_k)}, \quad k=-m+1,\ldots,im.$$

Since $\phi_{im},\psi_{im}\perp\mathcal{L}_{m-1,im-1}$ and

$$z^{-1}\phi_k(z),z^{-1}\psi_k(z)\in\mathcal{L}_{m-1,im-1}, \qquad k=-m+2,\ldots,i(m-1),$$

it follows that the only nonvanishing Fourier coefficients are related to the previous sets of $i+1$ Laurent polynomials, $\{\phi_{-m+1},\ldots,\phi_{im}\}$ and $\{\psi_{-m+1},\ldots,\psi_{im}\}$. We therefore obtain

$$\begin{aligned}c_{im,-m+1}\phi_{-m}(z)&=z^{-1}\phi_{im}(z)-a_{im,im}\phi_{im}(z)-a_{im,im-1}\phi_{im-1}(z)-\ldots\\&\quad-a_{im,i(m-1)+1}\phi_{i(m-1)+1}(z)-a_{im,-m+1}\phi_{-m+1}(z),\\d_{im,-m+1}\psi_{-m}(z)&=z^{-1}\psi_{im}(z)-b_{im,im}\psi_{im}(z)-b_{im,im-1}\psi_{im-1}(z)-\ldots\\&\quad-b_{im,i(m-1)+1}\psi_{i(m-1)+1}(z)-b_{im,-m+1}\psi_{-m+1}(z).\end{aligned}$$

This yields the $(i+2)$-term recursion formulas

$$\begin{aligned}\delta_{-m}\boldsymbol{v}_{-m}&=(A^{-1}-\zeta_{im,im}I_n)\boldsymbol{v}_{im}-\zeta_{im,im-1}\boldsymbol{v}_{im-1}-\ldots\\&\quad-\zeta_{im,i(m-1)+1}\boldsymbol{v}_{i(m-1)+1}-\zeta_{im,-m+1}\boldsymbol{v}_{-m+1},\\\gamma_{-m}\boldsymbol{w}_{-m}&=((A^T)^{-1}-\eta_{im,im}I_n)\boldsymbol{w}_{im}-\eta_{im,im-1}\boldsymbol{w}_{im-1}-\ldots\\&\quad-\eta_{im,i(m-1)+1}\boldsymbol{w}_{i(m-1)+1}-\eta_{im,-m+1}\boldsymbol{w}_{-m+1}\end{aligned} \quad (17)$$

with $\zeta_{j,k}:=\boldsymbol{w}_k^TA^{-1}\boldsymbol{v}_j$ and $\eta_{j,k}:=\boldsymbol{v}_k^T(A^{-T})\boldsymbol{w}_j$.

3.3 Computation of ϕ_{im+1} and ψ_{im+1}

We determine biorthogonal bases for $\mathcal{L}_{m,im+j}$ for $j = 1$. Regard the Laurent polynomials

$$c_{-m,im}\phi_{im+1}(z) - z\phi_{-m}(z), \quad d_{-m,im}\psi_{im+1}(z) - z\psi_{-m}(z) \in \mathcal{L}_{m,im}.$$

Analogously to the case $j = 0$, we express the Laurent polynomials (3.2) in terms of their Fourier expansions with Fourier coefficients

$$a_{-m,k} = \frac{(z\phi_{-m}, \psi_k)}{(\phi_k, \psi_k)}, \quad b_{-m,k} = \frac{(z\psi_{-m}, \phi_k)}{(\phi_k, \psi_k)}, \qquad k = -m, \ldots, im.$$

Note that $\phi_{-m}, \psi_{-m} \perp \mathcal{L}_{m-1,im}$ and

$$z\phi_k(z), z\psi_k(z) \in \mathcal{L}_{m-1,im}, \qquad k = -m+1, \ldots, im-1.$$

Therefore ϕ_{im+1} and ψ_{im+1} satisfy

$$\begin{aligned} c_{-m,im}\phi_{im+1}(z) &= z\phi_{-m}(z) - a_{-m,-m}\phi_{-m}(z) - a_{-m,im}\phi_{im}(z), \\ d_{-m,im}\psi_{im+1}(z) &= z\psi_{-m}(z) - b_{-m,-m}\psi_{-m}(z) - b_{-m,im}\psi_{im}(z). \end{aligned}$$

This gives the three-term recursion formulas

$$\begin{aligned} \delta_{im+1}\boldsymbol{v}_{im+1} &= (A - \alpha_{-m,-m}I_n)\boldsymbol{v}_{-m} - \alpha_{-m,im}\boldsymbol{v}_{im}, \\ \gamma_{im+1}\boldsymbol{w}_{im+1} &= (A^T - \beta_{-m,-m}I_n)\boldsymbol{w}_{-m} - \beta_{-m,im}\boldsymbol{w}_{im}, \end{aligned} \tag{18}$$

with $\alpha_{j,k} := \boldsymbol{w}_k^T A\boldsymbol{v}_j$ and $\beta_{j,k} := \boldsymbol{v}_k^T A^T\boldsymbol{w}_j$.

3.4 Computation of ϕ_{im+2} and ψ_{im+2}

We would like to determine biorthogonal bases for $\mathcal{L}_{m,im+2}$. Consider the functions

$$\phi_{im+2}(z) - z\phi_{im+1}(z), \quad \psi_{im+2}(z) - z\psi_{im+1}(z) \in \mathcal{L}_{m,im+1}.$$

The Fourier expansion of $\phi_{im+2}(z) - z\phi_{im+1}(z)$ has the coefficients

$$a_{im+1,k} = \frac{(z\phi_{im+1}, \psi_k)}{(\phi_k, \psi_k)}, \qquad k = -m, \ldots, im+1,$$

and the Fourier coefficients of $\psi_{im+2}(z) - z\psi_{im+1}(z)$ are given by

$$b_{im+1,k} = \frac{(z\psi_{im+1}, \phi_k)}{(\phi_k, \psi_k)}, \qquad k = -m, \ldots, im+1.$$

In view of that $\phi_{im+1}, \psi_{im+1} \perp \mathcal{L}_{m,im}$ and

$$z\phi_k(z), z\psi_k(z) \in \mathcal{L}_{m,im}, \qquad k = -m+1, \ldots, im-1,$$

it follows that ϕ_{im+2} and ψ_{im+2} satisfy

$$\begin{aligned} \phi_{im+2}(z) &= z\phi_{im+1}(z) - a_{im+1,im+1}\phi_{im+1}(z) \\ &\quad - a_{im+1,-m}\phi_{-m}(z) - a_{im+1,im}\phi_{im}(z), \\ \psi_{im+2}(z) &= z\psi_{im+1}(z) - b_{im+1,im+1}\psi_{im+1}(z) \\ &\quad - b_{im+1,-m}\psi_{-m}(z) - b_{im+1,im}\psi_{im}(z), \end{aligned}$$

which yields the four-term recursion formulas

$$\begin{aligned}\delta_{im+2}\boldsymbol{v}_{im+2} &= (A-\alpha_{im+1,im+1}I_n)\boldsymbol{v}_{im+1}\\ &\quad -\alpha_{im+1,-m}\boldsymbol{v}_{-m}-\alpha_{im+1,im}\boldsymbol{v}_{im},\\ \gamma_{im+2}\boldsymbol{w}_{im+2} &= (A^T-\beta_{im+1,im+1}I_n)\boldsymbol{w}_{im+1}\\ &\quad -\beta_{im+1,-m}\boldsymbol{w}_{-m}-\beta_{im+1,im}\boldsymbol{w}_{im}.\end{aligned} \tag{19}$$

3.5 Computation of ϕ_{im+j} and ψ_{im+j} for $j = 3, 4, \ldots, i$

We describe how to determine the remaining basis elements for the subspace $\mathcal{L}_{m,im+j}$ for $3 \leq j \leq i$. They can be computed with the aid of the nonsymmetric Lanczos recursions. We have

$$\begin{aligned}\delta_{im+j}\boldsymbol{v}_{im+j} &= (A-\alpha_{im+j-1,im+j-1}I_n)\boldsymbol{v}_{im+j-1}\\ &\quad -\alpha_{im+j-1,im+j-2}\boldsymbol{v}_{im+j-2},\\ \gamma_{im+j}\boldsymbol{w}_{im+j} &= (A^T-\beta_{im+j-1,im+j-1}I_n)\boldsymbol{w}_{im+j-1}\\ &\quad -\beta_{im+j-1,im+j-2}\boldsymbol{w}_{im+j-2}.\end{aligned} \tag{20}$$

This completes the computation of the basis for $\mathcal{L}_{m,i(m+1)}$.

3.6 Algorithm and biorthogonal projection

The following algorithm summarizes the computation of the biorthogonal bases for the extended Krylov subspaces $\mathbb{K}^{m+1,im+1}(A,\boldsymbol{v})$ and $\mathbb{K}^{m+1,im+1}(A^T,\boldsymbol{w})$. The algorithm is based on the recurrence relations for the biorthogonal bases for $\mathcal{L}_{m-1,im}$ derived in the previous subsections. Further details on the correspondence of the biorthogonal bases for $\mathbb{K}^{m+1,im+1}(A,\boldsymbol{v})$ and $\mathbb{K}^{m+1,im+1}(A^T,\boldsymbol{w})$, and for $\mathcal{L}_{m-1,im}$ can be found after the algorithm.

It is known that the nonsymmetric Lanczos algorithm may suffer from breakdown. This occurs when the inner products $\boldsymbol{r}^T\boldsymbol{s}$ or $\hat{\boldsymbol{r}}^T\hat{\boldsymbol{s}}$ in Algorithm 1 vanish, so that a coefficient δ_i or γ_i become zero. We will assume that m is small enough so that breakdown does not occur.

Algorithm 1 *(Computation of biorthogonal bases for* $\mathbb{K}^{m+1,im+1}(A,\boldsymbol{v})$ *and* $\mathbb{K}^{m+1,im+1}(A^T,\boldsymbol{w})$*.)*
Input: *integers* m, i, $\boldsymbol{v},\boldsymbol{w} \in \mathbb{R}^{n\times n}$ *such that* $(\boldsymbol{v},\boldsymbol{w}) = 1$*, functions for evaluating matrix-vector products and solve linear systems of equations with* $A, A^T \in \mathbb{R}^{n\times n}$*;*
Output: *biorthogonal bases* $\{\boldsymbol{v}_k\}_{k=-m}^{im}$ *for* $\mathbb{K}^{m+1,im+1}(A,\boldsymbol{v})$ *and* $\{\boldsymbol{w}_k\}_{k=-m}^{im}$ *for* $\mathbb{K}^{m+1,im+1}(A^T,\boldsymbol{w})$*;*
$\boldsymbol{v}_{-1} := \boldsymbol{0}$;
$\boldsymbol{w}_{-1} := \boldsymbol{0}$;
$\boldsymbol{v}_0 := \boldsymbol{v}$;
$\boldsymbol{w}_0 := \boldsymbol{w}/(\boldsymbol{w}^T\boldsymbol{v})$;
for $k = 0, 1, \ldots, m-1$ **do**
    $\boldsymbol{r} := A\boldsymbol{v}_{-k}$;
    $\boldsymbol{s} := A^T\boldsymbol{w}_{-k}$;

$\alpha_{-k,ik} := \boldsymbol{w}_{ik}^T\boldsymbol{r}$; $\boldsymbol{r} := \boldsymbol{r} - \alpha_{-k,ik}\boldsymbol{v}_{ik}$;
$\beta_{-k,ik} := \boldsymbol{v}_{ik}^T\boldsymbol{s}$; $\boldsymbol{s} := \boldsymbol{s} - \beta_{-k,ik}\boldsymbol{w}_{ik}$;
$\alpha_{-k,-k} := \boldsymbol{w}_{-k}^T\boldsymbol{r}$; $\boldsymbol{r} := \boldsymbol{r} - \alpha_{-k,-k}\boldsymbol{v}_{-k}$;
$\boldsymbol{s} := \boldsymbol{s} - \alpha_{-k,-k}\boldsymbol{w}_{-k}$;
$\delta_{ik+1} := |\boldsymbol{r}^T\boldsymbol{s}|^{1/2}$; $\boldsymbol{v}_{ik+1} := \boldsymbol{r}/\delta_{ik+1}$;
$\gamma_{ik+1} := \boldsymbol{r}^T\boldsymbol{s}/\delta_{ik+1}$; $\boldsymbol{w}_{ik+1} := \boldsymbol{s}/\gamma_{ik+1}$;
$\boldsymbol{r} := A\boldsymbol{v}_{ik+1}$;
$\boldsymbol{s} := A^T\boldsymbol{w}_{ik+1}$;
$\alpha_{ik+1,ik} := \boldsymbol{w}_{ik}^T\boldsymbol{r}$; $\boldsymbol{r} := \boldsymbol{r} - \alpha_{ik+1,ik}\boldsymbol{v}_{ik}$;
$\beta_{ik+1,ik} := \boldsymbol{v}_{ik}^T\boldsymbol{s}$; $\boldsymbol{s} := \boldsymbol{s} - \beta_{ik+1,ik}\boldsymbol{w}_{ik}$;
$\alpha_{ik+1,-k} := \boldsymbol{w}_{-k}^T\boldsymbol{r}$; $\boldsymbol{r} := \boldsymbol{r} - \alpha_{ik+1,-k}\boldsymbol{v}_{-k}$;
$\beta_{ik+1,-k} := \boldsymbol{v}_{-k}^T\boldsymbol{s}$; $\boldsymbol{s} := \boldsymbol{s} - \beta_{ik+1,-k}\boldsymbol{w}_{-k}$;
$\alpha_{ik+1,ik+1} := \boldsymbol{w}_{ik+1}^T\boldsymbol{r}$; $\boldsymbol{r} := \boldsymbol{r} - \alpha_{ik+1,ik+1}\boldsymbol{v}_{ik+1}$;
$\boldsymbol{s} := \boldsymbol{s} - \alpha_{ik+1,ik+1}\boldsymbol{w}_{ik+1}$;
$\delta_{ik+2} := |\boldsymbol{r}^T\boldsymbol{s}|^{1/2}$; $\boldsymbol{v}_{ik+2} := \boldsymbol{r}/\delta_{ik+2}$;
$\gamma_{ik+2} := \boldsymbol{r}^T\boldsymbol{s}/\delta_{ik+2}$; $\boldsymbol{w}_{ik+2} := \boldsymbol{s}/\gamma_{ik+2}$;
for $j = 3, \ldots, i$ **do**
  $\boldsymbol{r} := A\boldsymbol{v}_{ik+j-1}$;
  $\boldsymbol{s} := A^T\boldsymbol{w}_{ik+j-1}$;
  $\alpha_{ik+j-1,ik+j-2} := \boldsymbol{w}_{ik+j-2}^T\boldsymbol{r}$; $\boldsymbol{r} := \boldsymbol{r} - \alpha_{ik+j-1,ik+j-2}\boldsymbol{v}_{ik+j-2}$;
  $\beta_{ik+j-1,ik+j-2} := \boldsymbol{v}_{ik+j-2}^T\boldsymbol{s}$; $\boldsymbol{s} := \boldsymbol{s} - \beta_{ik+j-1,ik+j-2}\boldsymbol{w}_{ik+j-2}$;
  $\alpha_{ik+j-1,ik+j-1} := \boldsymbol{w}_{ik+j-1}^T\boldsymbol{r}$; $\boldsymbol{r} := \boldsymbol{r} - \alpha_{ik+j-1,ik+j-1}\boldsymbol{v}_{ik+j-1}$;
  $\boldsymbol{s} := \boldsymbol{s} - \alpha_{ik+j-1,ik+j-1}\boldsymbol{w}_{ik+j-1}$;
  $\delta_{ik+j} := |\boldsymbol{r}^T\boldsymbol{s}|^{1/2}$; $\boldsymbol{v}_{ik+j} := \boldsymbol{r}/\delta_{ik+j}$;
  $\gamma_{ik+j} := \boldsymbol{r}^T\boldsymbol{s}/\delta_{ik+j}$; $\boldsymbol{w}_{ik+j} := \boldsymbol{s}/\gamma_{ik+j}$;
end
$\hat{\boldsymbol{r}} := A^{-1}\boldsymbol{v}_{i(k+1)}$;
$\hat{\boldsymbol{s}} := A^{-T}\boldsymbol{w}_{i(k+1)}$;
$\zeta_{i(k+1),-k} := \boldsymbol{w}_{-k}^T\hat{\boldsymbol{r}}$; $\hat{\boldsymbol{r}} := \hat{\boldsymbol{r}} - \zeta_{i(k+1),-k}\boldsymbol{v}_{-k}$;
$\eta_{i(k+1),-k} := \boldsymbol{v}_{-k}^T\hat{\boldsymbol{s}}$; $\hat{\boldsymbol{s}} := \hat{\boldsymbol{s}} - \eta_{i(k+1),-k}\boldsymbol{w}_{-k}$;
for $j = 0, \ldots, i-1$ **do**
  $\zeta_{i(k+1),i(k+1)-j} := \boldsymbol{w}_{i(k+1)-j}^T\hat{\boldsymbol{r}}$; $\hat{\boldsymbol{r}} := \hat{\boldsymbol{r}} - \zeta_{i(k+1),i(k+1)-j}\boldsymbol{v}_{i(k+1)-j}$;
  $\eta_{i(k+1),i(k+1)-j} := \boldsymbol{v}_{i(k+1)-j}^T\hat{\boldsymbol{s}}$; $\hat{\boldsymbol{s}} := \hat{\boldsymbol{s}} - \eta_{i(k+1),i(k+1)-j}\boldsymbol{w}_{i(k+1)-j}$;
end
$\delta_{-(k+1)} := |\hat{\boldsymbol{r}}^T\hat{\boldsymbol{s}}|^{1/2}$; $\boldsymbol{v}_{-(k+1)} := \hat{\boldsymbol{r}}/\delta_{-(k+1)}$;
$\gamma_{-(k+1)} := \hat{\boldsymbol{r}}^T\hat{\boldsymbol{s}}/\delta_{-(k+1)}$; $\boldsymbol{w}_{-(k+1)} := \hat{\boldsymbol{s}}/\gamma_{-(k+1)}$;
end

The biorthogonal bases for the subspaces $\mathbb{K}^{m,im+1}(A,\boldsymbol{v})$ and $\mathbb{K}^{m,im+1}(A^T,\boldsymbol{w})$ determine the matrices

$$\begin{aligned}
V_{m(i+1)+1} &= [\boldsymbol{v}_0, \boldsymbol{v}_1, \ldots, \boldsymbol{v}_i, \boldsymbol{v}_{-1}, \ldots, \boldsymbol{v}_{-m+1}, \ldots, \boldsymbol{v}_{im}, \boldsymbol{v}_{-m}] \in \mathbb{R}^{n\times m(i+1)+1},\\
V_{m(i+1)+2} &= [V_{m(i+1)+1}, \boldsymbol{v}_{im+1}] \in \mathbb{R}^{n\times(m(i+1)+2)},\\
W_{m(i+1)+1} &= [\boldsymbol{w}_0, \boldsymbol{w}_1, \ldots, \boldsymbol{w}_i, \boldsymbol{w}_{-1}, \ldots, \boldsymbol{w}_{-m+1}, \ldots, \boldsymbol{w}_{im}, \boldsymbol{w}_{-m}] \in \mathbb{R}^{n\times m(i+1)+1},\\
W_{m(i+1)+2} &= [W_{m(i+1)+1}, \boldsymbol{w}_{im+1}] \in \mathbb{R}^{n\times(m(i+1)+2)}.
\end{aligned}$$

Equations (3.2), (3.3), (3.4), and (3.5) can be used to construct the matrix $\hat{H}_{m(i+1)+1} = [h_{j,k}] \in \mathbb{R}^{(m(i+1)+2)\times m(i+1)+1}$ such that

$$\begin{aligned} AV_{m(i+1)+1} &= V_{m(i+1)+2}\hat{H}_{m(i+1)+1}, \\ A^T W_{m(i+1)+1} &= W_{m(i+1)+2}\hat{H}^T_{m(i+1)+1}. \end{aligned}$$

The leading submatrix $H_{m(i+1)+1} \in \mathbb{R}^{(m(i+1)+1)\times(m(i+1)+1)}$ of $\hat{H}_{m(i+1)+1}$ satisfies

$$H_{m(i+1)+1} = W^T_{m(i+1)+1} AV_{m(i+1)+1}. \tag{21}$$

This matrix is analogous to the matrix T_m in the nonsymmetric Lanczos decomposition (2). It is pentadiagonal and its non-zero entries can be computed column-wise for the columns $(i+1)k+j$, $0 \le j \le i$, $0 \le k \le m-1$. We examine the columns corresponding to different values of j.

3.6.1 The case $j = 1$

The columns of $AV_{m(i+1)+1}$ and $A^T W_{m(i+1)+1}$ in this case correspond to $A\boldsymbol{v}_{-k}$ and $A^T\boldsymbol{w}_{-k}$, respectively. Equation (3.3) yields

$$\begin{aligned} A\boldsymbol{v}_{-k} &= \alpha_{-k,ik}\boldsymbol{v}_{ik} + \alpha_{-k,-k}\boldsymbol{v}_{-k} + \delta_{ik+1}\boldsymbol{v}_{ik+1}, \\ A^T\boldsymbol{w}_{-k} &= \beta_{-k,ik}\boldsymbol{w}_{ik} + \beta_{-k,-k}\boldsymbol{w}_{-k} + \gamma_{ik+1}\boldsymbol{w}_{ik+1}. \end{aligned}$$

Hence, the only nontrivial entries of the $((i+1)k+1)^{\text{th}}$ column of $H_{m(i+1)+1}$ are

$$\begin{aligned} &h_{(i+1)k,(i+1)k+1} = \alpha_{-k,ik}, \quad h_{(i+1)k+1,(i+1)k+1} = \alpha_{-k,-k}, \\ &h_{(i+1)k+2,(i+1)k+1} = \delta_{ik+1}. \end{aligned}$$

3.6.2 The case $j = 2$

The columns of $AV_{m(i+1)+2}$ and $A^T W_{m(i+1)+2}$ in this case correspond to $A\boldsymbol{v}_{ik+1}$ and $A^T\boldsymbol{w}_{ik+1}$, respectively. Equation (3.4) gives

$$\begin{aligned} A\boldsymbol{v}_{ik+1} &= \alpha_{ik+1,ik}\boldsymbol{v}_{ik} + \alpha_{ik+1,-k}\boldsymbol{v}_{-k} + \alpha_{ik+1,ik+1}\boldsymbol{v}_{ik+1} + \delta_{ik+2}\boldsymbol{v}_{ik+2}. \\ A^T\boldsymbol{w}_{ik+1} &= \beta_{ik+1,ik}\boldsymbol{w}_{ik} + \beta_{ik+1,-k}\boldsymbol{w}_{-k} + \beta_{ik+1,ik+1}\boldsymbol{w}_{ik+1} + \gamma_{ik+2}\boldsymbol{w}_{ik+2}. \end{aligned}$$

It follows that the only nontrivial entries of the $((i+1)k+2)^{\text{th}}$ column of $H_{m(i+1)+1}$ are

$$\begin{aligned} &h_{(i+1)k,(i+1)k+2} = \alpha_{ik+1,ik}, &&h_{(i+1)k+1,(i+1)k+2} = \alpha_{ik+1,-k}, \\ &h_{(i+1)k+2,(i+1)k+2} = \alpha_{ik+1,ik+1}, &&h_{(i+1)k+3,(i+1)k+2} = \delta_{ik+2}, \end{aligned}$$

where

$$\begin{aligned} \alpha_{ik+1,-k} &= (A\boldsymbol{v}_{ik+1}, \boldsymbol{w}_{-k}) \\ &= (\boldsymbol{v}_{ik+1}, A^T\boldsymbol{w}_{-k}) \\ &= (\boldsymbol{v}_{ik+1}, \beta_{-k,ik}\boldsymbol{w}_{ik} + \beta_{-k,-k}\boldsymbol{w}_{-k} + \gamma_{ik+1}\boldsymbol{w}_{ik+1}) \\ &= \gamma_{ik+1}. \end{aligned}$$

3.6.3 The cases $j = 3, 4, \ldots, i$

The columns of $AV_{m(i+1)+j}$ and $A^T W_{m(i+1)+j}$ in these cases correspond to $A\boldsymbol{v}_{ik+j-1}$ and $A^T\boldsymbol{w}_{ik+j-1}$, respectively. Equation (3.5) yields

$$\begin{aligned} A\boldsymbol{v}_{ik+j-1} &= \alpha_{ik+j-1,ik+j-2}\boldsymbol{v}_{ik+j-2} + \alpha_{ik+j-1,ik+j-1}\boldsymbol{v}_{ik+j-1} + \delta_{ik+j}\boldsymbol{v}_{ik+j}, \\ A^T\boldsymbol{w}_{ik+j-1} &= \beta_{ik+j-1,ik+j-2}\boldsymbol{w}_{ik+j-2} + \beta_{ik+j-1,ik+j-1}\boldsymbol{w}_{ik+j-1} + \gamma_{ik+j}\boldsymbol{w}_{ik+j}. \end{aligned}$$

The only nontrivial entries of the $((i+1)k+j)^{\text{th}}$ columns, for $j = 3, \ldots, i$, are

$$\begin{aligned} &h_{(i+1)k+j-1,(i+1)k+j} = \gamma_{ik+j-1}, \quad h_{(i+1)k+j,(i+1)k+j} = \alpha_{ik+j-1,ik+j-1}, \\ &h_{(i+1)k+1,(i+1)k+j} = \delta_{ik+j}. \end{aligned}$$

3.6.4 The case $j = 0$

The $((i+1)k)^{\text{th}}$ columns of $AV_{m(i+1)+1}$ and $A^T W_{m(i+1)+1}$ correspond to $A\boldsymbol{v}_{ik}$ and $A^T\boldsymbol{w}_{ik}$, respectively. The expressions for $A\boldsymbol{v}_{ik}$ and $A^T\boldsymbol{w}_{ik}$ can be obtained by multiplying the first and second equations in (3.2) by A and A^T, respectively, and making the appropriate substitutions for $A\boldsymbol{v}_{-m+1}, \ldots, A\boldsymbol{v}_{-m}$ and $A^T\boldsymbol{w}_{-m+1}, \ldots, A^T\boldsymbol{w}_{-m}$. Then, we simplify the resulting expressions using the facts that i) $\zeta_{ik,ik} \neq 0$ and ii) $\boldsymbol{w}_{ik}^T A^{-1}\boldsymbol{v}_r = 0,\ r = -k+1, \ldots, 0, \ldots, ik-2$. Hence,

$$\begin{aligned} A\boldsymbol{v}_{ik} &= h_{(i+1)k-1,(i+1)k}\boldsymbol{v}_{ik-1} + h_{(i+1)k,(i+1)k}\boldsymbol{v}_{ik} + \\ &\quad\ h_{(i+1)k+1,(i+1)k}\boldsymbol{v}_{-k} + h_{(i+1)k+2,(i+1)k}\boldsymbol{v}_{ik+1}, \\ A^T\boldsymbol{w}_{ik} &= h_{(i+1)k-1,(i+1)k}\boldsymbol{w}_{ik-1} + h_{(i+1)k,(i+1)k}\boldsymbol{w}_{ik} + \\ &\quad\ h_{(i+1)k+1,(i+1)k}\boldsymbol{w}_{-k} + h_{(i+1)k+2,(i+1)k}\boldsymbol{v}_{ik+1}, \end{aligned}$$

where

$$\begin{aligned} h_{(i+1)k-1,(i+1)k} &= \gamma_{ik}, \\ h_{(i+1)k+1,(i+1)k} &= \tfrac{-\delta_{-k}\alpha_{-k,-k}}{\zeta_{ik,ik}}, \\ h_{(i+1)k+2,(i+1)k} &= \tfrac{-\delta_{-k}\delta_{ik+1}}{\zeta_{ik,ik}}. \end{aligned}$$

The diagonal element is given by

$$h_{(i+1)k,(i+1)k} = \frac{1 - \zeta_{ik,ik-1}\delta_{ik} - \alpha_{-k,ik}\delta_{-k}}{\zeta_{ik,ik}}.$$

Example 3.1. Let $m = 3$ and $i = 3$. Then the matrix H_{13} is of the form

$$\begin{bmatrix}
\alpha_{0,0} & \gamma_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\delta_1 & \alpha_{1,1} & \gamma_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \delta_2 & \alpha_{2,2} & \gamma_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \delta_3 & h_{4,4} & \alpha_{-1,3} & \alpha_{4,3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & h_{5,4} & \alpha_{-1,-1} & \gamma_4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & h_{6,4} & \delta_4 & \alpha_{4,4} & \gamma_5 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \delta_5 & \alpha_{5,5} & \gamma_6 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \delta_6 & h_{8,8} & \alpha_{-2,6} & \alpha_{7,6} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & h_{9,8} & \alpha_{-2,-2} & \gamma_7 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & h_{10,8} & \delta_7 & \alpha_{7,7} & \gamma_8 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \delta_8 & \alpha_{8,8} & \gamma_9 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \delta_9 & h_{12,12} & \alpha_{-3,9} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & h_{13,12} & \alpha_{-3,-3}
\end{bmatrix}.$$

Let $G_{m(i+1)+1} \in \mathbb{R}^{(m(i+1)+1)\times(m(i+1)+1)}$ denote the projection of A^{-1} onto $\mathbb{K}^{m+1,im+1}(A,\boldsymbol{v})$ to $\mathbb{K}^{m+1,im+1}(A^T,\boldsymbol{w})$, that is

$$G_{m(i+1)+1} = W_{m(i+1)+1}^T A^{-1} V_{m(i+1)+1}. \tag{22}$$

The matrix $G_{m(i+1)+1}$ is a rank-one modification of $H_{m(i+1)+1}^{-1}$ and banded. Its non-vanishing entries form $(i+2)\times(i+2)$ blocks along the diagonal such that any two consecutive blocks overlap in one diagonal element; see [16] for a proof of this structure in the case when A is symmetric. This proof carries over to the present situation with obvious modifications.

4 Application to rational Gauss quadrature

This section discusses Gauss–Laurent quadrature rules for the approximation of functionals (1) based on quantities computed by Algorithm 1. Rational Gauss rules were first considered by Gonchar and López Lagomasino [11], and have subsequently received considerable attention; see, e.g., Gautschi [9, Section 3.1.4] as well as [6, 25] for discussions and references. An application of Gauss–Laurent rules to the computation of upper and lower bounds for certain symmetric matrix functionals is described in [15,16]. We consider the case $i \geq 1$ in (3).

Application of $\tau = m(i+1)$ steps of Algorithm 1 to the matrix A with initial vector $\boldsymbol{v}$ and $\boldsymbol{w}$, such that $\boldsymbol{v}^T\boldsymbol{w} = 1$, yields the decompositions

$$\begin{aligned}
AV_\tau &= V_\tau H_\tau + (h_{\tau+1,\tau}\boldsymbol{v}_{-m} + h_{\tau+2,\tau}\boldsymbol{v}_{im+1})\boldsymbol{e}_\tau^T, & (23)\\
A^{-1}V_\tau &= V_\tau G_\tau + \boldsymbol{v}_{-m}[g_{\tau+1,\tau-i}\boldsymbol{e}_{\tau-i},\ldots,g_{\tau+1,\tau-1}\boldsymbol{e}_{\tau-1},g_{\tau+1,\tau}\boldsymbol{e}_\tau]^T, & (24)\\
A^TW_\tau &= W_\tau H_\tau^T + (h_{\tau,\tau+1}\boldsymbol{w}_{-m} + h_{\tau,\tau+2}\boldsymbol{w}_{im+1})\boldsymbol{e}_\tau^T, & (25)\\
A^{-T}W_\tau &= W_\tau G_\tau^T + \boldsymbol{w}_{-m}[g_{\tau-i,\tau+1}\boldsymbol{e}_{\tau-i},\ldots,g_{\tau-1,\tau+1}\boldsymbol{e}_{\tau-1},g_{\tau,\tau+1}\boldsymbol{e}_\tau]^T, &
\end{aligned}$$

where the columns of $V_\tau, W_\tau \in \mathbb{R}^{n\times m(i+1)}$ form biorthogonal bases for $\mathbb{K}^{m,im+1}(A,\boldsymbol{v})$ and $\mathbb{K}^{m,im+1}(A^T,\boldsymbol{w})$, respectively. The matrices $H_\tau, G_\tau \in \mathbb{R}^{m(i+1)\times m(i+1)}$ generally are nonsymmetric and the matrix H_τ is pentadiagonal. The following example illustrates the structure of these matrices.

Example 4.1. The matrices H_τ and G_τ in the decompositions (4) and (4) for $i = 3$, $m = 3$, and $\tau = 12$ may have nonvanishing entries in the positions marked by "$*$":

$$H_{12} = \begin{bmatrix}
* & * & & & & & & & & & & \\
* & * & * & & & & & & & & & \\
& * & * & * & & & & & & & & \\
& & * & * & * & * & & & & & & \\
& & & * & * & * & & & & & & \\
& & & * & * & * & * & & & & & \\
& & & & & * & * & * & & & & \\
& & & & & & * & * & * & * & & \\
& & & & & & & * & * & * & & \\
& & & & & & & * & * & * & * & \\
& & & & & & & & & * & * & * \\
& & & & & & & & & & * & *
\end{bmatrix}, \qquad
G_{12} = \begin{bmatrix}
* & * & * & * & * & & & & & & & \\
* & * & * & * & * & & & & & & & \\
* & * & * & * & * & & & & & & & \\
* & * & * & * & * & & & & & & & \\
* & * & * & * & * & * & * & * & * & & & \\
& & & & * & * & * & * & * & & & \\
& & & & * & * & * & * & * & & & \\
& & & & * & * & * & * & * & & & \\
& & & & * & * & * & * & * & * & * & * \\
& & & & & & & & * & * & * & * \\
& & & & & & & & * & * & * & * \\
& & & & & & & & * & * & * & *
\end{bmatrix}.$$

We would like to establish that

$$\boldsymbol{w}^T f(A)\boldsymbol{v} = \boldsymbol{e}_1^T f(H_\tau)\boldsymbol{e}_1 \qquad \forall f \in \mathcal{L}_{2m-2,2im+1}, \tag{26}$$

where $A \in \mathbb{R}^{n\times n}$ is nonsingular and $\boldsymbol{w}, \boldsymbol{v} \in \mathbb{R}^n$ satisfy $\boldsymbol{w}^T\boldsymbol{v} = 1$. The right-hand side expression is a Gauss–Laurent quadrature rule for the approximation of the left-hand side. The quadrature rule on the right-hand side has τ nodes, which are the eigenvalues of H_τ. In order to show (4), we first need some auxiliary results on the properties of the matrices H_τ and G_τ. Analogous results for different spaces of Laurent polynomials have been shown by Schweitzer [28]. Related results for symmetric matrices can be found in [16].

Lemma 1 *Let $A \in \mathbb{R}^{n\times n}$ be positive or negative real, let $\boldsymbol{w}, \boldsymbol{v} \in \mathbb{R}^n$ satisfy $\boldsymbol{w}^T\boldsymbol{v} = 1$, and let the matrices H_τ and G_τ be defined by* (3.6) *and* (3.6.4)*, respectively, with the matrices V_τ, W_τ computed by Algorithm 1. Assume that $\tau := m(i+1) > 1$. Then*

$$\boldsymbol{w}^T p(A)\boldsymbol{v} = \boldsymbol{e}_1^T p(H_\tau)\boldsymbol{e}_1, \qquad p \in \mathbb{P}_{2im+1}, \tag{27}$$

$$\boldsymbol{w}^T q(A^{-1})\boldsymbol{v} = \boldsymbol{e}_1^T q(G_\tau)\boldsymbol{e}_1, \qquad q \in \mathbb{P}_{2m-1}. \tag{28}$$

Proof We first show (1) and note that it suffices to prove (1) for monomials $p(z) = z^j$, $j = 0, 1, \ldots, 2im+1$. For $j = 1$, we obtain from (4), using $V_\tau\boldsymbol{e}_1 = \boldsymbol{v}$, that

$$A\boldsymbol{v} = AV_\tau\boldsymbol{e}_1 = V_\tau H_\tau\boldsymbol{e}_1,$$

where the second term vanishes because $\boldsymbol{e}_\tau^T\boldsymbol{e}_1 = 0$. For increasing values of j, we obtain

$$A^j\boldsymbol{v} = A^jV_\tau\boldsymbol{e}_1 = V_\tau H_\tau^j\boldsymbol{e}_1 + \boldsymbol{z}_\tau\boldsymbol{e}_\tau^T H_\tau^{j-1}\boldsymbol{e}_1, \tag{29}$$

where

$$\boldsymbol{z}_\tau = h_{\tau+1,\tau}\boldsymbol{v}_{-m} + h_{\tau+2,\tau}\boldsymbol{v}_{im+1}.$$

Due to the structure of H_τ, the second term on the right-hand side of (4) vanishes, and for $j \le im$ we get

$$A^j\boldsymbol{v} = V_\tau H_\tau^j\boldsymbol{e}_1, \qquad j = 0, 1, \ldots, im. \tag{30}$$

Similarly, from (4) we have

$$(A^T)^j\boldsymbol{w} = W_\tau(H_\tau^T)^j\boldsymbol{e}_1, \qquad j = 0, 1, \ldots, im. \tag{31}$$

Combining (4) and (4) gives

$$\begin{aligned}
\boldsymbol{w}^T A^{2im+1}\boldsymbol{v} &= ((A^T)^{im}\boldsymbol{w})^T A(A^{im}\boldsymbol{v}) \\
&= (W_\tau(H_\tau^T)^{im}\boldsymbol{e}_1)^T A(V_\tau H_\tau^{im}\boldsymbol{e}_1) \\
&= \boldsymbol{e}_1^T H_\tau^{2im+1}\boldsymbol{e}_1.
\end{aligned}$$

The same conclusion can be drawn for lower powers of A. This shows (1). We can prove (1) in the same manner. $\square$

Next we will show a relation between positive powers of G_τ and negative powers of H_τ.

Lemma 2 *Let the assumptions of Lemma 1 be satisfied, and suppose that H_τ is nonsingular. Then*

$$\boldsymbol{e}_1^T p(G_\tau)\boldsymbol{e}_1 = \boldsymbol{e}_1^T p(H_\tau^{-1})\boldsymbol{e}_1, \qquad p \in \mathbb{P}_{2m-2}. \tag{32}$$

Proof Multiplying (4) by $W_\tau^T A$ from the left, we get

$$I = H_\tau G_\tau + W_\tau^T A\boldsymbol{v}_{-m}[g_{\tau+1,\tau-i}\boldsymbol{e}_{\tau-i}, \ldots, g_{\tau+1,\tau-1}\boldsymbol{e}_{\tau-1}, g_{\tau+1,\tau}\boldsymbol{e}_\tau]^T.$$

This implies that

$$H_\tau G_\tau \boldsymbol{e}_1 = \boldsymbol{e}_1.$$

We obtain by induction that

$$H_\tau^j G_\tau^j \boldsymbol{e}_1 = H_\tau^{j-1}(I - W_\tau^T A\boldsymbol{v}_{-m}[g_{\tau+1,\tau-i}\boldsymbol{e}_{\tau-i}, \ldots, g_{\tau+1,\tau}\boldsymbol{e}_\tau]^T)G_\tau^{j-1}\boldsymbol{e}_1$$

for $j = 0, 1, \ldots, m-1$. Observing that only the first $(2j-2)+i$ entries of $G_\tau^{j-1}\boldsymbol{e}_1$ may be nonzero, the above equation gives

$$H_\tau^j G_\tau^j \boldsymbol{e}_1 = H_\tau^{j-1} G_\tau^{j-1}\boldsymbol{e}_1 = \boldsymbol{e}_1, \quad j = 0, 1, \ldots, m-1.$$

Multiplying by H_τ^{-j} from the left shows that

$$G_\tau^j \boldsymbol{e}_1 = H_\tau^{-j}\boldsymbol{e}_1, \quad j = 0, 1, \ldots, m-1. \tag{33}$$

Similarly, we obtain

$$(G_\tau^T)^j \boldsymbol{e}_1 = (H_\tau^T)^{-j}\boldsymbol{e}_1, \quad j = 0, 1, \ldots, m-1. \tag{34}$$

Using (4) and (4) together gives

$$\boldsymbol{e}_1^T G_\tau^{2m-2}\boldsymbol{e}_1 = \boldsymbol{e}_1^T H_\tau^{-(2m-2)}\boldsymbol{e}_1.$$

A similar argument holds for lower powers of G_τ. This shows (2). □

We are now in a position to show that (4) holds.

Theorem 1 *The right-hand side of* (4) *is a Gauss–Laurent quadrature rule for the expression on the left-hand side.*

Proof Let $f \in \mathcal{L}_{2m-2,2im+1}$. Then $f(A) = p(A) + q(A^{-1})$ for some polynomials $p \in \mathbb{P}_{2im+1}$ and $q \in \mathbb{P}_{2m-2}$. We obtain from Lemma 1 that

$$\boldsymbol{w}^T f(A)\boldsymbol{v} = \boldsymbol{w}^T p(A)\boldsymbol{v} + \boldsymbol{w}^T q(A^{-1})\boldsymbol{v} = \boldsymbol{e}_1^T p(H_\tau)\boldsymbol{e}_1 + \boldsymbol{e}_1^T q(G_\tau)\boldsymbol{e}_1.$$

Applying Lemma 2 gives

$$\boldsymbol{w}^T f(A)\boldsymbol{v} = \boldsymbol{e}_1^T p(H_\tau)\boldsymbol{e}_1 + \boldsymbol{e}_1^T q(H_\tau^{-1})\boldsymbol{e}_1 = \boldsymbol{e}_1^T f(H_\tau)\boldsymbol{e}_1.$$

This shows (4). □

It is shown in [16] that for suitable integrands, appropriate pairs of Gauss–Laurent and Gauss–Laurent–Radau quadrature rules can be applied to determine upper and lower bounds for the functional (1) when the matrix A is symmetric. However, this approach is not guaranteed to furnish upper and lower bounds when the matrix A is nonsymmetric. We will show that in this situation, estimates of error bounds can be determined by evaluating appropriate pairs of Gauss–Laurent and anti-Gauss–Laurent quadrature rules.

Laurie [19] introduced the (standard) $(m+1)$-point anti-Gauss quadrature rule that gives an error of the same magnitude and of opposite sign as the (standard) m-point Gauss quadrature rule. The evaluation of the (standard) $(m+1)$-point anti-Gauss quadrature rule requires the computation of $m+1$ steps of the (standard) Lanczos process; see, e.g., [1, 2, 5] for details. We will show that anti-Gauss–Laurent rules can be computed in an analogous fashion.

Let

$$\tilde{\mathcal{G}}_{\tau+1} f := \sum_{j=1}^{\tau+1} f(\tilde{\lambda}_j)\tilde{\nu}_j\tilde{\nu}'_j$$

be the $(\tau+1)$-point anti-Gauss–Laurent rule associated with the Gauss–Laurent rule $\mathcal{G}_\tau f$ for the measure dw in (1). This anti-Gauss–Laurent rule is determined by the requirement that

$$(\mathcal{I} - \tilde{\mathcal{G}}_{\tau+1})f = -(\mathcal{I} - \mathcal{G}_\tau)f \qquad \forall f \in \mathcal{L}_{2m-2,2im+3}, \tag{35}$$

where $\mathcal{G}_\tau f$ is characterized by

$$\mathcal{G}_\tau f = \mathcal{I} f \qquad \forall f \in \mathcal{L}_{2m-2,2im+1}. \tag{36}$$

Relation (4) shows that $\tilde{\mathcal{G}}_{\tau+1}$ is the $(\tau+1)$-point Gauss–Laurent rule for the functional

$$\mathcal{J} f := (2\mathcal{I} - \mathcal{G}_\tau)f.$$

Introduce, analogously to (3.1) and (3.1), the vectors

$$\begin{aligned} \tilde{\boldsymbol{v}}_j &= \tilde{\phi}_j(A)\boldsymbol{v}, \\ \tilde{\boldsymbol{w}}_j &= \tilde{\psi}_j(A^T)\boldsymbol{w}, \end{aligned} \qquad j = -m+1, -m+2, \ldots, im+1,$$

where $\tilde{\phi}_j$ and $\tilde{\psi}_j$ are two families of biorthogonal Laurent polynomials with respect to the bilinear form

$$\{p, q\} := \mathcal{J}(pq),$$

i.e., $\{\tilde{\phi}_i, \tilde{\psi}_j\} = 0$ for all $i \neq j$ and $\{\tilde{\phi}_j, \tilde{\psi}_j\} = 1$ for all j. The biorthogonal bases $\tilde{V}_{\tau+1} = [\tilde{\boldsymbol{v}}_j]_{j=-m+1}^{im+1} \in \mathbb{R}^{n\times(\tau+1)}$ and $\tilde{W}_{\tau+1} = [\tilde{\boldsymbol{w}}_j]_{j=-m+1}^{im+1} \in \mathbb{R}^{n\times(\tau+1)}$ for the extended Krylov subspaces $\mathbb{K}^{m,im+2}(A, \boldsymbol{v})$ and $\mathbb{K}^{m,im+2}(A^T, \boldsymbol{w})$, respectively, with $\tilde{\boldsymbol{v}}_0 = \boldsymbol{v}$ and $\tilde{\boldsymbol{w}}_0 = \boldsymbol{w}$ satisfy the decompositions

$$\begin{aligned} A\tilde{V}_{\tau+1} &= \tilde{V}_{\tau+1}\tilde{H}_{\tau+1} + \tilde{h}_{\tau+2,\tau+1}\tilde{\boldsymbol{v}}_{im+2}\boldsymbol{e}_{\tau+1}^T, \\ A^T\tilde{W}_{\tau+1} &= \tilde{W}_{\tau+1}\tilde{H}_{\tau+1}^T + \tilde{h}_{\tau+1,\tau+2}\tilde{\boldsymbol{w}}_{im+2}\boldsymbol{e}_{\tau+1}^T, \end{aligned}$$

where $\tau = m(i+1)$ and the matrix $\tilde{H}_{\tau+1} = [\tilde{h}_{j,k}] \in \mathbb{R}^{(\tau+1)\times(\tau+1)}$ is a nonsymmetric and pentadiagonal. It follows from (4) and (4) that

$$\{\phi, \psi\} = [\phi, \psi] = \mathcal{I}(\phi\psi), \qquad \forall \phi\psi \in \mathcal{L}_{2m-2,2im+1}.$$

These equalities show that

$$\tilde{h}_{j,k} = h_{j,k}, \qquad j,k = 1,2,\ldots,\tau$$

Therefore, $\tilde{\phi}_j = \phi_j$ and $\tilde{\psi}_j = \psi_j$ for $j = -m+1, -m+2, \ldots, im$.

It follows from the structure of H_τ and relations (4) and (4), in view of (3.1) and (3.1), that the Laurent polynomials

$$\breve{\phi}_\tau(z) = h_{\tau+1,\tau}\phi_{-m}(z) + h_{\tau+2,\tau}\phi_{im+1}(z),$$
$$\breve{\psi}_\tau(z) = h_{\tau,\tau+1}\psi_{-m}(z) + h_{\tau,\tau+2}\psi_{im+1}(z),$$

for $i = 1$ can be computed with four-term recursion formulas

$$\breve{\phi}_\tau(z) = (z - h_{\tau,\tau})\phi_{im}(z) - h_{\tau-1,\tau}\phi_{-m+1}(z) - h_{\tau-2,\tau}\phi_{im-1}(z),$$
$$\breve{\psi}_\tau(z) = (z - h_{\tau,\tau})\psi_{im}(z) - h_{\tau,\tau-1}\psi_{-m+1}(z) - h_{\tau,\tau-2}\psi_{im-1}(z),$$

which can be written as

$$\breve{\phi}_\tau(z) = (z - \tilde{h}_{\tau,\tau})\tilde{\phi}_{im}(z) - \tilde{h}_{\tau-1,\tau}\tilde{\phi}_{-m+1}(z) - \tilde{h}_{\tau-2,\tau}\tilde{\phi}_{im-1}(z),$$
$$\breve{\psi}_\tau(z) = (z - \tilde{h}_{\tau,\tau})\tilde{\psi}_{im}(z) - \tilde{h}_{\tau,\tau-1}\tilde{\psi}_{-m+1}(z) - \tilde{h}_{\tau,\tau-2}\tilde{\psi}_{im-1}(z).$$

For $i > 1$, $\breve{\phi}_\tau$ and $\breve{\psi}_\tau$ can be determined with three-term recursion formulas

$$\breve{\phi}_\tau(z) = (z - h_{\tau,\tau})\phi_{im}(z) - h_{\tau-1,\tau}\phi_{im-1}(z),$$
$$\breve{\psi}_\tau(z) = (z - h_{\tau,\tau})\psi_{im}(z) - h_{\tau,\tau-1}\psi_{im-1}(z),$$

which can be expressed as

$$\breve{\phi}_\tau(z) = (z - \tilde{h}_{\tau,\tau})\tilde{\phi}_{im}(z) - \tilde{h}_{\tau-1,\tau}\tilde{\phi}_{im-1}(z),$$
$$\breve{\psi}_\tau(z) = (z - \tilde{h}_{\tau,\tau})\tilde{\psi}_{im}(z) - \tilde{h}_{\tau,\tau-1}\tilde{\psi}_{im-1}(z).$$

For all $i \geq 1$, we can determine Laurent polynomials $\breve{\phi}_{\tau+1}$ and $\breve{\psi}_{\tau+1} \in \mathcal{L}_{m-1,im+2}$ that are biorthogonal to $\mathcal{L}_{m-1,im+1}$ with three-term recursion formulas

$$\breve{\phi}_{\tau+1}(z) = (z - \alpha)\breve{\phi}_\tau(z) - \tilde{\gamma}_\tau\phi_{im}(z),$$
$$\breve{\psi}_{\tau+1}(z) = (z - \alpha)\breve{\psi}_\tau(z) - \tilde{\delta}_\tau\psi_{im}(z),$$

where

$$\tilde{\delta}_\tau\tilde{\gamma}_\tau = \{\breve{\phi}_\tau, \breve{\psi}_\tau\} = 2\mathcal{I}(\breve{\phi}_\tau\breve{\psi}_\tau) - \mathcal{G}_\tau(\breve{\phi}_\tau\breve{\psi}_\tau) = 2\mathcal{I}(\breve{\phi}_\tau\breve{\psi}_\tau) = 2[\breve{\phi}_\tau, \breve{\psi}_\tau] = 2\delta_\tau\gamma_\tau.$$

We may choose $\tilde{\delta}_\tau = \sqrt{2}\delta_\tau$ and $\tilde{\gamma}_\tau = \sqrt{2}\gamma_\tau$. It follows that the nonsymmetric pentadiagonal matrix associated with the anti-Gauss–Laurent rule $\tilde{\mathcal{G}}_{\tau+1}$ is given by

$$\tilde{H}_{\tau+1} = \begin{bmatrix} H_\tau & \sqrt{2}\gamma_\tau \\ \sqrt{2}\delta_\tau & \alpha \end{bmatrix} \in \mathbb{R}^{(\tau+1)\times(\tau+1)},$$

where the last diagonal coefficient can be determined from $\alpha = (z\breve{\phi}_\tau, \breve{\psi}_\tau)$. For $i > 1$, this coefficient can be evaluated by carrying out one additional "standard step" of Algorithm 1 that uses the three-term recurrence relation, i.e., we evaluate

$$\boldsymbol{r} := A\boldsymbol{v}_{im} - h_{\tau,\tau}\boldsymbol{v}_{im} - \gamma_{im}\boldsymbol{v}_{im-1};$$
$$\boldsymbol{s} := A^T\boldsymbol{w}_{im} - h_{\tau,\tau}\boldsymbol{w}_{im} - \delta_{im}\boldsymbol{w}_{im-1};$$

and then compute

$$\delta_{im+1} := |\boldsymbol{r}^T\boldsymbol{s}|^{1/2}; \quad \gamma_{im+1} := \boldsymbol{r}^T\boldsymbol{s}/\delta_{im+1}; \quad \boldsymbol{v}_{im+1} := \boldsymbol{r}/\delta_{im+1}; \quad \boldsymbol{w}_{im+1} := \boldsymbol{s}/\gamma_{im+1}.$$

Finally,

$$h_{\tau+1,\tau+1} = \alpha := \boldsymbol{w}_{im+1}^T A\boldsymbol{v}_{im+1};$$

Analogously to formula (4), the anti-Gauss–Laurent quadrature rule can be evaluated according to

$$\tilde{\mathcal{G}}_{\tau+1}f = e_1^T f(\tilde{H}_{\tau+1})e_1 \qquad \forall f \in \mathcal{L}_{2m-2,2im+3}.$$

We are now in a position to provide sufficient conditions for $\mathcal{G}_\tau f$ and $\tilde{\mathcal{G}}_{\tau+1}f$ to bracket $\mathcal{I}f$. Assume that we can carry out n steps of Algorithm 1 without breakdown. This yields biorthogonal bases $\{\boldsymbol{v}_j\}_{j=0}^{n-1}$ and $\{\boldsymbol{w}_j\}_{j=0}^{n-1}$ of $\mathbb{R}^n$ and associated sequences of Laurent polynomials $\{\phi_j, \psi_j\}_{j=0}^{n-1}$ defined by (3.1) and (3.1) that satisfy (2).

Theorem 2 *Let $\lambda(A)$ denote the spectrum of the matrix A. Consider the expansion of the integrand*

$$f(z) = \sum_{j=0}^{n-1} \mu_j\phi_j(z), \quad z \in \lambda(A), \tag{37}$$

in terms of the Laurent polynomials ϕ_j, and assume that the coefficients μ_j in (2) are such that

$$\left|\sum_{j=2im+2}^{2im+3} \mu_j\mathcal{G}_\tau\phi_j\right| \geq \max\left\{\left|\sum_{j=2im+4}^{n-1} \mu_j\mathcal{G}_\tau\phi_j\right|, \left|\sum_{j=2im+4}^{n-1} \mu_j\tilde{\mathcal{G}}_{\tau+1}\phi_j\right|\right\}. \tag{38}$$

Then the quadrature rules $\mathcal{G}_\tau f$ and $\tilde{\mathcal{G}}_{\tau+1}f$ bracket $\mathcal{I}f$.

Proof Since

$$\mathcal{I}f = \mu_0\mathcal{I}\phi_0, \qquad \mathcal{I}\phi_j = 0 \quad \forall j > 0$$

we have, in view of (4) and (4), that

$$\begin{aligned}\mathcal{G}_\tau f &= \sum_{j=0}^{n-1} \mu_j\mathcal{G}_\tau\phi_j = \sum_{j=0}^{2im+1} \mu_j\mathcal{G}_\tau\phi_j + \sum_{j=2im+2}^{n-1} \mu_j\mathcal{G}_\tau\phi_j \\ &= \mathcal{I}f + \mu_{2im+2}\mathcal{G}_\tau\phi_{2im+2} + \mu_{2im+3}\mathcal{G}_\tau\phi_{2im+3} + \sum_{j=2im+4}^{n-1} \mu_j\mathcal{G}_\tau\phi_j.\end{aligned} \tag{39}$$

$$\begin{aligned}\tilde{\mathcal{G}}_{\tau+1}f &= \sum_{j=0}^{n-1} \mu_j\tilde{\mathcal{G}}_{\tau+1}\phi_j = \sum_{j=0}^{2im+3} \mu_j(2\mathcal{I} - \mathcal{G}_\tau)\phi_j + \sum_{j=2im+4}^{n-1} \mu_j\tilde{\mathcal{G}}_{\tau+1}\phi_j \\ &= \mathcal{I}f - \mu_{2im+2}\mathcal{G}_\tau\phi_{2im+2} - \mu_{2im+3}\mathcal{G}_\tau\phi_{2im+3} + \sum_{j=2im+4}^{n-1} \mu_j\tilde{\mathcal{G}}_{\tau+1}\phi_j.\end{aligned} \tag{40}$$

combining (4) and (4) shows (2). $\square$

Theorem 2 shows that if the coefficients μ_j decay sufficiently rapidly with increasing j, then rational Gauss and anti-Gauss rules provide quadrature errors that are of opposite sign and of roughly the same magnitude. The following example illustrates the structure of the matrix $\tilde{H}_{\tau+1}$ for the cases $i = 1, 2, 3$.

Example 4.2. The matrix $\tilde{H}_{\tau+1}$ may have nonvanishing entries in the positions marked by "$*$" below. For instance, we have

$$\tilde{H}_7 = \begin{bmatrix} * & * & & & & & \\ * & * & * & * & & & \\ & * & * & * & & & \\ & * & * & * & * & * & \\ & & & * & * & * & \\ & & & * & * & * & * \\ & & & & & * & * \end{bmatrix} \qquad \text{for} \quad i = 1, m = 3, \tau = 6,$$

$$\tilde{H}_7 = \begin{bmatrix} * & * & & & & & \\ * & * & * & & & & \\ & * & * & * & * & & \\ & & * & * & * & & \\ & & * & * & * & * & \\ & & & & * & * & * \\ & & & & & * & * \end{bmatrix} \qquad \text{for} \quad i = 2, m = 2, \tau = 6,$$

and

$$\tilde{H}_{13} = \begin{bmatrix} * & * & & & & & & & & & & & \\ * & * & * & & & & & & & & & & \\ & * & * & * & & & & & & & & & \\ & & * & * & * & * & & & & & & & \\ & & & * & * & * & & & & & & & \\ & & & * & * & * & * & & & & & & \\ & & & & & * & * & * & & & & & \\ & & & & & & * & * & * & * & & & \\ & & & & & & & * & * & * & & & \\ & & & & & & & * & * & * & * & & \\ & & & & & & & & & * & * & * & \\ & & & & & & & & & & * & * & * \\ & & & & & & & & & & & * & * \end{bmatrix} \qquad \text{for} \quad i = 3, m = 3, \tau = 12.$$

5 Computed examples

In this section, we illustrate the performance of the Gauss–Laurent and associated anti-Gauss–Laurent rules when applied to several functionals (1). All computations were carried out using MATLAB R2017b on a 64-bit MacBook Pro personal computer with about 15 significant decimal digits.

The purpose of these examples is to compare the performance of the standard Gauss and Gauss–Laurent rules for the case $i = 3$. The last example illustrates the performance of these quadrature rules for $i = 1, 2$, and 3. Also, we show that pairs of Gauss–Laurent and anti-Gauss–Laurent quadrature rules provide upper and lower bounds for certain functionals (1). We compare the approximations obtained by the quadrature rules and the values computed by explicitly evaluating the functional (1). We choose $\tau = 0 \bmod 4$ and $\tau = 0 \bmod 3$ to ensure that the matrix H_τ defined by (4) is of the appropriate dimensions for $i = 1, 2, 3$. The table column headings $\boldsymbol{e}_1^T f(T)\boldsymbol{e}_1$, $\boldsymbol{e}_1^T f(H)\boldsymbol{e}_1$, and $\boldsymbol{e}_1^T f(\tilde{H})\boldsymbol{e}_1$ refer to standard Gauss, Gauss–Laurent, and anti-Gauss–Laurent quadrature rules, respectively.

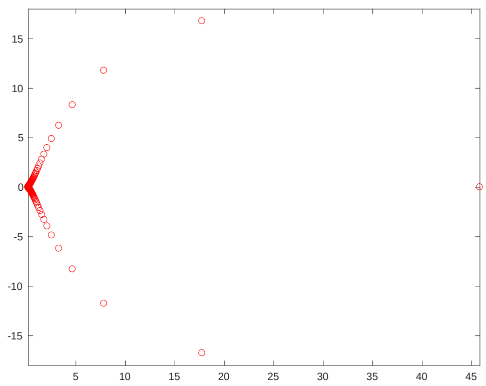

Fig. 1 Example 5.1: Spectrum of matrix A in $\mathbb{C}$. The eigenvalues are marked by "o". The horizontal axis shows the real parts of the eigenvalues, the vertical axis the imaginary parts.

Example 5.1. We would like to determine approximations of the functional

$$F(A) := \boldsymbol{w}^T \exp(-A)A^{-1/2}\boldsymbol{v},$$

where $A \in \mathbb{R}^{200\times 200}$ is a real nonsymmetric Toeplitz matrix with first row and column $[1, 1/2, \ldots, 1/200]$ and $[1, 1, \ldots, 1]^T$, respectively. The vectors $\boldsymbol{v}$ and $\boldsymbol{w}$ have normally distributed random entries with zero mean and are scaled so that $\boldsymbol{w}^T\boldsymbol{v} = 1$. Figure 1 shows the eigenvalues of A. The eigenvalue of largest magnitude is real-valued and about 45.8; the eigenvalues with the largest imaginary parts (in magnitude) are approximately $17.8 \pm 16.8i$, where $i = \sqrt{-1}$ is the imaginary unit. The eigenvalue of smallest magnitude is real and about 0.195.

We evaluate (1) as $\boldsymbol{w}^T \exp(-A)A^{-1/2}\boldsymbol{v}$, where the vector $A^{-1/2}\boldsymbol{v}$ is calculated by first computing the matrix square root and then solving a linear system of equations. The exact value of $F(A)$ is approximately 0.9990. We report this value to allow a reader to estimate the relative approximation error from Table 1.

The Gauss–Laurent rule is evaluated as

$$\boldsymbol{e}_1^T \exp(-H_\tau) G_\tau^{1/2} \boldsymbol{e}_1,$$

where $G_\tau^{1/2}\boldsymbol{e}_1$ is the first column of the inverse of the square root of the matrix H. It is determined by first computing the matrix square root and then solving a linear system of equations. The exponential is computed with the MATLAB function `expm`. The standard Gauss rule

$$\boldsymbol{e}_1^T \exp(-T_\tau) T_\tau^{-1/2} \boldsymbol{e}_1$$

is determined by first computing the inverse of the square root of the matrix T_τ and then solving a linear system of equations for the vector $T_\tau^{-1/2}\boldsymbol{e}_1$.

Columns 2 and 3 of Table 1 display the errors in approximations determined by standard Gauss and Gauss–Laurent rules for $i = 3$. We observe that the Gauss–Laurent rules yield higher accuracy than the standard Gauss rules when using the same number, τ, of quadrature nodes. Columns 3 and 4 of Table 1 show the errors in approximations obtained by Gauss–Laurent and associated anti-Gauss–Laurent rules to have opposite sign and to be of about the same magnitude for each value of τ. Therefore, the average rules

$$\frac{1}{2}(\boldsymbol{e}_1^T f(H_{i=3})\boldsymbol{e}_1 + \boldsymbol{e}_1^T f(\tilde{H}_{i=3})\boldsymbol{e}_1) \tag{41}$$

for the different τ-values determine more accurate approximations of $F(A)$ than the corresponding Gauss–Laurent rules. In applications, we use pairs of Gauss–Laurent and associated anti-Gauss–Laurent rules to determine estimates of upper and lower bounds for the functional $F(A)$, and use the averages rule as an approximation of $F(A)$. $\square$

τ	$\boldsymbol{e}_1^T f(T)\boldsymbol{e}_1$	$\boldsymbol{e}_1^T f(H_{i=3})\boldsymbol{e}_1$	$\boldsymbol{e}_1^T f(\tilde{H}_{i=3})\boldsymbol{e}_1$
12	$1.08 \cdot 10^{-1}$	$9.69 \cdot 10^{-4}$	$-8.69 \cdot 10^{-4}$
16	$3.15 \cdot 10^{-2}$	$2.69 \cdot 10^{-5}$	$-2.26 \cdot 10^{-5}$
20	$8.80 \cdot 10^{-3}$	$1.28 \cdot 10^{-6}$	$-1.48 \cdot 10^{-6}$

Table 1 Example 5.1: Errors for computed approximations of $F(A) = \boldsymbol{w}^T \exp(-A)A^{-1/2}\boldsymbol{v}$ with A a nonsymmetric Toeplitz matrix.

Example 5.2. This example determines approximations of the functional

$$F(A) := \boldsymbol{w}^T \ln(A)\boldsymbol{v},$$

with A the same matrix as in Example 5.1. We let $\boldsymbol{v} = [1, 1, \ldots, 1]^T \in \mathbb{R}^{200}$ and $\boldsymbol{w} = [1/200, 1/200, \ldots, 1/200]^T \in \mathbb{R}^{200}$ so that $\boldsymbol{w}^T\boldsymbol{v} = 1$. The exact value of $F(A)$ is approximately $2.924 \cdot 10^{-4}$. Columns 2 and 3 of Table 2 show the difference between the exact value and the approximations determined by the standard Gauss and Gauss–Laurent rules for $i = 3$ and the same number of nodes, τ. It can be seen that the quadrature error for the Gauss–Laurent rules is the smallest for all values of τ. Column 4 of Table 2 displays the errors achieved with the anti-Gauss–Laurent rules. We observe that the errors of these quadrature rules are of opposite sign and of about the same magnitude as the error in the corresponding Gauss–Laurent rules. Similarly as above, this indicates that the average rules (5) are more accurate than the corresponding Gauss–Laurent and anti-Gauss–Laurent rules. $\square$

τ	$\boldsymbol{e}_1^T f(T)\boldsymbol{e}_1$	$\boldsymbol{e}_1^T f(H_{i=3})\boldsymbol{e}_1$	$\boldsymbol{e}_1^T f(\tilde{H}_{i=3})\boldsymbol{e}_1$
8	$-1.10 \cdot 10^{-3}$	$-1.78 \cdot 10^{-5}$	$1.75 \cdot 10^{-5}$
12	$-9.71 \cdot 10^{-5}$	$-4.61 \cdot 10^{-8}$	$4.36 \cdot 10^{-8}$
16	$-7.58 \cdot 10^{-6}$	$-1.19 \cdot 10^{-10}$	$1.14 \cdot 10^{-10}$

Table 2 Example 5.2: Errors for computed approximations of $F(A) = \boldsymbol{w}^T \ln(A)\boldsymbol{v}$ with A a nonsymmetric Toeplitz matrix.

Example 5.3. In this example, we approximate the value

$$F(A) := \boldsymbol{w}^T A^{-1/2}\boldsymbol{v},$$

where $A \in \mathbb{R}^{1000\times1000}$ is the nonsymmetric tridiagonal Toeplitz matrix $[-1, 2, 1]$. The vectors $\boldsymbol{v}$ and $\boldsymbol{w}$ have normally distributed random entries with zero mean; they are scaled so that $\boldsymbol{w}^T\boldsymbol{v} = 1$. The eigenvalues of A all have real part 2 and their imaginary parts are zeros of a Chebyshev polynomial of the first kind of degree 1000 for the interval $[-2, 2]$. The exact value $F(A)$ is approximately 0.6201. Columns 2 and 3 of Table 3 display the errors in approximations obtained by the standard Gauss and Gauss–Laurent rules for $i = 3$. We find that Gauss–Laurent rules give significantly smaller approximations errors than the standard Gauss rules. Columns 4 of Table 3 shows the Gauss–Laurent and anti-Gauss–Laurent rules to bracket the exact value. This implies that the average (5) will be quite accurate. $\square$

τ	$\boldsymbol{e}_1^T f(T)\boldsymbol{e}_1$	$\boldsymbol{e}_1^T f(H_{i=3})\boldsymbol{e}_1$	$\boldsymbol{e}_1^T f(\tilde{H}_{i=3})\boldsymbol{e}_1$
8	$1.22 \cdot 10^{-7}$	$3.17 \cdot 10^{-10}$	$-3.13 \cdot 10^{-10}$
12	$9.41 \cdot 10^{-11}$	$1.22 \cdot 10^{-15}$	$-1.99 \cdot 10^{-15}$

Table 3 Example 5.3: Errors for computed approximations of $F(A) = \boldsymbol{w}^T A^{-1/2}\boldsymbol{v}$ with A a nonsymmetric tridiagonal Toeplitz matrix.

Example 5.4. In this example, we determine approximations of the functional

$$F(A) := \boldsymbol{w}^T (A^5 + A^{-6})\boldsymbol{v},$$

where $A \in \mathbb{R}^{1000\times1000}$ is the same matrix as in Example 5.3, $\boldsymbol{v} = [1, 1, \ldots, 1]^T$, and $\boldsymbol{w} = [1, 0, \ldots, 0]^T$. Thus, $\boldsymbol{w}^T\boldsymbol{v} = 1$. The value of $F(A)$ is approximately $7.340 \cdot 10^1$. Columns 2 and 3 of Table 4 display the errors in approximations determine by the standard Gauss and Gauss–Laurent rules for $i = 3$. Column 4 of Table 4 shows the approximations determine anti-Gauss-Laurent rules and illustrates that Gauss–Laurent and anti-Gauss–Laurent rules bracket the exact value. $\square$

τ	$\boldsymbol{e}_1^T f(T)\boldsymbol{e}_1$	$\boldsymbol{e}_1^T f(H_{i=3})\boldsymbol{e}_1$	$\boldsymbol{e}_1^T f(\tilde{H}_{i=3})\boldsymbol{e}_1$
8	$1.60 \cdot 10^{-5}$	$5.77 \cdot 10^{-7}$	$-5.77 \cdot 10^{-7}$
12	$8.75 \cdot 10^{-8}$	$1.08 \cdot 10^{-11}$	$-1.09 \cdot 10^{-11}$

Table 4 Example 5.4: Errors for computed approximations of $F(A) = \boldsymbol{w}^T(A^5 + A^{-6})\boldsymbol{v}$ with A a nonsymmetric tridiagonal Toeplitz matrix.

Example 5.5. In our last example, we approximate the value

$$F(A) := \boldsymbol{w}^T \ln(A)\boldsymbol{v},$$

where $\boldsymbol{v} = [1, 1, \ldots, 1]^T$, $\boldsymbol{w} = [1, 0, \ldots, 0]^T$, and the matrix A is obtained by discretizing the differential operator $-\Delta + \rho_1 \frac{\partial}{\partial x} + \rho_2 \frac{\partial}{\partial y}$. Here Δ denotes the two-dimensional Laplacian, which is discretized on the unit square by the standard 5-point stencil on a uniform mesh with grid size $h = \frac{1}{41}$. The discretization error is $O(h^2)$ as $h \searrow 0$. The partial first derivatives are discretized by the standard symmetric 2-point stencil with discretization error $O(h^2)$. Dirichlet boundary conditions are imposed. The coefficients ρ_i are defined below. This gives a nonsymmetric matrix $A \in \mathbb{R}^{1600\times1600}$ that can be represented as follows

$$A := -\frac{1}{h^2}(I_{40} \otimes C_1 + C_2 \otimes I_{40}),$$

where $I_{40} \in \mathbb{R}^{40\times40}$ is the identity matrix and

$$C_i = \begin{bmatrix} -2 & 1-\rho_i\frac{h}{2} & 0 & \cdots & 0 \\ 1+\rho_i\frac{h}{2} & -2 & 1-\rho_i\frac{h}{2} & 0 & \vdots \\ 0 & \ddots & \ddots & \ddots & 0 \\ \vdots & & 1+\rho_i\frac{h}{2} & -2 & 1-\rho_i\frac{h}{2} \\ 0 & \cdots & 0 & 1+\rho_i\frac{h}{2} & -2 \end{bmatrix} \in \mathbb{R}^{40\times40}.$$

see, e.g., [22,28]. The convection coefficients ρ_i are chosen such that the Péclet numbers $Pe_i = \frac{\rho_i h}{2}$ are equal to $Pe_1 = 0.2$ and $Pe_2 = 0.1$, respectively. All eigenvalues of A are real and positive; the extreme eigenvalues are $\lambda_1 = 1.04 \cdot 10^2$ and $\lambda_{1600} = 1.33 \cdot 10^4$.

Table 5 displays the difference between the exact value, $F(A) \approx 8.019$, and some approximations determined by the standard Gauss and Gauss–Laurent quadrature rules for $i = 1, 2, 3$. Since $\tau = m(i + 1)$, only certain combinations of i and m give quadrature rules with τ nodes. The entrries '–' mark combinations of m and i that do not correspond to quadrature rules with τ nodes. We note that Gauss–Laurent rules give the most accurate approximations of $F(A)$. Furthermore, the results achieved with Gauss–Laurent rules are fairly insensitive to the choice of $i \geq 1$. Therefore, it might be beneficial to use a value of i larger than one and in this manner reduce the computational cost. The Tables 6, 7, and 8 show the Gauss–Laurent and associated anti-Gauss–Laurent quadrature rules to give errors of about the same magnitude and of opposite sign. $\square$

τ	$\boldsymbol{e}_1^T f(T)\boldsymbol{e}_1$	$\boldsymbol{e}_1^T f(H_{i=1})\boldsymbol{e}_1$	$\boldsymbol{e}_1^T f(H_{i=2})\boldsymbol{e}_1$	$\boldsymbol{e}_1^T f(H_{i=3})\boldsymbol{e}_1$
6	$-3.40 \cdot 10^{-3}$	–	$-4.47 \cdot 10^{-4}$	–
8	$-1.10 \cdot 10^{-3}$	$-1.84 \cdot 10^{-5}$	–	$-9.11 \cdot 10^{-5}$
12	$-1.56 \cdot 10^{-4}$	$-9.59 \cdot 10^{-8}$	$-3.40 \cdot 10^{-7}$	$-1.08 \cdot 10^{-6}$
15	$-4.16 \cdot 10^{-5}$	–	$-8.66 \cdot 10^{-9}$	–
16	$-2.72 \cdot 10^{-5}$	$-3.50 \cdot 10^{-10}$	–	$-1.33 \cdot 10^{-8}$

Table 5 Example 5.5: Errors for computed approximations of $F(A) = \boldsymbol{w}^T \ln(A)\boldsymbol{v}$ for $i = 1, 2, 3$ when A is a discretization of a differential operator.

τ	$\boldsymbol{e}_1^T f(H_{i=1})\boldsymbol{e}_1$	$\boldsymbol{e}_1^T f(\tilde{H}_{i=1})\boldsymbol{e}_1$
8	$-1.84 \cdot 10^{-5}$	$1.82 \cdot 10^{-5}$
12	$-9.59 \cdot 10^{-8}$	$9.55 \cdot 10^{-8}$
16	$-3.50 \cdot 10^{-10}$	$3.49 \cdot 10^{-10}$

Table 6 Example 5.5: Errors for computed approximations of $F(A) = \boldsymbol{w}^T \ln(A)\boldsymbol{v}$ for $i = 1$, when A is a discretization of a differential operator.

τ	$\boldsymbol{e}_1^T f(H_{i=2})\boldsymbol{e}_1$	$\boldsymbol{e}_1^T f(\tilde{H}_{i=2})\boldsymbol{e}_1$
6	$-4.47 \cdot 10^{-4}$	$4.42 \cdot 10^{-4}$
12	$-3.40 \cdot 10^{-7}$	$3.39 \cdot 10^{-7}$
15	$-8.66 \cdot 10^{-9}$	$8.67 \cdot 10^{-9}$

Table 7 Example 5.5: Errors for computed approximations of $F(A) = \boldsymbol{w}^T \ln(A)\boldsymbol{v}$ for $i = 2$, when A is a discretization of a differential operator.

τ	$\boldsymbol{e}_1^T f(H_{i=3})\boldsymbol{e}_1$	$\boldsymbol{e}_1^T f(\tilde{H}_{i=3})\boldsymbol{e}_1$
8	$-9.11 \cdot 10^{-5}$	$9.06 \cdot 10^{-5}$
12	$-1.08 \cdot 10^{-6}$	$1.08 \cdot 10^{-6}$
16	$-1.33 \cdot 10^{-8}$	$1.34 \cdot 10^{-8}$

Table 8 Example 5.5: Errors for computed approximations of $F(A) = \boldsymbol{w}^T \ln(A)\boldsymbol{v}$ for $i = 3$, when A is a discretization of a differential operator.

6 Conclusion

It is known that Gauss–Laurent quadrature rules associated with a real nonnegative measure with support on the real axis are determined by symmetric pentadiagonal matrices. This paper extends the methods described in [16] to complex-valued measures with support in the complex plane. We investigate the structure of the matrices for Gauss–Laurent and associated anti-Gauss–Laurent quadrature rules and discuss properties of these quadrature rules. Computed examples show that Gauss–Laurent rules may give higher accuracy than standard Gauss rules with the same number of nodes. Moreover, they illustrate that pairs of Gauss–Laurent and anti-Gauss–Laurent rules provide upper and lower bounds for certain matrix functionals.

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