RECURSION RELATIONS FOR THE EXTENDED KRYLOV SUBSPACE METHOD

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Abstract. The evaluation of matrix functions of the form $f(A)\boldsymbol{v}$, where A is a large sparse or structured symmetric matrix, f is a nonlinear function, and $\boldsymbol{v}$ is a vector, is frequently subdivided into two steps: first an orthonormal basis of an extended Krylov subspace of fairly small dimension is determined, and then a projection onto this subspace is evaluated by a method designed for small problems. This paper derives short recursion relations for orthonormal bases of extended Krylov subspaces of the type $\mathbb{K}^{m,mi+1}(A) = \text{span}\{A^{-m+1}\boldsymbol{v}, \ldots, A^{-1}\boldsymbol{v}, \boldsymbol{v}, A\boldsymbol{v}, \ldots, A^{mi}\boldsymbol{v}\}$, $m = 1, 2, 3, \ldots$, with i a positive integer, and describes applications to the evaluation of matrix functions and the computation of rational Gauss quadrature rules.

Key words. extended Krylov subspace, orthogonal Laurent polynomial, recursion relation, matrix function evaluation, rational Gauss quadrature

1. Introduction.

Many problems in applied mathematics require the computation of expressions of the form

$$\boldsymbol{w} := f(A)\boldsymbol{v}, \tag{1.1}$$

where $A \in \mathbb{R}^{n\times n}$ is a large, sparse or structured, symmetric matrix, f is a nonlinear function defined on the spectrum of A, and $\boldsymbol{v} \in \mathbb{R}^n$. We will for simplicity assume that $\|\boldsymbol{v}\| = 1$, where $\|\cdot\|$ denotes the Euclidean vector norm. Functions of interest in applications include

$$f(t) := \exp(t), \qquad f(t) := \sqrt{t}, \qquad f(t) := \ln(t);$$

see [1, 2, 4, 5, 7, 8, 9, 11, 12, 13, 14, 18, 19, 20, 27] for applications and discussions on numerical methods for the evaluation of (1.1).

For matrices A of small to moderate size, the expression (1.1) can be evaluated by using the spectral factorization of A. However, when A is large the computation of the spectral factorization is prohibitively expensive. One then often seeks to determine an approximation of (1.1) by first projecting A to a small symmetric matrix T_m, with $m \ll n$, and then evaluating $f(T_m)$, e.g., by determining the spectral or Cholesky factorizations of T_m. For instance, m steps of the (standard) Lanczos process applied to A with initial vector $\boldsymbol{v}$ yield the decomposition

$$AV_m = V_mT_m + \boldsymbol{g}_m\boldsymbol{e}_m^T, \tag{1.2}$$

where $V_m = [\boldsymbol{v}_1, \boldsymbol{v}_2, \ldots, \boldsymbol{v}_m] \in \mathbb{R}^{n\times m}$, $V_m^TV_m = I_m$, $\boldsymbol{v}_1 := \boldsymbol{v}$, $T_m := V_m^TAV_m \in \mathbb{R}^{m\times m}$ is symmetric and tridiagonal, $\boldsymbol{g}_m \in \mathbb{R}^n$, and $V_m^T\boldsymbol{g}_m = \boldsymbol{0}$. Here and below $\boldsymbol{e}_j = [0, \ldots, 0, 1, 0, \ldots, 0]^T$ denotes the jth axis vector and I_m the identity matrix of order m. We tacitly assume that m is chosen small enough so that a decomposition of the form (1.2) exists. The expression (1.1) can be approximated by

$$\boldsymbol{w}_m := V_mf(T_m)\boldsymbol{e}_1. \tag{1.3}$$

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Since the columns of V_m form an orthonormal basis for the Krylov subspace

$$\mathbb{K}^m(A, \boldsymbol{v}) = \text{span}\{\boldsymbol{v}, A\boldsymbol{v}, \ldots, A^{m-1}\boldsymbol{v}\}, \tag{1.4}$$

the expression (1.3) is a polynomial approximant of (1.1) of degree at most $m-1$; see, e.g., [4, 11, 14, 19, 20, 26] for discussions of this approach. In particular, if f is a polynomial of degree at most $m-1$, then $\boldsymbol{w}_m = \boldsymbol{w}$; see [11, 26] for proofs.

If f cannot be approximated accurately by a polynomial of degree $m-1$ on the spectrum of A, then, generally, the expression (1.3) is a poor approximation of (1.1). For this reason Druskin and Knizhnerman [12] proposed the Extended Krylov Subspace (EKS) method, which allows for the approximation of f by a rational function with a fixed pole, say at the origin.

Assume that A is nonsingular and consider the extended Krylov subspace

$$\mathbb{K}^{\ell,m}(A, \boldsymbol{v}) = \text{span}\{A^{-\ell+1}\boldsymbol{v}, \ldots, A^{-1}\boldsymbol{v}, \boldsymbol{v}, A\boldsymbol{v}, \ldots, A^{m-1}\boldsymbol{v}\}. \tag{1.5}$$

Thus, $\mathbb{K}^{1,m}(A, \boldsymbol{v}) = \mathbb{K}^m(A, \boldsymbol{v})$. Druskin and Knizhnerman [12] showed that projecting the problem (1.1) onto the subspace (1.5), instead of onto (1.4), can be attractive for many functions f. An algorithm for computing such approximations is presented in [12]. In this algorithm ℓ is prespecified, but m can be increased until an analog of the expression (1.3) for the extended Krylov subspace (1.5) gives a sufficiently accurate approximation of (1.1).

Njåstad and Thron [24] showed that orthonormal bases for the sequence of nested rational Krylov subspaces

$$\mathbb{K}^{1,1}(A, \boldsymbol{v}) \subset \mathbb{K}^{2,2}(A, \boldsymbol{v}) \subset \ldots \subset \mathbb{K}^{m,m}(A, \boldsymbol{v}) \subset \ldots \subset \mathbb{R}^n \tag{1.6}$$

satisfy a short recursion relation, i.e., the number of terms of the recursion relation is bounded independently of m. Their derivation uses properties of orthogonal Laurent polynomials. A survey of this and related results is provided by Jones and Njåstad [21]. Recently, Simoncini [28] derived the recursion with linear algebra techniques. Error bounds for rational approximants are discussed in [4, 12, 13, 22].

An extension of the recursion relation discussed by Njåstad and Thron [24] to the sequence of rational Krylov subspaces

$$\mathbb{K}^{1,2}(A, \boldsymbol{v}) \subset \mathbb{K}^{2,4}(A, \boldsymbol{v}) \subset \ldots \subset \mathbb{K}^{m,2m}(A, \boldsymbol{v}) \subset \mathbb{R}^n \tag{1.7}$$

is described in [20], where we also mentioned our interest in ratios other than 2 of numerator and denominator degrees. It is the purpose of the present paper to describe recursion relations for orthonormal Laurent polynomial bases in the latter situation. Specifically, we consider sequences of nested rational Krylov subspaces of the form

$$\mathbb{K}^{1,i+1}(A, \boldsymbol{v}) \subset \mathbb{K}^{2,2i+1}(A, \boldsymbol{v}) \subset \ldots \subset \mathbb{K}^{m,mi+1}(A, \boldsymbol{v}) \subset \mathbb{R}^n, \tag{1.8}$$

where i is a positive integer. These spaces are of interest when the evaluation of $A^{-1}\boldsymbol{w}$ for vectors $\boldsymbol{w} \in \mathbb{R}^n$ is more cumbersome than the computation of $A\boldsymbol{w}$. This often is the case when $A^{-1}\boldsymbol{w}$ is computed by using a triangular factorization of A.

We apply the recursion relations to the computation of rational approximants of expressions (1.1). The error in the computed approximants depends on the value of $i \geq 1$. For some functions f, the choice $i > 1$ gives a smaller error than $i = 1$ for rational Krylov subspaces of the same dimension. This is illustrated in Section 5. We also discuss the computation of rational Gauss quadrature rules.

A different derivation of the recursion formulas in [20] and in the present paper recently has been provided by Díaz-Mendoza et al. [10], who do not require a sequence of the form (1.8) be used. Our linear algebra-based derivation also can be applied in this situation. However, this generality destroys the block-structure of the projection of A onto the rational Krylov subspace (1.8) and therefore is not pursued.

This paper is organized as follows. Section 2 discusses the recursions when A is symmetric positive definite. In Section 3, we are concerned with recursion relations when A is indefinite. Application to rational Gauss quadrature is described in Section 4, and Section 5 presents a few computed examples. Concluding remarks can be found in Section 6.

Many results on orthogonal rational functions can be found in the nice book by Bultheel et al. [6]. The possibly first application of rational Krylov subspaces reported in the literature is to eigenvalue problems; see Ruhe [25]. The extended Krylov subspace method of the present paper also can be applied in this context.

2. Recursions for positive definite matrices. We will use orthogonal Laurent polynomials to generate an orthonormal basis for the sequence of Krylov subspaces (1.8) corresponding to the ordering

$$\boldsymbol{v}, A\boldsymbol{v}, A^2\boldsymbol{v}, \ldots A^i\boldsymbol{v}, A^{-1}\boldsymbol{v}, A^{i+1}\boldsymbol{v}, \ldots, A^{2i}\boldsymbol{v}, A^{-2}\boldsymbol{v}, A^{2i+1}\boldsymbol{v}, \ldots \; .$$

Introduce the space of Laurent polynomials of denominator degree at most j and numerator degree at most k,

$$\mathcal{L}_{j,k} := \text{span}\{x^{-j}, x^{-j+1}, \ldots, 1, \ldots, x^{k-1}, x^k\}, \qquad x \in \mathbb{R}\backslash\{0\}.$$

Given Laurent polynomials $q,\ r \in \mathcal{L}_{j,k}$ and a symmetric positive definite matrix $A \in \mathbb{R}^{n\times n}$, we define the inner product on $\mathcal{L}_{j,k}$,

$$(q, r) := (q(A)\boldsymbol{v})^T(r(A)\boldsymbol{v}), \tag{2.1}$$

where we assume j and k to be sufficiently small so that (2.1) indeed is an inner product. Substituting the spectral decomposition of A into (2.1) shows that

$$(q, r) = \int q(x)r(x)d\mu(x) \tag{2.2}$$

for a nonnegative measure $d\mu$ on the real axis. The corresponding distribution function μ can be chosen to be piecewise constant on $\mathbb{R}$ with jumps at the eigenvalues of A.

Associated with the inner product (2.1), there is a sequence of monic orthogonal Laurent polynomials $\phi_0, \phi_1, \ldots, \phi_i, \phi_{-1}, \phi_{i+1}, \ldots, \phi_{2i}, \phi_{-2}, \ldots$ of the form

$$\phi_j(x) := \begin{cases} x^j + \displaystyle\sum_{k=-\lfloor (j-1)/i \rfloor}^{j-1} c_{j,k}x^k, & j = 1, 2, 3, \ldots\; , \\ x^j + \displaystyle\sum_{k=j+1}^{-ij} c_{j,k}x^k, & j = -1, -2, -3, \ldots\; . \end{cases}$$

with $\phi_0(x) := 1$. Thus,

$$(\phi_j, \phi_k) = 0, \qquad j \neq k. \tag{2.3}$$

Note that generating an orthogonal basis for $\mathcal{L}_{m-1,im}$ is equivalent to finding an orthogonal basis for the extended Krylov subspace $\mathbb{K}^{m,im+1}(A)$.

Suppose that an orthogonal basis

$$\{\phi_0, \phi_1, \ldots, \phi_i, \phi_{-1}, \phi_{i+1}, \ldots, \phi_{2i}, \phi_{-2}, \phi_{2i+1}, \ldots, \phi_{im}\} \tag{2.4}$$

for $\mathcal{L}_{m-1,im}$ is available. We describe how this basis can be complemented to yield orthogonal bases for the spaces $\mathcal{L}_{m,im+j}$, $j = 0, 1, \ldots, i$, starting with $j = 0$.

2.1. Computation of ϕ_{-m}. The evaluation of ϕ_{-m} corresponds to determining an orthogonal basis of $\mathcal{L}_{m,im}$. Consider the polynomial

$$c_{im,-m+1}\phi_{-m}(x) - x^{-1}\phi_{im}(x) \in \mathcal{L}_{m-1,im}. \tag{2.5}$$

The trailing coefficient, $c_{im,-m+1}$, of ϕ_{im} is nonvanishing by the properties of the inner product (2.1). Therefore

$$c_{im,-m+1}\phi_{-m}(x) - x^{-1}\phi_{im}(x) = -\sum_{k=-m+1}^{im} \gamma_{im,k}\phi_k(x),$$

where the Fourier coefficients are given by

$$\gamma_{im,k} = \frac{(x^{-1}\phi_{im}, \phi_k)}{(\phi_k, \phi_k)} = \frac{(\phi_{im}, x^{-1}\phi_k)}{(\phi_k, \phi_k)}. \tag{2.6}$$

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

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

it follows that the only nonvanishing Fourier coefficients are associated with the previous block of $i+1$ Laurent polynomials, $\phi_{-m+1}, \ldots, \phi_{im}$. We therefore obtain

$$\begin{aligned} c_{im,-m+1}\phi_{-m}(x) = x^{-1}\phi_{im}(x) &- \gamma_{im,im}\phi_{im}(x) - \gamma_{im,im-1}\phi_{im-1}(x) - \ldots \\ &- \gamma_{im,i(m-1)+1}\phi_{i(m-1)+1}(x) - \gamma_{im,-m+1}\phi_{-m+1}(x). \end{aligned} \tag{2.7}$$

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

$$\begin{aligned} \delta_{-m}\boldsymbol{v}_{-m} = (A^{-1} - \beta_{im,im}I_n)\boldsymbol{v}_{im} &- \beta_{im,im-1}\boldsymbol{v}_{im-1} - \ldots \\ &- \beta_{im,i(m-1)+1}\boldsymbol{v}_{i(m-1)+1} - \beta_{im,-m+1}\boldsymbol{v}_{-m+1} \end{aligned} \tag{2.8}$$

with $\beta_{j,k} := \boldsymbol{v}_j^T A^{-1}\boldsymbol{v}_k$.

2.2. Computation of ϕ_{im+1}. We determine a basis for $\mathcal{L}_{m,im+j}$ for $j = 1$. Regard

$$c_{-m,im}\phi_{im+1}(x) - x\phi_{-m}(x) \in \mathcal{L}_{m,im}. \tag{2.9}$$

Analogously to the case $j = 0$, we express (2.9) in terms of its Fourier expansion with Fourier coefficients

$$\gamma_{-m,k} = \frac{(\phi_{-m}, x\phi_k)}{(\phi_k, \phi_k)}, \qquad k = -m, \ldots, im.$$

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

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

Therefore ϕ_{im+1} satisfies

$$c_{-m,im}\phi_{im+1}(x) = x\phi_{-m}(x) - \gamma_{-m,-m}\phi_{-m}(x) - \gamma_{-m,im}\phi_{im}(x).$$

This yields the three-term recursion formula

$$\delta_{im+1}\boldsymbol{v}_{im+1} = (A - \alpha_{-m,-m}I_n)\boldsymbol{v}_{-m} - \alpha_{-m,im}\boldsymbol{v}_{im} \tag{2.10}$$

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

2.3. Computation of ϕ_{im+2}. We would like to determine a basis for $\mathcal{L}_{m,im+2}$. Therefore consider the function

$$\phi_{im+2}(x) - x\phi_{im+1}(x) \in \mathcal{L}_{m,im+1}. \tag{2.11}$$

Its Fourier expansion has the coefficients

$$\gamma_{im+1,k} = \frac{(\phi_{im+1}, x\phi_k)}{(\phi_k, \phi_k)}, \qquad k = -m, \ldots, im+1.$$

However, $\phi_{im+1} \perp \mathcal{L}_{m,im}$ and

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

It follows that ϕ_{im+2} satisfies

$$\begin{aligned} \phi_{im+2}(x) &= x\phi_{im+1}(x) - \gamma_{im+1,im+1}\phi_{im+1}(x) \\ &\quad -\gamma_{im+1,-m}\phi_{-m}(x) - \gamma_{im+1,im}\phi_{im}(x), \end{aligned}$$

which yields the four-term recursion formula

$$\begin{aligned} \delta_{im+2}\boldsymbol{v}_{im+2} &= (A - \alpha_{im+1,im+1}I_n)\boldsymbol{v}_{im+1} \\ &\quad -\alpha_{im+1,-m}\boldsymbol{v}_{-m} - \alpha_{im+1,im}\boldsymbol{v}_{im}. \end{aligned} \tag{2.12}$$

2.4. Computation of ϕ_{im+j} for $j = 3, 4, \ldots i$. We determine the remaining orthogonal basis elements for the spaces $\mathcal{L}_{m,im+j}$ for $3 \leq j \leq i$. They can be computed with the aid of the standard Lanczos recursions. We have

$$\begin{aligned} \delta_{im+j}\boldsymbol{v}_{im+j} &= (A - \alpha_{im+j-1,im+j-1}I_n)\boldsymbol{v}_{im+j-1} \\ &\quad -\alpha_{im+j-1,im+j-2}\boldsymbol{v}_{im+j-2}. \end{aligned} \tag{2.13}$$

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

2.5. Algorithm and orthogonal projection. The following algorithm summarizes the computation of the orthogonal basis for $\mathcal{L}_{m-1,im}$. The structure of the projected problem is discussed below.

ALGORITHM 2.1 (Orthogonalization process for $\mathbb{K}^{m,im+1}(A, \boldsymbol{v})$).
Input: *m, i, $\boldsymbol{v}$, functions for evaluating matrix-vector products and solving linear systems of equations with A;*
Output: *orthogonal basis $\{\boldsymbol{v}_k\}_{k=-m}^{im+1}$ of $\mathbb{K}^{m+1,im+1}(A, \boldsymbol{v})$;*
$\boldsymbol{v}_{-1} := \boldsymbol{0}$;

$\delta_0 := ||\boldsymbol{v}||$; $\boldsymbol{v}_0 := \boldsymbol{v}/\delta_0$;
for $k = 0, 1, \ldots, m-1$ **do**
  $\boldsymbol{u} := A\boldsymbol{v}_{-k}$;
  $\alpha_{-k,ik} := \boldsymbol{v}_{ik}^T\boldsymbol{u}$; $\boldsymbol{u} := \boldsymbol{u} - \alpha_{-k,ik}\boldsymbol{v}_{ik}$;
  $\alpha_{-k,-k} := \boldsymbol{v}_{-k}^T\boldsymbol{u}$; $\boldsymbol{u} := \boldsymbol{u} - \alpha_{-k,-k}\boldsymbol{v}_{-k}$;
  $\delta_{ik+1} := ||\boldsymbol{u}||$; $\boldsymbol{v}_{ik+1} := \boldsymbol{u}/\delta_{ik+1}$;
  $\boldsymbol{u} := A\boldsymbol{v}_{ik+1}$;
  $\alpha_{ik+1,ik} := \boldsymbol{v}_{ik}^T\boldsymbol{u}$; $\boldsymbol{u} := \boldsymbol{u} - \alpha_{2k+1,ik}\boldsymbol{v}_{ik}$;
  $\alpha_{ik+1,-k} := \boldsymbol{v}_{-k}^T\boldsymbol{u}$; $\boldsymbol{u} := \boldsymbol{u} - \alpha_{ik+1,-k}\boldsymbol{v}_{-k}$;
  $\alpha_{ik+1,ik+1} := \boldsymbol{v}_{ik+1}^T\boldsymbol{u}$; $\boldsymbol{u} := \boldsymbol{u} - \alpha_{ik+1,ik+1}\boldsymbol{v}_{ik+1}$;
  $\delta_{ik+2} := ||\boldsymbol{u}||$; $\boldsymbol{v}_{ik+2} := \boldsymbol{u}/\delta_{ik+2}$;
  for $j = 3, \ldots, i$ **do**
    $\boldsymbol{u} := A\boldsymbol{v}_{ik+j-1}$;
    $\alpha_{ik+j-1,ik+j-2} := \boldsymbol{v}_{ik+j-2}^T\boldsymbol{u}$; $\boldsymbol{u} := \boldsymbol{u} - \alpha_{ik+j-1,ik+j-2}\boldsymbol{v}_{ik+j-2}$;
    $\alpha_{ik+j-1,ik+j-1} := \boldsymbol{v}_{ik+j-1}^T\boldsymbol{u}$; $\boldsymbol{u} := \boldsymbol{u} - \alpha_{ik+j-1,ik+j-1}\boldsymbol{v}_{ik+j-1}$;
    $\delta_{ik+j} := \|\boldsymbol{u}\|$; $\boldsymbol{v}_{ik+j} := \boldsymbol{u}/\delta_{ik+j}$;
  end
  $\boldsymbol{w} := A^{-1}\boldsymbol{v}_{i(k+1)}$;
  $\beta_{i(k+1),-k} := \boldsymbol{v}_{-k}^T\boldsymbol{w}$; $\boldsymbol{w} := \boldsymbol{w} - \beta_{i(k+1),-k}\boldsymbol{v}_{-k}$;
  for $j = 0, \ldots, i-1$ **do**
    $\beta_{i(k+1),i(k+1)-j} := \boldsymbol{v}_{i(k+1)-j}^T\boldsymbol{w}$; $\boldsymbol{w} := \boldsymbol{w} - \beta_{i(k+1),i(k+1)-j}\boldsymbol{v}_{i(k+1)-j}$;
  end
  $\delta_{-(k+1)} := ||\boldsymbol{w}||$; $\boldsymbol{v}_{-(k+1)} := \boldsymbol{w}/\delta_{-(k+1)}$;
end

Given the orthonormal basis for the subspace $\mathbb{K}^{m,im+1}(A, \boldsymbol{v})$, we define the matrix

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

Equations (2.8), (2.10), (2.12), and (2.13) can be used to construct a matrix $H_{m(i+1)} = [h_{j,k}] \in \mathbb{R}^{m(i+1)\times m(i+1)}$, such that

$$AV_{m(i+1)} = V_{m(i+1)}H_{m(i+1)} + \boldsymbol{z}_{m(i+1)}\boldsymbol{e}_{m(i+1)}^T, \tag{2.14}$$

where

$$\boldsymbol{z}_{m(i+1)} = h_{m(i+1)+1,m(i+1)}\boldsymbol{v}_{-m} + h_{m(i+1)+2,m(i+1)}\boldsymbol{v}_{im+1}$$

and $H_{m(i+1)}$ satisfies

$$H_{m(i+1)} = V_{m(i+1)}^T AV_{m(i+1)}. \tag{2.15}$$

This matrix is analogous to the matrix T_m in the standard Lanczos decomposition (1.2). It is pentadiagonal and its non-zero entries can be determined column-wise for the columns $(i+1)k+1+j$, $0 \le j \le i$, $1 \le k \le m-1$. We examine the columns corresponding to different values of j.

2.5.1. The case $j = 1$. The column of $AV_{m(i+1)+1}$ in this case corresponds to $A\boldsymbol{v}_{-k}$. Equation (2.10) yields

$$A\boldsymbol{v}_{-k} = \alpha_{-k,ik}\boldsymbol{v}_{ik} + \alpha_{-k,-k}\boldsymbol{v}_{-k} + \delta_{ik+1}\boldsymbol{v}_{ik+1}.$$

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

$$h_{(i+1)k,(i+1)k+1} = \alpha_{-k,ik}, \qquad h_{(i+1)k+1,(i+1)k+1} = \alpha_{-k,-k},$$
$$h_{(i+1)k+2,(i+1)k+1} = \delta_{ik+1}.$$

2.5.2. The case $j = 2$. The column of $AV_{m(i+1)+1}$ in this case corresponds to $A\boldsymbol{v}_{ik+1}$. Equation (2.12) yields

$$A\boldsymbol{v}_{ik+1} = \alpha_{ik+1,ik}\boldsymbol{v}_{ik} + \alpha_{ik+1,-k}\boldsymbol{v}_{-k} + \alpha_{ik+1,ik+1}\boldsymbol{v}_{ik+1} + \delta_{ik+2}\boldsymbol{v}_{ik+2}.$$

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

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

2.5.3. The cases $j = 3, 4, \ldots, i$. The columns of $AV_{m(i+1)+1}$ in these cases correspond to $A\boldsymbol{v}_{ik+j-1}$. Equation (2.13) yields

$$A\boldsymbol{v}_{ik+j-1} = \alpha_{ik+j-1,ik+j-2}\boldsymbol{v}_{ik+j-2} + \alpha_{ik+j-1,ik+j-1}\boldsymbol{v}_{ik+j-1} + \delta_{ik+j}\boldsymbol{v}_{ik+j}.$$

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

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

2.5.4. The case $j = 0$. The $((i+1)k)^{\text{th}}$ column of $AV_{m(i+1)+1}$ corresponds to $A\boldsymbol{v}_{ik}$. In order to obtain an expression for $A\boldsymbol{v}_{ik}$, it is necessary to multiply (2.8) by A and make the appropriate substitutions for $A\boldsymbol{v}_{-m+1}, A\boldsymbol{v}_{i(m-1)+1}, \ldots, A\boldsymbol{v}_{im}, A\boldsymbol{v}_{-m}$. Simplification of the expression results from the facts that i) $\beta_{ik,ik} \neq 0$ by the properties of the inner product (2.1) and the positive definiteness of A, and ii) $\boldsymbol{v}_{ik}^T A\boldsymbol{v}_r = 0,\ r = -k+1, \ldots, 0, \ldots, ik-2$. Combining these properties yields

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

Symmetry immediately gives that

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

Finally, some arithmetic and the orthonormality of the vectors yield the diagonal element

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

Example 2.1. Let $m = 3$ and $i = 3$. Then the matrix H_{13} is of the form

$$\begin{bmatrix}
\alpha_{0,0} & \delta_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\delta_1 & \alpha_{1,1} & \delta_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & \delta_2 & \alpha_{2,2} & \delta_3 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & \delta_3 & h_{4,4} & \alpha_{-1,3} & \alpha_{4,3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \alpha_{-1,3} & \alpha_{-1,-1} & \delta_4 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \alpha_{4,3} & \delta_4 & \alpha_{4,4} & \delta_5 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & \delta_5 & \alpha_{5,5} & \delta_6 & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \delta_6 & h_{8,8} & \alpha_{-2,6} & \alpha_{7,6} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha_{-2,6} & \alpha_{-2,-2} & \delta_7 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha_{7,6} & \delta_7 & \alpha_{7,7} & \delta_8 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \delta_8 & \alpha_{8,8} & \delta_9 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \delta_9 & h_{12,12} & \alpha_{-3,9} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \alpha_{-3,9} & \alpha_{-3,-3}
\end{bmatrix}.$$

□

3. Recursions for indefinite matrices. The recursion formulas derived in Section 2 assume that A is definite. This assumption is not necessary, however, to the derivation of the recursion formulas presented in Sections 2.3 and 2.4. The only assumption necessary in these cases is that the vectors in the definition (1.5) of $\mathbb{K}^{m+1,im+1+j}(A, \boldsymbol{v})$, $j = 2, 3, \ldots, i$, remain independent. This assures that the positive degree of ϕ_{im+j} and the negative degree of ϕ_{-m} are $im + j$ and m, respectively.

The recursion formulas (2.8) and (2.10) presented in Sections 2.1 and 2.2 are derived under the assumption that the trailing coefficient, $c_{im,-m+1}$, of ϕ_{im} and the leading coefficient, $c_{-m,im}$, of ϕ_{-m} are nonvanishing. These conditions may not be satisfied for every value of m if A is indefinite. The indefinite case for $\ell = m$ is treated in [20], where it is explained that if the trailing or leading coefficient vanishes for some value m, then it is necessary to replace the three-term recursion formula with a five-term formula in this particular step. The situation is analogous when $\ell/m > 1$, but computionally unwieldy for the case $c_{im,-m+1} = 0$. This case and the case $c_{-m,im} = 0$ are discussed separately below. Example 5.3 in Section 5 illustrates the formulas of Section 2 applied to an indefinite matrix when a breakdown does not occur.

3.1. The case $c_{-m,im} = 0$. Assume that for some $m \geq 1$ the recursion formulas of Section 3 have been used to compute

$$\phi_0, \phi_1, \ldots, \phi_i, \phi_{-1}, \phi_{i+1}, \ldots, \phi_{2i}, \phi_{-2}, \phi_{2i+1}, \ldots, \phi_{im}, \phi_{-m},$$

and that the leading coefficient, $c_{-m,im}$, of ϕ_{-m} vanishes. Thus,

$$\phi_{-m}(x) = x^{-m} + c_{-m,im-2}x^{im-2} + \ldots + c_{-m,im-1}x^{im-1}.$$

Analogously to (2.7), we have

$$\begin{aligned}(3.1)\quad c_{im,-m+1}\phi_{-m}(x) = x^{-1}\phi_{im}(x) - \gamma_{im,im}\phi_{im}(x) - \gamma_{im,im-1}\phi_{im-1}(x) - \ldots \\ -\gamma_{im,i(m-1)+1}\phi_{i(m-1)+1}(x) - \gamma_{im,-m+1}\phi_{-m+1}(x),\end{aligned}$$

where the Fourier coefficients are given by (2.6), and

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

Comparing coefficients for the x^{im}-terms in the right-hand side and left-hand side of (3.1) shows that $\gamma_{im,im} = 0$. This is equivalent to $(x^{-1}\phi_{im}, \phi_{im}) = 0$; cf. (2.6).

Let $\psi \in \mathcal{L}_{m-1,im-1}$. Then

$$0 = (x^{-1}\phi_{im}, \phi_{im}) = (\phi_{im}, c_{im,-m+1}x^{-m} + \psi) = c_{im,-m+1}(\phi_{im}, x^{-m}).$$

Since $c_{im,-m+1} \neq 0$, we must have $(\phi_{im}, x^{-m}) = 0$. This condition implies that all the Fourier coefficients in (3.1) vanish and, therefore, the computation of ϕ_{-m} simplifies to

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

Correspondingly, using the relation (2.9), the computation of ϕ_{im+1} is most appropriately modified to

$$\phi_{im+1}(x) - x\phi_{im}(x) \in \mathcal{L}_{m,im}$$

along with a modification of the Fourier coefficients

$$\hat{\gamma}_{-m,k} = \frac{(\phi_{im}, x\phi_k)}{(\phi_k, \phi_k)}, \qquad k = -m, \ldots, im.$$

An argument similar to that of Section 2.2 shows that ϕ_{im+1} now satisfies a four-term recursion formula,

$$\begin{aligned}\phi_{im+1}(x) &= x\phi_{im}(x) - \hat{\gamma}_{-m,-m}\phi_{-m}(x) \\ &\quad - \hat{\gamma}_{-m,im}\phi_{im}(x) - \hat{\gamma}_{-m,im-1}\phi_{im-1}(x).\end{aligned}$$

The recursion formula (2.10), as well as the matrix $H_{m(i+1)+1}$, can be adjusted in a manner analogous to the modification for the indeterminate case described in [20].

3.2. The case $c_{im,-m+1} = 0$. The computation of ϕ_{-m} in Section 2.1 requires that $c_{im,-m+1} \neq 0$, cf. (2.5); that is, it is required that the trailing coefficient in

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

is nonvanishing. If this coefficient does vanish, then ϕ_{im} is deficient in the x^{-m+1} term and the expression (2.5) used to compute ϕ_{-m} must be modified. Further, the only indication of this deficiency in terms of the computed coefficients is that $(\phi_{im}, x^{-1}\phi_{im}) = 0$, a quantity that appears in the evaluation of ϕ_{-m} as expressed in (2.7). This is different from the situation when $c_{-m,im} = 0$ considered in Section 3.1, in which an indicator occurs in the evaluation of the previous vector.

If the trailing coefficient, $c_{im-1,-m+1}$, in

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

does not vanish, then the combination

$$c_{im-1,-m+1}\phi_{-m}(x) - x^{-1}\phi_{im-1}(x) \in \mathcal{L}_{m,im}$$

can be used to compute ϕ_{-m}. However, there is no guarantee that $c_{im-j,-m+1}$ does not vanish; that is, that $(\phi_{im-j}, x^{-1}\phi_{im-j}) \neq 0$, for any $j = 0, 1, \ldots, i-1$.

Under the assumption of linear independence of the extended Krylov vectors, ϕ_{-m} always can be computed from

$$\phi_{-m}(x) - x^{-1}\phi_{-m+1}(x) \in \mathcal{L}_{m,im}.$$

This is analogous to the case for $\ell = m$ presented in [20]. However, the quantities

$$(\phi_{-m+1}, x^{-1}\phi_j),$$

which appear in the computation of the Fourier coefficients, do not necessarily vanish for $j = -m+2, -m+1$ and for $j = i(m+2)+1, i(m+2)+2, \ldots, im$. Therefore the recursion formula that results has $2i+3$ terms. Even though ϕ_{-m+1} exists in the deficient case, an algorithm that accounts for this possibility is unwieldy for $i > 1$. We remark that an algorithm for the indefinite case when $i = 1$ ($\ell = m$) is presented in [20].

4. Application to rational Gauss quadrature. We first consider standard Gauss quadrature rules for the approximation of integrals

$$\mathcal{I}f := \int f(x)d\mu(x), \tag{4.1}$$

where $d\mu$ is the measure in (2.2) and the integrand f is assumed to be defined on the convex hull of the support of $d\mu$. Our approach to introduce Gauss rules follows Golub and Meurant [16], and generalizes to rational Gauss quadrature rules. It is convenient to express the integral (4.1) in the form

$$\mathcal{I}f = \boldsymbol{v}^T f(A)\boldsymbol{v}. \tag{4.2}$$

The following connection between the (standard) Lanczos decomposition (1.2) and the m-point Gauss quadrature rule for (4.1) is well known; see, e.g., Golub and Meurant [16]. We present a simple proof, which we subsequently generalize to rational Gauss rules.

THEOREM 4.1. *(Gauss quadrature) Let T_m be the symmetric tridiagonal matrix in the standard Lanczos decomposition (1.2). Then*

$$\mathcal{I}f = \boldsymbol{e}_1^T f(T_m)\boldsymbol{e}_1 \qquad \forall f \in \mathcal{L}_{0,2m-1}. \tag{4.3}$$

Thus, the right-hand side is an m-point Gauss quadrature rule for approximating the integral (4.1).

Proof. Let the matrices V_m and T_m be those of the standard Lanczos decomposition (1.2). The following equality can be established,

$$p(A)\boldsymbol{v} = V_m p(T_m)\boldsymbol{e}_1 \qquad \forall p \in \mathcal{L}_{0,m-1}, \tag{4.4}$$

by letting $p(t) := t^j$ for increasing $j \geq 0$; see, e.g., [11, 26] for details. Moreover,

$$A^m\boldsymbol{v} = AA^{m-1}\boldsymbol{v} = AV_m T_m^{m-1}\boldsymbol{e}_1 = V_m T_m^m \boldsymbol{e}_1 + \boldsymbol{g}_m\, \boldsymbol{e}_m^T T_m^{m-1}\boldsymbol{e}_1.$$

Therefore,

$$V_m^T q(A)\boldsymbol{v} = q(T_m)\boldsymbol{e}_1 \qquad \forall q \in \mathcal{L}_{0,m}.$$

Combining this with (4.4) yields

$$\boldsymbol{v}^T p(A)q(A)\boldsymbol{v} = \boldsymbol{e}_1^T p(T_m)q(T_m)\boldsymbol{e}_1 \qquad \forall p \in \mathcal{L}_{0,m-1}, \quad q \in \mathcal{L}_{0,m}.$$

This establishes (4.3). ∎

Substitution of the spectral decomposition of T_m into the right-hand side of (4.3) yields the "standard" representation of the Gauss rule in terms of its nodes and weights.

We turn to rational Gauss quadrature rules that are exact for certain Laurent polynomials. Rational Gauss rules were first considered by Gonchar and López Lagomasino [17], and have subsequently received considerable attention; see, e.g., Gautschi [15] for a recent discussion and references. An application of rational Gauss rules to the computation of upper and lower bounds for certain matrix functionals is described in [23].

We consider the case $i = 1$ in (1.8) and let the number of nodes be even. The analogue of the standard Lanczos decomposition are the two decompositions,

$$AV_{2m} = V_{2m}H_{2m} + \boldsymbol{z}_{2m}\boldsymbol{e}_{2m}^T, \tag{4.5}$$
$$A^{-1}V_{2m} = V_{2m}G_{2m} + \boldsymbol{v}_{-m}[g_{2m+1,2m-1}\boldsymbol{e}_{2m-1} + g_{2m+1,2m}\boldsymbol{e}_{2m}]^T, \tag{4.6}$$

where the columns of $V_{2m} \in \mathbb{R}^{n\times(2m)}$ form an orthonormal basis for $\mathbb{K}^{m,m+1}(A, \boldsymbol{v})$, the vectors $\boldsymbol{z}_{2m}, \boldsymbol{v}_{-m} \in \mathbb{R}^n$ are orthogonal to these columns, and $\boldsymbol{v} = V_{2m}\boldsymbol{e}_1$. The matrices $H_{2m}, G_{2m} \in \mathbb{R}^{(2m)\times(2m)}$ are symmetric block tridiagonal with 2×2 blocks; see [20] for details. The following example illustrates the structure of the subdiagonal blocks.

Example 4.1. The matrices H_{2m} and G_{2m} in the decompositions (4.5) and (4.6) may have nonzero entries at the positions marked by "$*$". The illustrations are for $m = 4$.

$$G_8 = \begin{bmatrix} * & * & * & & & & & \\ * & * & * & & & & & \\ * & * & * & * & * & & & \\ & & * & * & * & & & \\ & & * & * & * & * & * & \\ & & & & * & * & * & \\ & & & & * & * & * & * \\ & & & & & & * & * \end{bmatrix}, \qquad H_8 = \begin{bmatrix} * & * & & & & & & \\ * & * & * & * & & & & \\ & * & * & * & & & & \\ & * & * & * & * & * & & \\ & & & * & * & * & & \\ & & & * & * & * & * & * \\ & & & & & * & * & * \\ & & & & & * & * & * \end{bmatrix}.$$

The structure of the matrices H_k and G_k is shown in [20] for arbitrary sizes k. □

We would like to establish that

$$\boldsymbol{v}^T f(A)\boldsymbol{v} = \boldsymbol{e}_1^T f(H_{2m})\boldsymbol{e}_1 \qquad \forall f \in \mathcal{L}_{2m-2,2m+1}. \tag{4.7}$$

Substituting the spectral decomposition of H_{2m} into $\boldsymbol{e}_1^T f(H_{2m})\boldsymbol{e}_1$ shows that this expression can be considered a quadrature rule with $2m$ nodes for evaluating the left-hand side of (4.7). In view of (4.2), the latter equals (4.1). Since $\dim(\mathcal{L}_{2m-2,2m+1}) = 4m$, the property (4.7) would make the right-hand side a rational Gauss rule for the approximation of (4.1). A "standard" representation of this rule in terms of its nodes and weights can be obtained by replacing the matrix H_{2m} by its spectral decomposition. Thus, the nodes are the eigenvalues of H_{2m} and the weights are the square of the first component of normalized eigenvectors.

We will show (4.7) by first establishing some auxiliary results. It is convenient to require the matrix A to be definite. This secures the existence of the rational Gauss rule.

LEMMA 4.2. *Let H_{2m}, G_{2m}, and V_{2m} be the matrices in (4.5) and (4.6). Let $\boldsymbol{v} = V_{2m}\boldsymbol{e}_1$. Then*

$$\boldsymbol{v}^T A^j \boldsymbol{v} = \boldsymbol{e}_1^T H_{2m}^j \boldsymbol{e}_1, \qquad j = 0, 1, \ldots, 2m+1, \tag{4.8}$$

$$\boldsymbol{v}^T A^{-j} \boldsymbol{v} = \boldsymbol{e}_1^T G_{2m}^j \boldsymbol{e}_1, \qquad j = 0, 1, \ldots, 2m-1. \tag{4.9}$$

Proof. We first consider (4.8). The relation (4.5) and the structure of H_{2m}, illustrated in Example 4.1 and shown in [20], yield

$$A^j \boldsymbol{v} = V_{2m} H_{2m}^j \boldsymbol{e}_1, \qquad j = 0, 1, \ldots, m.$$

Moreover,

$$A^{m+1}\boldsymbol{v} = V_{2m} H_{2m}^{m+1} \boldsymbol{e}_1 + \boldsymbol{z}_{2m} \boldsymbol{e}_{2m}^T H_{2m}^m \boldsymbol{e}_1.$$

Combining these expressions and using that $V_{2m}^T \boldsymbol{z}_{2m} = \boldsymbol{0}$ shows (4.8).

The relation (4.6) and the structure of G_{2m}, illustrated in Example 4.1 and proved in [20], give

$$A^{-j}\boldsymbol{v} = V_{2m} G_{2m}^j \boldsymbol{e}_1, \qquad j = 0, 1, \ldots, m,$$

from which (4.9) follows. ◻

In order to show that (4.7) is a rational Gauss rule, it remains to relate the powers G_{2m}^j in (4.9) to the negative powers H_{2m}^{-j}. This is done in the following lemma.

LEMMA 4.3. *Let the matrices H_{2m} and G_{2m} be defined by (4.5) and (4.6), respectively, and let the matrix A be definite. Then*

$$\boldsymbol{e}_1^T G_{2m}^j \boldsymbol{e}_1 = \boldsymbol{e}_1^T H_{2m}^{-j} \boldsymbol{e}_1, \qquad j = 0, 1, \ldots, 2m-2. \tag{4.10}$$

Proof. According to [20, (2.16)], we have

$$H_{2m} G_{2m} = I_{2m} + \boldsymbol{e}_{2m} \boldsymbol{u}_{2m}^T, \tag{4.11}$$

where only the last two entries of $\boldsymbol{u}_{2m}$ may be nonvanishing. Multiplication of (4.11) by $\boldsymbol{e}_1$ from the right-hand side gives

$$H_{2m} G_{2m} \boldsymbol{e}_1 = \boldsymbol{e}_1.$$

Since A is definite, so is $H_{2m} = V_{2m}^T A V_{2m}$. Hence,

$$G_{2m}\boldsymbol{e}_1 = H_{2m}^{-1}\boldsymbol{e}_1.$$

Further, if $m \geq 3$, then

$$H_{2m}^2 G_{2m}^2 \boldsymbol{e}_1 = H_{2m}(I_{2m} + \boldsymbol{e}_{2m}\boldsymbol{u}_{2m}^T) G_{2m}\boldsymbol{e}_1 = H_{2m} G_{2m} \boldsymbol{e}_1 = \boldsymbol{e}_1,$$

where we have used that only the first three entries of the vector $G_{2m}\boldsymbol{e}_1$ may be nonzero. This follows from the structure of G_{2m}. Proceeding similarly for increasing values of j yields

$$H_{2m}^j G_{2m}^j \boldsymbol{e}_1 = \boldsymbol{e}_1, \qquad j = 0, 1, \ldots, m-1.$$

This shows (4.10). ◻

THEOREM 4.4. *(Rational Gauss quadrature) Equation (4.7) holds, i.e., the right-hand side is a rational Gauss quadrature rule for the approximation of (4.1).*

Proof. The result follows by combining (4.8)-(4.10). ◻

A result analogous to (4.7) can be shown in a similar fashion when the number of nodes is odd.

5. Numerical examples. The computations in this section are performed using MATLAB with about 15 significant decimal digits. In all examples, except when explicitly stated otherwise, $A \in \mathbb{R}^{1000\times 1000}$ and the vector $\boldsymbol{v} \in \mathbb{R}^{1000}$ have normally distributed random entries with mean zero and variance one. We will refer to the rational Lanczos method that uses the Krylov subspace $\mathbb{K}^{\ell,m}(A,\boldsymbol{v})$ as Lanczos(ℓ,m). The examples compare the performance of the standard Lanczos method with the rational Lanczos methods for the cases $\ell = m$, $\ell = 2m$, and $\ell = 3m$.

In all computed examples, we use Krylov subspaces of dimension $k = 12, 24, 36, 48$, and 60. These dimensions are divisible by both 2, 3, and 4, and assure that the denominator degree of the rational Lanczos methods considered increases by at least one in each step. We determine the actual value $\boldsymbol{w}$, given by (1.1), as well as approximations

$$\hat{\boldsymbol{w}}_k = V_k f(H_k)\boldsymbol{e}_1\|\boldsymbol{v}\|$$

where the pentadiagonal matrix H_k, defined by (2.15), depends on the ratio ℓ/m. For comparison, we also compute the approximation $\boldsymbol{w}_k$, given by (1.3), with $m = k$, evaluated with the aid of the standard Lanczos decomposition (1.2) with $m = k$. We refer to this method as Lanczos(k). The figures display the errors $\|\boldsymbol{w} - \hat{\boldsymbol{w}}_k\|$ in logarithmic scale for Lanczos(k), Lanczos$(k/2-1, k/2)$ ($\ell = m$), Lanczos$(k/3-1, 2k/3)$ ($\ell = 2m$), and Lanczos$(k/4-1, 3k/4)$ ($\ell = 3m$) for $k = 12, 24, 48, 60$, and a few functions f.

All matrix functions are computed by means of the spectral decomposition of the matrix. For the function $f(x) = \exp(x)/x$, we evaluate (1.1) as $\exp(A)A^{-1}\boldsymbol{v}$, where $A^{-1}\boldsymbol{v}$ is computed by solving a linear system of equations. The rational Lanczos methods yield approximations

$$\hat{\boldsymbol{w}}_k = V_k \exp(H_k)H_k^{-1}\boldsymbol{e}_1\|\boldsymbol{v}\|,$$

with a symmetric and pentadiagonal matrix H_k defined by (2.15). The vector $H_k^{-1}\boldsymbol{e}_1$ is determined by evaluating the first column of the pentadiagonal matrix G_k given by (4.6) for Lanczos$(k/2-1, k/2)$. For the other rational Lanczos methods, $H_k^{-1}\boldsymbol{e}_1$ is evaluated by solving a linear system of equations. The standard Lanczos(k) method determines the Lanczos decomposition (1.2) with $m = k$, which yields the approximation

$$\boldsymbol{w}_k = V_k \exp(T_k)T_k^{-1}\boldsymbol{e}_1\|\boldsymbol{v}\|.$$

This expression is evaluated by first solving a linear system of equations for the vector $T_k^{-1}\boldsymbol{e}_1$.

Examples 5.1–2. Let $A = [a_{i,j}]$ be the symmetric positive definite Toeplitz matrix with entries $a_{i,j} = 1/(1+|i-j|)$. Computed results are shown in Figures 5.1 and 5.2 for $f(x) = \exp(-x)/x$ and $f(x) = \log(x)$, respectively. We remark that fast direct solution methods are available for linear systems of equations with this kind of matrix; see, e.g., [3, 29]. Approximations of (1.1) determined by the rational Lanczos methods are seen to be of higher accuracy than approximations obtained with the standard

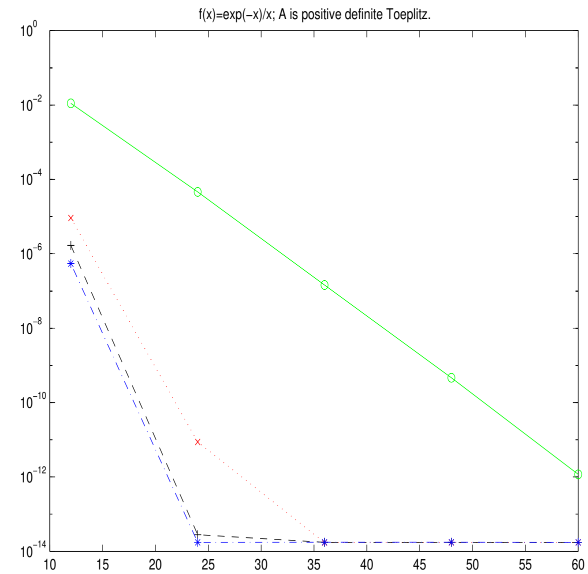

FIG. 5.1. *Example 5.1–2: Errors in approximations of $f(x) = \exp(-x)/x$ for Lanczos(k) ($\circ$–$\circ$), Lanczos$(k/2-1, k/2)$($\times \cdots \times$), Lanczos$(k/3-1, 2k/3)$($+ - - +$), and Lanczos$(k/4-1, 3k/4)$($* \cdot - *$) for subspaces of dimension $k = 12, 24, 36, 48, 60$.*

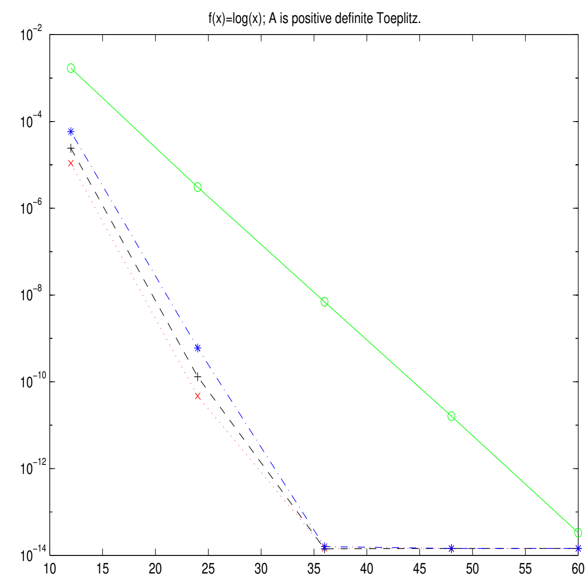

FIG. 5.2. *Example 5.1–2: Errors in approximations of $f(x) = \log(x)$ for Lanczos(k) ($\circ$–$\circ$), Lanczos$(k/2-1, k/2)$($\times \cdots \times$), Lanczos$(k/3-1, 2k/3)$($+ - - +$), and Lanczos$(k/4-1, 3k/4)$($* \cdot - *$) for subspaces of dimension $k = 12, 24, 36, 48, 60$.*

Lanczos method. Moreover, Krylov subspaces (1.8) for $i = 2$ and $i = 3$ yield smaller errors than Krylov subspaces for $i = 1$ of the same dimension. $\square$

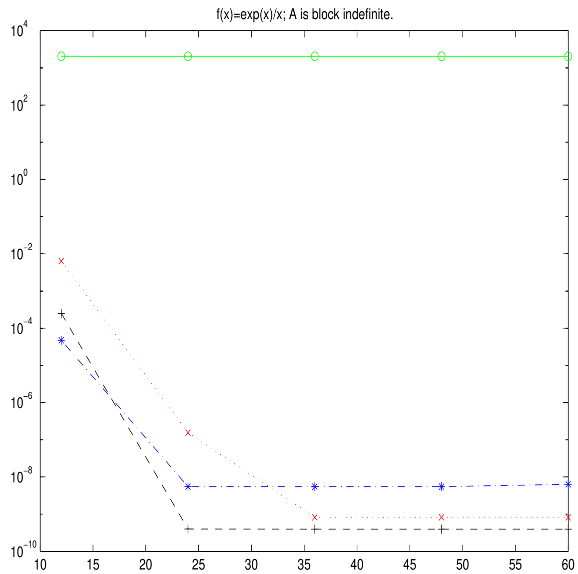

FIG. 5.3. *Example 5.3: Errors in approximations of $f(x) = \exp(-x)/x$ for Lanczos(k) ($\circ\!-\!\circ$), Lanczos$(k/2-1, k/2)$ ($\times \cdots \times$), Lanczos$(k/3-1, 2k/3)$ ($+--+$), and Lanczos$(k/4-1, 3k/4)$ ($*\!-\!*$) for subspaces of dimension $k = 12, 24, 36, 48, 60$.*

Example 5.3. The symmetric indefinite matrix of this example is of the form

$$A = \begin{bmatrix} B & C \\ C^T & -B \end{bmatrix},$$

where B is a tridiagonal symmetric Toeplitz matrix of order 500 with a typical row $[-1, 2, -1]$. All entries of $C \in \mathbb{R}^{500\times 500}$ are zero with the exception of the entry 1 in the lower left corner of the matrix. Figure 5.3 compares the errors in approximations of (1.1) for $f(t) = \exp(t)/t$ determined by the rational and standard Lanczos methods. The standard Lanczos method is seen to be unable to determine an accurate approximation. $\Box$

Examples 5.4–5. The matrix in this example is obtained by discretization of the self-adjoint differential operator $L(u) = \frac{1}{10}u_{xx} - 100u_{yy}$ in the unit square. Each derivative is approximated by the standard three-point stencil with 40 equally spaced interior nodes in each space dimension. Homogeneous boundary conditions are used. This yields a 1600×1600 symmetric positive definite matrix A. The initial vector $\boldsymbol{v}$ for the standard and rational Lanczos processes is chosen to be the unit vector with all entries $1/\sqrt{40}$. Figures 5.4 and 5.5 compare the errors in approximations of (1.1) determined by the standard and rational Lanczos methods for the functions $f(x) = \exp(x)/x$ and $f(x) = 1/\sqrt{x}$. $\Box$

6. Conclusion. Rational Lanczos methods for generating orthonormal bases of rational Krylov subspaces $\mathbb{K}^{m,mi+1}(A, \boldsymbol{v})$ can be implemented with short recursion relations. For all integers $i \geq 1$, the projected matrix $H_{m(i+1)+1}$, defined by (2.15), is pentadiagonal with a block-tridiagonal structure. Computed examples illustrate that the rational Krylov subspaces $\mathbb{K}^{m,mi+1}(A, \boldsymbol{v})$ may yield more accurate approximants for $i > 1$ than rational Krylov subspaces $\mathbb{K}^{m,mi+1}(A, \boldsymbol{v})$ with $i = 1$ or standard Krylov subspaces (1.4) of the same dimension.

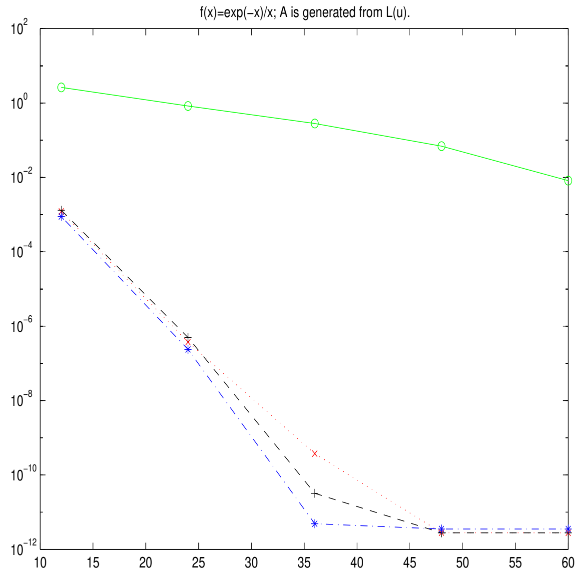

FIG. 5.4. *Example 5.4–5: Errors in approximations of* $f(x) = \exp(-x)/x$ *for Lanczos*(k) *(○–○), Lanczos*$(k/2-1, k/2)$ *(× ··· ×), Lanczos*$(k/3-1, 2k/3)$ *(+ – – +), and Lanczos*$(k/4-1, 3k/4)$ *(∗—∗) for subspaces of dimension* $k = 12, 24, 36, 48, 60$.

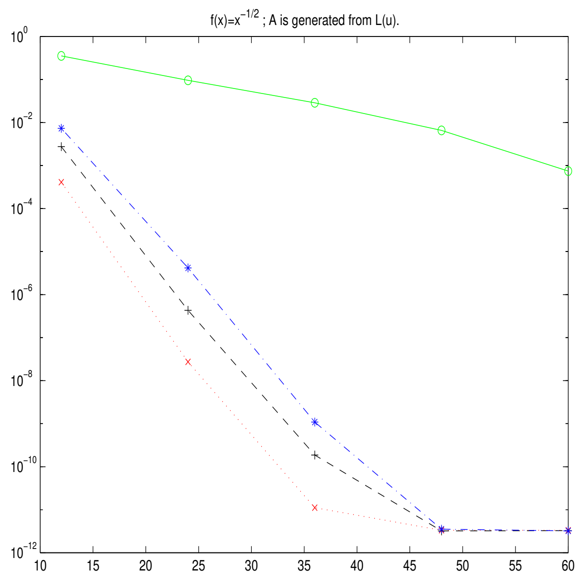

FIG. 5.5. *Example 5.4–5: Errors in approximations of* $f(x) = 1/\sqrt{x}$ *for Lanczos*(k) *(○–○), Lanczos*$(k/2-1, k/2)$ *(× ··· ×), Lanczos*$(k/3-1, 2k/3)$ *(+ – – +), and Lanczos*$(k/4-1, 3k/4)$ *(∗—∗) for subspaces of dimension* $k = 12, 24, 36, 48, 60$.

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