The extended global Lanczos method, Gauss–Radau quadrature, and matrix function approximation

In Memory of Bill Gragg.

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Abstract

The need to evaluate expressions of the form $\mathcal{I}(f) := \mathrm{trace}(W^T f(A)W)$, where the matrix $A \in \mathbb{R}^{n\times n}$ is symmetric, $W \in \mathbb{R}^{n\times k}$ with $1 \leq k \ll n$, and f is a function defined on the convex hull of the spectrum of A, arises in many applications including network analysis and machine learning. When the matrix A is large, the evaluation of $\mathcal{I}(f)$ by first computing $f(A)$ may be prohibitively expensive. In this situation it is attractive to compute an approximation of $\mathcal{I}(f)$ by first applying a few steps of a global Lanczos-type method to reduce A to a small matrix and then evaluating f at this reduced matrix. The computed approximation can be interpreted as a quadrature rule. The present paper generalizes the extended global Lanczos method introduced in [6] and discusses the computation of error-bounds and error estimates. Numerical examples illustrate the performance of the techniques described.

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1. Introduction

Let $A \in \mathbb{R}^{n\times n}$ be a large symmetric matrix, f a function defined on the convex hull of the spectrum of A, and $\boldsymbol{w} \in \mathbb{R}^n$ a vector of unit Euclidean norm. Application of $m \leq n$ steps of the (standard) Lanczos method to A with initial vector $\boldsymbol{w}$ yields the partial Lanczos decomposition

$$AV_m = V_m T_m + \boldsymbol{g}_m \boldsymbol{e}_m^T, \tag{1.1}$$

where the matrix $V_m \in \mathbb{R}^{n\times m}$ has orthonormal columns with initial column $\boldsymbol{w}$, $T_m \in \mathbb{R}^{m\times m}$ is a symmetric tridiagonal matrix, and $\boldsymbol{g}_m \in \mathbb{R}^n$ satisfies $V_m^T \boldsymbol{g}_m = \boldsymbol{0}$; see, e.g., [24, 39] for details on the Lanczos algorithm. Throughout this paper $\boldsymbol{e}_i$ denotes the ith column of the identity matrix of suitable order, and the superscript ^{T} stands for transposition. Generally, $m \ll n$ in applications of the Lanczos method. We assume that m is small enough so that the Lanczos decomposition (1.1) with the stated properties exists. This is the generic situation. Then

$$\text{range}(V_m) = \mathbb{K}_m(A, \boldsymbol{w}), \tag{1.2}$$

where the right-hand side denotes the Krylov subspace

$$\mathbb{K}_m(A, \boldsymbol{w}) := \text{span}\{\boldsymbol{w}, A\boldsymbol{w}, \ldots, A^{m-1}\boldsymbol{w}\}. \tag{1.3}$$

Introduce the spectral factorization

$$A = U\Lambda U^T, \quad \Lambda = \text{diag}[\lambda_1, \lambda_2, \ldots, \lambda_n] \in \mathbb{R}^{n\times n} \tag{1.4}$$

with an orthogonal matrix $U \in \mathbb{R}^{n\times n}$. Substituting the spectral factorization into

$$\mathcal{I}(f) := \boldsymbol{w}^T f(A) \boldsymbol{w}$$

gives

$$\mathcal{I}(f) = \boldsymbol{w}^T U f(\Lambda) U^T \boldsymbol{w} = \sum_{j=1}^{m} f(\lambda_j)\mu_j^2, \tag{1.5}$$

where $\mu_j = \boldsymbol{e}_j^T U^T \boldsymbol{w}$. The right-hand side of (1.5) can be written as a Stieltjes integral determined by a piece-wise constant non-decreasing distribution

function $\mu(\lambda)$ with jumps at the λ_j. Let $d\mu(\lambda)$ denote the measure associated with $\mu(\lambda)$. Then

$$\mathcal{I}(f) = \int f(\lambda) d\mu(\lambda). \tag{1.6}$$

We note for future reference that the measure $d\mu(\lambda)$ defines an inner product

$$(f, g) := \int f(\lambda) g(\lambda) d\mu(\lambda) \tag{1.7}$$

for polynomials f and g of low enough degree.

Golub and Meurant [22, 23] observed that the nontrivial entries of the symmetric tridiagonal matrix T_m in (1.1) are recursion coefficients for a sequence of orthonormal polynomials with respect to the inner product (1.7). In particular, the eigenvalues of T_m are the zeros of the orthonormal polynomial of degree m. This led Golub and Meurant [22, 23] to show that the expression

$$\mathcal{G}_m(f) := \boldsymbol{e}_1^T f(T_m) \boldsymbol{e}_1 \tag{1.8}$$

is the m-point Gauss quadrature rule for approximating the Stieltjes integral (1.6). Hence,

$$\mathcal{G}_m(f) = \mathcal{I}(f) \qquad \forall f \in \mathbb{P}_{2m-1}, \tag{1.9}$$

where $\mathbb{P}_{2m-1}$ denotes the set of polynomials of degree at most $2m-1$. Substituting the spectral factorization of T_m into (1.8) transforms the right-hand side into a sum of m terms and shows that the eigenvalues of T_m are the nodes and the square of the first component of normalized eigenvectors are the weights of the quadrature rule. This observation forms the basis for the Golub–Welsch algorithm [26] for the efficient computation of nodes and weights of a Gauss quadrature rule from T_m. However, we remark that it may not be necessary to first evaluate (1.8) by determining the nodes and weights of the Gauss rule and then compute f at the nodes. For some functions f, it may be more efficient to compute $f(T_m)$ directly by one of the methods discussed in [28]; see [15] for an illustration.

The quadrature rule (1.8) is obtained by applying m steps of the (standard) Lanczos method to A with initial vector $\boldsymbol{w}$. An analogous rule can be computed by applying the global Lanczos method to A with initial block vector $W \in \mathbb{R}^{n\times k}$ with block size $1 < k \ll n$. The global Lanczos method is a block Lanczos method with a particular inner product. It was first proposed and investigated by Elbouyahyaoui et al. [13] and Jbilou et al. [34]. The global block Lanczos method uses the inner product between block vectors

$$\langle W_1, W_2 \rangle := \operatorname{trace}(W_1^T W_2), \qquad W_1, W_2 \in \mathbb{R}^{n\times k}, \tag{1.10}$$

and the induced Frobenius norm

$$\|W_1\|_F := \langle W_1, W_1 \rangle^{1/2}.$$

This method can be applied to approximate expressions of the form

$$\mathcal{I}(f) := \mathrm{trace}(W^T f(A) W), \tag{1.11}$$

where $W \in \mathbb{R}^{n\times k}$ with $1 \leq k \ll n$.

The problem of estimating the trace of a matrix $f(A)$, without evaluating $f(A)$, is a classical problem in numerical linear algebra; see, e.g., [2, 3, 4, 5, 8, 9, 21, 25, 36]. The need to evaluate or approximate expressions of the type (1.11) arises in various applications, including in network analysis and when solving ill-posed problem; see, e.g., [5, 14, 16, 19, 25, 27] for discussions of these applications. An approximation of the trace of $f(A)$ can be computed by approximating expressions (1.11) for several block vectors $W := E_m$, $1 \leq m \leq n/k$, where the

$$E_m = [\boldsymbol{e}_{k(m-1)+1}, \ldots, \boldsymbol{e}_{km}] \in \mathbb{R}^{n\times k} \tag{1.12}$$

are block axis vectors. For notational simplicity, we here assume that n is a multiple of k; see [5] for details on the computations.

The method described in this paper for approximating expressions of the form (1.11) is particularly well suited for problems with a matrix A that allows efficient solution of linear systems of equations with this matrix. This includes semiseparable matrices [44] and, in particular, symmetric positive definite Toeplitz matrices [1].

This paper is organized as follows. Section 2 reviews the global Lanczos method. This method gives approximations of integrals that are exact when the integrand is a polynomial of low enough degree, analogously to (1.9). However, the error in the computed approximation may be large if the integrand cannot be well approximated by a polynomial of moderate degree. The extended global Lanczos method determines approximations of integrals that are exact when the integrand is a Laurent polynomial of low enough order. The method described in this paper may determine approximations of an integral with much higher accuracy than the (standard) global Lanczos method when the support of the measure includes points close to the origin, and the integrand has a singularity there. The extended global Lanczos method recently has been described in [6] for the special case when the numerator and denominator degrees of the Laurent polynomials that define the approximant are about the same. Section 3 extends this

method to allow more general Laurent polynomials. The method is derived by applying results in [31] for the extended Lanczos method. The computations with the method exploit that, analogously to computations with the standard Lanczos method, short recursion relations can be applied in the computations with the extended global Lanczos method. Section 4 is concerned with bounding the quadrature error of Gauss–Laurent quadrature rules associated with the extended global Lanczos method. These bounds require that certain derivatives of the integrand do not change sign on the convex hull of the support of the measure. A method that can be applied to evaluate error estimates is described in Section 5. This technique has been developed by Spalević [41, 42, 43] for estimating the error in Gauss quadrature rules. We describe an extension that can be applied to estimate the quadrature error in Gauss–Laurent rules. A few computed examples are presented in Section 6 and concluding remarks can be found in Section 7.

2. The global Lanczos algorithm and Gauss quadrature

Let $A \in \mathbb{R}^{n\times n}$ be a large symmetric matrix and $W \in \mathbb{R}^{n\times k}$ be a block vector with $1 \leq k \ll n$. Application of m steps of the global Lanczos algorithm gives the global Lanczos decomposition

$$A[V_1, V_2, \ldots, V_m] = [V_1, V_2, \ldots, V_m]\widehat{T}_{mk} + \beta_{m+1}V_{m+1}E_m^T, \qquad (2.1)$$

where the block columns $V_j \in \mathbb{R}^{n\times k}$ are orthonormal with respect to the inner product (1.10), i.e.,

$$\langle V_i, V_j\rangle = \begin{cases} 1, & i = j, \\ 0, & i \neq j. \end{cases}$$

The global Lanczos method simplifies to the standard Lanczos method when the block size k is one. Analogously to (1.2), the range of $[V_1, V_2, \ldots, V_m]$, given by $\left\{\sum_{j=1}^m \gamma_j V_j,\, \gamma_j \in \mathbb{R}\right\}$, is the block Krylov subspace

$$\mathbb{K}_m(A, W) = \text{span}\{W, AW, \ldots, A^{m-1}W\}.$$

The matrix $\widehat{T}_{mk} \in \mathbb{R}^{mk\times mk}$ in (2.1) can be expressed as

$$\widehat{T}_{mk} = T_m \otimes I_k, \qquad (2.2)$$

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

$$T_m = \begin{bmatrix} \alpha_1 & \beta_2 & & & & & \\ \beta_2 & \alpha_2 & \beta_3 & & & & \\ & \beta_3 & \ddots & \ddots & & & \\ & & \ddots & & & & \\ & & & & \ddots & & \\ & & & \ddots & \ddots & \beta_m & \\ & & & & \beta_m & \alpha_m & \end{bmatrix} \in \mathbb{R}^{m\times m}$$

is symmetric and tridiagonal. Its entries, as well as the block vectors in the decomposition (2.1), are determined by Algorithm 2.1 below. The symbol $\otimes$ in (2.2) denotes the Kronecker product. Moreover, E_m is the block axis vector (1.12) and $\beta_{m+1} > 0$ in (2.1). We assume that m is small enough so that the decomposition (2.1) with the stated properties exists.

Algorithm 2.1 (The global Lanczos method).

Input: *symmetric matrix $A \in \mathbb{R}^{n\times n}$, initial block vector $W \in \mathbb{R}^{n\times k}$, number of steps ℓ.*

Output: *global Lanczos decomposition (2.1).*

$V_0 = 0$, $\beta_1 = \|W\|_F$, $V_1 = W/\beta_1$

for $j = 1 : \ell$ **do**

$\widetilde{V} = AV_j - \beta_j V_{j-1}$, $\alpha_j = \langle V_j, \widetilde{V}\rangle$

$\widetilde{V} = \widetilde{V} - \alpha_j V_j$

$\beta_{j+1} = \|\widetilde{V}\|_F$, $V_{j+1} = \widetilde{V}/\beta_{j+1}$

end

The expression (1.11) can be written as

$$\mathcal{I}(f) = \|W\|_F^2 \,\mathrm{trace}(V_1^T f(A) V_1) = \|W\|_F^2 \,\mathrm{trace}(\widetilde{V}_1^T f(\Lambda)\widetilde{V}_1),$$

where we assume that $W \in \mathbb{R}^{n\times k}\backslash\{0\}$, $V_1 = W/\|W\|_F$, and $\widetilde{V}_1 = U^T V_1$; cf. (1.4). We define analogously to (1.6) the Stieltjes integrals

$$\mathcal{I}_i(f) := \boldsymbol{e}_i^T \widetilde{V}_1^T f(\Lambda)\widetilde{V}_1 \boldsymbol{e}_i = \int f(\lambda) d\mu_i(\lambda), \qquad i = 1, 2, \ldots, k,$$

where $\mu_i(\lambda)$ is a piece-wise constant non-decreasing distribution function that has jumps at the eigenvalues λ_j of A and $d\mu_i(\lambda)$ is the associated measure. Therefore,

$$\mathcal{I}(f) = \|W\|_F^2 \sum_{i=1}^{k} \mathcal{I}_i f = \|W\|_F^2 \int f(\lambda) d\mu(\lambda),$$

where

$$\mu(\lambda) := \sum_{i=1}^{k} \mu_i(\lambda) \tag{2.3}$$

is a piece-wise constant non-decreasing distribution function with jumps at the eigenvalues λ_j. The measure associated with $\mu(\lambda)$ defines the inner product

$$(f, g) := \int f(\lambda) g(\lambda) d\mu(\lambda) \tag{2.4}$$

for polynomials f and g of sufficiently small degree.

It is shown in [5] that the entries of the tridiagonal matrix T_m in (2.2) are recursion coefficients for orthonormal polynomials associated with the inner product (2.4). This provides the connection between the global Lanczos method and Gauss quadrature. A proof of the following result is provided in [5].

Proposition 2.1. *Let the symmetric tridiagonal matrix T_m in (2.2) be determined by Algorithm 2.1. Then*

$$\mathcal{G}_m(f) := \|W\|_F^2 \boldsymbol{e}_1^T f(T_m) \boldsymbol{e}_1 \tag{2.5}$$

is an m-point Gauss quadrature rule associated with the inner product (2.4) *defined by the distribution function* (2.3). *In particular, $\mathcal{G}_m(f) = \mathcal{I}(f)$ for all $f \in \mathbb{P}_{2m-1}$, where $\mathcal{I}(f)$ is defined by* (1.11). *Substituting the spectral factorization of T_m into (2.5) yields the quadrature rule in terms of its nodes and weights.*

Assume that the convex hull of the support of the measure $d\mu$ does not contain the origin. Gauss quadrature rules are well suited to approximate integrals with an integrand that allows accurate approximation by a polynomial of fairly low degree. However, when the integrand is non-differentiable on or close to the support of the measure, Gauss quadrature rules (2.5) may yield low accuracy also for fairly large values of m. In this situation, it may be beneficial to use quadrature rules that are exact for Laurent polynomials, which are rational functions of the form $p(x)/x^k$, where p is a polynomial and k is a positive integer. Further, Druskin and Knizhnerman [12] have shown that the approximation by Laurent polynomials may be beneficial, compared with polynomial approximation, also when approximating entire functions on an interval not containing the origin.

3. The extended global Lanczos algorithm and Gauss–Laurent rules

The extended global Lanczos method exploits that orthogonal Laurent polynomials associated with a non-negative measure on the real axis satisfy short recursion relations; see [10, 29, 30, 31, 35, 37, 40] for this and related results.

3.1. Recursion relations for extended Krylov subspaces

This section first reviews results in [31] on recursion relations of orthonormal bases for extended Krylov subspaces of the form

$$\mathbb{K}_{\ell,m}(A, \boldsymbol{w}) = \text{span}\{A^{-\ell+1}\boldsymbol{w}, \ldots, A^{-1}\boldsymbol{w}, \boldsymbol{w}, A\boldsymbol{w}, \ldots, A^{m-1}\boldsymbol{w}\}, \qquad (3.1)$$

and subsequently describes the extended global Lanczos process. We will in this section assume A to be symmetric and positive definite. Generically, $\mathbb{K}_{\ell,m}(A, \boldsymbol{w})$ is of dimension $m+\ell-1$. The space $\mathbb{K}_{1,m}(A, \boldsymbol{w})$ is the standard Krylov subspace (1.3).

Njåstad and Thron [37] showed that orthonormal bases for the sequence of nested extended Krylov subspaces

$$\mathbb{K}_{1,1}(A, \boldsymbol{w}) \subset \mathbb{K}_{2,2}(A, \boldsymbol{w}) \subset \cdots \subset \mathbb{K}_{m,m}(A, \boldsymbol{w}) \subset \mathbb{R}^n$$

satisfy a short recursion relation, i.e., the number of terms of the recursion relation can be bounded independently of m. The derivation of the recursion relations uses properties of orthogonal Laurent polynomials. A survey of this and related results is provided by Jones and Njåstad [35]. We remark that these references do not discuss Krylov subspaces; however, the results presented can be applied to Krylov subspace computations.

Generation of an orthonormal basis for the subspace $\mathbb{K}_{m,m}(A, \boldsymbol{w})$ requires the evaluation of $m-1$ matrix-vector products with the matrix A and the solution of $m-1$ linear systems of equations with A. For many matrices A, the evaluation of matrix-vector products with A can be carried out faster on modern computers than the solution of systems of equations with A, also when A already is available in factored form. This suggests that it may be interesting to choose m larger than ℓ in (3.1). In [31], short recursion formulas are derived for generating an orthonormal basis for a sequence of extended Krylov subspaces of the form

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

where i is a positive integer. The computation of this basis is based on the use of orthogonal Laurent polynomials. The recursion formulas generate orthogonal Laurent polynomials with respect to the inner product (1.7). This is equivalent to determining the vectors, in order,

$$\boldsymbol{v}_0, \boldsymbol{v}_1, \ldots, \boldsymbol{v}_i, \boldsymbol{v}_{-1}, \boldsymbol{v}_{i+1}, \ldots, \boldsymbol{v}_{2i}, \ldots, \boldsymbol{v}_{-m+1}, \ldots, \boldsymbol{v}_{im} \tag{3.2}$$

with $\boldsymbol{v}_0 = \boldsymbol{w}$, which make up an orthonormal basis for the extended Krylov subspace $\mathbb{K}_{m,im+1}(A, \boldsymbol{w})$. The meaning of the subscripts in the sequence (3.2) is that $\boldsymbol{v}_j$ for $j > 0$ is determined by multiplying the most recently generated vector by A and orthogonalizing the vector so obtained against selected already available vectors, while v_{-j} for $j \geq 1$ is computed by multiplying the most recently generated vector by A^{-1} and orthogonalizing the vector so obtained against selected already available vectors. Typically, the matrix A^{-1} is not explicitly formed; instead a linear system of equations with the matrix A is solved. The number of explicit orthogonalizations required for generating each vector $\boldsymbol{v}_j$, $j \in \mathbb{Z}$, can be bounded independently of the magnitude of j. Details are described in [31]. To facilitate the implementation, we describe an algorithm at the end of this section.

Introduce the matrix

$$V_\tau := [\boldsymbol{v}_0, \boldsymbol{v}_1, \ldots, \boldsymbol{v}_i, \boldsymbol{v}_{-1}, \boldsymbol{v}_{i+1}, \ldots, \boldsymbol{v}_{2i}, \ldots, \boldsymbol{v}_{-m+1}, \ldots, \boldsymbol{v}_{im}] \in \mathbb{R}^{n\times\tau},$$

where

$$\tau := m(i+1). \tag{3.3}$$

The recursion coefficients for generating the basis (3.2) as outlined determine a pentadiagonal matrix $H_\tau = [h_{j,k}] \in \mathbb{R}^{\tau\times\tau}$ such that

$$AV_\tau = V_\tau H_\tau + \boldsymbol{z}_\tau \boldsymbol{e}_\tau^T, \tag{3.4}$$

where

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

Thus,

$$H_\tau = V_\tau^T A V_\tau \tag{3.5}$$

is the orthogonal projection of A onto $\mathbb{K}_{m,im+1}(A, \boldsymbol{w})$. Since A is symmetric and positive definite, so is H_τ. We remark that the matrix H_τ is the analogue of the tridiagonal matrix T_m in (1.1).

Example 2.1. Consider the matrix H_τ for $i = 3$ and $m = 3$. Then $\tau = 12$. The matrix H_{12} may have non-vanishing entries in the positions marked by

"∗":

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

□

It is shown in [31] that the matrix (3.5) plays an analogous role for Gauss–Laurent quadrature rules, which are designed for the exact integration of functions in suitable spaces of Laurent polynomials, as the matrix T_m for Gauss rules.

Theorem 3.1. *(Gauss–Laurent quadrature) Let τ be given by (3.3) and define the quadrature rule*

$$\mathcal{H}_\tau(f) = \boldsymbol{e}_1^T f(H_\tau)\boldsymbol{e}_1. \tag{3.6}$$

Then

$$\mathcal{I}(f) = \mathcal{H}_\tau(f) \qquad \forall f \in \mathcal{L}_{2m-2,2mi+1},$$

where

$$\mathcal{L}_{2m-2,2mi+1} := span\{x^{-2m+2}, x^{-2m+3}, \ldots, 1, \ldots, x^{2mi}, x^{2mi+1}\}, \tag{3.7}$$

is a space of Laurent polynomials equipped with the inner product (1.7). We assume here that the dimension of the spaces (3.7) is small enough so that (1.7) indeed is an inner product.

The quadrature rule (3.6) has τ nodes. Its nodes and weights can be computed by a Golub–Welsch-type algorithm described in [31]. For some integrands f, e.g., for $f(t) = 1/t$, it may suffice to compute the Cholesky factorization of H_τ in order to evaluate the right-hand side of (3.6).

The discussion in this section has, so far, been concerned with the evaluation of Gauss–Laurent quadrature rules associated with the inner product (1.7), which is connected to the standard Lanczos algorithm. To instead evaluate Gauss–Laurent rules associated with the inner product (2.4), which

is connected to the extended global Lanczos algorithm, is straightforward: only the inner product has to be replaced. In particular, the structure of the matrix H_τ is the same for both inner products, but the value of the entries may differ. An algorithm for the extended global Lanczos method therefore can be based on the analysis presented in [31]. We conclude this section by describing such an algorithm.

3.2. Recursion relations for extended global Krylov method

Analogous to the global Lanczos method, we consider an initial block vector $W \in \mathbb{R}^{n\times k}$ with block size $1 \leq k \ll n$ and the inner product (2.4). The orthogonal block vectors equivalent to the orthogonal sequence in (3.2) are denoted by $V \in \mathbb{R}^{n\times k}$. The notation $V \in \mathcal{L}_{i,j}$ signifies that $V = \psi(A)V_0$ and that $\psi(x) \in \mathcal{L}_{i,j}$. The following discussion briefly describes the construction of H_τ in (3.5). The first $i+1$ block vectors satisfy the three-term recursion formulas for the Lanczos method,

$$\begin{aligned} AV_0 &= h_{1,1}V_0 + h_{2,1}V_1, \\ &\vdots \\ AV_{i-1} &= h_{i-1,i}V_{i-2} + h_{i,i}V_{i-1} + h_{i+1,i}V_i, \end{aligned}$$

where $h_{j,k} = \langle AV_j, V_k\rangle$. This concludes the computation of the first $i+1$ block vectors. Assume that for some $1 \leq j \leq m-1$, the block vectors

$$V_0, V_1, \ldots, V_i, V_{-1}, V_{i+1}, \ldots, V_{2i}, V_{-2}, \ldots, V_{ij},$$

have been computed. The following discusses the computation of the next $i+1$ block vectors beginning with V_{-j}; that is, with the incrementation of the reciprocal power. Let $\ell = (i+i)j$. Then

$$A^{-1}V_{ij} = g_{\ell-i,\ell}V_{-j+1} + g_{\ell-i+1,\ell}V_{ij-i+1} + \ldots + g_{\ell,\ell}V_{ij} + g_{\ell+1,\ell}V_{-j}, \quad (3.8)$$

where $g_{j,k} = \langle A^{-1}V_j, V_k\rangle$. Note that the computation of V_{-j} involves an expression with $i+2$ terms. (For $i = 1$, this reduces to a three-term recursion formula). It is necessary to find the entries of the ℓ^{th} column of H_τ pertaining to this step. The computation of $h_{\ell,\ell}$ and $h_{\ell,\ell+2}$ is discussed below. The $(\ell+1)^{\text{st}}$ column is determined by the requirment that $AV_{-j} \in \mathcal{L}_{j-1,ij+1} \perp \mathcal{L}_{j-1,ij-1}$, Hence, it satisfies a three-term recursion

$$AV_{-j} = h_{\ell,\ell+1}V_{ij} + h_{\ell+1,\ell+1}V_{-j} + h_{\ell+2,\ell+1}V_{ij+1}.$$

The $(\ell+2)^{\text{nd}}$ column of H_τ is determined by the requirement that $AV_{ij+1} \in \mathcal{L}_{j-1,ij+2} \perp \mathcal{L}_{j-1,ij-1}$. Observe that the numerator degree has increased

from the previous expression, but the orthogonality condition has not changed. This gives a four-term recursion,

$$AV_{ij+1} = h_{\ell,\ell+2}V_{ij} + h_{\ell+1,\ell+2}V_{-j} + h_{\ell+2,\ell+2}V_{ij+1} + h_{\ell+3,\ell+2}V_{ij+2}.$$

For $i > 2$, the entries in the next $i-1$ block columns correspond to $AV_{ij+2}, \ldots, AV_{\ell-1}$, which satisfy a standard three-term recursion formula

We return to the ℓ^{th} column of H_τ. It is determined by the requirement that $AV_{ij} \in \mathcal{L}_{j-2,ij+1} \perp \mathcal{L}_{j-1,ij-2}$ and satisfies a four-term recursion formula

$$AV_{ij} = h_{\ell-1,\ell}V_{ij-1} + h_{\ell,\ell}V_{ij} + h_{\ell+1,\ell}V_{-j} + h_{\ell+2,l}V_{ij+1}. \tag{3.9}$$

The recursion coefficients are obtained by multiplying equation (3.8) by A, which gives an equation in $g_{\ell,\ell}AV_{ij}$. Specifically, the known expressions for

$$AV_{-j+1}, AV_{ij-i+1}, \ldots, AV_{ij}, AV_{-j}$$

in terms of the Laurent orthogonal vectors are substituted into the modified expression and comparisons of like terms in the two formulas yield the coefficients in (3.9). The off-diagonal entries have been determined by symmetry for $i > 1$. The diagonal entry is given by

$$h_{\ell,\ell} = (1 - g_{\ell-1,\ell}h_{\ell,\ell-1} - g_{\ell+1,\ell}h_{\ell,\ell+1})/g_{\ell,\ell}.$$

For $i = 1$, we have

$$h_{\ell,\ell+2} = -g_{\ell+1,\ell}h_{\ell+2,\ell+1}/g_{\ell,\ell}.$$

These formulas are the basis for the following algorithm. We remark that even though the algorithm is formulated with the matrices A and A^{-1}, storage and computation of these matrices are not explicitly required. The algorithm needs functions for the evaluation of matrix-block-vector products with A and for the solution of linear systems of equations with the matrix A and k right-hand side vectors.

Algorithm 3.1 (Orthogonalization process for $\mathbb{K}^{m,im+1}(A,\boldsymbol{v})$).

Input: *m, i, $W \in \mathbb{R}^{n\times k}\backslash\{0\}$, $1 \le k \ll n$; functions for evaluating matrix-block-vector products with $A \in \mathbb{R}^{n\times n}$, and for solving linear systems of equations with A.*

Output: *orthogonal basis $\{V_k\}_{k=-m+1}^{im+1}$ for $\mathbb{K}^{m,im+1}(A,W)$, nontrivial entries h_{ij} of H_τ.*

$V_{-1} := 0 \in \mathbb{R}^{n\times k}$;
$h_{1,0} := ||W||_F$; $V_0 := W/h_{1,0}$; $h_{0,1} := h_{1,0}$;
for $j = 1 : i$ **do**
  $U := AV_{j-1} - h_{j-1,j}V_{j-2}$;
  $h_{j,j} := \langle V_{j-1}, U\rangle$; $U := U - h_{j,j}V_{j-1}$;
  $h_{j+1,j} := ||U||_F$; $V_j := U/h_{j+1,j}$; $h_{j,j+1} := h_{j+1,j}$;
end
for $j = 1 : m-1$ **do**
  $\ell := (1+i)j$;
  $\widehat{W} := A^{-1}V_{ij}$; $g_{\ell-i,\ell} := \langle V_{-j+1}, \widehat{W}\rangle$; $\widehat{W} := \widehat{W} - g_{\ell-i,\ell}V_{-j+1}$;
  for $k = 1 : i$ **do**
    $g_{\ell-i+k,\ell} := \langle V_{ij-i+k}, \widehat{W}\rangle$; $\widehat{W} := \widehat{W} - g_{\ell-i+k,\ell}V_{ij-i+k}$;
  end
  $g_{\ell+1,\ell} := ||\widehat{W}||_F$; $V_{-j} := \widehat{W}/g_{\ell+1,\ell}$;
  $U := AV_{-j}$; $h_{\ell,\ell+1} := \langle V_{ij}, U\rangle$; $U := U - h_{\ell,\ell+1}V_{ij}$;
  $h_{\ell+1,\ell+1} := \langle V_{-j}, U\rangle$; $U := U - h_{\ell+1,\ell+1}V_{-j}$;
  $h_{\ell+2,\ell+1} := ||U||_F$; $V_{ij+1} := U/h_{\ell+2,\ell+1}$;
  $h_{\ell+1,\ell} := h_{\ell,\ell+1}$; $h_{\ell+1,\ell+2} := h_{\ell+2,\ell+1}$;
  $h_{\ell,\ell} := (1 - g_{\ell-1,\ell}h_{\ell,\ell-1} - g_{\ell+1,\ell}h_{\ell,\ell+1})/g_{\ell,\ell}$;
  $h_{\ell,\ell+2} := -g_{\ell+1,\ell}h_{\ell+2,\ell+1}/g_{\ell,\ell}$; $h_{\ell+2,\ell} := h_{\ell,\ell+2}$;
  if $i > 1$ **do**
    $U := AV_{ij+1}$; $U := U - h_{\ell,\ell+2}V_{ij} - h_{\ell+1,\ell+2}V_{-j}$;
    $h_{\ell+2,\ell+2} := \langle V_{ij+1}, U\rangle$; $U := U - h_{\ell+2,\ell+2}V_{ij+1}$;
    $h_{\ell+3,\ell+2} := ||U||_F$; $V_{ij+2} := U/h_{\ell+3,\ell+2}$;
    $h_{\ell+2,\ell+3} := h_{\ell+3,\ell+2}$;
  end
  for $k = 3 : i$ **do**
    $U := AV_{ij+k-1} - h_{\ell+k-1,\ell+k}V_{ij+k-2}$;
    $h_{\ell+k,\ell+k} := \langle V_{ij+k-1}, U\rangle$; $U := U - h_{\ell+k,\ell+k}V_{ij+k-1}$;
    $h_{\ell+k+1,\ell+k} := ||U||_F$; $V_{ij+k} := U/h_{\ell+k+1,\ell+k}$;
    $h_{\ell+k,\ell+k+1} := h_{\ell+k+1,\ell+k}$;
  end
end
$U := AV_{(i+1)m}$; $h_{(i+1)m,(i+1)m} := \langle V_{(i+1)m}, U\rangle$;

Analogous to (3.4), Algorithm 3.1 produces a matrix $\mathbb{V}_\tau \in \mathbb{R}^{n\times k\tau}$ and a matrix of recursion coefficients $\widehat{H}_\tau \in \mathbb{R}^{k\tau\times k\tau}$ that satisfy the equation

$$A\mathbb{V}_\tau = \mathbb{V}_\tau\widehat{H}_\tau + \tilde{Z}_\tau E_\tau, \tag{3.10}$$

where

$$\mathbb{V}_\tau = [V_0, V_1, \dots V_i, V_{-1}, V_{i+1}, \dots, V_{2i}, \dots, V_{m+1}, \dots, V_{im}] \tag{3.11}$$

and

$$\begin{aligned} \widehat{H}_\tau &= H_\tau \otimes I_k, \\ \tilde{Z}_\tau &= h_{\tau+1,\tau} V_{-m} + h_{\tau+2,\tau} V_{im+1}, \\ E_\tau &= [0_{k\times(\tau-1)k}\ I_k]. \end{aligned} \tag{3.12}$$

We also define the vector of orthonormal Laurent polynomials,

$$\Phi_\tau(x) := [\phi_0(x), \dots, \phi_i(x), \phi_{-1}(x), \dots, \phi_{-m+1}(x), \dots, \phi_{im}(x)]^T, \tag{3.13}$$

with respect to the measure $d\mu(x)$. We have

$$V_j = \phi_j(A)V_0, \qquad j = 0, 1, \dots, i, -1, i+1, i+2, \dots\ .$$

The block vector $\tilde{Z}_\tau \in \mathbb{R}^{n\times k}$ in (3.10) is a linear combination of the orthonormal Laurent block vectors generated by Algorithm 3.1, but does not belong to the generated sequence. We denote the normalized block vector by $Z_\tau = \tilde{Z}/\tilde{h}_{\tau+1,\tau}$. The normalization factor, $\tilde{h}_{\tau+1,\tau} = \|\tilde{Z}\|$, may be derived from (3.12) and the orthogonality of the block vectors V_{-m} and V_{im+1}:

$$\tilde{h}_{\tau+1,\tau} = \sqrt{h_{\tau+1,\tau}^2 + h_{\tau+2,\tau}^2}. \tag{3.14}$$

We denote the polynomial associated with Z by $\psi_\tau \in \mathcal{L}_{m-1,im+1}$ in order to distinguish it from the sequence of polynomials in (3.13) generated by Algorithm 3.1. It satisfies

$$Z_\tau = \psi_\tau(A)V_0$$

and is orthogonal to $\mathcal{L}_{m-1,im}$ with respect to the inner product (2.4). This leads to the polynomial vector equivalent of (3.10),

$$x\Phi_\tau(x) = H_\tau\Phi_\tau(x) + \tilde{h}_{\tau+1,\tau}\psi_\tau(x)\boldsymbol{e}_\tau, \tag{3.15}$$

which we utilize in the next section when discussing Radau rules.

4. Bounds for Gauss–Laurent rules

The degree of $\psi_\tau \in \mathcal{L}_{m-1,im+1} \perp \mathcal{L}_{m-1,im}$ along with its orthogonality conditions guarantee that ψ_τ has τ distinct zeros, $\{x_j\}_{j=1}^\tau$. These zeros are eigenvalues of H_τ; see [31, Theorem 5.1]. Assume that f is differentiable.

Then the Laurent-Hermite interpolation polynomial, $\hat{L} \in \mathcal{L}_{2m-2,2im+1}$, that interpolates f and its derivative at the nodes x_j may be constructed. An expression for the approximation error $f - \hat{L} \in \mathcal{L}_{2m-2,2im+1}$ shown in [31, Theorem 5.4] can be used to derive the following error term for Gauss–Laurent quadrature.

Theorem 4.1. *Assume that f is 2τ times continuously differentiable in the convex hull of the support of the measure $d\mu$. Then the quadrature rule $\mathcal{H}_\tau$ defined in Theorem 3.1 satisfies*

$$(\mathcal{I} - \mathcal{H}_\tau)(f) = \frac{d^{2\tau}}{dt^{2\tau}} \left(t^{2m-2} f(t)\right)_{t=c} \frac{\mathcal{I}(\psi_\tau^2)}{a_\tau^2 (2\tau)!}$$

for some scalar c in the convex hull of the support of the measure $d\mu$ and where a_τ is the leading coefficient of ψ_τ.

Assume that f satisfies the conditions of Theorem 4.1 and that

$$\frac{d^{2\tau}}{dx^{2\tau}} \left(x^{2(m-1)} f(x)\right) \geq 0, \qquad a < x < b,$$

in some open interval (a, b) containing the spectrum of A. Then Theorem 4.1 gives a lower bound for $\mathcal{I}(f)$. We have

$$\mathcal{H}_\tau(f) \leq \mathcal{I}(f). \tag{4.1}$$

4.1. Bounds derived for Gauss–Laurent–Radau quadrature rules

A Gauss–Laurent–Radau rule can be implemented by using the following modification of the pentadiagonal matrix H_τ in (3.10),

$$\tilde{H}_{\tau+1}^a = \begin{bmatrix} H_\tau & \tilde{h}_{\tau+1,\tau} \boldsymbol{e}_\tau \\ \tilde{h}_{\tau+1,\tau} \boldsymbol{e}_\tau^T & \alpha_a \end{bmatrix} \in \mathbb{R}^{(\tau+1)\times(\tau+1)}. \tag{4.2}$$

The superscript a of $\tilde{H}_{\tau+1}^a$ is a value $a \leq \lambda_1$ and α_a denotes that the last diagonal element is a function of a. We obtain

$$A\mathbb{V}_{\tau+1} = \mathbb{V}_{\tau+1} \widehat{H}_{\tau+1}^a + \tilde{V}^a E_{\tau+1},$$

where $\mathbb{V}_{\tau+1} = [\mathbb{V}_\tau \ Z] \in \mathbb{R}^{n\times k(\tau+1)}$, and $\mathbb{V}_\tau$ and Z_τ are defined in (3.11) and (3.12), respectively. The trailing block vector, $\tilde{V}^a$, satisfies

$$\tilde{V}^a = \tilde{\psi}_{\tau+1}^a(A) V_0$$

for some Laurent polynomial $\tilde{\psi}_{\tau+1}^a \in \mathcal{L}_{m-1,im+2}$. Here $\tilde{V}^a$ is not chosen to satisfy an orthogonality condition, rather it is chosen so that $\tilde{\psi}_{\tau+1}^a(a) = 0$. This is the Radau condition. It guarantees that a is an eigenvalue of the modified recursion matrix (4.2). To determine the matrix (4.2), it suffices to consider the Radau modification of (3.15) with the partitioning

$$x \begin{bmatrix} \Phi_\tau(x) \\ \psi_\tau(x) \end{bmatrix} = \begin{bmatrix} H_\tau & \tilde{h}_{\tau+1,\tau} \boldsymbol{e}_\tau \\ \tilde{h}_{\tau+1,\tau} \boldsymbol{e}_\tau^T & \alpha_a \end{bmatrix} \begin{bmatrix} \Phi_\tau(x) \\ \psi_\tau(x) \end{bmatrix} + \begin{bmatrix} \mathbf{0} \\ \tilde{\psi}_{\tau+1}^a(x) \end{bmatrix}, \qquad \mathbf{0} \in \mathbb{R}^\tau.$$

The Radau condition with $x = a$ yields the linear system of equations

$$\begin{aligned} (H_\tau - aI)\Phi(a) &= -\tilde{h}_{\tau+1,\tau}\psi_\tau(a)\boldsymbol{e}_\tau, \\ \alpha_a \psi_\tau(a) &= a\psi_\tau(a) - \tilde{h}_{\tau+1,\tau}\boldsymbol{e}_\tau^T \Phi(a). \end{aligned}$$

Both equations are multiplied by $-\tilde{h}_{\tau+1,\tau}/\psi_\tau(a)$. The equation

$$(H_\tau - aI)\hat{\Phi}(a) = \tilde{h}_{\tau+1,\tau}^2 \boldsymbol{e}_\tau$$

then is solved for the vector $\hat{\Phi}(a)$, where $\hat{\Phi}(a) = -\tilde{h}_{\tau+1,\tau}\Phi(a)/\psi_\tau(a)$. It now follows from the second equation that

$$\alpha_a = a + \boldsymbol{e}_\tau^T \hat{\Phi}(a);$$

see [17, 18, 20, 22, 23, 31] for more details.

The value a in the above argument may be replaced by a value $b \geq \lambda_n$. This results in a modified recursion matrix $H_{\tau+1}^b$ with the trailing diagonal entry given by

$$\alpha_b = b + \boldsymbol{e}_\tau^T \hat{\Phi}(b).$$

In each case, the polynomials $\tilde{\psi}_{\tau+1}^a(x)$ and $\tilde{\psi}_{\tau+1}^b(x)$ have a zero at a and at b, respectively. The remaining τ zeros are distinct and lie in the interval (λ_1, λ_n); see [31]. This yields the $(\tau+1)$-point Gauss–Laurent–Radau rules $\boldsymbol{e}_1^T f(\hat{H}_{\tau+1}^a)\boldsymbol{e}_1$ and $\boldsymbol{e}_1^T f(\hat{H}_{\tau+1}^b)\boldsymbol{e}_1$ for the extended global Lanczos approximation of If defined by (1.11). The following bounds can be shown similarly as [31, Theorem 7.1].

Corollary 4.1. *Let f be a $2\tau+1$ times continuously differentiable function in the open interval (a, b). Assume that*

$$\frac{d^{2\tau+1}}{dx^{2\tau+1}} \left(x^{2(m-1)} f(x) \right) \geq 0$$

in this interval. Then

$$\boldsymbol{e}_1^T f(\hat{H}_{\tau+1}^a)\boldsymbol{e}_1 \leq \boldsymbol{v}^T f(A)\boldsymbol{v} \leq \boldsymbol{e}_1^T f(\hat{H}_{\tau+1}^b)\boldsymbol{e}_1. \tag{4.3}$$

The bounds will be illustrated in Section 6.

5. Estimating the error in Gauss–Laurent rules

Spalević [41, 42, 43] describes an approach to estimate the error in Gauss quadrature rules. Related results can be found in [11]. Extensions to Gauss–Szegő quadrature rules are discussed in [33]. This section presents an extension to Gauss–Laurent rules.

The matrices that arise in Spalević's approach to estimate the error in Gauss quadrature rules have the structure

$$\widehat{M} = \begin{bmatrix} M_1 & \beta_1 \boldsymbol{e}_\tau & O \\ \beta_1 \boldsymbol{e}_\tau^T & \alpha & \beta_2 \boldsymbol{e}_1^T \\ O & \beta_2 \boldsymbol{e}_1 & M_2 \end{bmatrix} \in \mathbb{R}^{(2\tau+1)\times(2\tau+1)}, \tag{5.1}$$

where $M_1, M_2 \in \mathbb{R}^{\tau\times\tau}$ are symmetric tridiagonal matrices with the same spectra and nonvanishing subdiagonal entries. Further, $\alpha, \beta_1, \beta_2 \in \mathbb{R}$ with $\beta_1\beta_2 \neq 0$, and $O \in \mathbb{R}^{\tau\times\tau}$ denotes the matrix of only zeros.

We will first discuss how the spectrum of the concatenated matrix $\widehat{M}$ relates to the spectrum of the matrix M_1. In our discussion, we will only require the matrices $M_1, M_2 \in \mathbb{R}^{\tau\times\tau}$ to be symmetric and have the same spectrum with distinct eigenvalues. To gain some insight into the spectrum of $\widehat{M}$, we apply a sequence of similarity transformations. Related transformations have been used by Borges and Gragg [7] in their development of a divide-and-conquer method for the computation of eigenvalues of a generalized eigenvalue problem with symmetric tridiagonal matrices. Basic results on arrowhead matrices, also referred to as bordered matrices, can be found in [45, pp. 94 ff.].

Theorem 5.1. *Let the matrix $\widehat{M} \in \mathbb{R}^{(2\tau+1)\times(2\tau+1)}$ have the structure* (5.1)*, where the symmetric matrices $M_1, M_2 \in \mathbb{R}^{\tau\times\tau}$ have the same spectra with distinct eigenvalues. Under suitable conditions on the eigenvectors of M_1 and M_2, the eigenvalues of M_1 are eigenvalues of $\widehat{M}$, and the remaining eigenvalues of $\widehat{M}$ interlace the eigenvalues of M_1.*

Proof. Introduce the spectral factorizations

$$M_1 = W_1 \Lambda W_1^T, \qquad M_2 = W_2 \Lambda W_2^T$$

with $\Lambda = \mathrm{diag}[\lambda_1, \lambda_2, \ldots, \lambda_\tau] \in \mathbb{R}^{\tau\times\tau}$ a diagonal matrix of eigenvalues and $W_1, W_2 \in \mathbb{R}^{\tau\times\tau}$ orthogonal matrices of eigenvectors. Define the block diagonal matrix

$$\widehat{W} = \begin{bmatrix} W_1 & & \\ & 1 & \\ & & W_2 \end{bmatrix} \in \mathbb{R}^{(2\tau+1)\times(2\tau+1)}$$

and the vectors $\boldsymbol{w}_1 = \beta_1 W_1^T \boldsymbol{e}_\tau$ and $\boldsymbol{w}_2 = \beta_2 W_2^T \boldsymbol{e}_1$. Here and below we do not explicitly mark zero-matrices. The matrix

$$\widehat{W}^T \widehat{M} \widehat{W} = \begin{bmatrix} \Lambda & \boldsymbol{w}_1 & \\ \boldsymbol{w}_1^T & \alpha & \boldsymbol{w}_2^T \\ & \boldsymbol{w}_2 & \Lambda \end{bmatrix} \tag{5.2}$$

is similar to (5.1) and has nontrivial entries only on the diagonal and in column and row $\tau + 1$. Clearly, if $\beta_1 = \beta_2 = 0$, then each eigenvalue of M_1 is an eigenvalue of $\widehat{M}$ of algebraic multiplicity two. In particular, the interlacing of eigenvalues in the statement of the theorem does not hold.

We turn to the situation when $\beta_1 \neq 0$ and $\beta_2 = 0$. Then, clearly, the eigenvalues of M_2 are eigenvalues of $\widehat{M}$. To secure that the remaining eigenvalues of $\widehat{M}$ interlace the eigenvalues of M_1, it suffices to require that all entries of the vector $\boldsymbol{w}_1$ are nonvanishing; see the discussion following eq. (5.5) below with the vector $\boldsymbol{w}$ replaced by $\boldsymbol{w}_1$.

The case when $\beta_1 = 0$ and $\beta_2 \neq 0$ can be treated similarly as above: we apply the permutation matrix

$$\widehat{P}_0 = [\boldsymbol{e}_{2\tau+1}, \boldsymbol{e}_{2\tau}, \ldots, \boldsymbol{e}_2, \boldsymbol{e}_1] \in \mathbb{R}^{(2\tau+1)\times(2\tau+1)}$$

from the right and from the left to the matrix (5.2) to obtain a matrix with the structure just considered. To secure that the eigenvalues of $\widehat{M}$ interlace the eigenvalues of M_1, it suffices to require that no entry of the vector $\boldsymbol{w}_2$ vanishes.

We turn to the situation when $\beta_1\beta_2 \neq 0$. Multiplication of the matrix (5.2) by the permutation matrix

$$\widehat{P} = [\boldsymbol{e}_1, \boldsymbol{e}_2, \ldots, \boldsymbol{e}_\tau, \boldsymbol{e}_{\tau+2}, \boldsymbol{e}_{\tau+3}, \ldots, \boldsymbol{e}_{2\tau+1}, \boldsymbol{e}_{\tau+1}] \in \mathbb{R}^{(2\tau+1)\times(2\tau+1)}$$

from the right and left gives the arrowhead matrix

$$\widehat{P}^T \widehat{W}^T \widehat{M} \widehat{W} \widehat{P} = \begin{bmatrix} \Lambda & & \boldsymbol{w}_1 \\ & \Lambda & \boldsymbol{w}_2 \\ \boldsymbol{w}_1^T & \boldsymbol{w}_2^T & \alpha \end{bmatrix}. \tag{5.3}$$

We now apply τ Givens rotations from the right to the columns j and $j + \tau$ of (5.3), for $j = 1, 2, \ldots, \tau$, to eliminate the vector $\boldsymbol{w}_1$ (and simultaneously modify the vector $\boldsymbol{w}_2$). The product of these Givens rotations is denoted by the matrix $\widehat{G} \in \mathbb{R}^{(2\tau+1)\times(2\tau+1)}$. We also multiply (5.3) by $\widehat{G}^T$ from the left. This defines a similarity transformation. The new matrix obtained is of the

form

$$\widehat{G}^T\widehat{P}^T\widehat{W}^T\widehat{M}\widehat{W}\widehat{P}\widehat{G} = \begin{bmatrix} \Lambda & & \mathbf{0} \\ & \Lambda & \boldsymbol{w} \\ \mathbf{0}^T & \boldsymbol{w}^T & \alpha \end{bmatrix}, \tag{5.4}$$

which shows that the eigenvalues of the matrix M_1 also are eigenvalues of $\widehat{M}$. The remaining $\tau+1$ eigenvalues of $\widehat{M}$ are the eigenvalues of the trailing $(\tau+1)\times(\tau+1)$ submatrix of (5.4). Assume that λ differs from all diagonal entries of Λ. Then

$$\begin{bmatrix} \Lambda & \boldsymbol{w} \\ \boldsymbol{w}^T & \alpha \end{bmatrix} - \lambda I = \begin{bmatrix} I & \mathbf{0} \\ \boldsymbol{w}^T(\Lambda-\lambda I)^{-1} & 1 \end{bmatrix} \begin{bmatrix} \Lambda-\lambda I & \boldsymbol{w} \\ \mathbf{0}^T & -s(\lambda) \end{bmatrix}, \tag{5.5}$$

where $s(\lambda)$ is the spectral function

$$s(\lambda) = \lambda - \alpha + \sum_{j=1}^{\tau} \frac{w_j^2}{\lambda_j - \lambda}, \qquad \boldsymbol{w} = [w_1, w_2, \ldots, w_\tau]^T. \tag{5.6}$$

The zeros of $s(\lambda)$ are eigenvalues of the matrix (5.5). If all entries w_j of $\boldsymbol{w}$ are nonvanishing, then $s(\lambda)$ has $\tau+1$ distinct zeros that interlace the diagonal entries of Λ. □

Borges and Gragg [7] considered the situation when the matrices M_1 and M_2 are symmetric and tridiagonal.

Corollary 5.2. *Let the matrices M_1 and M_2 be symmetric and tridiagonal with all subdiagonal entries nonvanishing. Let $\beta_1\beta_2 \neq 0$. Then the eigenvalues of M_1 are eigenvalues of $\widehat{M}$, and the remaining eigenvalues of $\widehat{M}$ interlace the eigenvalues of M_1.*

Proof. The eigenvectors of a symmetric tridiagonal matrix with non-vanishing subdiagonal entries have non-vanishing first and last entries. This secures that the function (5.6) has $\tau+1$ distinct zeros that interlace the eigenvalues of M_1. □

Spalević [41] obtained Corollary 5.2 from results by Peherstorfer [38] on orthogonal polynomials and quadrature. Theorem 5.1 is more general and provides an algebraic proof of Corollary 5.2.

The Gauss–Laurent quadrature rules of Section 3 are associated with pentadiagonal matrices H_τ, the entries of which are generated by Algorithm 3.1. The matrix associated with the generalized rule is

$$\widehat{H}_{2\tau+1} := \begin{bmatrix} H_\tau & \beta_1\boldsymbol{e}_\tau & O \\ \beta_1\boldsymbol{e}_\tau^T & \alpha & \beta_2\boldsymbol{e}_1^T \\ O & \beta_2\boldsymbol{e}_1 & PH_\tau P \end{bmatrix}, \tag{5.7}$$

where

$$P = [\boldsymbol{e}_\tau, \boldsymbol{e}_{\tau-1}, \boldsymbol{e}_{\tau-2}, \ldots, \boldsymbol{e}_2, \boldsymbol{e}_1].$$

It remains to determine the non-zero entries in the "cross" formed by the $(\tau+1)^{\text{st}}$ row and column of $\widehat{H}_{2\tau+1}$.

We first examine the Lanczos case, $i = 0$, developed by Spalević, in which H_τ is the tridiagonal Jacobi matrix. We denote the Lanczos polynomials by p_k, $k = 0, 1, \ldots, \tau, \tau+1$, where $p_k \in \mathbb{P}_k \perp \mathbb{P}_{k-1}$. The entries in the cross are determined by coefficients in the recursion formula for $p_{\tau+1}(x)$,

$$h_{\tau+1,\tau+2}p_{\tau+1}(x) = xp_\tau(x) - h_{\tau+1,\tau}p_{\tau-1}(x) - h_{\tau+1,\tau+1}p_\tau(x).$$

This yields

$$\alpha = h_{\tau+1,\tau+1}, \qquad \beta_1 = h_{\tau+1,\tau}, \qquad \beta_2 = h_{\tau+1,\tau+2}. \tag{5.8}$$

The matrix (5.7) contains the recursion coefficients for the polynomials

$$p_0, p_1, \ldots, p_{\tau+1}, \tilde{p}_{\tau+2}, \ldots, \tilde{p}_{2\tau+1}.$$

We refer to the polynomials $\tilde{p}_{\tau+2}, \tilde{p}_{\tau+3}, \ldots, \tilde{p}_{2\tau+1}$ as Spalević polynomials. Define the polynomial vector

$$\mathbf{P}_{2\tau+1}(x) = [p_0(x) \ldots p_{\tau+1}(x), \tilde{p}_{\tau+2}(x), \ldots, \tilde{p}_{2\tau}(x)]^T.$$

Our interest is in the orthogonality conditions satisfied by the Spalević polynomials. Consider the matrix formula

$$x\mathbf{P}_{2\tau+1}(x) = \widehat{H}_{2\tau+1}\mathbf{P}_{2\tau+1}(x) + \tilde{p}_{2\tau+1}(x)\boldsymbol{e}_{2\tau+1}.$$

Equating the $\tau+2, \tau+3, \ldots, 2\tau+1$ components on the left-hand side of the equation with those on the right-hand side yields the following recursion formulas:

$$\begin{aligned}
h_{\tau-1,\tau}\tilde{p}_{\tau+2}(x) &= xp_{\tau+1}(x) - h_{\tau+1,\tau+2}p_\tau(x) - h_{\tau,\tau}p_{\tau+1}(x), && (5.9)\\
h_{\tau-2,\tau-1}\tilde{p}_{\tau+3}(x) &= x\tilde{p}_{\tau+2}(x) - h_{\tau-1,\tau}p_{\tau+1}(x) \\
&\quad -h_{\tau-1,\tau-1}\tilde{p}_{\tau+2}(x), && (5.10)\\
&\vdots \\
h_{1,2}\tilde{p}_{2\tau}(x) &= x\tilde{p}_{2\tau-1}(x) - h_{2,3}\tilde{p}_{2\tau-2}(x) - h_{2,2}\tilde{p}_{2\tau-1}(x), \\
\tilde{p}_{2\tau+1}(x) &= x\tilde{p}_{2\tau}(x) - h_{1,2}\tilde{p}_{2\tau-1}(x) - h_{1,1}\tilde{p}_{2\tau}(x).
\end{aligned}$$

Consider the recursion relation (5.9) for $\tilde{p}_{\tau+2}(x)$:

$$\begin{aligned} h_{\tau-1,\tau}\tilde{p}_{\tau+2}(x) &= xp_{\tau+1}(x) - h_{\tau+1,\tau+2}p_\tau(x) - h_{\tau,\tau}p_{\tau+1}(x) \\ &= xp_{\tau+1}(x) - h_{\tau+1,\tau+2}p_\tau(x) - h_{\tau+2,\tau+2}p_{\tau+1}(x) \\ &\quad +(h_{\tau+2,\tau+2} - h_{\tau,\tau})p_{\tau+1}(x) \\ &= h_{\tau+1,\tau+2}p_{\tau+2}(x) + (h_{\tau+2,\tau+2} - h_{\tau,\tau})p_{\tau+1}(x), \end{aligned}$$

where we have used the recursion formula for the polynomial $p_{\tau+2}(x) \in \mathbb{P}_{\tau+2} \perp \mathbb{P}_{\tau+1}$ in the orthogonal Lanczos sequence. In other words, $\tilde{p}_{\tau+2}(x)$ is a linear combination of $p_{\tau+1}(x)$ and $p_{\tau+2}(x)$ and, hence, satisfies $\tilde{p}_{\tau+2}(x) \in \mathbb{P}_{\tau+2} \perp \mathbb{P}_\tau$.

Consider now the recursion formula (5.10) for $\tilde{p}_{\tau+3}(x)$. This polynomial is a linear combination of $x\tilde{p}_{\tau+2}(x)$, $p_{\tau+1}(x)$, and $\tilde{p}_{\tau+2}(x)$. Its degree and orthogonality conditions depend on $x\tilde{p}_{\tau+2}(x)$. Clearly, it is of degree $\tau+2$. The orthogonality condition satisfied by $\tilde{p}_{\tau+2}(x)$ is determined by

$$(q, x\tilde{p}_{\tau+2}(x)) = 0 \qquad q \in P_{\tau-1}.$$

But $(q, x\tilde{p}_{\tau+2}(x))$ is not necessarily 0 if $q \in \mathbb{P}_\tau$. Hence, $\tilde{p}_{\tau+3}(x) \in \mathbb{P}_{\tau+3} \perp \mathbb{P}_{\tau-1}$. The argument can be repeated with the remaining Spalević polynomials,

$$\tilde{p}_{\tau+k}(x) \in \mathbb{P}_{\tau+k} \perp \mathbb{P}_{\tau-k+2} \qquad k = 2, 3, \ldots, \tau+1.$$

This yields the following result.

Lemma 5.3. *The Spalević polynomial $\tilde{p}_{2\tau+1}(x)$ has degree $2\tau+1$ and is orthogonal to linear functions with respect to the measure $\mathrm{d}\mu(\lambda)$. Its zeros are the eigenvalues of $\widehat{H}_{2\tau+1}$; by Theorem 5.1, they are distinct. Denote them in increasing order by $x_1, x_2, \ldots, x_{2\tau}, x_{2\tau+1}$. Then $\tilde{p}_{2\tau+1}(x) = p_\tau(x)q(x)$ for some $q \in \mathbb{P}_{\tau+1}$. The interlacing property stated in Theorem 5.1 guarantees that the zeros of p_τ are those with even index and the ones of q are those with odd index.*

We proceed analogously when $i > 0$. The eigenvalues of H_τ are the zeros of $\psi_\tau \in \mathcal{L}_{m-1,im+1} \perp \mathcal{L}_{m-1,im}$ in (3.15). We have

$$\tilde{h}_{\tau+1,\tau}\psi_\tau = h_{\tau+1,\tau}\phi_{-m} + h_{\tau+2,\tau}\phi_{im+1}, \tag{5.11}$$

where $\tilde{h}_{\tau+1,\tau}$ is given by (3.14). The next polynomial in the orthogonal Laurent sequence is $\phi_{-m} \in \mathcal{L}_{m,im} \perp \mathcal{L}_{m-1,im}$, in which the denominator power is incremented. However, if we proceed by analogy, it is necessary

to determine the recursion coefficients used to compute a function $\psi_{\tau+1} \in \mathcal{L}_{m-1,im+2} \perp \mathcal{L}_{m-1,im+1}$. It will satisfy a three-term recursion formula

$$\tilde{h}_{\tau+2,\tau+1}\psi_{\tau+1} = x\psi_\tau - \tilde{h}_{\tau+1,\tau}\phi_{im} - \tilde{h}_{\tau+1,\tau+1}\psi_\tau. \tag{5.12}$$

The entries in the cross are the recursion coefficients

$$\alpha = \tilde{h}_{\tau+1,\tau+1}, \qquad \beta_1 = \tilde{h}_{\tau+1,\tau}, \qquad \beta_2 = \tilde{h}_{\tau+1,\tau+2},$$

where $\beta_1 = \tilde{h}_{\tau+1,\tau}$ is given by (3.14) and $\alpha = \tilde{h}_{\tau+1,\tau+1}$ equals $(x\psi_\tau, \psi_\tau)$. The latter can be determined by the orthogonality of the polynomials in the recursion formula (5.12),

$$\tilde{h}_{\tau+1,\tau+1} = (h^2_{\tau+1,\tau}h_{\tau+1,\tau+1}+2h_{\tau+1,\tau}h_{\tau+2,\tau}h_{\tau+1,\tau+2}+h^2_{\tau+2,\tau}h_{\tau+2,\tau+2})/\tilde{h}^2_{\tau+1,\tau}.$$

Observe that these assignments are equivalent to β_1 and α in (5.8) since in the case of $i = 0$, $h_{j,j+k} = 0$ for $|k| \geq 2$. The last entry in the cross, $\beta_2 = \tilde{h}_{\tau+2,\tau+1}$, is the norm of the monic polynomial $\psi_{\tau+1}$. This too is equivalent to the case $i = 0$, since $h_{\tau+2,\tau+1}$ is the norm of the $(\tau+1)^{\text{st}}$ monic orthogonal polynomial in the Lanczos sequence.

We denote the Laurent–Spalević polynomials by $\tilde{\psi}_{\tau+k}$, $k = 2, \ldots, \tau+1$. The denominator power of these polynomials remain a constant $m-1$. The numerator power increases by one at each step so that $\tilde{\psi}_{\tau+k} \in \mathcal{L}_{m-1,im+k+1}$, $k = 2, \ldots, \tau+1$. The analysis of these polynomials follows from considering the Lanczos polynomials $\breve{p}_k(x)$, which are orthogonal with respect to the positive measure $d\mu(x)/x^{m-1}$. They are of degree k and are orthogonal to $\mathcal{L}_{m-1,k-m}$ with respect to the original measure $d\mu(x)$. The non-zero entries of the tridiagonal Jacobi matrix, $\breve{T}_\tau$, are the recursion coefficients for $\breve{p}_k(x)$, $k = 0, 1, 2, \ldots, \tau-1$. Its eigenvalues are the zeros of $\breve{p}_\tau(x)$. It is shown in [32] that the spectra of $\breve{T}_\tau$ and H_τ are identical but differ for dimensions larger than τ. This is because the Laurent process increments the denominator power at the next step, whereas the denominator power remains constant in the rational Lanczos scheme. However, the denominator power is not incremented in the Spalević method. We conclude that the spectra of $\widehat{H}_{2\tau+1}$ and of the matrix $\widehat{M}$ of (5.1) are the same where M_1 and M_2 are constructed from $\breve{T}_\tau$ and the cross entries are determined from the recursion coefficients that generate $\breve{p}_{\tau+1}(x)$ as outlined in the case for $i = 0$. In particular, the zeros of the Spalević polynomial $\tilde{\psi}_{2\tau+1} \in \mathcal{L}_{m-1,im+\tau+2}$ are the eigenvalues of $\widehat{H}_{2\tau+1}$ and retain one degree of orthogonality with respect to $d\mu(x)$. This discussion yields the following theorem.

Theorem 5.4. *(Spalević–Laurent quadrature) Define the quadrature rule*

$$\widehat{\mathcal{H}}_{2\tau+1}(f) = \boldsymbol{e}_1^T f(\widehat{H}_{2\tau+1})\boldsymbol{e}_1. \tag{5.13}$$

Then

$$\mathcal{I}(f) = \widehat{\mathcal{H}}_{2\tau+1}(f) \qquad \forall f \in \mathcal{L}_{2m-2,2mi+4}, \tag{5.14}$$

Proof. The last Spalević polynomial in the sequence satisfies

$$\tilde{\psi}_{2\tau+1}(x) = \frac{P(x)}{x^{2m-1}}, \qquad P \in \mathbb{P}_{2\tau+1},$$

where the zeros of P are the eigenvalues of $\widehat{H}_{2\tau+1}$. By Theorem 5.1, it has $2\tau+1$ distinct zeros and, hence, the rule (5.13) is interpolatory. By Lemma 5.3, it is orthogonal to $\mathbb{P}_1$. Invoking [18, Theorem 1.45], the rule is exact for polynomials of degree $2\tau+1-1+2$ or $2\tau+2$ with respect to the measure $d\mu(x)/x^{m-1}$. This yields $2m-2$ denominator plus $2mi+4$ numerator degrees of accuracy with respect to the original measure $d\mu(x)$. □

Example 5.1. Consider the matrix $\widehat{H}_{2\tau+1}$ for $i = 1$ and $m = 2$. Then $\tau = 4$ and the rule $\boldsymbol{e}_1^T \widehat{H}_9 \boldsymbol{e}_1$ will be exact for Laurent polynomials in $\mathcal{L}_{2,8}$. The matrix $\widehat{H}_9$ may have non-vanishing entries in the positions marked by "$*$". The circled entries comprise the cross.

$$\widehat{H}_9 = \begin{bmatrix}
* & * & & & & & & & \\
* & * & * & * & & & & & \\
 & * & * & * & & & & & \\
 & * & * & * & \circledast & & & & \\
 & & & \circledast & \circledast & \circledast & & & \\
 & & & & \circledast & * & * & * & \\
 & & & & & * & * & * & \\
 & & & & & * & * & * & * \\
 & & & & & & & * & *
\end{bmatrix}.$$

□

6. Numerical examples

The computations in this section are performed using MATLAB with about 15 significant decimal digits. The first two examples compare the performance of the standard global Lanczos method ($i = 0$) with the global rational Lanczos methods for the cases $i = 1, 2, 3$. In all computed examples, we use Krylov subspaces of dimension $\tau = 12, 24, 36, 48$, and 60. These dimensions are divisible by 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 $\mathcal{I}f$, given by (1.11), as well as approximations $\mathcal{H}_\tau f$ given by (3.6). The figures display the errors $|\mathcal{I}f - \mathcal{H}_\tau f|$ in logarithmic scale for all methods. All matrix functions are computed by means of the spectral decomposition of the matrix.

Example 6.1. Let A be the symmetric positive definite tridiagonal Toeplitz matrix $[-1, 2, -1]$ of order 3000 and $f(x) = \exp(-x)/\sqrt{x}$. The block vector $W \in \mathbb{R}^{3000\times 4}$ has normally distributed random entries with mean zero and variance one. Figure 6.1 compares the errors in approximations of the different methods applied to the function $f(x) = \exp(-x)/\sqrt{x}$. The increase in the denominator power for each of the rational Lanczos methods speeds up the convergence, whereas the standard Lanczos method gives a much larger approximation error in the allotted number of iterations. □

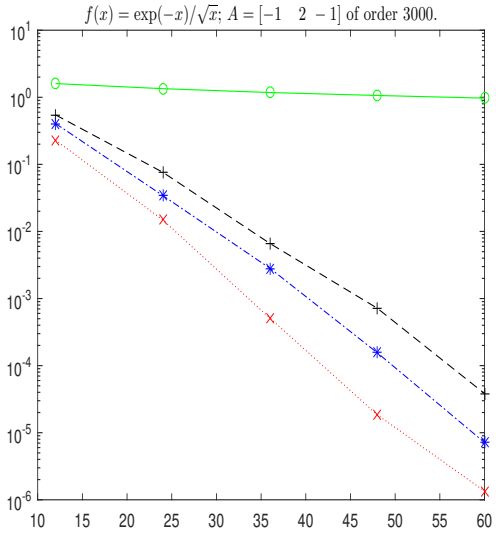

Figure 6.1: Example 6.1: Errors in approximations of $f(x) = \exp(-x)/\sqrt{x}$ for Lanczos ($\circ-\circ$), $i = 1(\times\cdots\times)$, $i = 2(+\,--+)$,and $i = 3(*-\cdot-*)$ for subspaces of dimension $\tau = 12, 24, 36, 48, 60$.

Example 6.2. 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 60 equally spaced interior nodes in each space dimension. Homogeneous boundary conditions are used. This yields a 3600×3600 symmetric positive definite matrix A. The initial block vector $W \in \mathbb{R}^{3600\times 4}$ for the standard

and rational Lanczos processes is chosen to be the unit vector with all entries $1/\sqrt{60}$. Figure 6.2 compares the errors in approximations of the different methods applied to the function $f(x) = \ln(x)$. As in the previous example, the increase in the denominator power for each of the rational Lanczos methods speeds up the convergence. The errors in approximations determined by the standard Lanczos method are decreasing, but much slower than the errors in approximations determined by the rational methods. □

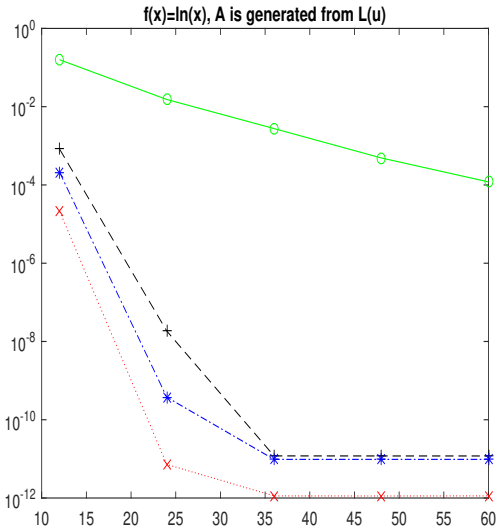

Figure 6.2: Example 6.2: Errors in approximations of $f(x) = \ln(x)$ for Lanczos ($\circ\!-\!\circ$), $i = 1(\times \cdots \times)$, $i = 2(+--+)$,and $i = 3(*-\!-\!*)$ for subspaces of dimension $\tau = 12, 24, 36, 48, 60$.

Example 6.3. The purpose of this example is to illustrate the bounds (4.1) and (4.3). The function $f(x) = \exp(x)$ satisfies the conditions stated in Theorem 4.1 and Corollary 4.1. We apply f to the symmetric positive definite Toeplitz matrix $A \in \mathbb{R}^{3000\times 3000}$ with entries $a_{j,k} = 1/(1 + |j - k|)$. The vector $W \in \mathbb{R}^{3000\times 4}$ has normally distributed random entries with mean zero and variance one. We remark that fast direct solution methods are available for linear systems of equations with this kind of matrix; see, e.g., [1, 44]. Table 6.1 displays the residuals

$$\mathrm{res}(H_i) = \mathcal{I}f - \boldsymbol{e}_1^T f(H_i)\boldsymbol{e}_1 \tag{6.1}$$

for $\tau = 4, 8, 12$, and for $i = 0$ (Lanczos) and $i = 1$. The column headings indicate the matrix used in the argument of res(·). The smallest eigenvalue

of A is $\lambda_1 = 0.3863$ and the largest one is $\lambda_{3000} = 14.3174$. We chose the Radau parameters $a = 0.3$ and $b = 14.5$. The order of the Radau matrices, H_i^a and H_i^b, is $\tau + 1$. The signs of the residuals are in accordance with the bounds of Section 4. □

τ	$H_{i=0}$	$\tilde{H}^a_{i=0}$	$\tilde{H}^b_{i=0}$	$H_{i=1}$	$\tilde{H}^a_{i=1}$	$\tilde{H}^b_{i=1}$
4	$1 \cdot 10^{2}$	$5 \cdot 10^{1}$	$-3 \cdot 10^{1}$	$5 \cdot 10^{2}$	$3 \cdot 10^{2}$	$-1 \cdot 10^{2}$
8	$9 \cdot 10^{-4}$	$2 \cdot 10^{-4}$	$-2 \cdot 10^{0}$	$3 \cdot 10^{0}$	$8 \cdot 10^{-1}$	$-3 \cdot 10^{1}$
12	$9 \cdot 10^{-11}$	$1 \cdot 10^{-11}$	$-3 \cdot 10^{-11}$	$2 \cdot 10^{-3}$	$5 \cdot 10^{-4}$	$-1 \cdot 10^{-3}$

Table 6.1: Example 6.3: Residuals in Gauss–Laurent and Gauss–Radau rules. The Radau nodes are fixed at $a = 0.3$ and $b = 14.5$. The matrix A is a positive definite Toeplitz matrix and $f(x) = \exp(x)$.

Example 6.4. We consider the Toeplitz matrix and initial vector, W, of Example 6.3 with the prescribed Radau nodes. The function $f(x) = \exp(x)/x$ has a pole at $x = 0$ and the derivatives change signs. Table 6.2 displays the residuals (6.1) in the approximations determined by the upper and lower Radau rules for $i = 0$, $i = 1$ and $i = 3$. The denominator power is the largest for $i = 1$, but $i = 3$ exhibits superior convergence properties for this example. □

τ	$\tilde{H}^a_{i=0}$	$\tilde{H}^b_{i=0}$	$\tilde{H}^a_{i=1}$	$\tilde{H}^b_{i=1}$	$\tilde{H}^a_{i=3}$	$\tilde{H}^b_{i=3}$
8	$-1 \cdot 10^{-2}$	$4 \cdot 10^{-3}$	$3 \cdot 10^{-2}$	$-7 \cdot 10^{-2}$	$1 \cdot 10^{-4}$	$-3 \cdot 10^{-4}$
12	$5 \cdot 10^{-3}$	$2 \cdot 10^{-4}$	$2 \cdot 10^{-6}$	$-4 \cdot 10^{-5}$	$7 \cdot 10^{-10}$	$-2 \cdot 10^{-9}$
16	$-2 \cdot 10^{-5}$	$9 \cdot 10^{-6}$	$2 \cdot 10^{-9}$	$-7 \cdot 10^{-9}$	$-2 \cdot 10^{-12}$	$1 \cdot 10^{-12}$

Table 6.2: Example 6.4: Residuals in Gauss–Laurent and Gauss–Radau rules. The Radau nodes are fixed at $a = 0.3$ and $b = 14.5$. The matrix A is a positive definite Toeplitz matrix and $f(x) = \exp(x)/x$.

Example 6.5. Table 6.3 compares the approximations of $\mathcal{I}(f)$ using the Gauss-Laurent methods for $i = 0$, $i = 2$, and $i = 5$ along with those resulting from the accompanying Spalević matrices for each case. The function $f(x) = 1/\sqrt{x}$ is applied to the matrix A resulting from the discretization of the $L(u)$ operator along with the block vector W defined in Example 6.2. The Gauss-Laurent matrices are denoted by $H_{i=j}$, $j = 0, 2, 5$, and the associated Spalević matrices are denoted by $\widehat{H}_{i=j}$. The values of τ are chosen so that τ is an integral multiple of six. This assures that the denominator degree of the rational Lanczos methods considered increases by at least one in each step.

The matrices $H_{i=0}$ and $H_{i=5}$ are identical for $\tau = 6$ since the denominator power is zero for the case $i = 5$ and for this value of τ. The Spalević rules match an additional moment and consequently perform slightly better. □

τ	$H_{i=0}$	$\widehat{H}_{i=0}$	$H_{i=2}$	$\widehat{H}_{i=2}$	$H_{i=5}$	$\widehat{H}_{i=5}$
6	$1 \cdot 10^{0}$	$4 \cdot 10^{-1}$	$2 \cdot 10^{-2}$	$7 \cdot 10^{-4}$	$1 \cdot 10^{0}$	$4 \cdot 10^{-1}$
12	$5 \cdot 10^{-1}$	$2 \cdot 10^{-1}$	$1 \cdot 10^{-4}$	$1 \cdot 10^{-5}$	$5 \cdot 10^{-3}$	$3 \cdot 10^{-4}$
18	$2 \cdot 10^{-1}$	$4 \cdot 10^{-2}$	$8 \cdot 10^{-6}$	$4 \cdot 10^{-9}$	$1 \cdot 10^{-4}$	$8 \cdot 10^{-6}$
24	$7 \cdot 10^{-2}$	$1 \cdot 10^{-2}$	$1 \cdot 10^{-10}$	$2 \cdot 10^{-11}$	$1 \cdot 10^{-6}$	$8 \cdot 10^{-8}$

Table 6.3: Example 6.5: Residuals in Gauss–Laurent and Spalević rules. The matrix $A \in \mathbb{R}^{3600\times 3600}$ is generated from the $L(u)$ operator and $f(x) = 1/\sqrt{x}$.

Example 6.6. This example retains the same function and matrix used in Example 6.5. Table 6.4 compares the difference

$$\mathcal{E}_{\tau}^{i=k} = \boldsymbol{e}_1^T \widehat{H}_{2\tau+1}^{i=k} \boldsymbol{e}_1 - \boldsymbol{e}_1^T H_{\tau+1}^{i=k} \boldsymbol{e}_1$$

for $i = 0$, $i = 2$, and $i = 5$. The matrix $H_{\tau+1}^{i=k}$ is of order $\tau + 1$ and its eigenvalues are the roots of $\psi_{\tau+1} \in \mathcal{L}_{m-1,im+2} \perp \mathcal{L}_{m-1,im+1}$ in (5.12). The rule $\boldsymbol{e}_1^T H_{\tau+1}^{i=k} \boldsymbol{e}_1$ will be exact for $f \in \mathcal{L}_{2m-2,2mi+3}$. □

τ	$\mathcal{E}_{\tau}^{i=0}$	$\mathcal{E}_{\tau}^{i=2}$	$\mathcal{E}_{\tau}^{i=5}$
6	$1 \cdot 10^{0}$	$1 \cdot 10^{-2}$	$1 \cdot 10^{0}$
12	$5 \cdot 10^{-1}$	$1 \cdot 10^{-4}$	$3 \cdot 10^{-3}$
18	$2 \cdot 10^{-1}$	$1 \cdot 10^{-7}$	$5 \cdot 10^{-5}$
24	$4 \cdot 10^{-2}$	$1 \cdot 10^{-10}$	$6 \cdot 10^{-7}$

Table 6.4: Example 6.6: Difference between rules $\boldsymbol{e}_1^T \widehat{H}_{2\tau+1}^{i=k}$ and $\boldsymbol{e}_1^T H_{\tau+1}^{i=k} \boldsymbol{e}_1$. The matrix $A \in \mathbb{R}^{3600\times 3600}$ is generated from the $L(u)$ operator and $f(x) = 1/\sqrt{x}$.

7. Conclusion

Recurrence relations for extended global Lanczos methods with the numerator degree roughly an arbitrary integer multiple of the denominator degree are described. Error bounds determined by pairs of Gauss–Laurent and Gauss–Laurent–Radau rules are discussed. These bounds apply to certain integrands. Error estimates for more general integrands are developed. These estimates generalize error estimates for Gauss quadrature rules developed by Spalević.

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