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Monotone convergence of the extended Krylov subspace method for Laplace–Stieltjes functions of Hermitian positive definite matrices☆

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Abstract

The extended Krylov subspace method is known to be very efficient in many cases in which one wants to approximate the action of a matrix function $f(A)$ on a vector $\boldsymbol{b}$, in particular when f belongs to the class of Laplace–Stieltjes functions. We prove that the Euclidean norm of the error decreases monotonically in this situation when A is Hermitian. Similar results are known for the (polynomial) Lanczos method for $f(A)\boldsymbol{b}$, and we demonstrate how the techniques of proof used in the polynomial Krylov case can be transferred to the extended Krylov case.

Keywords: matrix function, extended Krylov subspace, monotone convergence, Laplace–Stieltjes function, matrix exponential
2010 MSC: 65F30, 65F50, 65F60

1. Introduction

The extended Krylov subspace method has proven to be a very efficient method for approximating $f(A)\boldsymbol{b}$—the action of a matrix function on a vector—in many situations, see, e.g., [1–3] and the references therein. One situation in which extended Krylov subspace methods are particularly attractive and well-analyzed is when f is a *Cauchy–Stieltjes function*, i.e.,

$$f(z) = \int_0^\infty \frac{1}{z+t}\,\mathrm{d}\mu(t),$$

where μ is a nonnegative, monotonically increasing function, see, e.g., [2]. In this paper, we are concerned with the more general class of *Laplace–Stieltjes* functions [4, 5], which can be characterized as

$$f(z) = \int_0^\infty \exp(tz)\,\mathrm{d}\mu(t). \tag{1}$$

For examples of Cauchy–Stieltjes and Laplace–Stieltjes functions, see, e.g., [6–9] and the references therein. One can show that every Cauchy–Stieltjes function is a Laplace–Stieltjes function, but not vice versa, see, e.g, [6, 10]. The representation (1) allows us to base our results on an analysis of the extended Krylov subspace method for the exponential function. The main result of this paper is a proof that the extended Krylov subspace method for Hermitian positive definite A and f a Laplace–Stieltjes function always converges monotonically (i.e., the Euclidean norm of the error decreases monotonically from one iteration to the next). Results of this type are known for the (polynomial) Lanczos method, see [8, 11], and we will also transfer some of the techniques of proof from these papers to our situation.

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Algorithm 1: Extended Lanczos method from [15]

Input: $i, m \in \mathbb{N}$, $A \in \mathbb{C}^{n\times n}$ Hermitian positive definite, $\boldsymbol{b} \in \mathbb{C}^n$

Output: Orthonormal basis $(\boldsymbol{v}_k)_{k=-m,\dots,im+1}$ of $\mathcal{K}_m^{im+1}(A, \boldsymbol{b})$

$\boldsymbol{v}_{-1} \leftarrow \boldsymbol{0}$;
$\delta_0 \leftarrow \|\boldsymbol{b}\|_2$; $\boldsymbol{v}_0 \leftarrow \boldsymbol{b}/\delta_0$;
for $k = 0, \dots, m-1$ **do**
  $\boldsymbol{u} \leftarrow A\boldsymbol{v}_{-k}$;
  $\alpha_{-k,ik} \leftarrow \boldsymbol{v}_{ik}^H \boldsymbol{u}$; $\boldsymbol{u} \leftarrow \boldsymbol{u} - \alpha_{-k,ik}\boldsymbol{v}_{ik}$;
  $\alpha_{-k,-k} \leftarrow \boldsymbol{v}_{-k}^H \boldsymbol{u}$; $\boldsymbol{u} \leftarrow \boldsymbol{u} - \alpha_{-k,-k}\boldsymbol{v}_{-k}$;
  $\delta_{ik+1} = \|\boldsymbol{u}\|_2$; $\boldsymbol{v}_{ik+1} \leftarrow \boldsymbol{u}/\delta_{ik+1}$;
  if $i \geq 2$ **then**
    $\boldsymbol{u} \leftarrow A\boldsymbol{v}_{ik+1}$;
    $\alpha_{ik+1,ik} \leftarrow \boldsymbol{v}_{ik}^H \boldsymbol{u}$; $\boldsymbol{u} \leftarrow \boldsymbol{u} - \alpha_{ik+1,ik}\boldsymbol{v}_{ik}$;
    $\alpha_{ik+1,-k} \leftarrow \boldsymbol{v}_{-k}^H \boldsymbol{u}$; $\boldsymbol{u} \leftarrow \boldsymbol{u} - \alpha_{ik+1,-k}\boldsymbol{v}_{-k}$;
    $\alpha_{ik+1,ik+1} \leftarrow \boldsymbol{v}_{ik+1}^H \boldsymbol{u}$; $\boldsymbol{u} \leftarrow \boldsymbol{u} - \alpha_{ik+1,ik+1}\boldsymbol{v}_{ik+1}$;
    $\delta_{ik+2} = \|\boldsymbol{u}\|_2$; $\boldsymbol{v}_{ik+2} \leftarrow \boldsymbol{u}/\delta_{ik+2}$;
  for $j = 3, \dots, i$ **do**
    $\boldsymbol{u} \leftarrow A\boldsymbol{v}_{ik+j-1}$;
    $\alpha_{ik+j-1,ik+j-2} \leftarrow \boldsymbol{v}_{ik+j-2}^H \boldsymbol{u}$; $\boldsymbol{u} \leftarrow \boldsymbol{u} - \alpha_{ik+j-1,ik+j-2}\boldsymbol{v}_{ik+j-2}$;
    $\alpha_{ik+j-1,ik+j-1} \leftarrow \boldsymbol{v}_{ik+j-1}^H \boldsymbol{u}$; $\boldsymbol{u} \leftarrow \boldsymbol{u} - \alpha_{ik+j-1,ik+j-1}\boldsymbol{v}_{ik+j-1}$;
    $\delta_{ik+j} = \|\boldsymbol{u}\|_2$; $\boldsymbol{v}_{ik+j} \leftarrow \boldsymbol{u}/\delta_{ik+j}$;
  $\boldsymbol{w} \leftarrow A^{-1}\boldsymbol{v}_{i(k+1)}$;
  $\beta_{i(k+1),-k} \leftarrow \boldsymbol{v}_{-k}^H \boldsymbol{w}$; $\boldsymbol{w} \leftarrow \boldsymbol{w} - \beta_{i(k+1),-k}\boldsymbol{v}_{-k}$;
  for $j = 0, \dots, i-1$ **do**
    $\beta_{i(k+1),i(k+1)-j} \leftarrow \boldsymbol{v}_{i(k+1)-j}^H \boldsymbol{w}$; $\boldsymbol{w} \leftarrow \boldsymbol{w} - \beta_{i(k+1),i(k+1)-j}\boldsymbol{v}_{i(k+1)-j}$;
  $\delta_{-(k+1)} = \|\boldsymbol{w}\|_2$; $\boldsymbol{v}_{-(k+1)} \leftarrow \boldsymbol{w}/\delta_{-(k+1)}$;

The remainder of this paper is organized as follows. In Section 2, we introduce extended Krylov subspaces and review some basic facts about them on which our results are based. In Section 3 we prove our main result by investigating structural properties of the projection of A onto the Krylov subspace. Concluding remarks are given in Section 4.

2. Extended Krylov subspaces

Extended Krylov subspaces are a special case of *rational Krylov subspaces* [12, 13], in which only the shifts 0 and ∞ are used, i.e., they are built with respect to powers of A and A^{-1}. In the context of approximating matrix functions, they were first considered in [1] and have since then enjoyed much attention in the literature, see, e.g., [2, 3, 14–17].

The (p, q)th extended Krylov subspace with respect to $A \in \mathbb{C}^{n\times n}$ and $\boldsymbol{b} \in \mathbb{C}^n$ is defined by

$$\mathcal{K}_m^p(A, \boldsymbol{b}) = \{\phi(A)\boldsymbol{b} : \phi \in \mathcal{L}_m^p\},$$

where

$$\mathcal{L}_m^p = \operatorname{span}\{z^{-m}, z^{-m+1}, \dots, z^{-1}, 1, z, z^2, \dots, z^p\}$$

denotes the space of *Laurent polynomials* of denominator degree at most m and numerator degree at most p. Particular attention is devoted to the situation that $p = im + 1$ for some $i \in \mathbb{N}$ in the literature, see, e.g. [15]. In this case, an orthonormal basis of $\mathcal{K}_m^p(A, \boldsymbol{b})$ can efficiently be computed by a block-Lanczos-type method when A is Hermitian positive definite, see [15], given as Algorithm 1.

We collect the basis computed by Algorithm 1 in the matrix

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

and define

$$H_{m(i+1)} = V_{m(i+1)}^H A V_{m(i+1)}. \tag{2}$$

Then, $A, V_{m(i+1)}$ and $H_{m(i+1)}$ fulfill the extended Lanczos relation

$$AV_{m(i+1)} = V_{m(i+1)}H_{m(i+1)} + \boldsymbol{z}_{m(i+1)}\boldsymbol{e}_{m(i+1)}^H, \tag{3}$$

where $\boldsymbol{z}_{m(i+1)}$ is a linear combination of $\boldsymbol{v}_{-m}$ and $\boldsymbol{v}_{im+1}$; see [15].

In [15], recursion formulas for the entries $h_{j,k}$ of $H_{m(i+1)}$ are derived. Of particular interest in our situation are the formulas

$$\begin{aligned} h_{(i+1)k+j+1,(i+1)k+j} &= h_{(i+1)k+j,(i+1)k+j+1} = \delta_{ik+j} \quad &&, j = 1, \ldots, i, k = 0, \ldots, m-1 \\ h_{(i+1)k+1,(i+1)k} &= h_{(i+1)k,(i+1)k+1} \quad = \alpha_{-k,ik} &&, k = 1, \ldots, m-1 \\ h_{(i+1)k+2,(i+1)k} &= h_{(i+1)k,(i+1)k+2} \quad = \alpha_{ik+1,ik} &&, k = 1, \ldots, m-1 \end{aligned} \tag{4}$$

for the nonzero off-diagonal entries of $H_{m(i+1)}$. These provide information on the signs of the entries of $H_{m(i+1)}$, which we need to prove our main result in Section 3.

Proposition 1. *Let $A \in \mathbb{C}^{n\times n}$ be Hermitian positive definite, $\boldsymbol{b} \in \mathbb{C}^n$ and let $H_{m(i+1)}$ be given by* (2)*. Then all entries of $H_{m(i+1)}$ are real, all diagonal entries are nonnegative and the off-diagonal entries fulfill*

$$\begin{aligned} h_{(i+1)k+j+1,(i+1)k+j} &= h_{(i+1)k+j,(i+1)k+j+1} \geq 0, j = 1, \ldots, i, k = 0, \ldots, m-1 \\ h_{(i+1)k+1,(i+1)k} &= h_{(i+1)k,(i+1)k+1} \quad \leq 0, k = 1, \ldots, m-1 \\ h_{(i+1)k+2,(i+1)k} &= h_{(i+1)k,(i+1)k+2} \quad \leq 0, k = 1, \ldots, m-1 \end{aligned} \tag{5}$$

Proof. All diagonal entries of $H_{m(i+1)}$ are of the form $\boldsymbol{v}_i^H A\boldsymbol{v}_i$, which is nonnegative because A is Hermitian positive definite.

The first inequality in (5) follows directly from the first inequality in (4) by noting that δ_{ik+j} is defined as the norm of a vector in Algorithm 1. To prove the second inequality in (5), we use the recursion relation

$$\delta_{-k}\boldsymbol{v}_{-k} = A^{-1}\boldsymbol{v}_{ik} - \beta_{ik,-k}\boldsymbol{v}_{-(k-1)} - \sum_{j=0}^{i-1} \beta_{ik,ik-j}\boldsymbol{v}_{ik-j}$$

for the basis vectors in Algorithm 1. Left-multiplying by $\boldsymbol{v}_{ik+1}^H A$ gives

$$\delta_{-k}\boldsymbol{v}_{ik+1}^H A\boldsymbol{v}_{-k} = -\beta_{ik,-k}\boldsymbol{v}_{ik+1}^H A\boldsymbol{v}_{-(k-1)} - \sum_{j=0}^{i-1} \beta_{ik,ik-j}\boldsymbol{v}_{ik+1}^H A\boldsymbol{v}_{ik-j}. \tag{6}$$

Inserting recursion relations from Algorithm 1 again for all terms of the form $A\boldsymbol{v}_\ell$ in (6) and using the orthogonality of the basis vectors then gives

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

Again, $\delta_{-k} \geq 0, \delta_{ik+1} \geq 0$ is obvious, and $\beta_{ik} = \boldsymbol{v}_{ik}^H A^{-1}\boldsymbol{v}_{ik} \geq 0$ because A^{-1} is positive definite, so that $\alpha_{ik+1,ik} \leq 0$. Similarly,

$$\alpha_{-k,ik} = -\frac{\delta_{-k}\alpha_{-k}}{\beta_{ik,ik}},$$

and $\alpha_{-k,-k} = \boldsymbol{v}_{-k}^H A\boldsymbol{v}_{-k} \geq 0$ because A is positive definite. This concludes the proof of the proposition. □

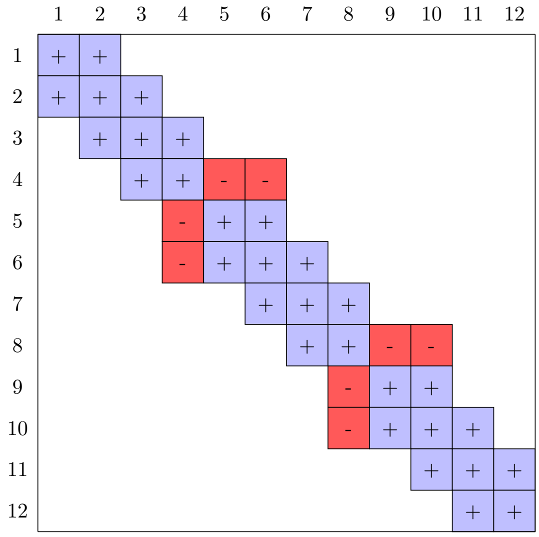

Figure 1: Sign structure of $H_{m(i+1)}$ for $m = 3, i = 3$.

The sign-structure of $H_{m(i+1)}$ given in Proposition 1 is illustrated in Figure 1 for $m = 3, i = 3$.

Given the quantities from the decomposition (3), one defines the extended Lanczos approximation for $f(A)\boldsymbol{b}$ as

$$\boldsymbol{f}_{m(i+1)} = \|\boldsymbol{b}\|_2 V_{m(i+1)} f(H_{m(i+1)}) \boldsymbol{e}_1. \tag{7}$$

When f is a Laplace–Stieltjes function of the form (1), we can rewrite this as

$$\boldsymbol{f}_{m(i+1)} = \|\boldsymbol{b}\|_2 V_{m(i+1)} \int_0^\infty \exp(tH_{m(i+1)}) \boldsymbol{e}_1 \, \mathrm{d}\mu(t). \tag{8}$$

In the next section, we prove that the approximation (8) converges monotonically to $f(A)\boldsymbol{b}$ for growing m.

3. Monotone convergence of the extended Krylov subspace method

In this section, we prove that the extended Lanczos approximations (7) converge monotonically to $f(A)\boldsymbol{b}$ when f is a Laplace–Stieltjes function and A is Hermitian positive definite, i.e., that

$$\|f(A)\boldsymbol{b} - \boldsymbol{f}_{m(i+1)}\|_2 \leq \|f(A)\boldsymbol{b} - \boldsymbol{f}_{(m-1)(i+1)}\|_2. \tag{9}$$

We begin by investigating the matrix exponential function $\exp(A)$.

Theorem 2. *Let $A \in \mathbb{C}^{n \times n}$ be Hermitian positive definite and let $\boldsymbol{b} \in \mathbb{C}^n$. Then the extended Lanczos approximations* (7) *converge monotonically to* $\exp(A)\boldsymbol{b}$ *in the sense of* (9).

Proof. Define a new basis $V^{\pm}_{m(i+1)} = V_{m(i+1)} S_{m(i+1)}$ of $\mathcal{K}_m^{im+1}(A, \boldsymbol{b})$ by right-multiplying the basis $V_{m(i+1)}$ by the signature matrix $S_{m(i+1)} = \operatorname{diag}(s_1, \ldots, s_{m(i+1)})$, where

$$s_j = \begin{cases} 1 & \text{if } \left\lfloor \frac{j-1}{i+1} \right\rfloor \text{ is even,} \\ -1 & \text{if } \left\lfloor \frac{j-1}{i+1} \right\rfloor \text{ is odd.} \end{cases}$$

Then

$$(V^{\pm}_{m(i+1)})^H A V^{\pm}_{m(i+1)} = S_{m(i+1)} H_{m(i+1)} S_{m(i+1)} =: H^{\pm}_{m(i+1)},$$

and

$$f(H^{\pm}_{m(i+1)}) = S_{m(i+1)} f(H_{m(i+1)}) S_{m(i+1)}$$

for any matrix function f, as $S_{m(i+1)} = S^{-1}_{m(i+1)}$. Therefore, using $S_{m(i+1)}\boldsymbol{e}_1 = \boldsymbol{e}_1$ and $S^2_{m(i+1)} = I_m$, we can also compute the extended Lanczos approximation (7) as

$$\boldsymbol{f}_{m(i+1)} = \|\boldsymbol{b}\|_2 V^{\pm}_{m(i+1)} f(H^{\pm}_{m(i+1)})\boldsymbol{e}_1 =: V^{\pm}_{m(i+1)} \boldsymbol{s}_{m(i+1)}. \tag{10}$$

By using Proposition 1 together with the definition of $S_{m(i+1)}$, one easily checks that $H^{\pm}_{m(i+1)}$ is a nonnegative matrix. Define the block diagonal matrix

$$\widehat{H}^{\pm}_{m(i+1)} = \left[\begin{array}{c|c} H^{\pm}_{(m-1)(i+1)} & O_{(m-1)(i+1)\times(i+1)} \\ \hline O_{(i+1)\times(m-1)(i+1)} & D_{i+1} \end{array}\right]$$

where $D_{i+1} = \mathrm{diag}(h^{\pm}_{(m-1)(i+1)+1,(m-1)(i+1)+1}, \ldots, h^{\pm}_{(i+1)m,(i+1)m})$ and $O_{k\times\ell} \in \mathbb{C}^{k\times\ell}$ denotes a matrix of all zeros. We then have

$$O_{m(i+1)\times m(i+1)} \leq \widehat{H}^{\pm}_{m(i+1)} \leq H^{\pm}_{m(i+1)}$$

and thus

$$O_{m(i+1)\times m(i+1)} \leq (\widehat{H}^{\pm}_{m(i+1)})^k \leq (H^{\pm}_{m(i+1)})^k \text{ for all } k \in \mathbb{N}. \tag{11}$$

Inserting (11) into the power series expansion of the exponential function, we find

$$\begin{aligned} O_{m(i+1)\times m(i+1)} \quad &\leq \quad \exp(\widehat{H}^{\pm}_{m(i+1)}) = \sum\nolimits_{k=0}^{\infty} \frac{1}{k!} \left(\widehat{H}^{\pm}_{m(i+1)}\right)^k \\ &\leq \quad \sum\nolimits_{k=0}^{\infty} \frac{1}{k!} \left(H^{\pm}_{m(i+1)}\right)^k = \exp(H^{\pm}_{m(i+1)}). \end{aligned} \tag{12}$$

By comparing the first columns of the matrices in (12) and noting that

$$\|\boldsymbol{b}\|_2 \exp(\widehat{H}^{\pm}_{m(i+1)})\boldsymbol{e}_1 = \begin{bmatrix} \boldsymbol{s}_{(m-1)(i+1)} \\ O_{(i+1)\times 1} \end{bmatrix},$$

we find

$$O_{m(i+1)\times 1} \leq \begin{bmatrix} \boldsymbol{s}_{(m-1)(i+1)} \\ O_{(i+1)\times 1} \end{bmatrix} \leq \boldsymbol{s}_{m(i+1)}. \tag{13}$$

Noting that by the finite termination property of the extended Krylov subspace method there exists some index m^* such that $\exp(A)\boldsymbol{b} = V^{\pm}_{m^*}\boldsymbol{s}_{m^*}$, we can rewrite the error of $\boldsymbol{f}_{m(i+1)}$ as

$$\exp(A)\boldsymbol{b} - \boldsymbol{f}_{m(i+1)} = V^{\pm}_{m^*}\left(\boldsymbol{s}_{m^*} - \begin{bmatrix} \boldsymbol{s}_{m(i+1)} \\ O_{(m^*-m(i+1))\times 1} \end{bmatrix}\right). \tag{14}$$

As the basis vectors in $V^{\pm}_{m(i+1)}$ are mutually orthogonal, the representation (14) directly implies

$$\|\exp(A)\boldsymbol{b} - \boldsymbol{f}_{m(i+1)}\|_2 = \left\|\boldsymbol{s}_{m^*} - \begin{bmatrix} \boldsymbol{s}_{m(i+1)} \\ O_{(m^*-m(i+1))\times 1} \end{bmatrix}\right\|_2. \tag{15}$$

From the monotonicity property (13), we get

$$\left\|\boldsymbol{s}_{m^*} - \begin{bmatrix} \boldsymbol{s}_{m(i+1)} \\ O_{(m^*-m(i+1))\times 1} \end{bmatrix}\right\|_2 \leq \left\|\boldsymbol{s}_{m^*} - \begin{bmatrix} \boldsymbol{s}_{(m-1)(i+1)} \\ O_{(m^*-(m-1)(i+1))\times 1} \end{bmatrix}\right\|_2,$$

which, together with (15), implies that the error norms in the extended Lanczos method are monotonically decreasing. In addition, one can easily show in the same way that the norms of the iterates are monotonically increasing. □

Using the result of Theorem 2, we can easily prove monotone convergence for the whole class of Laplace–Stieltjes functions.

Corollary 3. *Let $A \in \mathbb{C}^{n\times n}$ be Hermitian positive definite, let $\boldsymbol{b} \in \mathbb{C}^n$ and let f be a Laplace–Stieltjes function* (1)*. Then the extended Lanczos approximations* (7) *converge monotonically to $f(A)\boldsymbol{b}$ in the sense of* (9)*.*

Proof. Using (8) and (10), we can rewrite the extended Lanczos approximation to $f(A)\boldsymbol{b}$ as

$$\boldsymbol{f}_{m(i+1)} = V^{\pm}_{m(i+1)} \int_0^\infty \boldsymbol{s}_{m(i+1)}(t)\,\mathrm{d}\mu(t),$$

where $\boldsymbol{s}_{m(i+1)}(t)$ are the coefficients describing the Lanczos approximation to $\exp(tA)\boldsymbol{b}$ in the basis $V^{\pm}_{m(i+1)}$. As tA is Hermitian positive definite for all $t > 0$, the result of Theorem 2 holds for all these Lanczos approximations. We therefore have, using (13) and the monotonicity of μ,

$$O_{m(i+1)\times 1} \leq \int_0^\infty \begin{bmatrix} \boldsymbol{s}_{(m-1)(i+1)}(t) \\ O_{(i+1)\times 1} \end{bmatrix} \mathrm{d}\mu(t) \leq \int_0^\infty \boldsymbol{s}_{m(i+1)}(t)\,\mathrm{d}\mu(t),$$

from which the assertion follows. □

We just briefly remark that all results also apply for "intermediate" iterates with an index which is not a multiple of $i+1$ and can be proven in the same way (with obvious modifications), but we refrain from doing so here to avoid unnecessarily complicated notation.

4. Conclusions

We have proven that the error norm in the extended Krylov subspace method for approximating $f(A)\boldsymbol{b}$ is monotonically decreasing when A is Hermitian positive definite and f is a Laplace–Stieltjes function, thereby generalizing similar, known results for the polynomial Lanczos approximation. Similar to what was observed in the polynomial case, the developed results depend crucially on the orthogonality of the extended Krylov basis. Therefore the results do not hold any longer when the basis loses orthogonality. It is, however, still true that the coefficients $\boldsymbol{s}_{m(i+1)}$ describing the approximation in the Lanczos basis are monotonically increasing from one step to the next, we just cannot conclude anything about the norm of the approximation or the error any longer.

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