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Convergence of the block Lanczos method for eigenvalue clusters

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Abstract The Lanczos method is often used to solve a large scale symmetric matrix eigenvalue problem. It is well-known that the single-vector Lanczos method can only find one copy of any multiple eigenvalue (unless certain deflating strategy is incorporated) and encounters slow convergence towards clustered eigenvalues. On the other hand, the block Lanczos method can compute all or some of the copies of a multiple eigenvalue and, with a suitable block size, also compute clustered eigenvalues much faster. The existing convergence theory due to Saad for the block Lanczos method, however, does not fully reflect this phenomenon since the theory was established to bound approximation errors in each individual approximate eigenpairs. Here, it is argued that in the presence of an eigenvalue cluster, the entire approximate eigenspace associated with the cluster should be considered as a whole, instead of each individual approximate eigenvectors, and likewise for approximating clusters of eigenvalues. In this paper, we obtain error bounds on approximating eigenspaces and eigenvalue clusters. Our bounds are much sharper than the existing ones and expose true rates of convergence of the block Lanczos method towards eigenvalue clusters. Furthermore, their sharpness is independent of the closeness of eigenvalues within a cluster. Numerical examples are presented to support our claims.

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1 Introduction

The Lanczos method [15] is widely used for finding a small number of extreme eigenvalues and their associated eigenvectors of a symmetric matrix (or Hermitian matrix in the complex case). It requires only matrix-vector products to extract enough information to compute the desired solutions, and thus is very attractive in practice when the matrix is sparse and its size is too large to be solved by, e.g., the QR algorithm [8,21] or the matrix does not exist explicitly but in the form of a procedure that is capable of generating matrix-vector multiplications.

Let A be an $N \times N$ Hermitian matrix. Given an initial vector v_0, the single-vector Lanczos method begins by recursively computing an orthonormal basis $\{q_1, q_2, \ldots, q_n\}$ of the nth Krylov subspace of A on v_0:

$$\mathcal{K}_n(A, v_0) = \text{span}\{v_0, Av_0, \ldots, A^{n-1}v_0\} \tag{1.1}$$

and at the same time the projection of A onto $\mathcal{K}_n(A, v_0)$: $T_n = Q_n^{\mathrm{H}} A Q_n$, where $Q_n = [q_1, q_2, \ldots, q_n]$ and usually $n \ll N$. Afterwards some of the eigenpairs $(\tilde{\lambda}, w)$ of T_n:

$$T_n w = \tilde{\lambda} w,$$

especially the extreme ones, are used to construct approximate eigenpairs $(\tilde{\lambda}, Q_n w)$ of A. The number $\tilde{\lambda}$ is called a *Ritz value* and $Q_n w$ a *Ritz vector*. This procedure of computing approximate eigenpairs is not limited to Krylov subspaces but in general works for any given subspace. It is called the *Rayleigh–Ritz procedure*.

The single-vector Lanczos method may have difficulty in computing all copies of a multiple eigenvalue of A. In fact, only one copy of the eigenvalue can be found unless certain deflating strategy is incorporated. On the other hand, a block Lanczos method with a block size that is no smaller than the multiplicity of the eigenvalue can compute all copies of the eigenvalue at the same time. But perhaps the biggest problem for the single-vector Lanczos method is its effectiveness in handling eigenvalue clusters—slow convergence to each individual eigenvalue in the cluster. The closer the eigenvalues in the cluster are, the slower the convergence will be. It is well-known that a block version with a big enough block size will perform much better.

There are a few block versions, e.g., the ones introduced by Golub and Underwood [9], Cullum and Donath [5], and, more recently, by Ye [25] for an adaptive block Lanczos method (see also Cullum and Willoughby [6], Golub and van Loan [10]). The basic idea is to use an $N \times n_b$ matrix V_0, instead of a single vector v_0, and accordingly an orthonormal basis of the nth Krylov subspace of A on V_0:

$$\mathcal{K}_n(A, V_0) = \text{span}\{V_0, AV_0, \ldots, A^{n-1}V_0\} \tag{1.2}$$

will be generated, as well as the projection of A onto $\mathcal{K}_n(A, V_0)$. Afterwards the same Rayleigh-Ritz procedure is applied to compute approximate eigenpairs of A.

There has been a wealth of development, in both theory and implementation, for the Lanczos methods, mostly for the single-vector version. The most complete reference up to 1998 is Parlett [21]. This paper is concerned with the theoretical convergence theory of the block Lanczos method. Related past works include Kaniel [12], Paige [20], Saad [22], Li [18], as well as the potential-theoretic approach in Kuijlaars [13,14] who, from a very different perspective, investigated which eigenvalues are found first according to the eigenvalue distribution as $N \to \infty$, and what are their associated convergence rates as n goes to ∞ while n/N stays fixed. Results from these papers are all about the convergence of an individual eigenvalue and eigenvector, even in the analysis of Saad on the block Lanczos method.

The focus in this paper is, however, on the convergence of a cluster of eigenvalues, including multiple eigenvalues, and their associated eigenspace for the Hermitian eigenvalue problem. Our results distinguish themselves from those of Saad [22] in that they bound errors in approximate eigenpairs belonging to eigenvalue clusters together, rather than separately for each individual eigenpair. The consequence is much sharper bounds as our later numerical examples will demonstrate. These bounds are also independent of the closeness of eigenvalues within a cluster.

One of the key steps in analyzing the convergence of Lanczos methods is to pick (sub)optimal polynomials to minimize error bounds. For any eigenpair other than the first one, it is often the standard practice, as in [22], that each chosen polynomial has a factor to annihilate vector components in all proceeding eigenvector directions, resulting in a "bulky" factor in the form of the product involving all previous eigenvalues/Ritz values in the error bound. The factor can be big and likely is an artifact of the analyzing technique. We propose also a new kind of error bounds that do not have such a "bulky" factor, but require knowledge of the distance from the interested eigenspace to a Krylov subspace $\mathcal{K}_i$ of a lower order as a tradeoff.

The rest of this paper is organized as follows. Section 2 collects some necessary results on unitarily invariant norms and canonical angles between subspaces for our later use. Section 3 presents the (simplest) block Lanczos method whose convergence analysis that results in error bounds of the eigenspace/eigenvalue cluster type is done in Sect. 4 for eigenspaces and Sect. 5 for eigenvalues. In Sect. 6, we perform a brief theoretical comparison between our results and related results derived from those of Saad [22] and point out when Saad's bounds will overestimate the true rate of convergence. Numerical examples are given in Sect. 7 to support our comparison analysis. Section 8 establishes more bounds, based on the knowledge of Krylov subspaces of lower orders. Finally, we present our conclusion in Sect. 9.

Throughout this paper, A is an $N \times N$ Hermitian matrix, and has

$$\begin{array}{rl} \text{eigenvalues:} & \lambda_1 \geq \lambda_2 \geq \cdots \geq \lambda_N, \text{ and} \\ & \Lambda = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_N), \\ \text{orthonormal eigenvectors:} & u_1, u_2, \ldots, u_N, \text{ and} \\ & U = [u_1, u_2, \ldots, u_N], \\ \text{eigen-decomposition:} & A = U\Lambda U^{\mathrm{H}} \text{ and } U^{\mathrm{H}}U = I_N. \end{array} \tag{1.3}$$

$\mathbb{C}^{n\times m}$ is the set of all $n \times m$ complex matrices, $\mathbb{C}^n = \mathbb{C}^{n\times 1}$, and $\mathbb{C} = \mathbb{C}^1$. $\mathbb{P}_k$ is the set of polynomial of degree no bigger than k. I_n (or simply I if its dimension is clear

from the context) is the $n \times n$ identity matrix, and e_j is its jth column. The superscript ".H" takes the complex conjugate transpose of a matrix or vector. We shall also adopt MATLAB-like convention to access the entries of vectors and matrices. Let $i : j$ be the set of integers from i to j inclusive. For a vector u and a matrix X, $u_{(j)}$ is u's jth entry, $X_{(i,j)}$ is X's (i, j)th entry; X's submatrices $X_{(k:\ell,i:j)}$, $X_{(k:\ell,:)}$, and $X_{(:,i:j)}$ consist of intersections of row k to row ℓ and column i to column j, row k to row ℓ, and column i to column j, respectively. $\mathcal{R}(X)$ is the column space of X, i.e., the subspace spanned by the columns of X, and $\mathrm{eig}(X)$ denotes the set of all eigenvalues of a square matrix X. For matrices or scalars X_i, both $\mathrm{diag}(X_1, \ldots, X_k)$ and $X_1 \oplus \cdots \oplus X_k$ denote the same block diagonal matrix with the ith diagonal block X_i.

2 Preliminaries

2.1 Unitarily invariant norm

A matrix norm $|||\cdot|||$ is called a *unitarily invariant norm* on $\mathbb{C}^{m\times n}$ if it is a matrix norm and has the following two properties [1,23]

1. $|||X^{\mathrm{H}}BY||| = |||B|||$ for all unitary matrices X and Y of apt sizes and $B \in \mathbb{C}^{m\times n}$.
2. $|||B||| = \|B\|_2$, the spectral norm of B, if $\mathrm{rank}(B) = 1$.

Two commonly used unitarily invariant norms are

$$\begin{aligned} \text{the spectral norm: } \|B\|_2 &= \max_j \sigma_j, \\ \text{the Frobenius norm: } \|B\|_{\mathrm{F}} &= \sqrt{\textstyle\sum_j \sigma_j^2}, \end{aligned}$$

where $\sigma_1, \sigma_2, \ldots, \sigma_{\min\{m,n\}}$ are the singular values of B. The trace norm

$$|||B|||_{\mathrm{trace}} = \sum_j \sigma_j$$

is a unitarily invariant norm, too. In what follows, $|||\cdot|||$ denotes a general unitarily invariant norm.

In this article, for convenience, any $|||\cdot|||$ we use is generic to matrix sizes in the sense that it applies to matrices of all sizes. Examples include the matrix spectral norm $\|\cdot\|_2$, the Frobenius norm $\|\cdot\|_{\mathrm{F}}$, and the trace norm. One important property of unitarily invariant norms is

$$|||XYZ||| \le \|X\|_2 \cdot |||Y||| \cdot \|Z\|_2$$

for any matrices X, Y, and Z of compatible sizes.

Lemma 2.1 *Let H and M be two Hermitian matrices, and let S be a matrix of a compatible size as determined by the Sylvester equation $HY - YM = S$. If* $\mathrm{eig}(H) \cap \mathrm{eig}(M) = \emptyset$*, then the equation has a unique solution Y, and moreover*

$$|||Y||| \le \frac{c}{\eta}\,|||S|||,$$

where $\eta = \min|\mu - \omega|$ *over all* $\mu \in \mathrm{eig}(M)$ *and* $\omega \in \mathrm{eig}(H)$*, and the constant* c *lies between* 1 *and* $\pi/2$*, and it is* 1 *for the Frobenius norm, or if either* $\mathrm{eig}(H)$ *is in a closed interval that contains no eigenvalue of* M *or vice versa.*

This lemma for the Frobenius norm and for the case when either $\mathrm{eig}(H)$ is in a closed interval that contains no eigenvalue of M or vice versa is essentially in [7] (see also [23]), and it is due to [2,3] for the most general case: $\mathrm{eig}(H) \cap \mathrm{eig}(M) = \emptyset$ and any unitarily invariant norm.

2.2 Angles between subspaces

Consider two subspaces $\mathcal{X}$ and $\mathcal{Y}$ of $\mathbb{C}^N$ and suppose

$$k := \dim(\mathcal{X}) \le \dim(\mathcal{Y}) =: \ell. \tag{2.1}$$

Let $X \in \mathbb{C}^{N\times k}$ and $Y \in \mathbb{C}^{N\times \ell}$ be orthonormal basis matrices of $\mathcal{X}$ and $\mathcal{Y}$, respectively, i.e.,

$$X^{\mathrm{H}}X = I_k,\ \mathcal{X} = \mathcal{R}(X), \quad \text{and} \quad Y^{\mathrm{H}}Y = I_\ell,\ \mathcal{Y} = \mathcal{R}(Y),$$

and denote by σ_j for $1 \le j \le k$ in ascending order, i.e., $\sigma_1 \le \cdots \le \sigma_k$, the singular values of $Y^{\mathrm{H}}X$. The k *canonical angles* $\theta_j(\mathcal{X},\mathcal{Y})$ *from*[1] $\mathcal{X}$ *to* $\mathcal{Y}$ are defined by

$$0 \le \theta_j(\mathcal{X},\mathcal{Y}) := \arccos\sigma_j \le \frac{\pi}{2} \quad \text{for } 1 \le j \le k. \tag{2.2}$$

They are in descending order, i.e., $\theta_1(\mathcal{X},\mathcal{Y}) \ge \cdots \ge \theta_k(\mathcal{X},\mathcal{Y})$. Set

$$\Theta(\mathcal{X},\mathcal{Y}) = \mathrm{diag}(\theta_1(\mathcal{X},\mathcal{Y}),\ldots,\theta_k(\mathcal{X},\mathcal{Y})). \tag{2.3}$$

It can be seen that angles so defined are independent of the orthonormal basis matrices X and Y, which are not unique. A different way to define these angles is through the orthogonal projections onto $\mathcal{X}$ and $\mathcal{Y}$ [24].

When $k = 1$, i.e., X is a vector, there is only one canonical angle from $\mathcal{X}$ to $\mathcal{Y}$ and so we will simply write $\theta(\mathcal{X},\mathcal{Y})$.

In what follows, we sometimes place a vector or matrix in one or both arguments of $\theta_j(\cdot,\cdot)$, $\theta(\cdot,\cdot)$, and $\Theta(\cdot,\cdot)$ with the understanding that it is about the subspace spanned by the vector or the columns of the matrix argument.

Proposition 2.1 *Let* $\mathcal{X}$ *and* $\mathcal{Y}$ *be two subspaces in* $\mathbb{C}^N$ *satisfying* (2.1).

(a) *For any* $\widehat{\mathcal{Y}} \subseteq \mathcal{Y}$ *with* $\dim(\widehat{\mathcal{Y}}) = \dim(\mathcal{X}) = k$*, we have* $\theta_j(\mathcal{X},\mathcal{Y}) \le \theta_j(\mathcal{X},\widehat{\mathcal{Y}})$ *for* $1 \le j \le k$.

(b) *There exist an orthonormal basis* $\{x_1, x_2, \ldots, x_k\}$ *for* $\mathcal{X}$ *and an orthonormal basis* $\{y_1, y_2, \ldots, y_\ell\}$ *for* $\mathcal{Y}$ *such that*

[1] If $k = \ell$, we may say that these angles are *between* $\mathcal{X}$ and $\mathcal{Y}$.

$$\theta_j(\mathcal{X}, \mathcal{Y}) = \theta(x_j, y_j) \quad \textit{for} \quad 1 \le j \le k, \textit{ and}$$
$$x_i^{\mathrm{H}} y_j = 0 \qquad\qquad \textit{for} \quad 1 \le i \le k, k+1 \le j \le \ell.$$

In particular, $\Theta(\mathcal{X}, \mathcal{Y}) = \Theta(\mathcal{X}, \widehat{\mathcal{Y}})$*, where* $\widehat{\mathcal{Y}} = \mathrm{span}\{y_1, y_2, \ldots, y_k\}$*, and the subspace* $\widehat{\mathcal{Y}}$ *is unique if* $\theta_1(\mathcal{X}, \mathcal{Y}) < \pi/2$.

Proof Let $X \in \mathbb{C}^{N\times k}$ and $Y \in \mathbb{C}^{N\times \ell}$ be orthonormal basis matrices of $\mathcal{X}$ and $\mathcal{Y}$, respectively. If $\widehat{\mathcal{Y}} \subseteq \mathcal{Y}$ with $\dim(\widehat{\mathcal{Y}}) = \dim(\mathcal{X}) = k$, then there is $W \in \mathbb{C}^{\ell\times k}$ with orthonormal columns such that $\widehat{Y} = YW$ is an orthonormal basis matrix of $\widehat{\mathcal{Y}}$. Since $\cos\theta_j(\mathcal{X}, \widehat{\mathcal{Y}})$ for $1 \le j \le k$ are the singular values of $X^{\mathrm{H}}YW$ which are no bigger than the singular values of $X^{\mathrm{H}}Y$, i.e., $\cos\theta_j(\mathcal{X}, \widehat{\mathcal{Y}}) \le \cos\theta_j(\mathcal{X}, \mathcal{Y})$ individually, or equivalently, $\theta_j(\mathcal{X}, \widehat{\mathcal{Y}}) \ge \theta_j(\mathcal{X}, \mathcal{Y})$ for $1 \le j \le k$. This is item (a).

For item (b), let $X^{\mathrm{H}}Y = V\Sigma W^{\mathrm{H}}$ be the SVD of $X^{\mathrm{H}}Y$, where

$$\Sigma = [\mathrm{diag}(\sigma_1, \sigma_2, \ldots, \sigma_k), 0_{k\times(\ell-k)}].$$

Then XV and YW are orthonormal basis matrices of $\mathcal{X}$ and $\mathcal{Y}$, respectively, and their columns, denoted by x_i and y_j, respectively, satisfy the specified requirements in the theorem. If also $\theta_1(\mathcal{X}, \mathcal{Y}) < \pi/2$, then all $\sigma_i > 0$ and the first k columns of W spans $\mathcal{R}(Y^{\mathrm{H}}X)$ which is unique; so $\widehat{\mathcal{Y}}$ is unique for each given basis matrix Y. We have to prove that $\widehat{\mathcal{Y}}$ is independent of the choosing of Y. Let $\widetilde{Y}$ be another orthonormal basis matrix of $\mathcal{Y}$. Then $\widetilde{Y} = YZ$ for some $\ell \times \ell$ unitary matrix Z. Following the above construction for $\widehat{\mathcal{Y}}$, we will have a new $\widehat{\mathcal{Y}}_{\mathrm{new}} = \mathcal{R}(\widetilde{Y}\widetilde{W}_{(:,1:k)})$, where $\widetilde{W}$ is from the SVD $X^{\mathrm{H}}\widetilde{Y} = \widetilde{V}\Sigma\widetilde{W}^{\mathrm{H}}$. Notice

$$X^{\mathrm{H}}\widetilde{Y} = X^{\mathrm{H}}YZ = V\Sigma(W^{\mathrm{H}}Z)$$

which is yet another SVD of $X^{\mathrm{H}}\widetilde{Y}$. Thus the columns of $(Z^{\mathrm{H}}W)_{(:,1:k)} = Z^{\mathrm{H}}W_{(:,1:k)}$ span the column space of $\widetilde{Y}^{\mathrm{H}}X$ which is also spanned by the columns of $\widetilde{W}_{(:,1:k)}$. Hence $\widetilde{W}_{(:,1:k)} = Z^{\mathrm{H}}W_{(:,1:k)}M$ for some nonsingular matrix M, and

$$\widetilde{Y}\widetilde{W}_{(:,1:k)} = YW_{(:,1:k)}M$$

which implies $\widehat{\mathcal{Y}}_{\mathrm{new}} = \mathcal{R}(\widetilde{Y}\widetilde{W}_{(:,1:k)}) = \mathcal{R}(YW_{(:,1:k)}) = \widehat{\mathcal{Y}}$, as expected. □

Proposition 2.2 *Let* $\mathcal{X}$ *and* $\mathcal{Y}$ *be two subspaces in* $\mathbb{C}^N$ *satisfying* (2.1)*, and let* $X \in \mathbb{C}^{N\times k}$ *be an orthonormal basis matrix of* $\mathcal{X}$*, i.e.,* $X^{\mathrm{H}}X = I_k$*. Then*

$$\max_{1\le j\le k} \sin\theta(X_{(:,j)}, \mathcal{Y}) \le \|\sin\Theta(\mathcal{X}, \mathcal{Y})\| \le \sum_{j=1}^{k} \sin\theta(X_{(:,j)}, \mathcal{Y}), \tag{2.4}$$

$$\max_{1\le j\le k} \sin\theta(X_{(:,j)}, \mathcal{Y}) \le \|\sin\Theta(\mathcal{X}, \mathcal{Y})\|_{\mathrm{F}} = \sqrt{\sum_{j=1}^{k} \sin^2\theta(X_{(:,j)}, \mathcal{Y})}, \tag{2.5}$$

$$\|\sin\Theta(\mathcal{X}, \mathcal{Y})\| \le \|\tan\Theta(\mathcal{X}, \mathcal{Y})\| \le \frac{\|\sin\Theta(\mathcal{X}, \mathcal{Y})\|}{\sqrt{1 - \sin^2\theta_1(\mathcal{X}, \mathcal{Y})}}. \tag{2.6}$$

Proof Let $Y_\perp \in \mathbb{C}^{N\times(N-\ell)}$ be an orthonormal basis matrix of the orthogonal complement of $\mathcal{Y}$ in $\mathbb{C}^N$. We observe that $\sin\theta_j(\mathcal{X},\mathcal{Y})$ for $1 \le j \le k$ are the singular values of $X^{\mathrm{H}}Y_\perp$ and thus $\|\!|\sin\Theta(\mathcal{X},\mathcal{Y})|\!\| = \left\|\!\left| X^{\mathrm{H}}Y_\perp \right|\!\right\|$. Observe also $\sin\theta(X_{(:,j)},\mathcal{Y}) = \left\| X^{\mathrm{H}}_{(:,j)}Y_\perp \right\| = \|X^{\mathrm{H}}_{(:,j)}Y_\perp\|_2$. Therefore

$$\max_{1\le j\le k}\left\| X^{\mathrm{H}}_{(:,j)}Y_\perp \right\| \le \|\!|\sin\Theta(\mathcal{X},\mathcal{Y})|\!\| = \left\|\!\left| X^{\mathrm{H}}Y_\perp \right|\!\right\| \le \sum_{j=1}^{k}\|X^{\mathrm{H}}_{(:,j)}Y_\perp\|_2,$$

$$\max_{1\le j\le k}\left\| X^{\mathrm{H}}_{(:,j)}Y_\perp \right\|_{\mathrm{F}} \le \|\sin\Theta(\mathcal{X},\mathcal{Y})\|_{\mathrm{F}} = \|X^{\mathrm{H}}Y_\perp\|_{\mathrm{F}} = \sqrt{\sum_{j=1}^{k}\left\| X^{\mathrm{H}}_{(:,j)}Y_\perp \right\|_{\mathrm{F}}^2}.$$

They yield both (2.4) and (2.5). For (2.6), we notice

$$\sin\theta_j(\mathcal{X},\mathcal{Y}) \le \tan\theta_j(\mathcal{X},\mathcal{Y}) = \frac{\sin\theta_j(\mathcal{X},\mathcal{Y})}{\cos\theta_j(\mathcal{X},\mathcal{Y})} \le \frac{\sin\theta_j(\mathcal{X},\mathcal{Y})}{\cos\theta_1(\mathcal{X},\mathcal{Y})}$$

for $1 \le j \le k$. □

Proposition 2.3 *Let $\mathcal{X}$ and $\mathcal{Y}$ be two subspaces in $\mathbb{C}^N$ with equal dimension:* $\dim(\mathcal{X}) = \dim(\mathcal{Y}) = k$, *and let $X \in \mathbb{C}^{N\times k}$ be an orthonormal basis matrix of $\mathcal{X}$, i.e., $X^{\mathrm{H}}X = I_k$, and Y be a (not necessarily orthonormal) basis matrix of $\mathcal{Y}$ such that each column of Y is a unit vector, i.e., $\|Y_{(:,j)}\|_2 = 1$ for all j. Then*

$$\|\sin\Theta(\mathcal{X},\mathcal{Y})\|_{\mathrm{F}}^2 \le \|(Y^{\mathrm{H}}Y)^{-1}\|_2 \sum_{j=1}^{k}\sin^2\theta(X_{(:,j)},Y_{(:,j)}). \tag{2.7}$$

Proof Since $\sin^2\theta_j(\mathcal{X},\mathcal{Y})$ for $1 \le j \le k$ are the eigenvalues of

$$\begin{aligned} &I_k - \left[X^{\mathrm{H}}Y(Y^{\mathrm{H}}Y)^{-1/2}\right]^{\mathrm{H}}\left[X^{\mathrm{H}}Y(Y^{\mathrm{H}}Y)^{-1/2}\right] \\ &\quad = (Y^{\mathrm{H}}Y)^{-1/2}\left[Y^{\mathrm{H}}Y - (X^{\mathrm{H}}Y)^{\mathrm{H}}(X^{\mathrm{H}}Y)\right](Y^{\mathrm{H}}Y)^{-1/2}, \end{aligned}$$

we have

$$\begin{aligned} \|\sin\Theta(\mathcal{X},\mathcal{Y})\|_{\mathrm{F}}^2 &= \sum_{j=1}^{k}\sin^2\theta_j(\mathcal{X},\mathcal{Y}) \\ &= \left\|\!\left| I_k - \left[X^{\mathrm{H}}Y(Y^{\mathrm{H}}Y)^{-1/2}\right]^{\mathrm{H}}\left[X^{\mathrm{H}}Y(Y^{\mathrm{H}}Y)^{-1/2}\right] \right|\!\right\|_{\mathrm{trace}} \\ &\le \|(Y^{\mathrm{H}}Y)^{-1/2}\|_2 \left\|\!\left| Y^{\mathrm{H}}Y - (X^{\mathrm{H}}Y)^{\mathrm{H}}(X^{\mathrm{H}}Y) \right|\!\right\|_{\mathrm{trace}} \|(Y^{\mathrm{H}}Y)^{-1/2}\|_2 \\ &= \|(Y^{\mathrm{H}}Y)^{-1}\|_2 \,\mathrm{trace}\left(Y^{\mathrm{H}}Y - (X^{\mathrm{H}}Y)^{\mathrm{H}}(X^{\mathrm{H}}Y)\right) \end{aligned}$$

$$= \|(Y^{\mathrm{H}}Y)^{-1}\|_2 \sum_{j=1}^{k} \left[1 - Y_{(:,j)}^{\mathrm{H}} X X^{\mathrm{H}} Y_{(:,j)}\right]$$

$$\le \|(Y^{\mathrm{H}}Y)^{-1}\|_2 \sum_{j=1}^{k} \left[1 - Y_{(:,j)}^{\mathrm{H}} X_{(:,j)} X_{(:,j)}^{\mathrm{H}} Y_{(:,j)}\right]$$

$$= \|(Y^{\mathrm{H}}Y)^{-1}\|_2 \sum_{j=1}^{k} \sin^2\theta(X_{(:,j)}, Y_{(:,j)}), \tag{2.8}$$

as was to be shown. In obtaining (2.8), we have used

$$Y_{(:,j)}^{\mathrm{H}} X X^{\mathrm{H}} Y_{(:,j)} = \|X^{\mathrm{H}} Y_{(:,j)}\|_2^2 \ge Y_{(:,j)}^{\mathrm{H}} X_{(:,j)} X_{(:,j)}^{\mathrm{H}} Y_{(:,j)}$$

because $X_{(:,j)}^{\mathrm{H}} Y_{(:,j)}$ is the jth entry of the vector $X^{\mathrm{H}} Y_{(:,j)}$. □

Remark 2.1 The inequality (2.7) is about controlling the subspace angle $\Theta(\mathcal{X}, \mathcal{Y})$ by the individual angles between corresponding basis vectors. These individual angles depend on the selection of the basis vectors as well as their labelling. By Proposition 2.1(b), it is possible to find basis vectors for both $\mathcal{X}$ and $\mathcal{Y}$ and match them perfectly such that $\theta_j(\mathcal{X}, \mathcal{Y})$ collectively is the same as all individual angles between corresponding basis vectors. But, on the other hand, it is possible that for two close subspaces in the sense that $\Theta(\mathcal{X}, \mathcal{Y})$ is tiny there are unfortunately chosen and labelled basis vectors to make one or more individual angles between corresponding basis vectors near or even $\pi/2$. In fact, this can happen even when $\mathcal{X} = \mathcal{Y}$. Therefore in general the collection $\{\theta(X_{(:,j)}, Y_{(:,j)}),\ 1 \le j \le k\}$ cannot be controlled by $\Theta(\mathcal{X}, \mathcal{Y})$ without additional information.

Proposition 2.4 *Let $\mathcal{X}$ and $\mathcal{Y}$ be two subspaces in $\mathbb{C}^N$ with equal dimension:* $\dim(\mathcal{X}) = \dim(\mathcal{Y}) = k$. *Suppose $\theta_1(\mathcal{X}, \mathcal{Y}) < \pi/2$.*

(a) *For any $\widehat{\mathcal{Y}} \subseteq \mathcal{Y}$ of dimension $k_1 = \dim(\widehat{\mathcal{Y}}) \le k$, there is a unique $\widehat{\mathcal{X}} \subseteq \mathcal{X}$ of dimension k_1 such that $P_{\mathcal{Y}}\widehat{\mathcal{X}} = \widehat{\mathcal{Y}}$, where $P_{\mathcal{Y}}$ is the orthogonal projection onto $\mathcal{Y}$. Moreover*

$$\theta_{j+k-k_1}(\mathcal{X}, \mathcal{Y}) \le \theta_j(\widehat{\mathcal{X}}, \widehat{\mathcal{Y}}) \le \theta_j(\mathcal{X}, \mathcal{Y}) \quad \text{for } 1 \le j \le k_1 \tag{2.9}$$

which implies

$$\|\!| \sin\Theta(\widehat{\mathcal{X}}, \widehat{\mathcal{Y}}) |\!\| \le \|\!| \sin\Theta(\mathcal{X}, \mathcal{Y}) |\!\|.$$

(b) *For any set $\{y_1, y_2, \ldots, y_{k_1}\}$ of orthonormal vectors in $\mathcal{Y}$, there is a set $\{x_1, x_2, \ldots, x_{k_1}\}$ of linearly independent vectors in $\mathcal{X}$ such that $P_{\mathcal{Y}} x_j = y_j$ for $1 \le j \le k_1$. Moreover (2.9) holds for $\widehat{\mathcal{X}} = \mathrm{span}\{x_1, x_2, \ldots, x_{k_1}\}$ and $\widehat{\mathcal{Y}} = \mathrm{span}\{y_1, y_2, \ldots, y_{k_1}\}$.*

Proof Let $X \in \mathbb{C}^{N\times k}$ and $Y \in \mathbb{C}^{N\times k}$ be orthonormal basis matrices of $\mathcal{X}$ and $\mathcal{Y}$, respectively. $\widehat{\mathcal{Y}} \subseteq \mathcal{Y}$ can be represented by its orthonormal basis matrix $Y\widehat{Y}$, where $\widehat{Y} \in \mathbb{C}^{k\times k_1}$ satisfies $\widehat{Y}^{\mathrm{H}}\widehat{Y} = I_{k_1}$. We need to find a $\widehat{\mathcal{X}} \subseteq \mathcal{X}$ with the desired property. $\widehat{\mathcal{X}} \subseteq \mathcal{X}$ can be represented by its basis matrix (not necessary orthonormal) $X\widehat{X}$, where $\widehat{X} \in \mathbb{C}^{k\times k_1}$ is nonsingular and to be determined. The equation $P_{\mathcal{Y}}\widehat{\mathcal{X}} = \widehat{\mathcal{Y}}$ is the same as

$$YY^{\mathrm{H}}X\widehat{X} = Y\widehat{Y} \quad \Leftrightarrow \quad Y^{\mathrm{H}}X\widehat{X} = \widehat{Y} \quad \Leftrightarrow \quad \widehat{X} = (Y^{\mathrm{H}}X)^{-1}\widehat{Y} \tag{2.10}$$

because $\theta_1(\mathcal{X}, \mathcal{Y}) < \pi/2$ implies $Y^{\mathrm{H}}X$ is nonsingular. This proves the existence of $\widehat{\mathcal{X}} = \mathcal{R}(X\widehat{X})$. Following the argument, one can also prove that this $\widehat{\mathcal{X}}$ is independent of how the orthonormal basis matrices X and Y are chosen, and thus unique. To prove (2.9), we note that $\hat{\sigma}_j := \cos\theta_j(\widehat{\mathcal{X}}, \widehat{\mathcal{Y}})$ for $1 \le j \le k_1$ are the singular values of

$$\begin{aligned}(Y\widehat{Y})^{\mathrm{H}}(X\widehat{X})[(X\widehat{X})^{\mathrm{H}}(X\widehat{X})]^{-1/2} &= \widehat{Y}^{\mathrm{H}}Y^{\mathrm{H}}X\widehat{X}[\widehat{X}^{\mathrm{H}}\widehat{X}]^{-1/2} \\ &= \left[\widehat{Y}^{\mathrm{H}}(Y^{\mathrm{H}}X)^{-\mathrm{H}}(Y^{\mathrm{H}}X)^{-1}\widehat{Y}\right]^{-1/2}.\end{aligned}$$

So the eigenvalues of $\widehat{Y}^{\mathrm{H}}(Y^{\mathrm{H}}X)^{-\mathrm{H}}(Y^{\mathrm{H}}X)^{-1}\widehat{Y}$ are $\hat{\sigma}_j^{-2}$ for $1 \le j \le k_1$. On the other hand, $\sigma_j := \cos\theta_j(\mathcal{X}, \mathcal{Y})$ for $1 \le j \le k$ are the singular values of $Y^{\mathrm{H}}X$. So the eigenvalues of $(Y^{\mathrm{H}}X)^{-\mathrm{H}}(Y^{\mathrm{H}}X)^{-1}$ are σ_j^{-2} for $1 \le j \le k$. Use the Cauchy interlacing inequalities [21] to conclude that

$$\sigma_j^{-2} \ge \hat{\sigma}_j^{-2} \ge \sigma_{j+k-k_1}^{-2} \quad \text{for } 1 \le j \le k_1$$

which yield (2.9). This proves item (a).

To prove item (b), we pick the orthonormal basis matrix Y above in such a way that its first k_1 columns are $y_1, y_2, \ldots, y_{k_1}$. In (2.10), let $\widehat{Y} = [e_1, e_2, \ldots, e_{k_1}]$, i.e., $\widehat{\mathcal{Y}} = \mathrm{span}\{y_1, y_2, \ldots, y_{k_1}\}$, and let $\widehat{X} = (Y^{\mathrm{H}}X)^{-1}\widehat{Y}$. Then $[x_1, x_2, \ldots, x_{k_1}] := X\widehat{X}$ gives what we need because of (2.10). □

Remark 2.2 The part of Proposition 2.4 on the existence of $\widehat{\mathcal{X}}$ in the case of $k_1 = 1$ is essentially taken from [22, Lemma 4].

Remark 2.3 The canonical angles are defined under the standard inner product $\langle x, y\rangle = x^{\mathrm{H}}y$ in $\mathbb{C}^N$. In a straightforward way, they can be defined under any given M-inner product $\langle x, y\rangle_M = x^{\mathrm{H}}My$, where $M \in \mathbb{C}^{N\times N}$ is Hermitian and positive definite. We will call these angles the *M-canonical angles*. All results we have proved in this section are valid in slightly different forms for the M-canonical angles. Details are omitted.

3 Block Lanczos method

Given $V_0 \in \mathbb{C}^{N\times n_b}$ with $\mathrm{rank}(V_0) = n_b$, the block Lanczos process [5,9] of Algorithm 1 is the simplest version and will generate an orthonormal basis of the Krylov subspace $\mathcal{K}_n(A, V_0)$ as well as a projection of A onto the Krylov subspace. It is

Algorithm 1 Simple Block Lanczos Process

Given Hermitian $A \in \mathbb{C}^{N\times N}$ and $V_0 \in \mathbb{C}^{N\times n_b}$ with $\mathrm{rank}(V_0) = n_b$, this generic block Lanczos process performs a partial tridiagonal reduction on A.

1: perform orthogonalization on given $V_0 \in \mathbb{C}^{N\times n_b}$ ($\mathrm{rank}(V_0) = n_b$) to obtain $V_0 = V_1 B_0$ (e.g., via modified Gram-Schmit), where $V_1 \in \mathbb{C}^{N\times n_b}$ satisfying $V_1^{\mathrm{H}} V_1 = I_{n_b}$, and $B_0 \in \mathbb{C}^{n_b\times n_b}$;
2: $Z = AV_1$, $A_1 = V_1^{\mathrm{H}} Z$;
3: $Z = Z - V_1 A_1$;
4: perform orthogonalization on Z to obtain $Z = V_2 B_1$, where $V_2 \in \mathbb{C}^{N\times n_b}$ satisfying $V_2^{\mathrm{H}} V_2 = I_{n_b}$ and $B_1 \in \mathbb{C}^{n_b\times n_b}$;
5: **for** $j = 2$ to n **do**
6: $Z = AV_j$, $A_j = V_j^{\mathrm{H}} Z$;
7: $Z = Z - V_j A_j - V_{j-1} B_{j-1}^{\mathrm{H}}$;
8: perform orthogonalization on Z to obtain $Z = V_{j+1} B_j$, $V_{j+1} \in \mathbb{C}^{N\times n_b}$ satisfying $V_{j+1}^{\mathrm{H}} V_{j+1} = I_{n_b}$ and $B_j \in \mathbb{C}^{n_b\times n_b}$;
9: **end for**

simplest because we assume all Z at Lines 4 and 8 there have full column rank n_b for all j. Then $V_j \in \mathbb{C}^{N\times n_b}$, and

$$\mathcal{K}_n := \mathcal{K}_n(A, V_0) = \mathcal{R}(V_1) \oplus \cdots \oplus \mathcal{R}(V_n), \tag{3.1}$$

the direct sum of $\mathcal{R}(V_j)$ for $j = 1, 2, \ldots, n$.

A fundamental relation of the process is

$$AQ_n = Q_n T_n + [0_{N\times nn_b}, V_{n+1} B_n], \tag{3.2}$$

where

$$Q_n = [V_1, V_2, \ldots, V_n] \in \mathbb{C}^{N\times nn_b}, \quad \text{and} \tag{3.3a}$$

$$T_n = Q_n^{\mathrm{H}} A Q_n = \begin{bmatrix} A_1 & B_1^{\mathrm{H}} & & & \\ B_1 & A_2 & B_2^{\mathrm{H}} & & \\ & \ddots & \ddots & \ddots & \\ & & B_{n-2} & A_{n-1} & B_{n-1}^{\mathrm{H}} \\ & & & B_{n-1} & A_n \end{bmatrix} \in \mathbb{C}^{nn_b\times nn_b}. \tag{3.3b}$$

$T_n = Q_n^{\mathrm{H}} A Q_n$ is the so-called *Rayleigh* quotient matrix with respect to $\mathcal{K}_n$ and it is the projection of A onto $\mathcal{K}_n$, too. Let

$$\Pi_n = Q_n Q_n^{\mathrm{H}} \tag{3.4}$$

which is the orthogonal projection onto $\mathcal{K}_n$. In particular $\Pi_1 = Q_1 Q_1^{\mathrm{H}} = V_1 V_1^{\mathrm{H}}$ is the orthogonal projection onto $\mathcal{R}(V_0) = \mathcal{R}(V_1)$.

Basically the block Lanczos method is this block Lanczos process followed by solving the eigenvalue problem for T_n to obtain approximate eigenpairs for A: any

eigenpair $(\tilde{\lambda}_j, w_j)$ of T_n gives an approximate eigenpair $(\tilde{\lambda}_j, Q_n w_j)$ for A. The number $\tilde{\lambda}_j$ is called a *Ritz value* and $\tilde{u}_j := Q_n w_j$ a *Ritz vector*.

We introduce the following notation for T_n that will be used in the next two sections:

$$\begin{array}{rl}
\text{eigenvalues (also Ritz values):} & \tilde{\lambda}_1 \geq \tilde{\lambda}_2 \geq \cdots \geq \tilde{\lambda}_{nn_b}, \text{ and} \\
& \Omega = \operatorname{diag}(\tilde{\lambda}_1, \tilde{\lambda}_2, \ldots, \tilde{\lambda}_{nn_b}), \\
\text{orthonormal eigenvectors:} & w_1, w_2, \ldots, w_{nn_b}, \text{ and} \\
& W = [w_1, w_2, \ldots, w_{nn_b}], \\
\text{eigen-decomposition:} & T_n W = W\Omega \text{ and } W^{\mathrm{H}} W = I_{nn_b}, \\
\text{Ritz vectors:} & \tilde{u}_j = Q_n w_j \text{ for } 1 \leq j \leq nn_b, \text{ and} \\
& \widetilde{U} = [\tilde{u}_1, \tilde{u}_2, \ldots, \tilde{u}_{nn_b}].
\end{array} \tag{3.5}$$

Note the dependency of $\tilde{\lambda}_j,\ w_j, W$ on n is suppressed for convenience.

As in Saad [22], there is no loss of generality in assuming that all eigenvalues of A are of multiplicity not exceeding n_b. In fact, let P_j be the orthogonal projections onto the eigenspaces corresponding to the distinct eigenvalues of A. Then

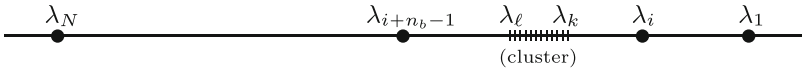
$$\mathcal{U} := \bigoplus_j \mathcal{R}(P_j V_0)$$

is an invariant subspace of A, and $A_{|\mathcal{U}}$, the restriction of A onto $\mathcal{U}$, has the same distinct eigenvalues as A and the multiplicity of any distinct eigenvalue of $A_{|\mathcal{U}}$ is no bigger than n_b. Since $\mathcal{K}_n(A, V_0) \subseteq \mathcal{U}$, what the block Lanczos method does is essentially to approximate some of the eigenpairs of $A_{|\mathcal{U}}$.

When $n_b = 1$, Algorithm 1 reduces to the single-vector Lanczos process.

4 Convergence of eigenspaces

Recall Π_n in (3.4), and in particular, $\Pi_1 = Q_1 Q_1^{\mathrm{H}} = V_1 V_1^{\mathrm{H}}$. For the rest of this and the next section, each of i, k, and ℓ will be reserved for one assignment only: we are considering the ith to $(i + n_b - 1)$st eigenpairs of A among which the kth to ℓth eigenvalues may form a cluster as in



where

$$1 \leq i < n, \quad i \leq k \leq \ell \leq i + n_b - 1.$$

Recall (1.3). We are interested in bounding

1. the canonical angles from the invariant subspace $\mathcal{R}(U_{(:,k:\ell)})$ to the Krylov subspace $\mathcal{K}_n \equiv \mathcal{K}_n(A, V_0)$,
2. the canonical angles between the invariant subspace $\mathcal{R}(U_{(:,k:\ell)})$ and $\operatorname{span}\{\tilde{u}_k, \ldots, \tilde{u}_\ell\}$ (which we call a *Ritz subspace*),

3. the differences between the eigenvalues λ_j and the Ritz values $\tilde{\lambda}_j$ for $k \le j \le \ell$.

In doing so, we will use the jth Chebyshev polynomial of the first kind $\mathscr{T}_j(t)$:

$$\mathscr{T}_j(t) = \cos(j \arccos t) \qquad \text{for} \quad |t| \le 1, \tag{4.1a}$$

$$= \frac{1}{2}\left[\left(t + \sqrt{t^2-1}\right)^j + \left(t + \sqrt{t^2-1}\right)^{-j}\right] \qquad \text{for} \quad t \ge 1. \tag{4.1b}$$

It frequently shows up in numerical analysis and computations because of its numerous nice properties, for example $|\mathscr{T}_j(t)| \le 1$ for $|t| \le 1$ and $|\mathscr{T}_j(t)|$ grows extremely fast[2] for $|t| > 1$. We will also need [17]

$$\left|\mathscr{T}_j\left(\frac{1+t}{1-t}\right)\right| = \left|\mathscr{T}_j\left(\frac{t+1}{t-1}\right)\right| = \frac{1}{2}\left[\Delta_t^j + \Delta_t^{-j}\right] \quad \text{for } 1 \ne t > 0, \tag{4.2}$$

where

$$\Delta_t := \frac{\sqrt{t}+1}{|\sqrt{t}-1|} \quad \text{for} \quad t > 0. \tag{4.3}$$

In the rest of this section and the entire next section, we will always assume

$$\operatorname{rank}(V_0^{\mathrm{H}} U_{(:,i:i+n_b-1)}) = \operatorname{rank}(V_1^{\mathrm{H}} U_{(:,i:i+n_b-1)}) = n_b, \tag{4.4}$$

and $X_{i,k,\ell} \in \mathbb{C}^{N\times(\ell-k+1)}$ is to be defined by (4.5) below. Consider an application of Proposition 2.4(b) with $k_1 = \ell - k + 1$,

$$\mathcal{X} = \mathcal{R}(V_0) = \mathcal{R}(V_1), \quad \mathcal{Y} = \mathcal{R}(U_{(:,i:i+n_b-1)}), \quad [y_1, y_2, \ldots, y_{k_1}] = [u_k, u_{k+1}, \ldots, u_\ell].$$

The application yields a unique

$$X_{i,k,\ell} := [x_1, x_2, \ldots, x_{k_1}] \tag{4.5}$$

such that $\mathcal{R}(X_{i,k,\ell}) \subseteq \mathcal{R}(V_0)$ and

$$U_{(:,i:i+n_b-1)} U_{(:,i:i+n_b-1)}^{\mathrm{H}} X_{i,k,\ell} = U_{(:,k:\ell)} \equiv [u_k, u_{k+1}, \ldots, u_\ell]. \tag{4.6}$$

Moreover, by Proposition 2.4(a),

$$\left\|\sin\Theta(U_{(:,k:\ell)}, X_{i,k,\ell})\right\| \le \left\|\sin\Theta(U_{(:,i:i+n_b-1)}, V_0)\right\|, \tag{4.7}$$

$$\left\|\tan\Theta(U_{(:,k:\ell)}, X_{i,k,\ell})\right\| \le \left\|\tan\Theta(U_{(:,i:i+n_b-1)}, V_0)\right\|. \tag{4.8}$$

They show that the chosen $\mathcal{R}(X_{i,k,\ell})$ has a significant component in the eigenspace $\mathcal{R}(U_{(:,k:\ell)})$ of interest if the initial $\mathcal{R}(V_0)$ has a significant component in the eigenspace $\mathcal{R}(U_{(:,i:i+n_b-1)})$.

[2] In fact, a result due to Chebyshev himself says that if $p(t)$ is a polynomial of degree no bigger than j and $|p(t)| \le 1$ for $-1 \le t \le 1$, then $|p(t)| \le |\mathscr{T}_j(t)|$ for any t outside $[-1, 1]$ [4, p. 65].

The matrix $X_{i,k,\ell}$ defined in (4.5) obviously depends on n_b as well. This dependency is suppressed because n_b is reserved throughout this article. The idea of picking such $X_{i,k,\ell}$ is essentially borrowed from [22, Lemma 4] (see Remark 2.2).

Theorem 4.1 *For any unitarily invariant norm $|||\cdot|||$, we have*

$$\left|\left|\left|\tan\Theta(U_{(:,k:\ell)}, \mathcal{K}_n)\right|\right|\right| \le \frac{\xi_{i,k}}{\mathscr{T}_{n-i}(\kappa_{i,\ell,n_b})} \left|\left|\left|\tan\Theta(U_{(:,k:\ell)}, X_{i,k,\ell})\right|\right|\right|, \tag{4.9}$$

$$\left|\left|\left|\sin\Theta(U_{(:,k:\ell)}, \widetilde{U}_{(:,k:\ell)})\right|\right|\right| \le \gamma \left|\left|\left|\sin\Theta(U_{(:,k:\ell)}, \mathcal{K}_n)\right|\right|\right| \tag{4.10}$$

$$\le \frac{\gamma\,\xi_{i,k}}{\mathscr{T}_{n-i}(\kappa_{i,\ell,n_b})} \left|\left|\left|\tan\Theta(U_{(:,k:\ell)}, X_{i,k,\ell})\right|\right|\right|, \tag{4.11}$$

where $X_{i,k,\ell}$ is defined by (4.5), $\widetilde{U}$ by (3.5), and[3]

$$\xi_{i,k} = \prod_{j=1}^{i-1} \frac{\lambda_j - \lambda_N}{\lambda_j - \lambda_k}, \quad \delta_{i,\ell,n_b} = \frac{\lambda_\ell - \lambda_{i+n_b}}{\lambda_\ell - \lambda_N}, \quad \kappa_{i,\ell,n_b} = \frac{1+\delta_{i,\ell,n_b}}{1-\delta_{i,\ell,n_b}}, \tag{4.12}$$

$$\gamma = 1 + \frac{c}{\eta}\,\|\Pi_n A(I-\Pi_n)\|_2, \tag{4.13}$$

and the constant c lies between 1 and $\pi/2$, and it is[4] *1 for the Frobenius norm or if $\tilde{\lambda}_{k-1} > \lambda_k$, and*

$$\eta = \min_{\substack{k\le j\le \ell \\ p<k,\ \text{or}\ p>\ell}} |\lambda_j - \tilde{\lambda}_p|. \tag{4.14}$$

For the Frobenius norm, γ in (4.13) can be improved to

$$\gamma = \sqrt{1 + \left(\frac{1}{\eta}\,\|\Pi_n A(I-\Pi_n)\|_2\right)^2}. \tag{4.15}$$

Proof Write

$$U = \overset{\quad i-1 \quad n_b \quad N-n_b-i+1}{\left[\begin{array}{ccc} U_1 & U_2 & U_3 \end{array}\right]}, \quad \Lambda = \begin{array}{c} i-1 \\ n_b \\ N-n_b-i+1 \end{array} \overset{\quad i-1 \quad n_b \quad N-n_b-i+1}{\left[\begin{array}{ccc} \Lambda_1 & & \\ & \Lambda_2 & \\ & & \Lambda_3 \end{array}\right]}, \tag{4.16a}$$

$$\check{U}_2 = U_{(:,k:\ell)} = (U_2)_{(:,k-i+1:\ell-i+1)} = [u_k, \ldots, u_\ell], \tag{4.16b}$$

$$\check{\Lambda}_2 = \Lambda_{(k:\ell,k:\ell)} = (\Lambda_2)_{(k-i+1:\ell-i+1,k-i+1:\ell-i+1)} = \mathrm{diag}(\lambda_k, \ldots, \lambda_\ell). \tag{4.16c}$$

[3] By convention, $\prod_{j=1}^{0}(\cdots) \equiv 1$.

[4] A by-product of this is that $c = 1$ if $k = \ell$.

For convenience, let's drop the subscripts to $X_{i,k,\ell}$ because i, k, ℓ do not change in this proof. We have

$$\begin{aligned} X &= UU^{\mathrm{H}}X = U_1U_1^{\mathrm{H}}X + U_2U_2^{\mathrm{H}}X + U_3U_3^{\mathrm{H}}X \\ &= U_1U_1^{\mathrm{H}}X + \check{U}_2\check{U}_2^{\mathrm{H}}X + U_3U_3^{\mathrm{H}}X \end{aligned} \tag{4.17}$$

by (4.6). Let $X_0 = X(X^{\mathrm{H}}X)^{-1/2}$ which has orthonomal columns. We know that

$$\mathcal{R}(f(A)X_0) \subset \mathcal{K}_n \quad \text{for any } f \in \mathbb{P}_{n-1},$$

since $\mathcal{R}(X_0) = \mathcal{R}(X) \subseteq \mathcal{R}(V_0)$. By (4.17),

$$Y := f(A)X_0 = U_1 f(\Lambda_1)U_1^{\mathrm{H}}X_0 + \check{U}_2 f(\check{\Lambda}_2)\check{U}_2^{\mathrm{H}}X_0 + U_3 f(\Lambda_3)U_3^{\mathrm{H}}X_0. \tag{4.18}$$

By (4.6), $\check{U}_2^{\mathrm{H}}X = I_{\ell-k+1}$ and thus $\check{U}_2^{\mathrm{H}}X_0$ is nonsingular. Now if also $f(\check{\Lambda}_2)$ is nonsingular (which is true for the selected f later), then

$$\begin{aligned} Y\left(\check{U}_2^{\mathrm{H}}X_0\right)^{-1}[f(\check{\Lambda}_2)]^{-1} &= U_1 f(\Lambda_1)U_1^{\mathrm{H}}X_0\left(\check{U}_2^{\mathrm{H}}X_0\right)^{-1}[f(\check{\Lambda}_2)]^{-1} \\ &\quad + \check{U}_2 + U_3 f(\Lambda_3)U_3^{\mathrm{H}}X_0\left(\check{U}_2^{\mathrm{H}}X_0\right)^{-1}[f(\check{\Lambda}_2)]^{-1}, \end{aligned} \tag{4.19}$$

and consequently by Proposition 2.1

$$\begin{aligned} \left\|\tan\Theta(\check{U}_2, \mathcal{K}_n)\right\| &\le \left\|\tan\Theta(\check{U}_2, Y)\right\| \\ &= \left\| \begin{bmatrix} f(\Lambda_1)U_1^{\mathrm{H}}X_0\left(\check{U}_2^{\mathrm{H}}X_0\right)^{-1}[f(\check{\Lambda}_2)]^{-1} \\ f(\Lambda_3)U_3^{\mathrm{H}}X_0\left(\check{U}_2^{\mathrm{H}}X_0\right)^{-1}[f(\check{\Lambda}_2)]^{-1} \end{bmatrix} \right\| \\ &= \left\| \begin{bmatrix} f(\Lambda_1) & \\ & f(\Lambda_3) \end{bmatrix} \begin{bmatrix} U_1^{\mathrm{H}}X_0\left(\check{U}_2^{\mathrm{H}}X_0\right)^{-1} \\ U_3^{\mathrm{H}}X_0\left(\check{U}_2^{\mathrm{H}}X_0\right)^{-1} \end{bmatrix} [f(\check{\Lambda}_2)]^{-1} \right\| \\ &\le \max_{\substack{1\le j\le i-1 \\ i+n_b\le j\le N}} |f(\lambda_j)| \times \max_{k\le j\le \ell} \frac{1}{|f(\lambda_j)|} \times \left\|\tan\Theta(\check{U}_2, X_0)\right\|. \end{aligned} \tag{4.20}$$

We need to pick an $f \in \mathbb{P}_{n-1}$ to make the right-hand side of (4.20) as small as we can. To this end for the case $i = 1$, we choose

$$f(t) = \mathscr{T}_{n-1}\left(\frac{2t - (\lambda_{n_b+1} + \lambda_N)}{\lambda_{n_b+1} - \lambda_N}\right) \Big/ \mathscr{T}_{n-1}(\kappa_{1,\ell,n_b}) \tag{4.21}$$

for which

$$\min_{k\le j\le \ell} f(\lambda_j) = f(\lambda_\ell) = 1, \quad \max_{n_b+1\le j\le N} |f(\lambda_j)| \le \frac{1}{\mathscr{T}_{n-1}(\kappa_{1,\ell,n_b})}. \tag{4.22}$$

This, together with (4.20), concludes the proof of (4.9) for $i = 1$.

In general for $i > 1$, we shall consider polynomials of form

$$f(t) = (\lambda_1 - t)\cdots(\lambda_{i-1} - t) \times g(t), \tag{4.23}$$

and search a $g \in \mathbb{P}_{n-i}$ such that $\max_{i+n_b\le j\le N} |g(\lambda_j)|$ is made as small as we can while $\min_{k\le j\le \ell} |g(\lambda_j)| = g(\lambda_\ell) = 1$. To this end, we choose

$$g(t) = \mathscr{T}_{n-i}\left(\frac{2t - (\lambda_{i+n_b} + \lambda_N)}{\lambda_{i+n_b} - \lambda_N}\right) \Big/ \mathscr{T}_{n-i}(\kappa_{i,\ell,n_b}), \tag{4.24}$$

for which

$$\min_{k\le j\le \ell} g(\lambda_j) = g(\lambda_\ell) = 1, \quad \max_{i+n_b\le j\le N} |g(\lambda_j)| \le \frac{1}{\mathscr{T}_{n-i}(\kappa_{i,\ell,n_b})}. \tag{4.25}$$

This, together with (4.20) and (4.23), concludes the proof of (4.9) for $i > 1$.

Next we prove (4.10) with an argument influenced by [11]. Recall (4.16). Let $Q_\perp \in \mathbb{C}^{N\times(N-nn_b)}$ such that $[Q_n, Q_\perp]$ is unitary, and write

$$\check{U}_2 = Q_n Z + Q_\perp Z_\perp, \tag{4.26}$$

where $Z = Q_n^{\mathrm{H}}\check{U}_2$, $Z_\perp = Q_\perp^{\mathrm{H}}\check{U}_2$. Then

$$\left\|\!\left|\cos\Theta(\check{U}_2, \mathcal{K}_n)\right|\!\right\| = \|\!|Z|\!\|, \quad \left\|\!\left|\sin\Theta(\check{U}_2, \mathcal{K}_n)\right|\!\right\| = \|\!|Z_\perp|\!\|. \tag{4.27}$$

Keeping in mind that $A\check{U}_2 = \check{U}_2\check{\Lambda}_2$, $Q_n^{\mathrm{H}} A Q_n = T_n$, and $T_n W = W\Omega$ from (3.5), we have

$$\begin{aligned} & Q_n^{\mathrm{H}} A\,[Q_n, Q_\perp][Q_n, Q_\perp]^{\mathrm{H}}\check{U}_2 = Q_n^{\mathrm{H}}\check{U}_2\check{\Lambda}_2 \\ \Rightarrow\ & [T_n, Q_n^{\mathrm{H}} A Q_\perp]\begin{bmatrix} Z \\ Z_\perp \end{bmatrix} = Z\check{\Lambda}_2 \\ \Rightarrow\ & T_n Z - Z\check{\Lambda}_2 = -Q_n^{\mathrm{H}} A Q_\perp Z_\perp. \end{aligned} \tag{4.28}$$

Similarly to (4.16), partition W and Ω as

$$W = \overset{\begin{matrix} k-1 & \ell-k+1 & nn_b-\ell \end{matrix}}{\begin{bmatrix} W_1 & W_2 & W_3 \end{bmatrix}}, \quad \Omega = \overset{\begin{matrix} k-1 \\ \ell-k+1 \\ nn_b-\ell \end{matrix}}{\overset{\begin{matrix} k-1 & \ell-k+1 & nn_b-\ell \end{matrix}}{\begin{bmatrix} \Omega_1 & & \\ & \Omega_2 & \\ & & \Omega_3 \end{bmatrix}}},$$

and set $W_{1,3} := [W_1, W_3]$ and $\Omega_{1,3} := \Omega_1 \oplus \Omega_3$. Multiply (4.28) by W^{H} from the left to get $\Omega W^{\mathrm{H}} Z - W^{\mathrm{H}} Z \check{\Lambda}_2 = -W^{\mathrm{H}} Q_n^{\mathrm{H}} A Q_\perp Z_\perp$, and thus we have

$$\Omega_{1,3} W_{1,3}^{\mathrm{H}} Z - W_{1,3}^{\mathrm{H}} Z \check{\Lambda}_2 = -W_{1,3}^{\mathrm{H}} Q_n^{\mathrm{H}} A Q_\perp Z_\perp. \tag{4.29}$$

By Lemma 2.1, we conclude that

$$\left\| W_{1,3}^{\mathrm{H}} Z \right\| \le \frac{c}{\eta} \left\| W_{1,3}^{\mathrm{H}} Q_n^{\mathrm{H}} A Q_\perp Z_\perp \right\| \le \frac{c}{\eta} \|\Pi_n A (I - \Pi_n)\|_2 \, |||Z_\perp|||. \tag{4.30}$$

Let $\widetilde{U}_{1,3} = Q_n W_{1,3}$. It can be verified that

$$W_{1,3}^{\mathrm{H}} Z = (\widetilde{U}_{1,3})^{\mathrm{H}} (Q_n Z) = (\widetilde{U}_{1,3})^{\mathrm{H}} (\check{U}_2 - Q_\perp Z_\perp) = (\widetilde{U}_{1,3})^{\mathrm{H}} \check{U}_2$$

by (4.26). Therefore

$$\begin{aligned} \left\| \sin \Theta(\check{U}_2, \widetilde{U}_{(:,k:\ell)}) \right\| &= \left\| [\widetilde{U}_{1,3}, Q_\perp]^{\mathrm{H}} \check{U}_2 \right\| \\ &\le \left\| (\widetilde{U}_{1,3})^{\mathrm{H}} \check{U}_2 \right\| + \left\| Q_\perp^{\mathrm{H}} \check{U}_2 \right\| \\ &= \left\| W_{1,3}^{\mathrm{H}} Z \right\| + |||Z_\perp||| \end{aligned} \tag{4.31}$$

which, for the Frobenius norm, can be improved to an identity

$$\| \sin \Theta(\check{U}_2, \widetilde{U}_{(:,k:\ell)}) \|_{\mathrm{F}} = \sqrt{\| W_{1,3}^{\mathrm{H}} Z \|_{\mathrm{F}}^2 + \| Z_\perp \|_{\mathrm{F}}^2}.$$

The inequality (4.10) is now a consequence of (4.27), (4.30), and (4.31). □

Remark 4.1 Although the appearance of three integers, i, k, and ℓ makes Theorem 4.1 awkward and more complicated than simply taking $i = k$ or $i + n_b - 1 = \ell$, it provides the flexibility when it comes to apply (4.9) with balanced $\xi_{i,k}$ (which should be made as small as possible) and δ_{i,ℓ,n_b} (which should be made as large as possible). In fact, for given k and ℓ, both $\xi_{i,k}$ and δ_{i,ℓ,n_b} increase with i. But the right-hand side of (4.9) increases as $\xi_{i,k}$ increases and decreases (rapidly) as δ_{i,ℓ,n_b} increases. So we would like to make $\xi_{i,k}$ as small as we can and δ_{i,ℓ,n_b} as large as we can. In particular, if $k \le \ell \le n_b$, one can always pick $i = 1$ so that (4.9) gets used with $\xi_{1,k} = 1$; but then if δ_{1,ℓ,n_b} is tiny, (4.9) is better used with some $i > 1$. A general guideline is to make sure $\{\lambda_j\}_{j=k}^{\ell}$ is a cluster and the rest of λ_j are relatively far away.

5 Convergence of eigenvalues

In this section, we will bound the differences between the eigenvalues λ_j and the Ritz values $\tilde{\lambda}_j$ for $k \le j \le \ell$.

Theorem 5.1 *Let $k = i$. For any unitarily invariant norm, we have*

$$\begin{aligned}&\left\|\operatorname{diag}(\lambda_i - \tilde{\lambda}_i, \lambda_{i+1} - \tilde{\lambda}_{i+1}, \ldots, \lambda_\ell - \tilde{\lambda}_\ell)\right\| \\ &\le (\lambda_i - \lambda_N)\left[\frac{\zeta_i}{\mathscr{T}_{n-i}(\kappa_{i,\ell,n_b})}\right]^2 \left\|\tan^2\Theta(U_{(:,k:\ell)}, X_{i,k,\ell})\right\|,\end{aligned} \tag{5.1}$$

where κ_{i,ℓ,n_b} is the same as the one in (4.12), and

$$\zeta_i = \max_{i+1\le p\le N} \prod_{j=1}^{i-1} \left|\frac{\tilde{\lambda}_j - \lambda_p}{\tilde{\lambda}_j - \lambda_i}\right|. \tag{5.2}$$

In particular, if also $\tilde{\lambda}_{i-1} \ge \lambda_i$, then

$$\zeta_i = \prod_{j=1}^{i-1} \left|\frac{\tilde{\lambda}_j - \lambda_N}{\tilde{\lambda}_j - \lambda_i}\right|. \tag{5.3}$$

Proof Upon shifting A by $\lambda_i I$ to $A - \lambda_i I_N$, we may assume $\lambda_i = 0$. Doing so doesn't change the Krylov subspace $\mathcal{K}_n(A, V_0) = \mathcal{K}_n(A - \lambda_i I, V_0)$ and doesn't change any eigenvector and any Ritz vector of A, but it does shift all eigenvalues and Ritz values of A by the same amount, i.e., λ_i, and thus all differences $\lambda_p - \lambda_j$ and $\lambda_p - \tilde{\lambda}_j$ remain unchanged. Suppose $\lambda_i = 0$ and thus $\lambda_{i-1} \ge \lambda_i = 0 \ge \lambda_{i+1}$.

Recall (3.5), and adopt the proof of Theorem 4.1 up to (4.19). Take f as

$$f(t) = (\tilde{\lambda}_1 - t)\cdots(\tilde{\lambda}_{i-1} - t) \times g(t), \tag{5.4}$$

where $g \in \mathbb{P}_{n-i}$. We claim $Y^{\mathrm{H}} Q_n w_j = 0$ for $1 \le j \le i-1$. This is because Y can be represented by $Y = (A - \tilde{\lambda}_j I)\widehat{Y}$ for some matrix $\widehat{Y} \in \mathbb{C}^{N\times(\ell-i+1)}$ with $\mathcal{R}(\widehat{Y}) \subseteq \mathcal{K}_n$ which further implies $\widehat{Y} = Q_n \check{Y}$ for some matrix $\check{Y} \in \mathbb{C}^{nn_b\times(\ell-i+1)}$. Thus $Y = (A - \tilde{\lambda}_j I) Q_n \check{Y}$ and

$$Y^{\mathrm{H}} Q_n w_j = \check{Y}^{\mathrm{H}} Q_n^{\mathrm{H}} (A - \tilde{\lambda}_j I) Q_n w_j = \check{Y}^{\mathrm{H}} (T_n - \tilde{\lambda}_j I) w_j = 0.$$

Set

$$Y_0 = Y\left(\check{U}_2^{\mathrm{H}} X_0\right)^{-1} [f(\check{\Lambda}_2)]^{-1} = U_1 R_1 + \check{U}_2 + U_3 R_3, \tag{5.5}$$

where $R_j = f(\Lambda_j) U_j^{\mathrm{H}} X_0 \left(\check{U}_2^{\mathrm{H}} X_0\right)^{-1} [f(\check{\Lambda}_2)]^{-1}$.

Let $Z = Y_0 (Y_0^{\mathrm{H}} Y_0)^{-1/2}$, and denote by $\mu_1 \ge \cdots \ge \mu_{\ell-i+1}$ the eigenvalues of $Z^{\mathrm{H}} A Z$ which depends on f in (5.4) to be determined for best error bounds. Note

$$Z^{\mathrm{H}} Q_n [w_1, \ldots, w_{i-1}] = 0, \quad \mathcal{R}(Z) \subseteq \mathcal{K}_n, \quad Z^{\mathrm{H}} Z = I_{\ell-i+1}. \tag{5.6}$$

Write $Z = Q_n\widehat{Z}$ because $\mathcal{R}(Z) \subseteq \mathcal{K}_n$, where $\widehat{Z}$ has orthonormal columns. Apply Cauchy's interlace inequalities to $Z^{\mathrm{H}}AZ = \widehat{Z}^{\mathrm{H}}(Q_n^{\mathrm{H}}AQ_n)\widehat{Z}$ and $Q_n^{\mathrm{H}}AQ_n$ to get $\tilde{\lambda}_{i+j-1} \geq \mu_j$ for $1 \leq j \leq \ell - i + 1$, and thus

$$0 \leq \lambda_{i+j-1} - \tilde{\lambda}_{i+j-1} \leq \lambda_{i+j-1} - \mu_j \quad \text{for } 1 \leq j \leq \ell - i + 1. \tag{5.7}$$

In particular, this implies $\mu_j \leq \lambda_{i+j-1} \leq \lambda_i \leq 0$ and consequently $Y_0^{\mathrm{H}}AY_0$ is negative semidefinite. Therefore for any nonzero vector $y \in \mathbb{C}^{\ell-i+1}$,

$$\begin{aligned} 0 \geq y^{\mathrm{H}}Y_0^{\mathrm{H}}AY_0y &= y^{\mathrm{H}}R_1^{\mathrm{H}}\Lambda_1R_1y + y^{\mathrm{H}}\check{\Lambda}_2y + y^{\mathrm{H}}R_3^{\mathrm{H}}\Lambda_3R_3y \\ &\geq y^{\mathrm{H}}\check{\Lambda}_2y + y^{\mathrm{H}}R_3^{\mathrm{H}}\Lambda_3R_3y, \\ y^{\mathrm{H}}Y_0^{\mathrm{H}}Y_0y &= y^{\mathrm{H}}R_1^{\mathrm{H}}R_1y + y^{\mathrm{H}}y + y^{\mathrm{H}}R_3^{\mathrm{H}}R_3y \\ &\geq y^{\mathrm{H}}y, \end{aligned}$$

where we have used $y^{\mathrm{H}}R_1^{\mathrm{H}}\Lambda_1R_1y \geq 0$, $y^{\mathrm{H}}R_1^{\mathrm{H}}R_1y \geq 0$, and $y^{\mathrm{H}}R_3^{\mathrm{H}}R_3y \geq 0$. Therefore

$$0 \geq \frac{y^{\mathrm{H}}Y_0^{\mathrm{H}}AY_0y}{y^{\mathrm{H}}Y_0^{\mathrm{H}}Y_0y} \geq \frac{y^{\mathrm{H}}Y_0^{\mathrm{H}}AY_0y}{y^{\mathrm{H}}y} \geq \frac{y^{\mathrm{H}}(\check{\Lambda}_2 + R_3^{\mathrm{H}}\Lambda_3R_3)y}{y^{\mathrm{H}}y}. \tag{5.8}$$

Denote by $\hat{\mu}_1 \geq \cdots \geq \hat{\mu}_{\ell-i+1}$ the eigenvalues of $\check{\Lambda}_2 + R_3^{\mathrm{H}}\Lambda_3R_3$. By (5.8), we know $\mu_j \geq \hat{\mu}_j$ for $1 \leq j \leq \ell - i + 1$ which, together with (5.7), lead to

$$0 \leq \lambda_{i+j-1} - \tilde{\lambda}_{i+j-1} \leq \lambda_{i+j-1} - \hat{\mu}_j \quad \text{for } 1 \leq j \leq \ell - i + 1. \tag{5.9}$$

Hence for any unitarily invariant norm [16,23]

$$\begin{aligned} &\left|\left|\left|\mathrm{diag}(\lambda_i - \tilde{\lambda}_i, \lambda_{i+1} - \tilde{\lambda}_{i+1}, \ldots, \lambda_\ell - \tilde{\lambda}_\ell)\right|\right|\right| \\ &\leq \left|\left|\left|\mathrm{diag}(\lambda_i - \hat{\mu}_1, \lambda_{i+1} - \hat{\mu}_2, \ldots, \lambda_\ell - \hat{\mu}_{\ell-i+1})\right|\right|\right| \\ &\leq \left|\left|\left| R_3^{\mathrm{H}}\Lambda_3R_3 \right|\right|\right| \\ &\leq (\lambda_i - \lambda_N)\left|\left|\left| R_3^{\mathrm{H}}R_3 \right|\right|\right|, \end{aligned} \tag{5.10}$$

where the last inequality is true because (1) $R_3^{\mathrm{H}}\Lambda_3R_3$ is negative semi-definite, (2) we shifted A by $\lambda_i I$, and (3) the jth largest eigenvalue of $R_3^{\mathrm{H}}(\lambda_i I - \Lambda_3)R_3$ which is positive semi-definite is bounded by the jth largest eigenvalue of $(\lambda_i - \lambda_N)R_3^{\mathrm{H}}R_3$.

Denote by σ_j (in descending order) for $1 \leq j \leq \ell - i + 1$ the singular values of $R_3 = f(\Lambda_3)U_3^{\mathrm{H}}X_0\left(\check{U}_2^{\mathrm{H}}X_0\right)^{-1}[f(\check{\Lambda}_2)]^{-1}$, and by $\hat{\sigma}_j$ (in descending order) for $1 \leq j \leq \ell - i + 1$ the singular values of $U_3^{\mathrm{H}}X_0\left(\check{U}_2^{\mathrm{H}}X_0\right)^{-1}$. Then $\hat{\sigma}_j$ is less than or equal to the jth largest singular value of $\begin{bmatrix} U_1^{\mathrm{H}}X_0\left(\check{U}_2^{\mathrm{H}}X_0\right)^{-1} \\ U_3^{\mathrm{H}}X_0\left(\check{U}_2^{\mathrm{H}}X_0\right)^{-1} \end{bmatrix}$, which is $\tan\theta_j(\check{U}_2, X)$. We have

$$\sigma_j \le \max_{i+n_b \le j \le N} |f(\lambda_j)| \times \max_{i \le j \le \ell} \frac{1}{|f(\lambda_j)|} \times \hat{\sigma}_j$$
$$\le \max_{i+n_b \le j \le N} |f(\lambda_j)| \times \max_{i \le j \le \ell} \frac{1}{|f(\lambda_j)|} \times \tan\theta_j(\check{U}_2, X). \tag{5.11}$$

What remains to be done is to pick $f \in \mathbb{P}_{n-1}$ to make the right-hand side of (5.11) as small as we can.

For the case of $i = 1$, we choose f as in (4.21), and then (4.22) holds. Finally combining (5.10) and (5.11) with (4.22) leads to (5.1) for the case $i = 1$.

In general for $i > 1$, we take $f(t)$ as in (5.4) with $g(t)$ given by (4.24) satisfying (4.25), together again with (5.10) and (5.11), to conclude the proof. □

Remark 5.1 In Theorem 5.1, $k = i$ always, unlike lin Theorem 4.1, because we need the first equation in (5.6) for our proof to work.

6 A comparison with the existing results

The existing results related to our results in the previous two sections include those by Kaniel [12], Paige [20], and Saad [22] (see also Parlett [21]). The most complete and strongest ones are in Saad [22].

In comparing ours with Saad's results, the major difference is that ours are of the eigenspace/eigenvalue cluster type while Saad's results are of the single-vector/eigenvalue type. When specialized to an individual eigenvector/eigenvalue, our results reduce to those of Saad. Specifically, for $k = \ell = i$ the inequality (4.9) becomes Saad [22, Theorem 5] and Theorem 5.1 becomes Saad [22, Theorem 6]. Certain parts of our proofs bear similarities to Saad's proofs for the block case, but there are subtleties in our proofs that cannot be handled in a straightforward way following Saad's proofs.

It is well-known [7] that eigenvectors associated with eigenvalues in a tight cluster are sensitive to perturbations/rounding errors while the whole invariant subspace associated with the cluster is not so much. Therefore it is natural to treat the entire invariant subspace as a whole, instead of each individual eigenvectors in the invariant subspace separately.

In what follows, we will perform a brief theoretical comparison between our results and those of Saad, and point out when Saad's bounds may be too large. Numerical examples in the next section support this comparison.

As mentioned, Saad's bounds are of the single-vector/eigenvalue type. So a direct comparison cannot be done. But it is possible to derive some bounds for eigenspaces/eigenvalue clusters from Saad's bounds, except that these derived bounds are less elegant and (likely) less sharp (which we will demonstrate numerically in Sect. 7). One possible derivation based on [22, Theorem 5] may be as follows. By Proposition 2.2,

$$\max_{k \le j \le \ell} \sin\theta(u_j, \mathcal{K}_n) \le \left\| \sin\Theta(U_{(:,k:\ell)}, \mathcal{K}_n) \right\| \le \sum_{j=k}^{\ell} \sin\theta(u_j, \mathcal{K}_n), \tag{6.1}$$

$$\max_{k\le j\le \ell} \sin\theta(u_j,\mathcal{K}_n) \le \|\sin\Theta(U_{(:,k:\ell)},\mathcal{K}_n)\|_{\mathrm{F}} \le \sqrt{\sum_{j=k}^{\ell}\sin^2\theta(u_j,\mathcal{K}_n)}\,. \tag{6.2}$$

These inequalities imply that the largest $\sin\theta(u_j,\mathcal{K}_n)$ is comparable to $\sin\Theta(U_{(:,k:\ell)},\mathcal{K}_n)$, and thus finding good bounds for all $\sin\theta(u_j,\mathcal{K}_n)$ is comparably equivalent to finding a good bound for $\sin\Theta(U_{(:,k:\ell)},\mathcal{K}_n)$.

The right-most sides of (6.1) and (6.2) can be bounded, using [22, Theorem 5] (i.e., the inequality (4.9) for the case $k=\ell=i$). In the notation of Theorem 4.1, we have, for $k\le j\le \ell$,

$$\tan\theta(u_j,\mathcal{K}_n) \le \frac{\xi_{j,j}}{\mathscr{T}_{n-j}(\kappa_{j,j,n_b})}\tan\theta(u_j,X_{j,j,j}) \tag{6.3}$$

and use $\sin\theta\le\tan\theta$ to get

$$\left\|\sin\Theta(U_{(:,k:\ell)},\mathcal{K}_n)\right\| \le \sum_{j=k}^{\ell}\frac{\xi_{j,j}}{\mathscr{T}_{n-j}(\kappa_{j,j,n_b})}\tan\theta(u_j,X_{j,j,j}), \tag{6.4}$$

$$\|\sin\Theta(U_{(:,k:\ell)},\mathcal{K}_n)\|_{\mathrm{F}} \le \sqrt{\sum_{j=k}^{\ell}\left[\frac{\xi_{j,j}}{\mathscr{T}_{n-j}(\kappa_{j,j,n_b})}\tan\theta(u_j,X_{j,j,j})\right]^2}, \tag{6.5}$$

where $X_{j,j,j}\in\mathbb{C}^N$ are as defined right before Theorem 4.1, and κ_{j,j,n_b} are as defined in Theorem 4.1. If $\theta_1(U_{(:,k:\ell)},\mathcal{K}_n)$ is not too close to $\pi/2$ which we will assume, the left-hand sides of (4.9), (6.4), and (6.5) are comparable by Proposition 2.2, but there isn't any easy way to compare their right-hand sides. Nevertheless, we argue that the right-hand side of (4.9) is preferable. First it is much simpler; Second, it is potentially much sharper for two reasons:

1. One or more $\xi_{j,j}$ for $k\le j\le\ell$ in (6.4) and (6.5) may be much bigger than $\xi_{i,k}$ in (4.9).
2. By Proposition 2.3, $\Theta(U_{(:,k:\ell)},[X_{k,k,k},\ldots,X_{\ell,\ell,\ell}])$ can be bounded in terms of the angles in $\{\theta(u_j,X_{j,j,j}),\ k\le j\le\ell\}$ but not the other way around, i.e., together $\{\theta(u_j,X_{j,j,j}),\ k\le j\le\ell\}$ cannot be bounded by something in terms of

$$\Theta(U_{(:,k:\ell)},[X_{k,k,k},\ldots,X_{\ell,\ell,\ell}])$$

in general as we argued in Remark 2.1.

For bounding errors between eigenvectors u_j and Ritz vectors $\tilde{u}_j$, the following inequality was established in [22, Theorem3] (which is also true for the block Lanczos method as commented there [22, p. 703]):

$$\sin\theta(u_j,\tilde{u}_j)\le\chi_j\ \sin\theta(u_j,\mathcal{K}_n)\quad\text{with}\quad \chi_j=\sqrt{1+\left(\frac{\|\Pi_n A(I-\Pi_n)\|_2}{\min_{p\ne j}|\lambda_j-\tilde{\lambda}_p|}\right)^2}. \tag{6.6}$$

This inequality can grossly overestimate $\sin\theta(u_j, \tilde{u}_j)$ even with the "exact" (i.e., computed) $\sin\theta(u_j, \mathcal{K}_n)$ for the ones associated with a cluster of eigenvalues due to possibly extremely tiny gap $\min_{p\neq j}|\lambda_j - \tilde{\lambda}_p|$, not to mention after using (6.3) to bound $\sin\theta(u_j, \mathcal{K}_n)$. By Proposition 2.3, we have

$$\begin{aligned}\|\sin\Theta(U_{(:,k:\ell)}, \widetilde{U}_{(:,k:\ell)})\|_{\mathrm{F}} &\leq \sqrt{\sum_{j=k}^{\ell}\sin^2\theta(u_j, \tilde{u}_j)} \\ &\leq \sqrt{\sum_{j=k}^{\ell}\chi_j^2\,\sin^2\theta(u_j, \mathcal{K}_n)} \qquad (6.7)\\ &\leq \sqrt{\sum_{j=k}^{\ell}\left[\frac{\chi_j\xi_{j,j}}{\mathscr{T}_{n-j}(\kappa_{j,j,n_b})}\tan\theta(u_j, X_{j,j,j})\right]^2}. \qquad (6.8)\end{aligned}$$

Inherently any bound derived from bounds for all $\sin^2\theta(u_j, \tilde{u}_j)$ likely very much overestimates $\|\sin\Theta(U_{(:,k:\ell)}, \widetilde{U}_{(:,k:\ell)})\|_{\mathrm{F}}^2$ because there is no simply way to bound $\sum_{j=k}^{\ell}\sin^2\theta(u_j, \tilde{u}_j)$ in terms of $\|\sin\Theta(U_{(:,k:\ell)}, \widetilde{U}_{(:,k:\ell)})\|_{\mathrm{F}}^2$, i.e., the former may already be much bigger than the latter, as we argued in Remark 2.1. So we anticipate the bounds of (6.7) and (6.8) to be bad when λ_j with $k \leq j \leq \ell$ form a tight cluster.

Saad [22, Theorem 6] provides a bound on $\lambda_j - \tilde{\lambda}_j$ individually. The theorem is the same as our Theorem 5.1 for the case $k = \ell = i$. Concerning the eigenvalue cluster $\{\lambda_k, \ldots, \lambda_\ell\}$, Saad's theorem gives

$$\sqrt{\sum_{j=k}^{\ell}(\lambda_j - \tilde{\lambda}_j)^2} \leq \sqrt{\sum_{j=k}^{\ell}(\lambda_j - \lambda_N)^2\left[\frac{\zeta_j}{\mathscr{T}_{n-j}(\kappa_{j,j,n_b})}\tan\theta(u_j, X_{j,j,j})\right]^4}. \qquad (6.9)$$

This bound, too, could be much bigger than the one of (5.1) because of one or more ζ_j with $k = i \leq j \leq \ell$ are much bigger than ζ_i.

7 Numerical examples

In this section, we shall numerically test the effectiveness of our upper bounds on the convergence of the block Lanczos method in the case of a cluster. In particular, we will demonstrate that our upper bounds are preferable to those of the single-vector/eigenvalue type in Saad [22], especially in the case of a tight cluster. Specifically,

(a) the subspace angle $\Theta(U_{(:,k:\ell)}, X_{i,k,\ell})$ used in our bounds is more reliable than the individual angles in $\{\theta(u_j, X_{j,j,j}),\ k \leq j \leq \ell\}$ together to bound $\Theta(U_{(:,k:\ell)}, \mathcal{K}_n)$ (see remarks in Sect. 6), and
(b) our upper bounds are much sharper than those derived from Saad's bounds in the presence of tight clusters of eigenvalues.

We point out that the worst individual bound of (6.3) or (6.6) or for $\lambda_j - \tilde{\lambda}_j$ is at the same magnitude as the derived bound of (6.5) or (6.8) or (6.9), respectively. So if a derived bound is bad, the worst corresponding individual bound cannot be much better. For this reason, we shall focus on comparing our bounds to the derived bounds in Sect. 6.

Our first example below is intended to illustrate the first point (a), while the second example supports the second point (b). The third example is essentially taken from [22], again to show the effectiveness of our upper bounds.

We implemented the block Lanczos method within MATLAB, with full reorthogonalization to simulate the block Lanczos method in exact arithmetic. This is the best one can do in a floating point environment. In our tests, without loss of generality, we take

$$A = \mathrm{diag}(\lambda_1, \ldots, \lambda_N)$$

with special eigenvalue distributions to be specified later. Although we stated our theorems in unitarily invariant norms for generality, our numerical results are presented in terms of the Frobenius norm for easy understanding (and thus for Theorem 4.1, γ by (4.15) is used). No breakdown was encountered during all Lanczos iterations.

We will measure the following errors: (in all examples, $k = i = 1$ and $\ell = n_b = 3$)

$$\epsilon_1 = \sqrt{\sum_{j=k}^{\ell} |\tilde{\lambda}_j - \lambda_j|^2}, \tag{7.1a}$$

$$\epsilon_2 = \| \sin \Theta(U_{(:,k:\ell)}, \widetilde{U}_{(:,k:\ell)}) \|_{\mathrm{F}}, \tag{7.1b}$$

$$\epsilon_3 = \| \sin \Theta(U_{(:,k:\ell)}, \mathcal{K}_n) \|_{\mathrm{F}}, \tag{7.1c}$$

$$\epsilon_4 = \| \tan \Theta(U_{(:,k:\ell)}, \mathcal{K}_n) \|_{\mathrm{F}}, \tag{7.1d}$$

for their numerically observed values (considered as "exact"), bounds of Theorems 4.1 and 5.1, and derived bounds of (6.9), (6.8) and (6.5) considered as "Saad's bounds" for comparison purpose. Rigorously speaking, these are not Saad's bounds.

For very tiny $\theta_1(U_{(:,k:\ell)}, \mathcal{K}_n)$, $\epsilon_3 \approx \epsilon_4$ since

$$\epsilon_3 \le \epsilon_4 \le \epsilon_3 / \sqrt{1 - \sin^2 \theta_1(U_{(:,k:\ell)}, \mathcal{K}_n)}.$$

Indeed in the examples that follows, the difference between ϵ_3 and ϵ_4 is so tiny that we can safely ignore their difference. Therefore we will be focusing on ϵ_1, ϵ_2, and ϵ_3, but not ϵ_4.

Example 7.1 We take $N = 600$, the number of Lanczos steps $n = 20$, and

$$\lambda_1 = 3.5,\ \lambda_2 = 3,\ \lambda_3 = 2.5, \quad \lambda_j = 1 - \frac{5j}{N}, \quad j = 4, \ldots, N,$$

and set $i = k = 1, \ell = 3$ and $n_b = 3$. There are two eigenvalue clusters: $\{\lambda_1, \lambda_2, \lambda_3\}$ and $\{\lambda_4, \ldots, \lambda_N\}$. We are seeking approximations related to the first cluster $\{\lambda_1, \lambda_2, \lambda_3\}$. The gap 0.5 between eigenvalues within the first cluster is to ensure

Table 1 Example 7.1: $N = 600, n = 20, i = k = 1, \ell = 3, n_b = 3$, and V_0 as in (7.2)

$\sqrt{\sum_{j=k}^{\ell} \lvert\tilde{\lambda}_j - \lambda_j\rvert^2}$			$\lVert \sin\Theta(U_{(:,k:\ell)}, \widetilde{U}_{(:,k:\ell)})\rVert_{\mathrm{F}}$			$\lVert \sin\Theta(U_{(:,k:\ell)}, \mathcal{K}_n)\rVert_{\mathrm{F}}$		
Observed	Bound of (5.1)	Saad bound of (6.9)	Observed	Bound of (4.11)	Saad bound of (6.8)	Observed	Bound of (4.9)	Saad bound of (6.5)
1.9×10^{-14}	4.4×10^{-14}	4.2×10^{-3}	3.5×10^{-8}	1.3×10^{-7}	6.8×10^{-2}	3.3×10^{-8}	1.0×10^{-7}	2.5×10^{-2}

that our investigation for our point (a) will not be affected too much by the eigenvalue closeness in the cluster. The effect of the closeness is, however, the subject of Example 7.2.

Our first test run is with a special V_0 given by

$$V_0 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ \frac{1}{N} & \sin 1 & \cos 1 \\ \vdots & \vdots & \vdots \\ \frac{N-n_b}{N} & \sin(N-n_b) & \cos(N-n_b) \end{bmatrix}. \tag{7.2}$$

Table 1 reports ϵ_1, ϵ_2, and ϵ_3 and their bounds. Our bounds are very sharp—comparable to the observed ones, but the ones by (6.9), (6.8) and (6.5) overestimate the true errors too much to be of much use. Looking at (6.5) carefully, we find two contributing factors that make the resulting bound too big. The first contributing factor is the constants

$$\xi_{1,1} = 1, \quad \xi_{2,2} = 15, \quad \xi_{3,3} = 105. \tag{7.3}$$

The second contributing factor is the angles $\theta(u_j, X_{j,j,j})$ for $k \le j \le \ell$:

j	1	2	3
$\theta_j(U_{(:,k:\ell)}, X_{i,k,\ell})$	1.51299	1.51298	1.49976
$\theta(u_j, X_{j,j,j})$	1.49976	1.57066	1.57069

What we see is that the canonical angles $\theta_j(U_{(:,k:\ell)}, X_{i,k,\ell})$ are bounded away from $\pi/2$ but the last two of the angles $\theta(u_j, X_{j,j,j})$ are nearly $\pi/2 = 1.57080$. This of course has something to do with the particular initial V_0 in (7.2). But given the exact eigenvectors are e_1, e_2, e_3, this V_0 should not be considered a deliberate choice so as to simply make our bounds look good.

Similar reasons explain why the upper bounds of (6.9) and (6.8) are poor as well. In fact, now the first contributing factor is

$$\zeta_1 = 1, \quad \zeta_2 = 15 - 1.5 \cdot 10^{-13} \approx 15, \quad \zeta_3 = 105 - 3.8 \cdot 10^{-12} \approx 105, \tag{7.4}$$

$$\chi_1 \approx \chi_2 \approx \chi_3 \approx 2.6860, \tag{7.5}$$

Table 2 Example 7.1: averages over 20 random V_0

$\sqrt{\sum_{j=k}^{\ell} \lvert\tilde{\lambda}_j - \lambda_j\rvert^2}$			$\lVert \sin\Theta(U_{(:,k:\ell)}, \widetilde{U}_{(:,k:\ell)})\rVert_{\mathrm{F}}$			$\lVert \sin\Theta(U_{(:,k:\ell)}, \mathcal{K}_n)\rVert_{\mathrm{F}}$		
Observed	Bound of (5.1)	Saad bound of (6.9)	Observed	Bound of (4.11)	Saad bound of (6.8)	Observed	Bound of (4.9)	Saad bound of (6.5)
1.2×10^{-14}	2.5×10^{-13}	8.2×10^{-8}	5.9×10^{-8}	2.5×10^{-7}	2.7×10^{-4}	5.6×10^{-8}	2.0×10^{-7}	9.9×10^{-5}

and then again the set of angles $\theta(u_j, X_{j,j,j})$ for $k \le j \le \ell$ is the second contributing factor.

Next we test random initial V_0 as generated by `randn`(N, n_b) in MATLAB. Table 2 reports the averages of the same errors/bounds as reported before over 20 test runs. The bounds of (6.9), (6.8) and (6.5) are much better now, but still about 1,000 times bigger than ours. The following table displays the canonical angles $\theta_j(U_{(:,k:\ell)}, X_{i,k,\ell})$ as well as $\theta(u_j, X_{j,j,j})$.

j	1	2	3
$\theta_j(U_{(:,k:\ell)}, X_{i,k,\ell})$	1.5497	1.5183	1.4712
$\theta(u_j, X_{j,j,j})$	1.5481	1.5359	1.5281

It shows that the randomness in V_0 makes none of $\theta(u_j, X_{j,j,j})$ for $k \le j \le \ell$ as close to $\pi/2$ as V_0 in (7.2) does. In fact, they are about at the same level as the canonical angles $\theta_j(U_{(:,k:\ell)}, X_{i,k,\ell})$. Therefore, the sole contributing factor that makes the bounds of (6.9), (6.8), and (6.5), worse than ours are the ξ's and ζ's in (7.3) and (7.4).

Example 7.2 Let $N = 1{,}000$, $n = 25$, and

$$\lambda_1 = 2 + \delta,\ \lambda_2 = 2,\ \lambda_3 = 2 - \delta, \quad \lambda_j = 1 - \frac{5j}{N}, \quad j = 4, \ldots, N,$$

and again set $i = k = 1, \ell = 3, n_b = 3$. We will adjust the parameter $\delta > 0$ to control the tightness among eigenvalues within the cluster $\{\lambda_1, \lambda_2, \lambda_3\}$ and to see how it affects the upper bounds and the convergence rate of the block Lanczos method. We will demonstrate that our bounds which are of the eigenspace/eigenvalue cluster type are insensitive to δ and barely change as δ goes to 0, while "Saad's bounds" are very sensitive and quickly become useless as δ goes to 0. We randomly generate initial V_0 and investigate the average errors/bounds over 20 test runs. Since the randomness will reduce the difference in contributions by $\Theta(U_{(:,k:\ell)}, X_{i,k,\ell})$ and by $\theta(u_j, X_{j,j,j})$ as we have seen in Example 7.1, the gap δ within the cluster and the gap between the cluster and the rest of the eigenvalues are the only contributing factor for approximation errors ϵ_i.

Table 3 reports the averages of the errors defined in 7.1 and the averages of their bounds of Theorems 4.1 and 5.1 and "Saad's bounds" of (6.9), (6.8) and (6.5) over 20 test runs. From the table, we observed that

Table 3 Example 7.2: averages over 20 random V_0

δ	$\sqrt{\sum_{j=k}^{\ell} \lvert\tilde{\lambda}_j - \lambda_j\rvert^2}$			$\lVert \sin\Theta(U_{(:,k:\ell)}, \widetilde{U}_{(:,k:\ell)})\rVert_{\mathrm{F}}$			$\lVert \sin\Theta(U_{(:,k:\ell)}, \mathcal{K}_n)\rVert_{\mathrm{F}}$		
	Observed	Bound of (5.1)	Saad bound of (6.9)	Observed	Bound of (4.11)	Saad bound of (6.8)	Observed	Bound of (4.9)	Saad bound of (6.5)
10^{-1}	5.6×10^{-15}	2.6×10^{-13}	2.6×10^{-6}	7.3×10^{-8}	3.8×10^{-7}	8.9×10^{-3}	6.6×10^{-8}	2.2×10^{-7}	6.7×10^{-4}
10^{-2}	1.8×10^{-13}	5.4×10^{-12}	8.9×10^{-3}	4.1×10^{-7}	1.5×10^{-6}	$4.9 \times 10^{+0}$	3.8×10^{-7}	3.8×10^{-7}	3.8×10^{-2}
10^{-3}	6.1×10^{-15}	2.5×10^{-14}	$6.1 \times 10^{+2}$	3.4×10^{-8}	1.2×10^{-7}	$4.1 \times 10^{+3}$	3.2×10^{-8}	7.2×10^{-8}	$3.2 \times 10^{+1}$
10^{-4}	2.3×10^{-14}	5.1×10^{-14}	$1.7 \times 10^{+6}$	4.7×10^{-8}	1.6×10^{-7}	$6.7 \times 10^{+6}$	4.3×10^{-8}	1.0×10^{-7}	$5.3 \times 10^{+2}$
10^{-5}	4.0×10^{-15}	3.7×10^{-14}	$6.2 \times 10^{+10}$	4.9×10^{-8}	1.5×10^{-7}	$1.3 \times 10^{+10}$	4.5×10^{-8}	9.7×10^{-8}	$1.0 \times 10^{+5}$

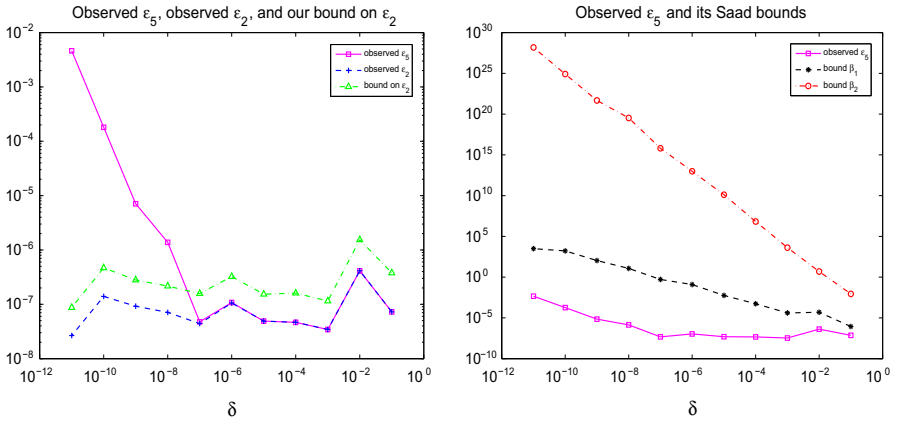


Fig. 1 Observed ϵ_5 deteriorates as δ goes to 0 while ϵ_2 seems to remain unchanged in magnitude. "Saad's bounds" on ϵ_5 are not included in the *left plot* in order not to obscure the radical difference between ϵ_2 and ϵ_5 for tiny δ

(i) all of our bounds which are of the eigenspace/eigenvalue cluster type are rather sharp—comparable to the observed ("exact") errors, and moreover, they seem to be independent of the parameter δ as it becomes tinier and tinier;
(ii) as δ gets tinier and tinier, the "Saad's bounds" of (6.9), (6.8), and (6.5) increase dramatically and quickly contain no useful information for $\delta = 10^{-3}$ or smaller.

To explain the observation (ii), we first note that $\xi_{j,j}$ in (6.5) are given by

$$\xi_{1,1} = 1, \quad \xi_{2,2} = 1 + \frac{6}{\delta}, \quad \text{and} \quad \xi_{3,3} = \frac{6}{\delta} + \frac{36}{\delta^2}.$$

They grow uncontrollably to ∞ as δ goes to 0. Therefore, the "Saad's bound" of (6.5) is about $\mathcal{O}(\delta^{-2})$ for tiny δ. Similarly, since $\xi_{j,j}$ and ζ_j are almost of the same level, it can be seen from (6.9) that the "Saad's bound" for ϵ_1 is about $\mathcal{O}(\delta^{-4})$. For (6.8), when n is moderate, χ_j is about $\mathcal{O}(\delta^{-1})$, and therefore, "Saad's bound" for ϵ_2 is about $\mathcal{O}(\delta^{-3})$ for tiny δ.

We argued in Sect. 6 that Saad's bound on $\theta(u_j, \tilde{u}_j)$ can be poor in a tight cluster of eigenvalues. Practically, it is also unreasonable to expect it to go as tiny as the machine's unit roundoff $\boldsymbol{u}$ as the number of Lanczos steps increases. For this example, by the Davis-Kahan $\sin\theta$ theorem [7] (see also [23]), we should expect, for $1 \le j \le 3$,

$$\text{(observed)} \ \sin\theta(u_j, \tilde{u}_j) = \mathcal{O}(\text{Lanczos approximation error}) + \mathcal{O}(\boldsymbol{u}/\delta),$$

where $\mathcal{O}(\boldsymbol{u}/\delta)$ is due to machine's roundoff and can dominate the Lanczos approximation error after certain number of Lanczos steps. To illustrate this point, we plot, in Fig. 1,

$$\epsilon_5 = \sqrt{\sum_{j=k}^{\ell} \sin^2\theta(u_j, \tilde{u}_j)}$$

Table 4 Example 7.3: $N = 900, n = 12, i = k = 1, \ell = 3, n_b = 3$

$\sqrt{\sum_{j=k}^{\ell} \lvert\tilde{\lambda}_j - \lambda_j\rvert^2}$			$\lVert \sin\Theta(U_{(:,k:\ell)}, \widetilde{U}_{(:,k:\ell)})\rVert_{\mathrm{F}}$			$\lVert \sin\Theta(U_{(:,k:\ell)}, \mathcal{K}_n)\rVert_{\mathrm{F}}$		
Observed	Bound of (5.1)	Saad bound of (6.9)	Observed	Bound of (4.11)	Saad bound of (6.8)	Observed	Bound of (4.9)	Saad bound of (6.5)
9.4×10^{-10}	1.5×10^{-8}	4.8×10^{-4}	3.9×10^{-5}	1.3×10^{-4}	3.0×10^{-2}	3.7×10^{-5}	1.1×10^{-4}	1.9×10^{-2}

as δ varies from 10^{-1} down to 10^{-11}. Also plotted are its two upper bounds β_1 and β_2 of (6.7) and (6.8)

$$\epsilon_5 \le \beta_1 := \sqrt{\sum_{j=k}^{\ell} \chi_j^2 \sin^2\theta(u_j, \mathcal{K}_n)}$$
$$\le \beta_2 := \sqrt{\sum_{j=k}^{\ell} \left[\frac{\chi_j \xi_{j,j}}{\mathcal{T}_{n-j}(\kappa_{j,j,n_b})} \tan\theta(u_j, X_{j,j,j}) \right]^2},$$

as well as the observed values of $\epsilon_2 = \lVert \sin\Theta(U_{(:,k:\ell)}, \widetilde{U}_{(:,k:\ell)})\rVert_{\mathrm{F}}$ defined in (7.1b) and its upper bounds of (4.11). From the figure, we see that the observed ϵ_5 is about 10^{-7} for $\delta \ge 10^{-7}$ and then starts to deteriorate from about 10^{-7} up to 10^{-3} as δ goes down to 10^{-8} or smaller. At the same time, the magnitudes of ϵ_2 and its bound of (4.11) remain unchanged around 10^{-7}. This supports our point that one should measure the convergence of the entire invariant subspace corresponding to tightly clustered eigenvalues rather than their each individual eigenvector within the subspace.

Example 7.3 Our last example is from [22]:

$$\lambda_1 = 2,\ \lambda_2 = 1.6,\ \lambda_3 = 1.4, \quad \lambda_j = 1 - \frac{j-3}{N}, \quad j = 4, \ldots, N,$$
$$V_0 = \begin{bmatrix} 1 & 1 & 1 & \cdots & 1 & 1 & 1 \\ 1 & 0 & -1 & \cdots & 1 & 0 & -1 \\ 1 & -2 & 1 & \cdots & 1 & -2 & 1 \end{bmatrix}^{\mathrm{H}}.$$

Since the first three eigenvalues are in a cluster, we take $i = k = 1$, $\ell = 3$ and $n_b = 3$. Saad [22] tested this problem for $N = 60$ and $n = 12$. We ran our code with various N, including $N = 60$ and saw little variations in observed errors and their bounds. What we report in Table 4 is for $N = 900$ and $n = 12$.

The table shows that our bounds very much agree with the corresponding observed values but "Saad's bounds" are much bigger — about the square roots of the observed values and our bounds. This is due mainly to the small gap between λ_2 and λ_3 since we observed that $\theta_j(U_{(:,k:\ell)}, X_{i,k,\ell}) \approx \theta(u_j, X_{j,j,j}) \approx 1.51303$ for $j = 1, 2, 3$.

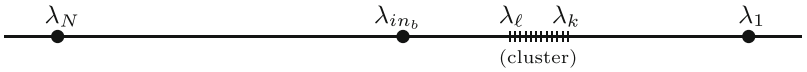
8 More bounds

The numerical examples in the previous section indicate that $\xi_{i,k}$ in Theorem 4.1 and ζ_i in Theorem 5.1 can worsen the error bounds, especially in the case of tightly clustered eigenvalues. However, both can be made 1 if only the first n_b eigenpairs are considered (see Remark 4.1). To use Theorems 4.1 or 5.1 for eigenvalues/eigenvectors involving eigenpairs beyond the first n_b ones, we have to have $\xi_{i,k}$ or ζ_i in the mix. Thus potentially the resulting bounds may overestimate too much to be indicative.

Another situation in which the bounds of Theorems 4.1 or 5.1 would overestimate the actual quantities (by too much) is when there are clustered eigenvalues with cluster sizes bigger than n_b, because then δ_{i,ℓ,n_b} is very tiny for any choices of i, k, and ℓ. Ye [25] proposed an adaptive strategy to use variable n_b aiming at updating n_b adaptively so that it is bigger than or equal to the biggest cluster size of interest.

In what follows, we propose more error bounds with $\xi_{i,k}$ and ζ_i always 1. However, it requires the knowledge of the canonical angles from the interested eigenspace to $\mathcal{K}_i(A, V_0)$, where $i < n$ is a positive integer. Roughly speaking, the new results show that if the eigenspace is not too far from $\mathcal{K}_i(A, V_0)$ for some $i < n$ (in the sense that no canonical angle is too near $\pi/2$), the canonical angles from the eigenspace to $\mathcal{K}_n(A, V_0)$ are reduced by a factor purely depending upon the optimal polynomial reduction.

To proceed, we let $i < n$. Now we are considering the 1st to (in_b)th eigenpairs of A among which the kth to ℓth eigenvalues may form a cluster as in



where

$$1 \le k < \ell \le in_b, \quad 1 \le i < n.$$

Suppose $\theta_1(U_{(:,1:in_b)}, Q_i) = \theta_1(U_{(:,1:in_b)}, \mathcal{K}_i(A, V_0)) < \pi/2$, i.e.,

$$\operatorname{rank}(Q_i^{\mathrm{H}} U_{(:,1:in_b)}) = in_b. \tag{8.1}$$

Consider an application of Proposition 2.4(b) with $k_1 = \ell - k + 1$,

$$\mathcal{X} = \mathcal{R}(Q_i), \quad \mathcal{Y} = \mathcal{R}(U_{(:,1:in_b)}), \quad [y_1, y_2, \ldots, y_{k_1}] = [u_k, u_{k+1}, \ldots, u_\ell].$$

The application yields a unique

$$Z_{i,k,\ell} := [x_1, x_2, \ldots, x_{k_1}] \tag{8.2}$$

such that $\mathcal{R}(Z_{i,k,\ell}) \subseteq \mathcal{R}(Q_i)$ and

$$U_{(:,1:in_b)} U_{(:,1:in_b)}^{\mathrm{H}} Z_{i,k,\ell} = U_{(:,k:\ell)} \equiv [u_k, u_{k+1}, \ldots, u_\ell]. \tag{8.3}$$

Moreover

$$\left\|\sin\Theta(U_{(:,k:\ell)}, Z_{i,k,\ell})\right\| \le \left\|\sin\Theta(U_{(:,1:in_b)}, Q_i)\right\|, \tag{8.4}$$

$$\left\|\tan\Theta(U_{(:,k:\ell)}, Z_{i,k,\ell})\right\| \le \left\|\tan\Theta(U_{(:,1:in_b)}, Q_i)\right\|. \tag{8.5}$$

Finally, we observe that

$$\mathcal{K}_{n-i+1}(A, Q_i) = \mathcal{K}_n(A, V_0). \tag{8.6}$$

The rest is the straightforward application of Theorems 4.1 and 5.1 to $\mathcal{K}_{n-i+1}(A, Q_i)$.

Theorem 8.1 *For any unitarily invariant norm $\|\cdot\|$, we have*

$$\left\|\tan\Theta(U_{(:,k:\ell)}, \mathcal{K}_n)\right\| \le \frac{1}{\mathcal{T}_{n-i}(\hat{\kappa}_{i,\ell,n_b})} \left\|\tan\Theta(U_{(:,k:\ell)}, Z_{i,k,\ell})\right\|, \tag{8.7}$$

$$\left\|\sin\Theta(U_{(:,k:\ell)}, \widetilde{U}_{(:,k:\ell)})\right\| \le \gamma \left\|\sin\Theta(U_{(:,k:\ell)}, \mathcal{K}_n)\right\| \tag{8.8}$$

$$\le \frac{\gamma}{\mathcal{T}_{n-i}(\hat{\kappa}_{i,\ell,n_b})} \left\|\tan\Theta(U_{(:,k:\ell)}, Z_{i,k,\ell})\right\|, \tag{8.9}$$

where $Z_{i,k,\ell}$ is defined by (8.2), $\widetilde{U}$ by (3.5), and

$$\hat{\delta}_{i,\ell,n_b} = \frac{\lambda_\ell - \lambda_{in_b+1}}{\lambda_\ell - \lambda_N}, \quad \hat{\kappa}_{i,\ell,n_b} = \frac{1+\hat{\delta}_{i,\ell,n_b}}{1-\hat{\delta}_{i,\ell,n_b}}, \tag{8.10}$$

and γ takes the same form as in (4.13) with, again, the constant c lying between 1 and $\pi/2$ and being 1 for the Frobenius norm or if $\tilde{\lambda}_{k-1} > \lambda_k$, and with η being the same as the one in (4.14). For the Frobenius norm, γ can be improved to the one in (4.15).

Theorem 8.2 *Let $k = 1$. For any unitarily invariant norm, we have*

$$\left\|\mathrm{diag}(\lambda_1 - \tilde{\lambda}_1, \lambda_2 - \tilde{\lambda}_2, \ldots, \lambda_\ell - \tilde{\lambda}_\ell)\right\|$$

$$\le (\lambda_1 - \lambda_N)\left[\frac{1}{\mathcal{T}_{n-i}(\hat{\kappa}_{i,\ell,n_b})}\right]^2 \left\|\tan^2\Theta(U_{(:,1:\ell)}, Z_{i,1,\ell})\right\|, \tag{8.11}$$

where $\hat{\kappa}_{i,\ell,n_b}$ is the same as the one in (8.10).

9 Conclusions

We have established a new convergence theory for solving large scale Hermitian eigenvalue problem by the block Lanczos method from a perspective of bounding approximation errors in the entire eigenspace associated with all eigenvalues in a tight cluster, in contrast to bounding errors in each individual approximate eigenvector as was done in Saad [22]. In a way, this is a natural approach to follow because the block Lanczos method is known to be capable of computing multiple/cluster eigenvalues

much faster than the single-vector Lanczos method (which will miss all but one copy of each multiple eigenvalue). The outcome is three error bounds on

1. the canonical angles from the eigenspace to the generated Krylov subspace,
2. the canonical angles between the eigenspace and its Ritz approximate subspace,
3. the total differences between the eigenvalues in the cluster and their corresponding Ritz values.

These bounds are much sharper than the existing ones and expose true rates of convergence of the block Lanczos method towards eigenvalue clusters, as illustrated by numerical examples. Furthermore, their sharpness is independent of the closeness of eigenvalues within a cluster.

As is well-known, the (block) Lanczos method favors the eigenvalues at both ends of the spectrum. So far, we have only focused on the convergence of the few largest eigenvalues and their associated eigenspaces, but as is usually done, applying what we have established to the eigenvalue problem for $-A$ will lead to various convergence results for the few smallest eigenvalues and their associated eigenspaces.

All results are stated in terms of unitarily invariant norms for generality, but specializing them to the spectral norm and the Frobenius norm will be sufficient for all practical purposes. Those results can also be extended to the generalized eigenvalue problem without much difficulty [19, Sect. 9].

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