

MAJORIZATION BOUNDS FOR RITZ VALUES OF SELF-ADJOINT MATRICES*

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Abstract. A priori, a posteriori, and mixed type upper bounds for the absolute change in Ritz values of self-adjoint matrices in terms of submajorization relations are obtained. Some of our results prove recent conjectures by Knyazev, Argentati, and Zhu, which extend several known results for one dimensional subspaces to arbitrary subspaces. In addition, we improve Nakatsukasa's version of the $\tan \Theta$ theorem of Davis and Kahan. As a consequence, we obtain new quadratic a posteriori bounds for the absolute change in Ritz values.

Key words. principal angles, Ritz values, Rayleigh quotients, majorization

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1. Introduction. The study of sensitivity of Ritz values and Rayleigh quotients of self-adjoint matrices (i.e., the changes in the eigenvalues of compressions of a self-adjoint matrix) is a well established and active research field in applied mathematics [1, 3, 7, 8, 9, 10, 12, 14, 17, 18, 19, 20]. Specifically, given a $d \times d$ complex self-adjoint matrix A and isometries X, Y of size $d \times k$, with ranges \mathcal{X} and \mathcal{Y} , respectively, we are interested in computing upper and lower bounds for

$$|\lambda(\rho(X)) - \lambda(\rho(Y))| = (|\lambda_i(\rho(X)) - \lambda_i(\rho(Y))|)_{i \in \mathbb{I}_k} \in \mathbb{R}_{\geq 0}^k,$$

where $\rho(X) = X^*AX$, $\rho(Y) = Y^*AY$ are $k \times k$ complex self-adjoint matrices known as Rayleigh quotients (RQ) of A , and $\lambda(\rho(X)), \lambda(\rho(Y)) \in \mathbb{R}^k$ are the eigenvalues (counting multiplicities and arranged in nonincreasing order) also known as Ritz values.

Typically, the bounds for the absolute change in the Ritz values are obtained in terms of the residuals $R_X = AX - X\rho(X)$ and $R_Y = AY - Y\rho(Y)$ or in terms of the principal angles between subspaces (PABS) denoted by $\Theta(\mathcal{X}, \mathcal{Y}) \in [0, \pi/2]^k$. Upper bounds are classified according to which parameters are used to bound the change in Ritz values (see [18]). Indeed, the a priori bounds are those obtained in terms of PABS; the a posteriori bounds are those obtained in terms of (singular values of) residuals while the *mixed type* bounds are obtained in terms of both PABS and residuals. It is worth pointing out that PABS appearing in a priori bounds may not be readily available in practice. On the other hand, a posteriori bounds are based on computable singular values of residual matrices. Moreover, bounds based on residuals (i.e., both a posteriori and mixed type) are particularly convenient in case one of the spaces, say \mathcal{X} , is A -invariant (as in this case $R_X = 0$), as opposed to (autonomous) a priori bounds.

The abstract matrix analysis formulation of the sensitivity problem stated above makes it possible to apply this theory in a variety of different research areas such

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as graph matching [8] in terms of spectral analysis of the graphs; signal distinction in signal processing, where Ritz values serve as harmonic signature to differentiate subspaces; finite element methods (FEM) [7] for approximation of subspaces corresponding to fundamental modes; and matrix analysis, e.g., for bounds for eigenvalues after matrix additive perturbations. Also, bounds for changes in Ritz values play a central role in the analysis of algorithms for simultaneous approximation of eigenvalues based on Rayleigh–Ritz methods (see [15, 16] and the references therein). The crucial role of submajorization in obtaining bounds for the change of Ritz values (recognized in the seminal paper [8]) is well known; this partial preorder relation is a powerful tool in this context, as bounds in terms of submajorization imply a whole family of inequalities with respect to unitarily invariant norms and with respect to the class of nondecreasing convex functions [11].

In this work we obtain *a priori*, *a posteriori*, and mixed type upper bounds for the absolute change in Ritz values of self-adjoint matrices in terms of submajorization. Some of our results prove recent conjectures from [7, 18, 19] which extend several known results for one dimensional subspaces to arbitrary subspaces. In addition, we improve Nakatsukasa’s version of the $\tan \Theta$ theorem [13] of Davis and Kahan [4]. We have included some (rather simple) examples to establish comparisons with previous work (for a detailed exposition of the context, previous work, our results, and some applications, see section 3). We will consider further applications of the results herein elsewhere.

This paper is organized as follows. In section 2 we introduce preliminary results in majorization theory and PABS. In section 3 we develop our main results; our approach to obtaining these results is based on methods from abstract matrix analysis, so we delay the proofs of some technical results until the appendix. Section 3 is divided into three subsections: In section 3.1 we prove a mixed type upper bound for the change of the Ritz values that is conjectured in [19] and show that this bound is sharp. We have also included some comments with a comparison of our results with previous works and with future applications of the results of this subsection. In section 3.2 we establish a link between the results from section 3.1 and an *a priori* upper bound for Ritz values conjectured from [7]. Although the results in this section are not sharp, they can be applied in quite general situations and capture the order of approximation conjectured in [7]. In section 3.3 we revisit Nakatsukasa’s version of the $\tan \Theta$ theorem of Davis and Kahan and obtain an improved version of this result; we include an example that shows that this new version of the $\tan \Theta$ theorem is sharp in cases in which the classical result is not. As an application, we obtain improved quadratic *a posteriori* error bounds for Ritz values. The paper ends with an appendix (section A) in which we include a detailed background on majorization theory and present the proofs of some technical results needed in section 3.

2. Preliminaries.

Throughout our work we use the following.

Notation and terminology. We let $\mathcal{M}_{d,k}(\mathbb{C})$ be the space of complex $d \times k$ matrices and write $\mathcal{M}_{d,d}(\mathbb{C}) = \mathcal{M}_d(\mathbb{C})$ for the algebra of $d \times d$ complex matrices. We denote by $\mathcal{H}(d) \subset \mathcal{M}_d(\mathbb{C})$ the set of self-adjoint matrices and by $\mathcal{M}_d(\mathbb{C})^+$ the cone of positive semidefinite matrices. Also, $\mathcal{G}l(d) \subset \mathcal{M}_d(\mathbb{C})$ and $\mathcal{U}(d)$ denote the groups of invertible and unitary matrices, respectively, and $\mathcal{G}l(d)^+ = \mathcal{G}l(d) \cap \mathcal{M}_d(\mathbb{C})^+$. On the other hand, given a subspace $\mathcal{Z} \subset \mathbb{C}^d$, we let $\mathcal{L}(\mathcal{Z})$ denote the space of linear operators acting on \mathcal{Z} .

For $d \in \mathbb{N}$, let $\mathbb{I}_d = \{1, \dots, d\}$. Given a vector $x \in \mathbb{C}^d$ we denote by D_x the diagonal matrix in $\mathcal{M}_d(\mathbb{C})$ whose main diagonal is x . Given $x = (x_i)_{i \in \mathbb{I}_d} \in \mathbb{R}^d$,

we denote by $x^\downarrow = (x_i^\downarrow)_{i \in \mathbb{I}_d}$ the vector obtained by rearranging the entries of x in nonincreasing order. We also use the notation $(\mathbb{R}^d)^\downarrow = \{x \in \mathbb{R}^d : x = x^\downarrow\}$, $R_{\geq 0} = \{x \in \mathbb{R} : x \geq 0\}$, and $(\mathbb{R}_{\geq 0}^d)^\downarrow = \{x \in \mathbb{R}_{\geq 0}^d : x = x^\downarrow\}$. For $r \in \mathbb{N}$, we let $\mathbf{1}_r = (1, \dots, 1) \in \mathbb{R}^r$.

Given a matrix $A \in \mathcal{H}(d)$ we denote by $\lambda(A) = (\lambda_i(A))_{i \in \mathbb{I}_d} \in (\mathbb{R}^d)^\downarrow$ the eigenvalues of A counting multiplicities and arranged in nonincreasing order. For $B \in \mathcal{M}_d(\mathbb{C})$ we let $s(B) = \lambda(|B|)$ denote the singular values of B , i.e., the eigenvalues of $|B| = (B^*B)^{1/2} \in \mathcal{M}_d(\mathbb{C})^+$. We use the abbreviation ONB for “orthonormal basis.”

Arithmetic operations with vectors are performed entrywise; i.e., in case $x = (x_i)_{i \in \mathbb{I}_k}$ and $y = (y_i)_{i \in \mathbb{I}_k} \in \mathbb{C}^k$, then $x + y = (x_i + y_i)_i$ and, following the notational convention of the principal references on these matters,

$$xy = (x_i y_i)_i \quad \text{and (assuming that } y_i \neq 0, \text{ for } i \in \mathbb{I}_k\text{)} \quad \frac{x}{y} = (x_i/y_i)_i ,$$

where all of these vectors lie in \mathbb{C}^k . Moreover, if we assume further that $x, y \in \mathbb{R}^k$, then we write $x \leq y$ whenever $x_i \leq y_i$, for $i \in \mathbb{I}_k$.

Next, we recall the notion of majorization between vectors that will play a central role throughout our work.

DEFINITION 2.1. Let $x, y \in \mathbb{R}^k$. We say that x is submajorized by y , and write $x \prec_w y$, if

$$\sum_{i=1}^j x_i^\downarrow \leq \sum_{i=1}^j y_i^\downarrow \quad \text{for } j \in \mathbb{I}_k .$$

If $x \prec_w y$ and $\text{tr } x \stackrel{\text{def}}{=} \sum_{i=1}^k x_i = \text{tr } y$, then we say that x is majorized by y , and write $x \prec y$.

There are many fundamental results in matrix theory that are stated in terms of submajorization relations. In what follows, we mention some elementary properties of submajorization that we will need in section 3 (for detailed expositions on majorization theory, including proofs of the results mentioned below, see [2, 6, 11]). We will consider some further properties and results on majorization theory in section A. Given $f : [a, b] \rightarrow \mathbb{R}$, where $[a, b] \subset \mathbb{R}$ is an interval and $z = (z_i)_{i \in \mathbb{I}_k} \in [a, b]^k$, we denote $f(z) = (f(z_i))_{i \in \mathbb{I}_k} \in \mathbb{R}^k$.

Remark 2.2. Let $[a, b] \subset \mathbb{R}$ be an interval, and let $f : [a, b] \rightarrow \mathbb{R}$ be a convex function. Then we present the following:

1. If $x, y \in [a, b]^k$ satisfy $x \prec y$, then $f(x) \prec_w f(y)$.
2. If $x, y \in [a, b]^k$ only satisfy $x \prec_w y$, but f is further nondecreasing in $[a, b]$, then $f(x) \prec_w f(y)$.

DEFINITION 2.3. A norm N in $\mathcal{M}_d(\mathbb{C})$ is unitarily invariant (briefly u.i.n.) if $N(UAV) = N(A)$ for every $A \in \mathcal{M}_d(\mathbb{C})$ and $U, V \in \mathcal{U}(d)$.

Well known examples of u.i.n. are the spectral norm $\|\cdot\|_{sp}$ and the Schatten p -norms $\|\cdot\|_p$ for $p \geq 1$.

Remark 2.4. It is well known that (sub)majorization relations between singular values of matrices are intimately related with inequalities with respect to u.i.n.’s. Indeed, given $A, B \in \mathcal{M}_d(\mathbb{C})$ the following statements are equivalent:

1. For every u.i.n. N in $\mathcal{M}_d(\mathbb{C})$ we have that $N(A) \leq N(B)$.
2. $s(A) \prec_w s(B)$.

Principal angles between subspaces. Let $\mathcal{X}, \mathcal{Y} \subset \mathbb{C}^d$ denote subspaces with $\dim \mathcal{X} = h$ and $\dim \mathcal{Y} = k$. Let $X \in \mathcal{M}_{d,h}$ and $Y \in \mathcal{M}_{d,k}$ be such that their columns form orthonormal bases of \mathcal{X} and \mathcal{Y} , respectively. Then, the principal angles between \mathcal{X} and \mathcal{Y} , denoted $\pi/2 \geq \Theta_1(\mathcal{X}, \mathcal{Y}) \geq \dots \geq \Theta_m(\mathcal{X}, \mathcal{Y}) \geq 0$, where $m = \min\{h, k\}$, are determined by

$$\cos(\Theta_{m-i+1}(\mathcal{X}, \mathcal{Y})) = s_i(X^*Y) \quad \text{for } i \in \mathbb{I}_m.$$

We further write $\Theta(\mathcal{X}, \mathcal{Y}) = (\Theta_i(\mathcal{X}, \mathcal{Y}))_{i \in \mathbb{I}_m} \in (\mathbb{R}^m)^\downarrow$ for the vector of principal angles between \mathcal{X} and \mathcal{Y} . Principal angles are a useful tool in describing the relative position and several geometric and metric aspects related with the subspaces \mathcal{X} and \mathcal{Y} in \mathbb{C}^d (see [4, 5] and the references therein).

3. Main results. In this section we develop our main results. This section is divided into three parts. First, we prove [19, Conjecture 2.1], which establishes a mixed type bound for the error in the (absolute) change of the Ritz values. In the second part, we establish connections between the mixed type bounds of the first section and some a priori bounds for the change of Ritz values conjectured in [7, 9]. Finally, we take a closer look at Nakatsukasa's $\tan \Theta$ theorem under relaxed conditions from [13] and obtain an improved version of this result. As a consequence we obtain quadratic a posteriori error bounds for the change of the Ritz values that improve several known bounds. Our approach to obtaining these results is based on methods from abstract matrix analysis, so we delay the proofs of some technical results until Appendix A, where we have also included several classical results of this area that we will refer to in this section.

We begin by introducing the following setting.

Setting 3.1. Throughout this section we consider the following notation and terminology:

1. $\mathcal{X}, \mathcal{Y} \subset \mathbb{C}^d$ denote two subspaces of dimension k . We fix $X, Y \in \mathcal{M}_{d,k}(\mathbb{C})$ such that their columns form orthonormal bases of \mathcal{X} and \mathcal{Y} , respectively.
2. $\Theta(\mathcal{X}, \mathcal{Y}) \in (\mathbb{R}_{\geq 0}^k)^\downarrow$ denotes the vector of principal angles between the subspaces \mathcal{X} and \mathcal{Y} . In this case,

$$\cos(\Theta^\uparrow(\mathcal{X}, \mathcal{Y})) = s(X^*Y) = (s_1(X^*Y), \dots, s_k(X^*Y)) \in (\mathbb{R}_{\geq 0}^k)^\downarrow.$$

3. For a (fixed) self-adjoint $A \in \mathcal{H}(d)$ we set $\rho(X) = X^*AX \in \mathcal{M}_k(\mathbb{C})$, $R_X = AX - X\rho(X) \in \mathcal{M}_{d,k}(\mathbb{C})$, and similarly, $\rho(Y)$ and R_Y for Y . Notice that

$$R_X = AX - XX^*AX = AX - P_{\mathcal{X}}AX = P_{\mathcal{X}^\perp}AX \in \mathcal{M}_{d,k}(\mathbb{C}),$$

where $P_{\mathcal{X}} \in \mathcal{M}_d(\mathbb{C})$ denotes the orthogonal projection onto \mathcal{X} , and \mathcal{X}^\perp denotes the orthogonal complement of \mathcal{X} . We consider similar notation and identities for \mathcal{Y} .

4. Let $X_\perp \in \mathcal{M}_{d,d-k}(\mathbb{C})$ be such that its columns form an ONB of \mathcal{X}^\perp . Then, the matrix $(X, X_\perp) \in \mathcal{U}(d)$ and we get

$$\tilde{A} = (X, X_\perp) \ A \ (X, X_\perp)^* = \begin{pmatrix} \rho(X) & R_X^* X_\perp \\ X_\perp^* R_X & \rho(X_\perp) \end{pmatrix}.$$

Note that, since $R_X = (I - P_{\mathcal{X}})R_X$, then $s(R_X) = s(X_\perp^* R_X)$, so that we can think of R_X (up to an isometric factor) as the $(2, 1)$ -block of \tilde{A} , in the block matrix representation of (the unitary conjugate of A) \tilde{A} as above.

3.1. Rayleigh–Ritz majorization error bounds of the mixed type. We adopt Setting 3.1; moreover, in this subsection we further assume that \mathcal{X} and \mathcal{Y} are such that $\Theta_1(\mathcal{X}, \mathcal{Y}) < \frac{\pi}{2}$, that is, that $X^*Y \in \mathcal{G}l(k)$ is invertible.

Our first result concerns a submajorization error bound for the distance of eigenvalue lists of self-adjoint matrices.

THEOREM 3.2. *Let $C, D \in \mathcal{H}(k)$, and let $T \in \mathcal{G}l(k)$. Then,*

$$(3.1) \quad |\lambda(C) - \lambda(D)| \prec_w s(T^{-1}) s(CT - TD).$$

Proof. See Appendix A for the proof. \square

The following result is [19, Conjecture 2.1] (see also Corollary 3.4).

THEOREM 3.3. *Under Setting 3.1, if $\Theta_1(\mathcal{X}, \mathcal{Y}) < \frac{\pi}{2}$, then*

$$(3.2) \quad |\lambda(\rho(X)) - \lambda(\rho(Y))| \prec_w \frac{s(P_{\mathcal{Y}} R_X) + s(P_{\mathcal{X}} R_Y)}{\cos(\Theta(\mathcal{X}, \mathcal{Y}))} \quad \text{and}$$

$$(3.3) \quad |\lambda(\rho(X)) - \lambda(\rho(Y))| \prec_w [s(P_{\mathcal{X}+\mathcal{Y}} R_X) + s(P_{\mathcal{X}+\mathcal{Y}} R_Y)] \tan(\Theta(\mathcal{X}, \mathcal{Y})).$$

Proof. Set $T = X^*Y$ and notice that, since $\Theta_1(\mathcal{X}, \mathcal{Y}) < \frac{\pi}{2}$, $T \in \mathcal{M}_k(\mathbb{C})$ is invertible. Using Theorem 3.2 we get that

$$(3.4) \quad |\lambda(\rho(X)) - \lambda(\rho(Y))| \prec_w s(T^{-1}) s(\rho(X)T - T\rho(Y)),$$

where $\rho(X) = X^*AX$, $\rho(Y) = Y^*AY \in \mathcal{H}(k)$. By construction we have that

$$(3.5) \quad s(T^{-1}) = \frac{1}{\cos(\Theta(\mathcal{X}, \mathcal{Y}))} \in (\mathbb{R}_{>0})^\downarrow.$$

Arguing as in [19, Thm. 4.1] we notice that

$$\begin{aligned} \rho(X)T - T\rho(Y) &= X^*A X X^*Y - X^*Y Y^*A Y = X^*A P_{\mathcal{X}} Y - X^*P_{\mathcal{Y}} A Y \\ &= X^*A (I - P_{\mathcal{X}^\perp})Y - X^*(I - P_{\mathcal{Y}^\perp})A Y \\ &= X^*A Y - X^*A P_{\mathcal{X}^\perp} Y - X^*A Y + X^*P_{\mathcal{Y}^\perp} A Y \\ &= -X^*A P_{\mathcal{X}^\perp} Y + X^*P_{\mathcal{Y}^\perp} A Y. \end{aligned}$$

Using that $s(C) = s(C^*)$ for $C \in \mathcal{M}_k(\mathbb{C})$, we see that

$$s(X^*A P_{\mathcal{X}^\perp} Y) = s(Y^*P_{\mathcal{X}^\perp} A X) = s(P_{\mathcal{Y}} P_{\mathcal{X}^\perp} A X) = s(P_{\mathcal{Y}} R_X) \in (\mathbb{R}_{\geq 0})^\downarrow.$$

Analogously $s(X^*P_{\mathcal{Y}^\perp} A Y) = s(P_{\mathcal{X}} R_Y)$. The previous facts, together with the subadditivity property of singular values (item 1 in Theorem A.1), imply that

$$(3.6) \quad s(\rho(X)T - T\rho(Y)) = s(-X^*A P_{\mathcal{X}^\perp} Y + X^*P_{\mathcal{Y}^\perp} A Y) \prec_w s(P_{\mathcal{X}} R_Y) + s(P_{\mathcal{Y}} R_X).$$

Now, if we apply (3.5) and (3.6) to (3.4), together with item 4 in Lemma A.3, we get (3.2).

In order to show (3.3) we point out that by [19, Lemma 4.1] we get that

$$(3.7) \quad s(P_{\mathcal{X}} R_Y) \prec_w s(P_{\mathcal{X}+\mathcal{Y}} R_Y) \sin(\Theta(\mathcal{X}, \mathcal{Y})).$$

Since the entries of these vectors are ordered downwards, by Lemma A.3 we deduce that

$$(3.8) \quad s(P_{\mathcal{X}} R_Y) + s(P_{\mathcal{Y}} R_X) \prec_w (s(P_{\mathcal{X}+\mathcal{Y}} R_Y) + s(P_{\mathcal{X}+\mathcal{Y}} R_X)) \sin(\Theta(\mathcal{X}, \mathcal{Y})).$$

Hence, using (3.2) and (3.8) together with Lemma A.3, we see that (3.3) holds. \square

The fact that (3.2) implies (3.3) was already observed in [19]; we have included the proof of this fact for the benefit of the reader.

COROLLARY 3.4. *Consider Setting 3.1 and assume that $\Theta_1(\mathcal{X}, \mathcal{Y}) < \frac{\pi}{2}$. If we further assume that \mathcal{X} is A -invariant, then*

$$(3.9) \quad |\lambda(\rho(X)) - \lambda(\rho(Y))| \prec_w \frac{s(P_{\mathcal{X}} R_Y)}{\cos(\Theta(\mathcal{X}, \mathcal{Y}))} \quad \text{and}$$

$$(3.10) \quad |\lambda(\rho(X)) - \lambda(\rho(Y))| \prec_w s(P_{\mathcal{X}+\mathcal{Y}} R_Y) \tan(\Theta(\mathcal{X}, \mathcal{Y})).$$

Proof. In case that \mathcal{X} is A -invariant, notice that $R_X = 0$. The result now follows from Theorem 3.3. \square

It is natural to wonder whether we can improve the bounds in the previous results. As shown in the following example, the submajorization bounds in Theorem 3.3 and Corollary 3.4 are *sharp*.

Example 3.5. Let $\lambda = (a, b, c, d) \in \mathbb{R}^4$, where $a < b < c < d$, and consider $A \in \mathcal{H}(4)$ given by $A = D_\lambda$, i.e., A is the diagonal matrix with main diagonal λ .

Let \mathcal{X} be the A -invariant subspace $\mathcal{X} = \text{span}\{e_1, e_2\}$ spanned by the first two elements of the canonical basis of \mathbb{C}^4 . For $\theta \in (0, \pi/2)$ let $f_\theta = \cos \theta e_2 + \sin \theta e_3$ and set $\mathcal{Y}_\theta = \text{span}\{e_1, f_\theta\}$. Then, the principal angles are given by $\Theta(\mathcal{X}, \mathcal{Y}_\theta) = (\theta, 0)$. Let

$$X = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad X_\perp = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \text{and} \quad Y_\theta = \begin{pmatrix} 1 & 0 \\ 0 & \cos \theta \\ 0 & \sin \theta \\ 0 & 0 \end{pmatrix}.$$

It is straightforward to check that $\lambda(X^* A X) = (b, a)$ and that $\lambda(Y_\theta^* A Y_\theta) = (b \cos^2 \theta + c \sin^2(\theta), a)$. Again, simple computations show that

$$R_{Y_\theta} = \begin{pmatrix} 0 & 0 \\ 0 & (b-c) \cos \theta \sin^2 \theta \\ 0 & (c-b) \cos^2 \theta \sin \theta \\ 0 & 0 \end{pmatrix}, \quad P_{\mathcal{X}} R_{Y_\theta} = \begin{pmatrix} 0 & 0 \\ 0 & (b-c) \cos \theta \sin^2 \theta \\ 0 & 0 \\ 0 & 0 \end{pmatrix}.$$

Hence, $s(P_{\mathcal{X}} R_{Y_\theta}) = ((c-b) \cos \theta \sin^2 \theta, 0)$. Now,

$$(3.11) \quad |\lambda(X^* A X) - \lambda((Y_\theta)^* A Y_\theta)| = ((c-b) \sin^2 \theta, 0),$$

$$(3.12) \quad \frac{s(P_{\mathcal{X}} R_{Y_\theta})}{\cos(\Theta(\mathcal{X}, \mathcal{Y}_\theta))} = ((c-b) \sin^2 \theta, 0).$$

That is, (3.9) in Corollary 3.4 becomes an equality in this case. This also shows that (3.2) is sharp, since (3.9) above is a particular case (when \mathcal{X} is A -invariant).

Notice that $\mathcal{X} + \mathcal{Y}_\theta = \text{span}\{e_1, e_2, e_3\}$. Therefore, since $P_{\mathcal{X}+\mathcal{Y}_\theta} R_{Y_\theta} = R_{Y_\theta}$ and $s(R_{Y_\theta}) = ((c-b) \cos \theta \sin \theta, 0)$,

$$(3.13) \quad s(P_{\mathcal{X}+\mathcal{Y}_\theta} R_{Y_\theta}) \tan(\Theta(\mathcal{X}, \mathcal{Y}_\theta)) = ((c-b) \sin^2 \theta, 0).$$

By (3.11) and (3.13) we now see that (3.10) in Corollary 3.4 becomes an equality in this case. This also shows that (3.3) is sharp, since (3.10) above is a particular case (when \mathcal{X} is A -invariant).

Remark 3.6 (relations between our work and previous results). In the vector case, when \mathcal{X} and \mathcal{Y} are one dimensional spaces, Theorem 3.3 implies the upper bounds in [18, Theorem 3.7], which is one of the main results of that work (see also Corollary 3.24 and Remark 3.25).

In [19] Zhu and Knyazev obtained several bounds for the absolute change of the Ritz values. Using Setting 3.1, the authors show (see [19, Theorem 4.2 and Corollary 4.4]) that

$$(3.14) \quad |\lambda(\rho(X)) - \lambda(\rho(Y))|^2 \prec_w \frac{\{s(P_Y R_X) + s(P_X R_Y)\}^2}{\cos^2(\Theta(\mathcal{X}, \mathcal{Y}))} \quad \text{and}$$

$$(3.15) \quad |\lambda(\rho(X)) - \lambda(\rho(Y))|^2 \prec_w \{s(P_{\mathcal{X}+\mathcal{Y}} R_X) + s(P_{\mathcal{X}+\mathcal{Y}} R_Y)\}^2 \tan^2(\Theta(\mathcal{X}, \mathcal{Y})).$$

Using the fact that $f : \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}_{\geq 0}$ given by $f(x) = x^2$ is an increasing and convex function, Remark 2.2 shows that (3.14) and (3.15) follow from (3.2) and (3.3) from Theorem 3.3. Similarly, using that $\cos \Theta_1(\mathcal{X}, \mathcal{Y}) = \cos \Theta_{\max}(\mathcal{X}, \mathcal{Y}) \leq \cos \Theta_i(\mathcal{X}, \mathcal{Y})$, for $i \in \mathbb{I}_k$, we get that Theorem 3.3 implies [19, Theorems 4.1 and 4.3].

In [19] the authors show that their results can be applied in several situations such as first order and quadratic a posteriori majorization bounds and bounds for eigenvalues after matrix additive perturbations. The previous remarks show that our bounds can also be applied in these settings. Moreover, Theorem 3.3 allows one to formalize the arguments related with bounds for eigenvalues after matrix additive perturbations, and, in particular, with bounds for eigenvalues after discarding off-diagonal blocks from [19, section 5] (see the detailed discussion there).

The bounds in Theorem 3.3 can be used to perform a detailed analysis and obtain better convergence rates for iterative algorithms related with the Rayleigh–Ritz method (see [15, 16, 20]). We will consider such applications elsewhere.

3.2. Applications: A priori majorization error bounds for Ritz values.

In this section we establish a link between the majorization error bounds of the mixed type obtained in the previous section and some a priori majorization error bounds considered in [7, 9].

DEFINITION 3.7. Let $A \in \mathcal{H}(d)$, and let $\mathcal{Z} \subset \mathbb{C}^d$ be a subspace with $\dim \mathcal{Z} = p$. We define the (spectral) spread of A relative to \mathcal{Z} , denoted $\text{Spr}(A, \mathcal{Z})$, given by

$$\text{Spr}(A, \mathcal{Z}) = \lambda(A_{\mathcal{Z}}) - \lambda^{\dagger}(A_{\mathcal{Z}}) = (\lambda_i(A_{\mathcal{Z}}) - \lambda_{p-i+1}(A_{\mathcal{Z}}))_{i \in \mathbb{I}_p} \in (\mathbb{R}^p)^{\downarrow},$$

where $A_{\mathcal{Z}} = P_{\mathcal{Z}} A|_{\mathcal{Z}} \in \mathcal{L}(\mathcal{Z})$ is a self-adjoint operator (defined in the obvious way). In case $\mathcal{Z} = \mathbb{C}^d$, we write $\text{Spr}(A, \mathbb{C}^d) = \text{Spr}(A)$.

Remark 3.8. Let $A \in \mathcal{H}(d)$, and let $\mathcal{X}, \mathcal{Y} \subset \mathbb{C}^d$ with $\dim(\mathcal{X}) = \dim(\mathcal{Y}) = k$. Denote $p = \dim \mathcal{X} + \mathcal{Y}$. In what follows we consider the vector

$$\text{Spr}(A, \mathcal{X} + \mathcal{Y}) \sin(\Theta(\mathcal{X}, \mathcal{Y})) = ((\lambda_i(A_{\mathcal{X}+\mathcal{Y}}) - \lambda_{p-i+1}(A_{\mathcal{X}+\mathcal{Y}})) \sin(\Theta_i(\mathcal{X}, \mathcal{Y})))_{i \in \mathbb{I}_k}.$$

We point out that this vector has nonnegative entries, which are arranged in nonincreasing order (in particular, $\sin(\Theta_i(\mathcal{X}, \mathcal{Y})) = 0$ whenever $\lambda_i(A_{\mathcal{X}+\mathcal{Y}}) - \lambda_{p-i+1}(A_{\mathcal{X}+\mathcal{Y}}) < 0$ for $i \in \mathbb{I}_k$); hence, $\text{Spr}(A, \mathcal{X} + \mathcal{Y}) \sin(\Theta(\mathcal{X}, \mathcal{Y})) \in (\mathbb{R}_{\geq 0}^k)^{\downarrow}$ (see [19]). This fact becomes relevant for the conjectures posed in (3.16) and (3.17).

Remark 3.9 (a priori error bounds for changes of Ritz values: conjectures and previous work). Let $A \in \mathcal{H}(d)$, and let $\mathcal{X}, \mathcal{Y} \subset \mathbb{C}^d$ with $\dim(\mathcal{X}) = \dim(\mathcal{Y}) = k$. In [7]

the authors conjectured that, in general, the following submajorization bound for the Ritz values holds:

$$(3.16) \quad |\lambda(\rho(X)) - \lambda(\rho(Y))| \prec_w \text{Spr}(A, \mathcal{X} + \mathcal{Y}) \sin(\Theta(\mathcal{X}, \mathcal{Y})).$$

Moreover, in case that \mathcal{X} is A -invariant, the authors conjectured that

$$(3.17) \quad |\lambda(\rho(X)) - \lambda(\rho(Y))| \prec_w \text{Spr}(A, \mathcal{X} + \mathcal{Y}) \sin(\Theta(\mathcal{X}, \mathcal{Y}))^2.$$

These conjectures are natural extensions of results from [9] (that were obtained for $k = 1$). Although [7, Conjecture 2.1] claims the validity of (3.16) and (3.17) for arbitrary subspaces \mathcal{X} and \mathcal{Y} such that $\dim \mathcal{X} = \dim \mathcal{Y}$, these bounds would become relevant in the particular case when the subspace \mathcal{Y} is a (small) perturbation of the subspace \mathcal{X} . In this case, the validity of (3.16) and (3.17) would reveal the different orders of approximation of $\rho(X)$ by $\rho(Y)$ in terms of PABS as well as in terms of the spectral spread of A (i.e., when considering A as well as \mathcal{X} and \mathcal{Y} as variables). Notice that these results would have immediate applications in the study of numerical stability and convergence of iterative methods related with the Rayleigh–Ritz type algorithms.

In [7, Theorem 2.1] the authors showed that, in general,

$$(3.18) \quad |\lambda(\rho(X)) - \lambda(\rho(Y))| \prec_w (\lambda_{\max}(A_{\mathcal{X}+\mathcal{Y}}) - \lambda_{\min}(A_{\mathcal{X}+\mathcal{Y}})) \sin(\Theta(\mathcal{X}, \mathcal{Y})),$$

while, in case \mathcal{X} is A -invariant,

$$(3.19) \quad |\lambda(\rho(X)) - \lambda(\rho(Y))| \prec_w (\lambda_{\max}(A_{\mathcal{X}+\mathcal{Y}}) - \lambda_{\min}(A_{\mathcal{X}+\mathcal{Y}})) \sin(\Theta(\mathcal{X}, \mathcal{Y}))^2,$$

where $A_{\mathcal{X}+\mathcal{Y}} = P_{\mathcal{X}+\mathcal{Y}} A|_{\mathcal{X}+\mathcal{Y}} \in \mathcal{L}(\mathcal{X} + \mathcal{Y})$; moreover, in [7, Theorem 2.2] they showed that in the particular case in which \mathcal{X} is the A -invariant subspace corresponding to the k largest eigenvalues of A , then

$$(3.20) \quad 0 \leq \lambda(\rho(X)) - \lambda(\rho(Y)) \prec_w (\lambda_i(A_{\mathcal{X}+\mathcal{Y}}) - \lambda_{\min}(A_{\mathcal{X}+\mathcal{Y}}))_{i \in \mathbb{I}_k} \sin(\Theta(\mathcal{X}, \mathcal{Y}))^2.$$

Notice that (3.20) is a stronger bound than that in (3.19); yet, it is weaker than the bound conjectured in (3.17), since $\text{Spr}_i(A, \mathcal{X} + \mathcal{Y}) \leq \lambda_i(A_{\mathcal{X}+\mathcal{Y}}) - \lambda_{\min}(A_{\mathcal{X}+\mathcal{Y}})$ for $i \in \mathbb{I}_k$.

In what follows we apply Theorem 3.3 and obtain some results related with the conjectures from [7] described in (3.16) and (3.17). In order to obtain these results, we take a closer look at the quantity $s(P_{\mathcal{X}} R_Y)$ for arbitrary \mathcal{X} and \mathcal{Y} , as well as in the case where \mathcal{X} is A -invariant.

PROPOSITION 3.10. *Let $A \in \mathcal{H}(d)$, and let $\mathcal{X}, \mathcal{Y} \subset \mathbb{C}^d$ with $\dim(\mathcal{X}) = \dim(\mathcal{Y}) = k$. Then*

$$(3.21) \quad s(P_{\mathcal{X}} R_Y) \prec_w \text{Spr}(A, \mathcal{X} + \mathcal{Y}) \sin(\Theta(\mathcal{X}, \mathcal{Y})).$$

Proof. See Appendix A for the proof. \square

THEOREM 3.11. *Let $A \in \mathcal{H}(d)$, $\mathcal{X}, \mathcal{Y} \subset \mathbb{C}^d$ subspaces, $\dim(\mathcal{X}) = \dim(\mathcal{Y}) = k$. If $\Theta_1(\mathcal{X}, \mathcal{Y}) < \frac{\pi}{2}$, then*

$$(3.22) \quad |\lambda(\rho(X)) - \lambda(\rho(Y))| \prec_w \frac{2 \text{Spr}(A, \mathcal{X} + \mathcal{Y}) \sin(\Theta(\mathcal{X}, \mathcal{Y}))}{\cos(\Theta(\mathcal{X}, \mathcal{Y}))}.$$

Proof. Theorem 3.3 establishes that

$$|\lambda(\rho(X)) - \lambda(\rho(Y))| \prec_w \frac{s(P_{\mathcal{X}}R_Y) + s(P_{\mathcal{Y}}R_X)}{\cos(\Theta(\mathcal{X}, \mathcal{Y}))}.$$

Proposition 3.10 together with Lemma A.3 imply that

$$\frac{s(P_{\mathcal{X}}R_Y) + s(P_{\mathcal{Y}}R_X)}{\cos(\Theta(\mathcal{X}, \mathcal{Y}))} \prec_w \frac{2 \operatorname{Spr}(A, \mathcal{X} + \mathcal{Y}) \sin(\Theta(\mathcal{X}, \mathcal{Y}))}{\cos(\Theta(\mathcal{X}, \mathcal{Y}))}.$$

The result follows from combining these last two inequalities. \square

The next result illustrates the quadratic dependance of $s(P_{\mathcal{X}}R_Y)$ from $\sin(\Theta(\mathcal{X}, \mathcal{Y}))$ in case that \mathcal{X} is A -invariant.

PROPOSITION 3.12. *Let $A \in \mathcal{H}(d)$, $\mathcal{X}, \mathcal{Y} \subset \mathbb{C}^d$ subspaces with $\dim(\mathcal{X}) = \dim(\mathcal{Y}) = k$. Assume that \mathcal{X} is A -invariant. Then,*

$$(3.23) \quad s(P_{\mathcal{X}}R_Y) \prec_w 2 (\lambda_i(A_{\mathcal{X}+\mathcal{Y}}) - \lambda_{\min}(A_{\mathcal{X}+\mathcal{Y}}))_{i \in \mathbb{I}_k} \sin^2(\Theta(\mathcal{X}, \mathcal{Y})).$$

Proof. See Appendix A for the proof. \square

THEOREM 3.13. *Let $A \in \mathcal{H}(d)$, $\mathcal{X}, \mathcal{Y} \subset \mathbb{C}^d$ subspaces, $\dim(\mathcal{X}) = \dim(\mathcal{Y}) = k$, and assume that \mathcal{X} is A -invariant. If $\Theta_1(\mathcal{X}, \mathcal{Y}) < \frac{\pi}{2}$, then*

$$(3.24) \quad |\lambda(\rho(X)) - \lambda(\rho(Y))| \prec_w \frac{2 (\lambda_i(A_{\mathcal{X}+\mathcal{Y}}) - \lambda_{\min}(A_{\mathcal{X}+\mathcal{Y}}))_{i \in \mathbb{I}_k} \sin^2(\Theta(\mathcal{X}, \mathcal{Y}))}{\cos(\Theta(\mathcal{X}, \mathcal{Y}))}.$$

Proof. The result follows from Corollary 3.4 and Proposition 3.12 with an argument similar to that in the proof of Theorem 3.11 above. \square

COROLLARY 3.14. *Let $A \in \mathcal{H}(d)$, $\mathcal{X}, \mathcal{Y} \subset \mathbb{C}^d$ subspaces, $\dim(\mathcal{X}) = \dim(\mathcal{Y}) = k$. If $\Theta_1(\mathcal{X}, \mathcal{Y}) < \frac{\pi}{2}$, then*

$$|\lambda(\rho(X)) - \lambda(\rho(Y))| \prec_w \frac{2}{\cos(\Theta_1(\mathcal{X}, \mathcal{Y}))} \operatorname{Spr}(A, \mathcal{X} + \mathcal{Y}) \sin(\Theta(\mathcal{X}, \mathcal{Y})).$$

If we assume further that \mathcal{X} is A -invariant, then

$$|\lambda(\rho(X)) - \lambda(\rho(Y))| \prec_w \frac{2}{\cos(\Theta_1(\mathcal{X}, \mathcal{Y}))} (\lambda_i(A_{\mathcal{X}+\mathcal{Y}}) - \lambda_{\min}(A_{\mathcal{X}+\mathcal{Y}}))_{i \in \mathbb{I}_k} \sin^2(\Theta(\mathcal{X}, \mathcal{Y})).$$

We end this section with some remarks concerning the relations among Theorems 3.11 and 3.13, Corollary 3.14, and the conjectured bounds in (3.16) and (3.17). As already mentioned in Remark 3.9, the bounds in (3.16) and (3.17) would be particularly relevant in case that \mathcal{Y} is a (small) perturbation of \mathcal{X} or, in other words, in case \mathcal{X} and \mathcal{Y} are close subspaces (e.g., $\Theta_1(\mathcal{X}, \mathcal{Y})$ is small). In order to simplify the discussion, let us assume that $\Theta_1(\mathcal{X}, \mathcal{Y}) \leq \pi/4$. We point out that this assumption holds in a number of significant situations (see, for example, [19, section 5.2]). In this case, if $A \in \mathcal{H}(d)$, then Corollary 3.14 implies that

$$(3.25) \quad |\lambda(\rho(X)) - \lambda(\rho(Y))| \prec_w (2\sqrt{2}) \operatorname{Spr}(A, \mathcal{X} + \mathcal{Y}) \sin(\Theta(\mathcal{X}, \mathcal{Y})).$$

Hence, under the present assumptions ($\Theta_1(\mathcal{X}, \mathcal{Y}) \leq \pi/4$), the upper bound in (3.25) has the conjectured order of approximation (when considering A as well as the subspaces \mathcal{X} and \mathcal{Y} as variables), up to the constant factor $2\sqrt{2}$.

If we further assume that \mathcal{X} is A -invariant, then by the same result we get that

$$(3.26) \quad |\lambda(\rho(X)) - \lambda(\rho(Y))| \prec_w (2\sqrt{2}) (\lambda_i(A_{\mathcal{X}+\mathcal{Y}}) - \lambda_{\min}(A_{\mathcal{X}+\mathcal{Y}}))_{i \in \mathbb{I}_k} \sin^2(\Theta(\mathcal{X}, \mathcal{Y})).$$

Again, the upper bound in (3.26) has the conjectured order of approximation (when considering A as well as the subspaces \mathcal{X} and \mathcal{Y} as variables), up to the constant factor $2\sqrt{2}$. Moreover, notice that this bound holds for an arbitrary A -invariant subspace \mathcal{X} (as opposed to the bound in (3.20) from [7] that is shown to hold for special choices of A -invariant subspaces \mathcal{X}).

3.3. The $\tan \Theta$ theorem revisited: Improved quadratic a posteriori error bounds. In this section we revisit Nakatsukasa's extension of the Davis–Kahan $\tan(\theta)$ theorem. Our motivation is the study of an improved version of this result conjectured in [19] (see Corollary 3.22). We first recall the separation hypothesis for Nakatsukasa's result. As before, in this section we adopt Setting 3.1.

DEFINITION 3.15. Let $A \in \mathcal{H}(d)$, and let $\mathcal{X}, \mathcal{Y} \subset \mathbb{C}^d$ be subspaces with $\dim \mathcal{X} = \dim \mathcal{Y} = k$, such that \mathcal{X} is A -invariant. Let $[X, X_\perp], [Y, Y_\perp] \in \mathcal{U}(d)$ be unitary matrices such that the columns of (the $d \times k$ matrices) X and Y form ONBs of \mathcal{X} and \mathcal{Y} , respectively. Given $\delta > 0$ we say that $(A, \mathcal{X}, \mathcal{Y}, \delta)$ satisfies the Davis–Kahan–Nakatsukasa (DKN) separation property if there exist $a \leq b$ such that

1. $\lambda_i(X_\perp^* A X_\perp) = \lambda_i(P_{\mathcal{X}^\perp} A P_{\mathcal{X}^\perp}) \in [a, b]$ for $i \in \mathbb{I}_{d-k}$;
2. $\lambda_i(Y^* A Y) = \lambda_i(P_{\mathcal{Y}} A P_{\mathcal{Y}}) \in (\infty, a - \delta] \cup [b + \delta, \infty)$ for $i \in \mathbb{I}_k$.

Next, we state Nakatsukasa's $\tan \Theta$ theorem under relaxed conditions.

THEOREM 3.16 (see [13]). Let $A \in \mathcal{H}(d)$, let $\mathcal{X}, \mathcal{Y} \subset \mathbb{C}^d$, and let $\delta > 0$ be such that $(A, \mathcal{X}, \mathcal{Y}, \delta)$ satisfies the DKN separation property. Then, $\Theta_1(\mathcal{X}, \mathcal{Y}) < \pi/2$ and

$$\delta \|\tan(\Theta(\mathcal{X}, \mathcal{Y}))\| \leq \|R_Y\|$$

for every u.n.i. norm $\|\cdot\|$. Equivalently, $\delta \tan(\Theta(\mathcal{X}, \mathcal{Y})) \prec_w s(R_Y)$.

Remark 3.17. Theorem 3.16 requires knowledge of the full matrix A in order to bound the (norm of the) vector $\tan(\Theta(\mathcal{X}, \mathcal{Y}))$ from above. Instead, it would be interesting to bound the vector $\tan(\Theta(\mathcal{X}, \mathcal{Y}))$ from above (only) in terms of the self-adjoint operator $A_{\mathcal{X}+\mathcal{Y}} = P_{\mathcal{X}+\mathcal{Y}} A |_{\mathcal{X}+\mathcal{Y}} \in \mathcal{L}(\mathcal{X} + \mathcal{Y})$ (defined in the obvious way). In the next result we show that the $\tan \Theta$ theorem mentioned above allows one to obtain such a result. Moreover, we will also see that it is possible to describe separation hypotheses for $(A_{\mathcal{X}+\mathcal{Y}}, \mathcal{X}, \mathcal{Y})$ that are more general than the DKN separation hypothesis for $(A, \mathcal{X}, \mathcal{Y})$, for which the $\tan \Theta$ theorem holds; arguing in terms of interlacing inequalities, we can show that these separation hypotheses on $A_{\mathcal{X}+\mathcal{Y}}$ provide better separation constants than the DKN separation hypotheses on the matrix A .

We formalize the content of the previous remark—with a small variation on the notation—in the following result. First, we recall some facts related with the relative position of two subspaces.

Remark 3.18. Let $\mathcal{X}, \mathcal{Y} \subset \mathbb{C}^d$ be two subspaces with $\dim \mathcal{X} = \dim \mathcal{Y} = k$. Consider the mutually orthogonal subspaces

$$\mathcal{H}_{00} = \mathcal{X}^\perp \cap \mathcal{Y}^\perp, \quad \mathcal{H}_{10} = \mathcal{X} \cap \mathcal{Y}^\perp, \quad \mathcal{H}_{01} = \mathcal{X}^\perp \cap \mathcal{Y}, \quad \mathcal{H}_{11} = \mathcal{X} \cap \mathcal{Y},$$

and $\mathcal{H}_g = \mathbb{C}^d \ominus (\mathcal{H}_{00} \oplus \mathcal{H}_{10} \oplus \mathcal{H}_{01} \oplus \mathcal{H}_{11})$, which is called the *generic part* of the pair $(\mathcal{X}, \mathcal{Y})$. Each of these five (possible zero) subspaces reduces each projection $P_{\mathcal{X}}$ and $P_{\mathcal{Y}}$. Moreover, the subspaces $\mathcal{X}_g = \mathcal{X} \cap \mathcal{H}_g$ and $\mathcal{Y}_g = \mathcal{Y} \cap \mathcal{H}_g$ are in *generic*

position so that $\mathcal{H}_g = \mathcal{X}_g + \mathcal{Y}_g$. For details of this well-known construction and several fundamental results, see [5].

THEOREM 3.19. *Let $A \in \mathcal{H}(d)$, and let $\mathcal{X}, \mathcal{Y} \subset \mathbb{C}^d$ be such that $\dim \mathcal{X} = \dim \mathcal{Y} = k$. Let $A_{\mathcal{X}+\mathcal{Y}} = S^* AS \in \mathcal{H}(p)$, where $S \in \mathcal{M}_{d,p}(\mathbb{C})$ is such that its columns form an ONB for $\mathcal{X} + \mathcal{Y}$. Then we present the following:*

1. *If $\delta > 0$ is such that $(A, \mathcal{X}, \mathcal{Y}, \delta)$ satisfies the DKN separation property, then there exists $\delta' \geq \delta$ such that $(A_{\mathcal{X}+\mathcal{Y}}, S^* \mathcal{X}, S^* \mathcal{Y}, \delta')$ satisfies the DKN separation property.*
2. *If $\delta' > 0$ is such that $(A_{\mathcal{X}+\mathcal{Y}}, S^* \mathcal{X}, S^* \mathcal{Y}, \delta')$ satisfies the DKN separation property, then*

$$(3.27) \quad \delta' \|\tan(\Theta(\mathcal{X}, \mathcal{Y}))\| \leq \|A_{\mathcal{X}+\mathcal{Y}} Y_S - Y_S (Y_S^* A_{\mathcal{X}+\mathcal{Y}} Y_S)\| = \|P_{\mathcal{X}+\mathcal{Y}} R_Y\|$$

for every u.n.i. norm $\|\cdot\|$, where $Y_S = S^* Y \in \mathcal{M}_{p,k}(\mathbb{C})$.

Proof. We first show item 1. Let $X, Y \in \mathcal{M}_{d,k}(\mathbb{C})$ be such that their columns form orthonormal bases of \mathcal{X} and \mathcal{Y} , respectively. By hypothesis, there exist $a \leq b$ such that for $i \in \mathbb{I}_{d-k}$ and $j \in \mathbb{I}_k$

$$\lambda_i(X_{\perp}^* AX_{\perp}) \in [a, b] \quad \text{and} \quad \lambda_j(Y^* AY) \in (\infty, a - \delta] \cup [b + \delta, \infty),$$

where $X_{\perp} \in \mathcal{M}_{d,d-k}(\mathbb{C})$ is such that its columns form an ONB for \mathcal{X}^{\perp} . Let $\mathcal{Z} = \mathcal{X} + \mathcal{Y}$, and notice that $S \in \mathcal{M}_{d,p}(\mathbb{C})$ is an isometry from \mathbb{C}^p onto \mathcal{Z} . Moreover, the matrix $S^* AS \in \mathcal{H}(p)$. Similarly, $X_S = S^* X$, $Y_S = S^* Y \in \mathcal{M}_{p,k}$ are isometries from \mathbb{C}^k onto $S^* \mathcal{X}$, $S^* \mathcal{Y} \subseteq \mathbb{C}^p$, respectively. Consider the mutually orthogonal subspaces

$$\mathcal{H}_{11} = \mathcal{X} \cap \mathcal{Y}, \quad \mathcal{X}_g = \mathcal{H}_g \cap \mathcal{X}, \quad \text{and} \quad \mathcal{X}_{g^{\perp}} = \mathcal{H}_g \ominus \mathcal{X}_g,$$

where \mathcal{H}_g is the subspace of \mathbb{C}^d corresponding to the generic part of the pair $(\mathcal{X}, \mathcal{Y})$ (see Remark 3.18). By Theorem 3.16 we have that $\Theta_1(\mathcal{X}, \mathcal{Y}) < \pi/2$, so then $\mathcal{X}^{\perp} \cap \mathcal{Y} = \{0\} = \mathcal{X} \cap \mathcal{Y}^{\perp}$. Thus,

$$\mathcal{X} = \mathcal{H}_{11} \oplus \mathcal{X}_g, \quad \mathcal{Z} = \mathcal{H}_{11} \oplus \mathcal{X}_g \oplus \mathcal{X}_{g^{\perp}}, \quad \text{and} \quad \mathcal{X}_{g^{\perp}} = \mathcal{Z} \ominus \mathcal{X}.$$

Let $X' \in \mathcal{M}_{d,(p-k)}(\mathbb{C})$ be such that its columns form an orthonormal basis of $\mathcal{X}_{g^{\perp}} \subset \mathcal{X}^{\perp}$. Then, $X'_S = S^* X' \in \mathcal{M}_{p,(p-k)}(\mathbb{C})$ is an isometry from \mathbb{C}^{p-k} onto $S^* \mathcal{X}_{g^{\perp}} = (S^* \mathcal{X})^{\perp} \subseteq \mathbb{C}^p$. To check the DKN separation property for $(A_{\mathcal{X}+\mathcal{Y}}, S^* \mathcal{X}, S^* \mathcal{Y})$, we consider the eigenvalues of

$$(X'_S)^*(S^* AS) X'_S = (X')^* S S^* A S S^* X' = (X')^* A X' \in \mathcal{H}(p-k),$$

since $SS^* = P_{\mathcal{Z}} \in \mathcal{M}_d(\mathbb{C})$, $P_{\mathcal{Z}} X' = X'$, and $(X')^* P_{\mathcal{Z}} = (X')^*$. Hence, we now see that

$$\lambda_i((X'_S)^*(S^* AS) X'_S) = \lambda_i(P_{\mathcal{X}_{g^{\perp}}} A P_{\mathcal{X}_{g^{\perp}}}) \quad \text{for } i \in \mathbb{I}_{p-k}.$$

Since $\mathcal{X}_{g^{\perp}} \subset \mathcal{X}^{\perp}$ we have that $P_{\mathcal{X}_{g^{\perp}}} A P_{\mathcal{X}_{g^{\perp}}}$ is a compression of $P_{\mathcal{X}^{\perp}} A P_{\mathcal{X}^{\perp}}$. Using the interlacing inequalities for compressions of self-adjoint matrices (see [2]), we get that if $\lambda_i((P_{\mathcal{X}^{\perp}} A P_{\mathcal{X}^{\perp}})) \in [a, b]$ for $i \in \mathbb{I}_{d-k}$, then

$$(3.28) \quad \lambda_i(P_{\mathcal{X}_{g^{\perp}}} A P_{\mathcal{X}_{g^{\perp}}}) \in [a, b] \quad \text{for } i \in \mathbb{I}_{p-k}.$$

On the other hand, notice that

$$Y_S^* (S^* AS) Y_S = Y^* P_{\mathcal{Z}} A P_{\mathcal{Z}} Y = Y^* A Y$$

since, as before, $SS^* = P_{\mathcal{Z}}$, $P_{\mathcal{Z}}Y = Y$, and $Y^*P_{\mathcal{Z}} = Y^*$. Therefore, we get that

$$(3.29) \quad \lambda_i(Y_S^*(S^*AS)Y_S) = \lambda_i(Y^*AY) \in (\infty, a - \delta] \cup [b + \delta, \infty) \quad \text{for } i \in \mathbb{I}_k.$$

Item 1 now follows from (3.28) and (3.29) and the fact that $S^*\mathcal{X} \subseteq \mathbb{C}^p$ is, by construction, an $A_{\mathcal{X}+\mathcal{Y}}$ -invariant subspace.

In order to show item 2, we fix a u.n.i. norm $\|\cdot\|$. Using that $\mathcal{X}, \mathcal{Y} \subset \mathcal{Z}$ and the fact that S^* is an isometry from \mathcal{Z} onto \mathbb{C}^p , we see that $\Theta(\mathcal{X}, \mathcal{Y}) = \Theta(S^*\mathcal{X}, S^*\mathcal{Y})$. Then, an application of Nakatsukasa's tan Θ theorem (Theorem 3.16) to the self-adjoint matrix $S^*AS \in \mathcal{H}(p)$ and subspaces $S^*\mathcal{X}, S^*\mathcal{Y} \subseteq \mathbb{C}^p$ shows that

$$\delta' \|\tan(\Theta(\mathcal{X}, \mathcal{Y}))\| \leq \|A_{\mathcal{X}+\mathcal{Y}}Y_S - Y_S(Y_S^*A_{\mathcal{X}+\mathcal{Y}}Y_S)\|,$$

where $Y_S = S^*Y \in \mathcal{M}_{p,k}$ is an isometry from \mathbb{C}^k onto $S^*\mathcal{Y}$. We notice that

$$\begin{aligned} A_{\mathcal{X}+\mathcal{Y}}Y_S - Y_S(Y_S^*A_{\mathcal{X}+\mathcal{Y}}Y_S) &= S^*AS S^*Y - S^*Y(Y^*S(S^*AS)S^*Y) \\ &= S^*(AY - Y(Y^*AY)), \end{aligned}$$

where we have used that $SS^* = P_{\mathcal{Z}}$, $P_{\mathcal{Z}}Y = Y$, and $Y^*P_{\mathcal{Z}} = Y^*$. Hence, it follows that

$$\|A_{\mathcal{X}+\mathcal{Y}}Y_S - Y_S(Y_S^*A_{\mathcal{X}+\mathcal{Y}}Y_S)\| = \|P_{\mathcal{Z}}(AY - Y(Y^*AY))\| = \|P_{\mathcal{X}+\mathcal{Y}}R_Y\|,$$

thus completing the proof. \square

Remark 3.20. With the notation of Theorem 3.19 and using Remark 2.4, (3.27) is equivalent to the majorization relation

$$\delta' \tan(\Theta(\mathcal{X}, \mathcal{Y})) \prec_w s(A_{\mathcal{X}+\mathcal{Y}}Y_S - Y_S(Y_S^*A_{\mathcal{X}+\mathcal{Y}}Y_S)) = s(P_{\mathcal{X}+\mathcal{Y}}R_Y)$$

in terms of the separation constant δ' for $A_{\mathcal{X}+\mathcal{Y}} = S^*AS$, $S^*\mathcal{X}$, and $S^*\mathcal{Y}$.

Consider the notation in Theorem 3.19. Let $\delta > 0$ be such that $(A, \mathcal{X}, \mathcal{Y}, \delta)$ satisfies the DKN separation property. Given a u.n.i. norm $\|\cdot\|$, Theorem 3.16 allows one to bound $\|\tan \Theta(\mathcal{X}, \mathcal{Y})\|$ from above by

$$(3.30) \quad \|\tan \Theta(\mathcal{X}, \mathcal{Y})\| \leq \frac{\|R_Y\|}{\delta}.$$

On the other hand, by item 2 in Theorem 3.19 there exists $\delta' \geq \delta > 0$ such that $(A_{\mathcal{X}+\mathcal{Y}}, S^*\mathcal{X}, S^*\mathcal{Y}, \delta')$ satisfies the DKN separation property, so that we get the upper bound

$$(3.31) \quad \|\tan \Theta(\mathcal{X}, \mathcal{Y})\| \leq \frac{\|P_{\mathcal{X}+\mathcal{Y}}R_Y\|}{\delta'}.$$

Since $\|P_{\mathcal{X}+\mathcal{Y}}R_Y\| \leq \|R_Y\|$ and $\delta \leq \delta'$, we immediately see that the upper bound in (3.31) improves the classical bound in (3.30). In order to compare these two bounds in some more detail, let us consider the following example.

Example 3.21. Let $\tilde{\lambda} = (a, b, d, c) \in \mathbb{R}^4$, where $a < b < c < d$, and let $\tilde{A} \in \mathcal{H}(4)$ be given by $\tilde{A} = D_{\tilde{\lambda}}$. For the purposes of this example, we consider the real parameter $c \in (b, d)$ as variable (while a, b, d are fixed).

Let $\mathcal{X}, \mathcal{Y}_\theta \subset \mathbb{C}^4$ be as in Example 3.5, i.e., $\mathcal{X} = \text{span}\{e_1, e_2\}$ and $\mathcal{Y}_\theta = \text{span}\{e_1, f_\theta\}$. Recall that $\Theta(\mathcal{X}, \mathcal{Y}_\theta) = (\theta, 0)$. In particular, $\tan \Theta(\mathcal{X}, \mathcal{Y}_\theta) = (\tan \theta, 0)$ in this case.

It is clear that $\mathcal{X} + \mathcal{Y}_\theta = \text{span}\{e_1, e_2, e_3\}$. Let

$$X = \begin{pmatrix} 1 & 0 \\ 0 & 1 \\ 0 & 0 \\ 0 & 0 \end{pmatrix}, \quad X_\perp = \begin{pmatrix} 0 & 0 \\ 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \text{and} \quad Y_\theta = \begin{pmatrix} 1 & 0 \\ 0 & \cos \theta \\ 0 & \sin \theta \\ 0 & 0 \end{pmatrix}.$$

Then, we have that $\lambda(Y_\theta^* \tilde{A} Y_\theta) = (b \cos^2 \theta + d \sin^2(\theta), a)$, while $\lambda(X_\perp^* \tilde{A} X_\perp) = (d, c)$. Therefore, if we let $\theta_0(c) = \theta_0 = \arcsin\left(\sqrt{\frac{c-b}{d-b}}\right)$ and set

$$\delta_\theta = c - (b \cos^2 \theta + d \sin^2 \theta) > 0 \quad \text{for } 0 < \theta < \theta_0,$$

then $(\tilde{A}, \mathcal{X}, \mathcal{Y}_\theta, \delta_\theta)$ satisfies the DKN separation property, and δ_θ is the optimal (largest) separation constant and the separation property holds only for $0 < \theta < \theta_0$ in this case. Again, simple computations show that $s(R_{Y_\theta}) = ((d-b) \cos \theta \sin \theta, 0)$.

Now, (3.30) obtained from Theorem 3.16 becomes

$$(3.32) \quad \tan \theta \leq \frac{(d-b) \cos \theta \sin \theta}{c - (b \cos^2 \theta + d \sin^2 \theta)} \quad \text{for } 0 < \theta < \theta_0.$$

Notice that $\lim_{c \rightarrow b^+} \theta_0 = 0$, i.e., the range of θ for which we can apply the bound in (3.32) tend to become small. In the limit case in which $b = c$ (i.e., multiple eigenvalues) we cannot apply the bound (3.32) (the separation constant in this case is $\delta_0 = 0$). Finally, if we consider the limit case in which θ becomes small, then the upper bound is comparable with the upper bound $(\frac{d-b}{c-b}) \tan \theta (> \tan \theta)$.

On the other hand, $\mathcal{X} + \mathcal{Y}_\theta \ominus \mathcal{X} = \mathbb{C} e_3$, the subspace spanned by e_3 . In this case, if we let $X' = (0, 0, 1, 0)^t$, it is clear that $\lambda((X'_S)^* \tilde{A} X'_S) = d$. Therefore, if we let $\delta'_\theta = d - (b \cos^2 \theta + d \sin^2 \theta) = (d-b) \cos^2 \theta > 0$ for $\theta \in (0, \pi/2)$, we get that $(\tilde{A}_{\mathcal{X}+\mathcal{Y}_\theta}, S^* \mathcal{X}, S^* \mathcal{Y}_\theta, \delta'_\theta)$ satisfies the DKN separation property, where $S \in \mathcal{M}_{4,3}(\mathbb{C})$ is the matrix whose columns are the first three elements in the canonical basis. In this case we have that

$$\frac{s_1(P_{\mathcal{X}+\mathcal{Y}_\theta} R_{Y_\theta})}{\delta'_\theta} = \frac{(d-b) \cos \theta \sin \theta}{(d-b) \cos^2 \theta} = \tan \theta,$$

and hence, the upper bound in (3.31) coincides with $\tan \theta$ (where $\tan \Theta(\mathcal{X}, \mathcal{Y}_\theta) = (\tan \theta, 0)$), i.e., the upper bound is sharp. Notice that this bound is applicable for every $\theta \in (0, \pi/2)$.

The following result was conjectured in [19].

COROLLARY 3.22. *Let $A \in \mathcal{H}(d)$, let $\mathcal{X}, \mathcal{Y} \subset \mathbb{C}^d$, and let $\delta > 0$ be such that $(A, \mathcal{X}, \mathcal{Y}, \delta)$ satisfies the DKN separation property. Then,*

$$\delta \| \tan(\Theta(\mathcal{X}, \mathcal{Y})) \| \leq \| P_{\mathcal{X}+\mathcal{Y}} R_Y \|$$

for every u.n.i. norm $\| \cdot \|$.

Proof. Let $S \in \mathcal{M}_{d,p}(\mathbb{C})$ be such that its columns form an ONB for $\mathcal{X} + \mathcal{Y}$. By item 1 in Theorem 3.19, there exists $\delta' \geq \delta$ such that $(S^* A S, S^* \mathcal{X}, S^* \mathcal{Y}, \delta')$ satisfies the DKN separation property. By item 2 of the same result, we have that

$$\delta \| \tan(\Theta(\mathcal{X}, \mathcal{Y})) \| \leq \delta' \| \tan(\Theta(\mathcal{X}, \mathcal{Y})) \| \leq \| P_{\mathcal{X}+\mathcal{Y}} R_Y \|.$$

Finally, we get the following quadratic a posteriori error bound for the simultaneous approximation of eigenvalues of A by the Ritz values corresponding to Rayleigh quotients for which a DKN separation property holds.

THEOREM 3.23. *Let $A \in \mathcal{H}(d)$, $\mathcal{X}, \mathcal{Y} \subset \mathbb{C}^d$, and let $\delta > 0$ be such that $(A, \mathcal{X}, \mathcal{Y}, \delta)$ satisfies the DKN separation property. Then, for every u.n.i. norm $\|\cdot\|$ we have that*

$$\|\lambda(\rho(X)) - \lambda(\rho(Y))\| \leq \frac{\|P_{\mathcal{X}+\mathcal{Y}} R_Y\|^2}{\delta}.$$

Proof. This is a consequence of Corollary 3.4 and Theorem 3.19. \square

Theorem 3.23 allows one to obtain the following extension of [18, Theorem 5.3] (see Remark 3.25) which is a quadratic a posteriori majorization error bound for simultaneous approximation of consecutive eigenvalues.

COROLLARY 3.24. *Let $A \in \mathcal{H}(d)$, and let $\mathcal{Y} \subset \mathbb{C}^d$ be such that*

1. $\lambda_1(Y^*AY) < \lambda_j(A)$, where $j \in \mathbb{I}_{d-k}$ is the smallest such index;
2. $\lambda_i(Y^*AY) \geq \lambda_{i+j}(A)$ for $i \in \mathbb{I}_k$.

*Let \mathcal{U} be the A -invariant space spanned by the eigenvectors associated with $\lambda_i(A)$ for $1 \leq i \leq j$, and set $\mathcal{X} = (I - P_{\mathcal{U}})\mathcal{Y}$. If $\eta = \lambda_j(A) - \lambda_1(Y^*AY) > 0$, then*

$$\|(\lambda_{i+j}(A))_{i \in \mathbb{I}_k} - \lambda(\rho(Y))\| \leq \frac{\|P_{\mathcal{X}+\mathcal{Y}} R_Y\|^2}{\eta}$$

for every u.n.i. norm $\|\cdot\|$.

Proof. Let $\mathcal{V} = \mathcal{U} + \mathcal{Y}$ and notice that $\mathcal{U} \cap \mathcal{Y} = \{0\}$; hence, $p = \dim \mathcal{V} = \dim \mathcal{U} + k$ i.e., $j = \dim \mathcal{U} = p - k$. Moreover, $\mathcal{V} \ominus \mathcal{U} = (I - P_{\mathcal{U}})\mathcal{Y} = \mathcal{X}$; then, in particular, $\dim \mathcal{X} = \dim \mathcal{Y}$ and $\mathcal{V} \ominus \mathcal{X} = \mathcal{U}$. Also notice that $\Theta_1(\mathcal{X}, \mathcal{Y}) < \pi/2$ or, otherwise, we would have that $\mathcal{U} \cap \mathcal{Y} \neq \{0\}$, since $\mathcal{V} \ominus \mathcal{X} = \mathcal{U}$.

Let $V \in \mathcal{M}_{d,p}(\mathbb{C})$ be such that its columns form an ONB of \mathcal{V} , and set $A_V = V^*AV \in \mathcal{H}(p)$. Similarly, let $X, Y \in \mathcal{M}_{d,k}(\mathbb{C})$, $U \in \mathcal{M}_{d,p-k}(\mathbb{C})$ be such that their columns form ONBs of \mathcal{X} , \mathcal{Y} , and \mathcal{U} , respectively; set $X_V = V^*X$, $Y_V = V^*Y \in \mathcal{M}_{p,k}(\mathbb{C})$, and $U_V = V^*U \in \mathcal{M}_{p,p-k}(\mathbb{C})$. Then, the columns of U_V span $\mathcal{U}_V \subset \mathbb{C}^p$, an A -invariant space of A_V . In particular, the columns of X_V span $\mathcal{X}_V \subset \mathbb{C}^p$ which is also an A -invariant space of A_V . In this case $\mathcal{X}_V^\perp = \mathcal{U}_V$ and $\Theta_1(\mathcal{X}_V, \mathcal{Y}_V) = \Theta_1(\mathcal{X}, \mathcal{Y}) < \pi/2$, where $\mathcal{Y}_V \subset \mathbb{C}^p$ is the space spanned by the columns of Y_V . Notice that, by construction $\lambda_i(Y_V^* A_V Y_V) = \lambda_i(Y^* A Y)$ for $i \in \mathbb{I}_k$. Since $\mathcal{X} \subset \mathcal{U}^\perp$ by the interlacing inequalities for compressions of self-adjoint matrices and item 2 above, we get that for $i \in \mathbb{I}_k$,

$$(3.33) \quad \lambda_i(X_V^* A_V X_V) = \lambda_i(X^* A X) \leq \lambda_i(A_{U^\perp}) = \lambda_{j+i}(A) \leq \lambda_i(Y_V^* A_V Y_V),$$

where $U_\perp \in \mathcal{M}_{d,d-j}(\mathbb{C})$ is such that its columns form an ONB for \mathcal{U}^\perp . On the other hand, by hypothesis $(A_V, \mathcal{X}_V, \mathcal{Y}_V, \eta)$ satisfies the DKN separation property (recall that $\mathcal{X}_V^\perp = \mathcal{U}_V$). Hence, by Theorem 3.23 we conclude that

$$(3.34) \quad \|\lambda(X_V^* A_V X_V) - \lambda(Y_V^* A_V Y_V)\| \leq \frac{\|P_{\mathcal{X}_V+\mathcal{Y}_V} (A_V Y_V - Y_V (Y_V^* A_V Y_V))\|^2}{\eta}.$$

By (3.33) we get that

$$|(\lambda_{i+j}(A))_{i \in \mathbb{I}_k} - \lambda(Y_V^* A_V Y_V)| \prec_w |\lambda(X_V^* A_V X_V) - \lambda(Y_V^* A_V Y_V)|.$$

On the other hand, arguing as in the proof of Theorem 3.19, we see that

$$\| P_{\mathcal{X}_V + \mathcal{Y}_V} (A_V Y_V - Y_V (Y_V^* A_V Y_V)) \| = \| P_{\mathcal{X} + \mathcal{Y}} R_Y \|.$$

The result follows from these last facts together with (3.34) and Remark 2.4. \square

Remark 3.25. We mention that the hypothesis in item 1 in Corollary 3.24 is that there exists an eigenvalue β of A such that $\lambda_1(Y^* A Y) < \beta$. Indeed, in this case we can apply the interlacing inequalities and get that $\lambda_i(Y^* A Y) \geq \lambda_{d-k+i}(A)$ for $i \in \mathbb{I}_k$. Therefore, $\beta = \lambda_j(A)$ for some $1 \leq j \leq d - k$.

The hypothesis in item 2 is rather restrictive and difficult to check in general. Nevertheless, we mention two cases in which the hypotheses in Corollary 3.24 can be easily checked:

1. In case that the hypothesis in item 1 holds for $j = d - k$, by the interlacing inequalities we have

$$\lambda_i(Y^* A Y) \geq \lambda_{i+d-k}(A) \quad \text{for } i \in \mathbb{I}_k,$$

so the hypothesis in item 2 automatically holds.

2. In case $k = 1$, that is, if $\mathcal{Y} = \mathbb{C} y$ for a unit norm vector $y \in \mathbb{C}^d$, the hypotheses become the existence of $j \in \mathbb{I}_{d-1}$ such that $\lambda_{j+1}(A) \leq \langle A y, y \rangle < \lambda_j(A)$; then, Corollary 3.24 implies that

$$0 \leq \langle A y, y \rangle - \lambda_{j+1}(A) \leq \frac{\| P_{\mathcal{X} + \mathcal{Y}}(A y - \langle A y, y \rangle y) \|}{\lambda_j(A) - \langle A y, y \rangle},$$

where $\mathcal{X} = \mathbb{C} x$ for $x = (I - P_U)y \in \mathbb{C}^d$; this is [18, Theorem 5.3]. As explained in [18], Corollary 3.24 encodes several known bounds related with eigenvalues estimation even when $k = 1$.

Appendix A. Here we collect several well-known results about majorization used throughout our work. The first result deals with submajorization relations between singular values of arbitrary matrices in $\mathcal{M}_d(\mathbb{C})$. For detailed proofs of these results and general references in majorization theory, see [2, 6, 11]. For $A \in \mathcal{M}_d(\mathbb{C})$ we denote $\text{re}(A) = \frac{A+A^*}{2} \in \mathcal{H}(d)$.

THEOREM A.1. *Let $C, D \in \mathcal{M}_d(\mathbb{C})$. Then,*

1. $s(C + D) \prec_w s(C) + s(D)$ *(Lidskii's additive property);*
2. $s(\text{re}(C)) \prec_w s(C)$;
3. $s(CD) \prec_w s(C)s(D)$ *(Lidskii's multiplicative property);*
4. *if we assume that $CD \in \mathcal{H}(d)$, then $s(CD) \prec_w s(\text{re}(DC))$.*

For Hermitian matrices we have the following majorization relations.

THEOREM A.2. *Let $C, D \in \mathcal{H}(d)$. Then,*

1. $\lambda(C) - \lambda(D) \prec \lambda(C - D) \prec \lambda(C) - \lambda^\uparrow(D)$;
2. $|\lambda(C) - \lambda(D)| \prec_w s(C - D)$;
3. *let $\mathcal{P} = \{P_j\}_{j=1}^r$ be a system of projections (i.e., they are mutually orthogonal projections on \mathbb{C}^d such that $\sum_{i=1}^r P_i = I$). If $C_{\mathcal{P}}(C) = \sum_{i=1}^r P_i C P_i$, then $\lambda(C_{\mathcal{P}}(C)) \prec \lambda(C)$.*

In the next result we describe elementary but useful properties of (sub)majorization between real vectors.

LEMMA A.3. *Let $x, y, z \in \mathbb{R}^k$. Then,*

1. $x^\downarrow + y^\uparrow \prec x + y \prec x^\downarrow + y^\downarrow$;
2. if $x \prec_w y$ and $y, z \in (\mathbb{R}^k)^\downarrow$, then $x + z \prec_w y + z$.

If we assume further that $x, y, z \in \mathbb{R}_{\geq 0}^k$, then

3. $x^\downarrow y^\uparrow \prec_w x y \prec_w x^\downarrow y^\downarrow$;
4. if $x \prec_w y$ and $y, z \in (\mathbb{R}_{\geq 0}^k)^\downarrow$, then $x z \prec_w y z$.

PROPOSITION A.4. Let $1 \leq k < d$, and let $E \in \mathbb{M}_{k,(d-k)}(\mathbb{C})$. Then

$$\hat{E} = \begin{pmatrix} 0 & E \\ E^* & 0 \end{pmatrix} \in \mathcal{H}(d) \quad \text{and} \quad \lambda(\hat{E}) = (s(E), -s(E^*)^\downarrow) \in (\mathbb{R}^d)^\downarrow.$$

THEOREM A.5 (see [7]). Let $\mathcal{X}, \mathcal{Y} \subset \mathbb{C}^d$ be such that $\dim(\mathcal{X}) = \dim(\mathcal{Y}) = k$. Then

$$\lambda(P_{\mathcal{X}} P_{\mathcal{Y}^\perp} P_{\mathcal{X}}) = s(P_{\mathcal{X}} P_{\mathcal{Y}^\perp} P_{\mathcal{X}}) = s^2(P_{\mathcal{Y}} P_{\mathcal{X}^\perp}) = s^2(P_{\mathcal{X}^\perp} P_{\mathcal{Y}}) = (\sin^2(\Theta(\mathcal{X}, \mathcal{Y})), 0_{d-k}).$$

Notice that item 2 below is Theorem 3.2 from section 3.

THEOREM A.6. Let $C, D \in \mathcal{H}(k)$. Then,

1. if $T \in \mathcal{G}l(k)^+$, then $s(C - D) \prec_w s(T^{-1}) s(CT - TD)$;
2. if $T \in \mathcal{G}l(k)$, then $|\lambda(C) - \lambda(D)| \prec_w s(T^{-1}) s(CT - TD)$.

Proof. We first show item 1. Since T is positive and invertible, using Theorem A.2 (item 3) we get that

$$\begin{aligned} s(C - D) &= s(CT^{\frac{1}{2}}T^{-\frac{1}{2}} - T^{-\frac{1}{2}}T^{\frac{1}{2}}D) = s(T^{-\frac{1}{2}}(T^{\frac{1}{2}}CT^{\frac{1}{2}} - T^{\frac{1}{2}}DT^{\frac{1}{2}})T^{-\frac{1}{2}}) \\ &\prec_w s(T^{-\frac{1}{2}})^2 s(T^{\frac{1}{2}}CT^{\frac{1}{2}} - T^{\frac{1}{2}}DT^{\frac{1}{2}}) = s(T^{-1}) s(T^{\frac{1}{2}}(C - D)T^{\frac{1}{2}}). \end{aligned}$$

By Theorem A.1 (items 2 and 4) and the fact that $\text{re}(DT) = \text{re}(TD)$ we obtain that

$$(A.1) \quad s(T^{\frac{1}{2}}(C - D)T^{\frac{1}{2}}) \prec_w s(\text{re}[(C - D)T]) = s(\text{re}[CT - TD]) \prec_w s(CT - TD).$$

By the previous inequalities and Lemma A.3 we see that

$$(A.2) \quad s(C - D) \prec_w s(T^{-1}) s(CT - TD).$$

In order to show item 2, consider a representation of T given by $T = U\Sigma V^*$, where $U, V \in \mathcal{U}(k)$ are unitary matrices and $\Sigma \in \mathcal{M}_k(\mathbb{C})$ is the diagonal matrix with main diagonal $s(T) \in \mathbb{R}_{\geq 0}^k$ (notice that such representation follows from the SVD decomposition of T); note that Σ is definite positive and invertible. Using item 2 in Theorem A.2 and (the already proved) item 1 of the statement, we get

$$\begin{aligned} |\lambda(C) - \lambda(D)| &= |\lambda(U^*CU) - \lambda(V^*DV)| \prec_w s(U^*CU - V^*DV) \\ &\prec_w s(\Sigma^{-1}) s(U^*CU\Sigma - \Sigma V^*DV) = s(T^{-1}) s(U^*(CT - TD)V) \\ &= s(T^{-1}) s(CT - TD). \end{aligned} \quad \square$$

In what follows we restate and prove two propositions of section 3.2.

PROPOSITION 3.10. Let $A \in \mathcal{H}(d)$, and let $\mathcal{X}, \mathcal{Y} \subset \mathbb{C}^d$ with $\dim(\mathcal{X}) = \dim(\mathcal{Y}) = k$. Then,

$$(A.3) \quad s(P_{\mathcal{X}} R_Y) \prec_w \text{Spr}(A, \mathcal{X} + \mathcal{Y}) \sin(\Theta(\mathcal{X}, \mathcal{Y})).$$

Proof. We begin with a simple reduction argument. In order to describe this reduction it will be convenient to consider matrices in terms of the linear operators that they induce. Hence, given $A \in \mathcal{M}_d(\mathbb{C})$, we consider $A \in \mathcal{L}(\mathbb{C}^d)$ (defined in the obvious way). The advantage in considering $A \in \mathcal{L}(\mathbb{C}^d)$ is that we can get different block matrix representations of A (considered as an operator) with respect to orthogonal decompositions $\mathbb{C}^d = \mathcal{V} \oplus \mathcal{V}^\perp$ for a (proper) subspace $\mathcal{V} \subset \mathbb{C}^d$, in the usual manner. We now proceed as follows: Let $\mathcal{Z} = \mathcal{X} + \mathcal{Y}$ with $\dim \mathcal{Z} = p$, and consider the matrix representations with respect to the decomposition $\mathbb{C}^d = \mathcal{Z} \oplus \mathcal{Z}^\perp$:

$$P_{\mathcal{X}} = \begin{pmatrix} P^{\mathcal{X}} & 0 \\ 0 & 0 \end{pmatrix}, \quad P_{\mathcal{Y}} = \begin{pmatrix} P^{\mathcal{Y}} & 0 \\ 0 & 0 \end{pmatrix}, \quad \text{and} \quad A = \begin{pmatrix} A_{\mathcal{Z}} & * \\ * & * \end{pmatrix},$$

where $P^{\mathcal{X}}$, $P^{\mathcal{Y}}$, $A_{\mathcal{Z}} = P_{\mathcal{Z}}A|_{\mathcal{Z}} \in \mathcal{L}(\mathcal{Z})$ are self-adjoint operators. In this case we have

$$P_{\mathcal{X}}(AP_{\mathcal{Y}} - P_{\mathcal{Y}}AP_{\mathcal{Y}}) = \begin{pmatrix} P^{\mathcal{X}}(A_{\mathcal{Z}}P^{\mathcal{Y}} - P^{\mathcal{Y}}A_{\mathcal{Z}}P^{\mathcal{Y}}) & 0 \\ 0 & 0 \end{pmatrix}.$$

On the other hand, a simple calculation shows that

$$(s(P_{\mathcal{X}}R_Y), 0_{d-k}) = s(P_{\mathcal{X}}(AP_{\mathcal{Y}} - P_{\mathcal{Y}}AP_{\mathcal{Y}})) \in (\mathbb{R}_{\geq 0}^d)^\perp.$$

Hence, $(s(P_{\mathcal{X}}R_Y), 0_{p-k}) = s(P^{\mathcal{X}}(A_{\mathcal{Z}}P^{\mathcal{Y}} - P^{\mathcal{Y}}A_{\mathcal{Z}}P^{\mathcal{Y}})) = s(P^{\mathcal{X}}(I_{\mathcal{Z}} - P^{\mathcal{Y}})A_{\mathcal{Z}}P^{\mathcal{Y}})$. Thus, we can assume further that $\mathbb{C}^d = \mathcal{Z} = \mathcal{X} + \mathcal{Y}$ and show that

$$(A.4) \quad (s(P_{\mathcal{X}}R_Y), 0_{d-k}) = s(P_{\mathcal{X}}(P_{\mathcal{Y}^\perp}AP_{\mathcal{Y}})) \prec_w (\text{Spr}(A) \sin(\Theta(\mathcal{X}, \mathcal{Y})), 0_{d-k}).$$

Now using item 3 of Theorem A.1 (Lidskii's multiplicative property),

$$(A.5) \quad s(P_{\mathcal{X}}P_{\mathcal{Y}^\perp}AP_{\mathcal{Y}}) = s(P_{\mathcal{X}}P_{\mathcal{Y}^\perp}P_{\mathcal{Y}^\perp}AP_{\mathcal{Y}}) \prec_w s(P_{\mathcal{X}}P_{\mathcal{Y}^\perp})s(P_{\mathcal{Y}^\perp}AP_{\mathcal{Y}}).$$

First notice that by Theorem A.5, we have that $s(P_{\mathcal{X}}P_{\mathcal{Y}^\perp}) = (\sin(\Theta(\mathcal{X}, \mathcal{Y})), 0_{d-k})$. On the other hand, consider the matrix representation induced by the decomposition $\mathbb{C}^d = \mathcal{Y} \oplus \mathcal{Y}^\perp$:

$$(A.6) \quad A = \begin{pmatrix} A_{11} & A_{21}^* \\ A_{21} & A_{22} \end{pmatrix} \quad \text{and set} \quad A_1 := \begin{pmatrix} A_{11} & 0 \\ 0 & A_{22} \end{pmatrix}, \quad A_2 := \begin{pmatrix} 0 & A_{21}^* \\ A_{21} & 0 \end{pmatrix}.$$

Then, we have that $A = A_1 + A_2$. Now, A_1 is a pinching of A (associated with the system of projections $\{P_{\mathcal{Y}}, P_{\mathcal{Y}^\perp}\}$) so $\lambda(A_1) \prec \lambda(A)$, so then

$$(A.7) \quad -\lambda^\uparrow(A_1) \prec -\lambda^\uparrow(A).$$

Using Lidskii's additive property for $A_2 = A - A_1$ (see item 1 in Theorem A.2),

$$(A.8) \quad \lambda(A_2) \prec \lambda(A) - \lambda^\uparrow(A_1).$$

Combining (A.7) and (A.8), we obtain

$$(A.9) \quad \lambda(A_2) \prec \lambda(A) - \lambda^\uparrow(A) = \text{Spr}(A) \in \mathbb{R}^d.$$

By Proposition A.4, we get that $\lambda(A_2) = (s(A_{21}), -s(A_{21}^*))^\perp$; in particular, $s(A_{21}) = (\lambda_i(A_2))_{i \in \mathbb{I}_k}$. Now, $s(P_{\mathcal{Y}^\perp}AP_{\mathcal{Y}}) = (s(A_{21}), 0_{d-k})$; thus, we see that

$$(A.10) \quad s(P_{\mathcal{Y}^\perp}AP_{\mathcal{Y}}) = (s(A_{21}), 0_{d-k}) = ((\lambda_i(A_2))_{i \in \mathbb{I}_k}, 0_{d-k}) \prec_w ((\text{Spr}_i(A))_{i \in \mathbb{I}_k}, 0_{d-k}),$$

where $\text{Spr}(A) = (\text{Spr}_i(A))_{i \in \mathbb{I}_d}$. Using (A.5) and (A.10) together with Lemma A.3, we finally get that

$$s(P_{\mathcal{X}}P_{\mathcal{Y}^\perp}AP_{\mathcal{Y}}) \prec_w (\text{Spr}(A) \sin(\Theta(\mathcal{X}, \mathcal{Y})), 0_{d-k}) \in (\mathbb{R}_{\geq 0}^d)^\downarrow.$$

Now the result follows from the last submajorization relation, by considering the first k entries of both vectors. \square

PROPOSITION 3.12. *Let $A \in \mathcal{H}(d)$, $\mathcal{X}, \mathcal{Y} \subset \mathbb{C}^d$ subspaces with $\dim(\mathcal{X}) = \dim(\mathcal{Y}) = k$. Assume that \mathcal{X} is A -invariant. Then,*

$$(A.11) \quad s(P_{\mathcal{X}}R_Y) \prec_w 2(\lambda_i(A_{\mathcal{X}+\mathcal{Y}}) - \lambda_{\min}(A_{\mathcal{X}+\mathcal{Y}}))_{i \in \mathbb{I}_k} \sin^2(\Theta(\mathcal{X}, \mathcal{Y})).$$

Proof. Arguing as in the proof of Proposition 3.10, we can assume further that $\mathbb{C}^d = \mathcal{X} + \mathcal{Y}$. With this assumption, we consider first the case where $A \in \mathcal{M}_d(\mathbb{C})^+$ and show that

$$(A.12) \quad s(P_{\mathcal{X}}R_Y) \prec_w 2(\lambda_i(A))_{i \in \mathbb{I}_k} \sin^2(\Theta(\mathcal{X}, \mathcal{Y})).$$

Indeed, the A -invariance of \mathcal{X} allows us to write $A = P_{\mathcal{X}}AP_{\mathcal{X}} + P_{\mathcal{X}^\perp}AP_{\mathcal{X}^\perp}$. With this decomposition in mind and using the fact that $(s(P_{\mathcal{X}}R_Y), 0_{d-k}) = s(P_{\mathcal{X}}P_{\mathcal{Y}^\perp}AP_{\mathcal{Y}})$, we have that

$$\begin{aligned} s(P_{\mathcal{X}}P_{\mathcal{Y}^\perp}AP_{\mathcal{Y}}) &= s(P_{\mathcal{X}}P_{\mathcal{Y}^\perp}P_{\mathcal{X}}AP_{\mathcal{X}}P_{\mathcal{Y}} + P_{\mathcal{X}}P_{\mathcal{Y}^\perp}P_{\mathcal{X}^\perp}AP_{\mathcal{X}^\perp}P_{\mathcal{Y}}) \\ &\prec_w s(P_{\mathcal{X}}P_{\mathcal{Y}^\perp}P_{\mathcal{X}}AP_{\mathcal{X}}P_{\mathcal{Y}}) + s(P_{\mathcal{X}}P_{\mathcal{Y}^\perp}AP_{\mathcal{X}^\perp}P_{\mathcal{Y}}) \stackrel{\text{def}}{=} M. \end{aligned}$$

Using item 3 of Theorem A.1 (Lidskii's multiplicative property), the fact that $0_d \leq s(P_{\mathcal{X}}P_{\mathcal{Y}}) \leq \mathbb{1}_d$, and Theorem A.5, we get

$$\begin{aligned} M &\prec_w s(P_{\mathcal{X}}P_{\mathcal{Y}^\perp}P_{\mathcal{X}})s(A) + s(P_{\mathcal{X}}P_{\mathcal{Y}^\perp})s(A)s(P_{\mathcal{X}^\perp}P_{\mathcal{Y}}) \\ &\prec_w 2\lambda(A)(\sin^2(\Theta(\mathcal{X}, \mathcal{Y})), 0_{d-k}) \in (\mathbb{R}_{\geq 0}^d)^\downarrow, \end{aligned}$$

since $A \in \mathcal{M}_d(\mathbb{C})^+$ is positive semidefinite. The result now follows from the previous facts.

In general, for $A \in \mathcal{H}(d)$ consider the auxiliary matrix $\tilde{A} = A - \lambda_{\min(A)}I \in \mathcal{M}_d(\mathbb{C})^+$. Notice that

$$R_Y(\tilde{A}) = \tilde{A}Y - Y(Y^*\tilde{A}Y) = AY - Y(Y^*AY) = R_Y,$$

and $\lambda(\tilde{A}) = \lambda(A) - \lambda_{\min(A)}\mathbb{1}_d$. The result now follows from these facts and from (A.12) applied to \tilde{A} . \square

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