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Between Subspaces, Ritz values, and
graph Laplacian spectra**

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MAJORIZATION FOR CHANGES IN ANGLES BETWEEN SUBSPACES, RITZ VALUES, AND GRAPH LAPLACIAN SPECTRA*

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Abstract. Many inequality relations between real vector quantities can be succinctly expressed as “weak (sub)majorization” relations using the symbol \prec_w . We explain these ideas and apply them in several areas: angles between subspaces, Ritz values, and graph Laplacian spectra, which we show are all surprisingly related.

Let $\Theta(\mathcal{X}, \mathcal{Y})$ be the vector of principal angles in nondecreasing order between subspaces \mathcal{X} and \mathcal{Y} of a finite dimensional space \mathcal{H} with a scalar product. We consider the change in principal angles between subspaces \mathcal{X} and \mathcal{Z} , where we let \mathcal{X} be perturbed to give \mathcal{Y} . We measure the change using the weak majorization. We prove that $|\cos^2 \Theta(\mathcal{X}, \mathcal{Z}) - \cos^2 \Theta(\mathcal{Y}, \mathcal{Z})| \prec_w \sin \Theta(\mathcal{X}, \mathcal{Y})$, and give similar results for differences of cosines, i.e. $|\cos \Theta(\mathcal{X}, \mathcal{Z}) - \cos \Theta(\mathcal{Y}, \mathcal{Z})| \prec_w \sin \Theta(\mathcal{X}, \mathcal{Y})$, and of sines, and of sines squared, assuming $\dim \mathcal{X} = \dim \mathcal{Y}$.

We observe that $\cos^2 \Theta(\mathcal{X}, \mathcal{Z})$ can be interpreted as a vector of Ritz values, where the Rayleigh-Ritz method is applied to the orthogonal projector on \mathcal{Z} using \mathcal{X} as a trial subspace. Thus, our result for the squares of cosines can be viewed as a bound on the change in the Ritz values with the change of the trial subspace for the particular case, where the Rayleigh-Ritz method is applied to an orthogonal projector. We then extend it to prove a general result for Ritz values for an arbitrary Hermitian operator A , not necessarily a projector: let $\Lambda(P_{\mathcal{X}}A|_{\mathcal{X}})$ be the vector of Ritz values in nonincreasing order for operator A on a trial subspace \mathcal{X} , which is perturbed to give another trial subspace \mathcal{Y} , then $|\Lambda(P_{\mathcal{X}}A|_{\mathcal{X}}) - \Lambda(P_{\mathcal{Y}}A|_{\mathcal{Y}})| \prec_w (\lambda_{\max} - \lambda_{\min}) \sin \Theta(\mathcal{X}, \mathcal{Y})$, where the constant is the difference between the largest and the smallest eigenvalues of A . This confirms our previous conjecture that the square root of two factor, which has been present in the constant of our earlier estimate, can be eliminated. Our present proof is based on a classical but rarely used result of extending a Hermitian operator in \mathcal{H} to an orthogonal projector in the “double” space \mathcal{H}^2 .

An application of our Ritz values weak majorization result for Laplacian graph spectra comparison is suggested, based on the possibility to interpret eigenvalues of the edge Laplacian of a given graph as Ritz values of the edge Laplacian of the complete graph. We prove that $\sum_k |\lambda_k^1 - \lambda_k^2| \leq nl$, where λ_k^1 and λ_k^2 are all ordered elements of the Laplacian spectra of two graphs with the same n vertices and with the number of differences between the edges equal to l .

Key words. Majorization, principal angles, canonical angles, canonical correlations, subspace, orthogonal projection, perturbation analysis, Ritz values, Rayleigh–Ritz method, graph spectrum, graph vertex Laplacian, graph edge Laplacian.

1. Introduction. Many inequality relations between real vector quantities can be succinctly expressed as “weak (sub)majorization” relations using the symbol \prec_w . The importance of weak majorization can be seen from the classical statement that for two real vectors x and y the following two conditions are equivalent: $x \prec_w y$ and $\sum \phi(x) \leq \sum \phi(y)$ for all nondecreasing convex functions ϕ . Thus, a single weak majorization result implies a great variety of inequalities. We explain these ideas and apply them in several areas: angles between subspaces, Ritz values, and graph Laplacian spectra, which we show are all surprisingly related.

The concept of principal angles, also referred to as canonical angles between subspaces is one of the classical mathematical ideas originated from Jordan [13] with

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many applications. In functional analysis, the gap between subspaces, which is related to the sine of the largest principal angle, bounds the perturbation of a closed linear operator by measuring the change in its graph, while the smallest nontrivial principal angle between two subspaces determines if the sum of the subspaces is closed. In numerical analysis, principal angles appear naturally to estimate how close an approximate eigenspace is to the true eigenspace. The chordal distance, the Frobenius norm of the sine of the principal angles, on the Grassmannian space of finite dimensional subspaces is used, e.g., for subspace packing with applications in control theory. In statistics, the cosines of principal angles are called canonical correlations and have applications in information retrieval and data visualization.

Let \mathcal{H} be a real or complex $n < \infty$ dimensional vector space equipped with an inner product (x, y) and a vector norm $\|x\| = (x, x)^{1/2}$. The acute angle between two non-zero vectors x and y is defined as

$$\theta(x, y) = \arccos \frac{|(x, y)|}{\|x\|\|y\|} \in [0, \pi/2].$$

For three nonzero vectors x, y, z , we have a bound of the change in the angle

$$(1.1) \quad |\theta(x, z) - \theta(y, z)| \leq \theta(x, y),$$

a bound for the sine

$$(1.2) \quad |\sin(\theta(x, z)) - \sin(\theta(y, z))| \leq \sin(\theta(x, y)),$$

a bound for the cosine

$$(1.3) \quad |\cos(\theta(x, z)) - \cos(\theta(y, z))| \leq \sin(\theta(x, y)),$$

and an estimate for the sine or cosine squared

$$(1.4) \quad |\cos^2(\theta(x, z)) - \cos^2(\theta(y, z))| = |\sin^2(\theta(x, z)) - \sin^2(\theta(y, z))| \leq \sin(\theta(x, y)).$$

Let us note that we can project the space \mathcal{H} into the $\text{span}\{x, y, z\}$ without changing the angles, i.e. the inequalities above present essentially the case of a $3D$ space.

Inequality (1.1) is proved in Qiu et al. [29]. We note that (1.2) follows from (1.1), since the sine function is increasing and subadditive, see Qiu et al. [29].

It is instructive to provide a simple geometry-based proof of the sine inequality (1.2) using orthogonal projectors. Let $P_{\mathcal{X}}, P_{\mathcal{Y}}, P_{\mathcal{Z}}$ be, respectively, the orthogonal projectors onto the subspaces spanned by the vectors x, y , and z , and let $\|\cdot\|$ also denote the induced operator norm. When we are dealing with $1D$ subspaces, we have the following elementary formula $\sin(\theta(x, y)) = \|P_{\mathcal{X}} - P_{\mathcal{Y}}\|$. Then the sine (1.2) inequality is equivalent to $|\|P_{\mathcal{X}} - P_{\mathcal{Z}}\| - \|P_{\mathcal{Y}} - P_{\mathcal{Z}}\|| \leq \|P_{\mathcal{X}} - P_{\mathcal{Y}}\|$.

In this paper, we replace $1D$ subspaces spanned by the vectors x, y and z , with multi-dimensional subspaces \mathcal{X}, \mathcal{Y} and \mathcal{Z} , and we use the concept of principal angles between subspaces. Principal angles are very well studied in the literature, however, some important gaps still remain. Here, we are interested in generalizing inequalities (1.2)-(1.4) above to multi-dimensional subspaces to include all principal angles, using weak majorization.

Let us denote by $\Theta(\mathcal{X}, \mathcal{Y})$ the vector of principal angles in nondecreasing order between subspaces \mathcal{X} and \mathcal{Y} . Let $\dim \mathcal{X} = \dim \mathcal{Y}$, and let another subspace \mathcal{Z} be given. We prove that $|\cos^2 \Theta(\mathcal{X}, \mathcal{Z}) - \cos^2 \Theta(\mathcal{Y}, \mathcal{Z})| \prec_w \sin \Theta(\mathcal{X}, \mathcal{Y})$, and give similar

results for differences of cosines, i.e. $|\cos \Theta(\mathcal{X}, \mathcal{Z}) - \cos \Theta(\mathcal{Y}, \mathcal{Z})| \prec_w \sin \Theta(\mathcal{X}, \mathcal{Y})$, and of sines, and of sines squared. This is the first main result of the present paper, see Section 3. The proof of weak majorization for sines is a direct generalization of the 1D proof above. Our proofs of weak majorization for cosines and sines or cosines squared do not have such simple 1D analogs.

Our second main result, see Section 4, concerns proximity of the Ritz values with a change of the trial subspace. We attack the problem by first discovering a simple, but deep, connection between the principal angles and the Rayleigh–Ritz method.

We observe that the cosines squared $\cos^2 \Theta(\mathcal{X}, \mathcal{Z})$ of principal angles between subspaces \mathcal{X} and \mathcal{Z} can be interpreted as a vector of Ritz values, where the Rayleigh–Ritz method is applied to the orthogonal projector $P_{\mathcal{Z}}$ onto \mathcal{Z} using \mathcal{X} as a trial subspace. Let us illustrate this connection for one–dimensional $\mathcal{X} = \text{span}\{x\}$ and $\mathcal{Z} = \text{span}\{z\}$, where it becomes trivial:

$$\cos^2(\theta(x, z)) = \frac{(x, P_{\mathcal{Z}}x)}{(x, x)}.$$

The ratio on the right is the Rayleigh quotient for $P_{\mathcal{Z}}$ — the one dimensional analog of the Ritz value. In this notation, estimate (1.4) turns into

$$(1.5) \quad \left| \frac{(x, P_{\mathcal{Z}}x)}{(x, x)} - \frac{(y, P_{\mathcal{Z}}y)}{(y, y)} \right| \leq \sin(\theta(x, y)),$$

which clearly now is a particular case of a general estimate of proximity of the Rayleigh quotient, cf. Knyazev and Argentati [16],

$$(1.6) \quad \left| \frac{(x, Ax)}{(x, x)} - \frac{(y, Ay)}{(y, y)} \right| \leq (\lambda_{\max} - \lambda_{\min}) \sin(\theta(x, y)),$$

where A is a Hermitian operator and $\lambda_{\max} - \lambda_{\min}$ is the spread of its spectrum.

We show that the multi–dimensional analog of (1.5) can be interpreted as a bound on the proximity of the Ritz values with the change of the trial subspace, in a particular case where the Rayleigh–Ritz method is applied to an orthogonal projector. We then extend it to prove a general result for Ritz values for an arbitrary Hermitian operator A , not necessarily a projector: let $\Lambda(P_{\mathcal{X}}A|_{\mathcal{X}})$ be the vector of Ritz values in nonincreasing order for the operator A on a trial subspace \mathcal{X} , which is perturbed to give another trial subspace \mathcal{Y} , then $|\Lambda(P_{\mathcal{X}}A|_{\mathcal{X}}) - \Lambda(P_{\mathcal{Y}}A|_{\mathcal{Y}})| \prec_w (\lambda_{\max} - \lambda_{\min}) \sin \Theta(\mathcal{X}, \mathcal{Y})$, which is a multi–dimensional analog of (1.6). Our present proof is based on a classical but rarely used idea of extending a Hermitian operator in \mathcal{H} to an orthogonal projector in the “double” space \mathcal{H}^2 preserving its Ritz values.

An application of our Ritz values weak majorization result for Laplacian graph spectra comparison is suggested in Section 5, based on the possibility to interpret eigenvalues of the edge Laplacian of a given graph as Ritz values of the edge Laplacian of the complete graph. We prove that $\sum_k |\lambda_k^1 - \lambda_k^2| \leq nl$, where λ_k^1 and λ_k^2 are all ordered elements of the Laplacian spectra of two graphs with the same n vertices and with the number of differences between the edges equal to l .

The rest of the paper is organized as follows. In Section 2, we provide some background, definitions and several statements concerning weak majorization, principal angles between subspaces, and extensions of Hermitian operators to projectors. In Section 3, we prove in Theorems 3.2 and 3.3 that the absolute value of the change in (the squares of) the sines and cosines is weakly majorized by the sines of the angles

between the original and perturbed subspaces. In Section 4, we prove in Theorem 4.3 that a change in the Ritz values in the Rayleigh-Ritz method with respect to the change in the trial subspaces is weakly majorized by the sines of the principal angles between the original and perturbed trial subspaces times a constant. In Section 5 we apply our Ritz values weak majorization result to Laplacian graphs spectra comparison.

This paper is related to several different subjects: majorization, principal angles, Rayleigh-Ritz method, and Laplacian graph spectra. In most cases, whenever possible, we cite books rather than the original works in order to keep our already quite long list of references within the reasonable size.

The results of the paper were presented at the 12th ILAS Conference in Canada in June 2005 at the mini-symposium ‘‘Canonical Angles Between Subspaces: Theory and Applications.’’

2. Definitions and Preliminaries. In this section we introduce some definitions, basic concepts and mostly known results for later use.

2.1. Weak Majorization. Majorization is a well known, e.g., Hardy et al. [11], Marshall and Olkin [21], important mathematical concept with numerous applications.

For real vector $x = [x_1, \dots, x_n]$ let x^\downarrow be the vector obtained by rearranging the entries of x in the algebraically non-increasing order, $x_1^\downarrow \geq \dots \geq x_n^\downarrow$. We denote $[|x_1|, \dots, |x_n|]$ by $|x|$. We say that vector y weakly majorizes vector x and we use the notation $[x_1, \dots, x_n] \prec_w [y_1, \dots, y_n]$ or $x \prec_w y$ if $\sum_{i=1}^k x_i^\downarrow \leq \sum_{i=1}^k y_i^\downarrow$, $k = 1, \dots, n$. Two vectors of different lengths may be compared weakly by simply appending zeroes to increase the size of the smaller vector to make the vectors the same length.

Weak majorization is a powerful tool for estimates involving eigenvalues and singular values and is covered in many graduate textbooks, e.g., Bhatia [1] and Horn and Johnson [12]. In the present paper, we use several well known statements below. We follow and refer the reader to Gohberg and Kreĭn [7] and Bhatia [1], where references to the original works and all necessary proofs can be found.

Let $S(A)$ denote the vector of all singular values of $A : \mathcal{H} \rightarrow \mathcal{H}$ in nonincreasing order, i.e. $S(A) = S^\downarrow(A)$, while individual singular values of A numerated in the nonincreasing order are denoted by $s_i(A)$. For Hermitian A let $\Lambda(A)$ denote the vector of all eigenvalues of A in nonincreasing order, i.e. $\Lambda(A) = \Lambda^\downarrow(A)$, while individual eigenvalues of A numerated in the nonincreasing order are denoted by $\lambda_i(A)$.

The starting point for weak majorization results we use in this paper is

THEOREM 2.1. $\Lambda(A + B) \prec_w \Lambda(A) + \Lambda(B)$ for Hermitian A and B ,

which follows easily from the Ky Fan’s trace maximum principle and the fact that the maximum of a sum is bounded from above by the sum of the maxima. A more delicate and stronger result is the following Lidskii theorem, which can be proved using the Wielandt maximum principle,

THEOREM 2.2. For Hermitian A and B and a set of indices $1 \leq i_1 < \dots < i_k \leq n = \dim \mathcal{H}$, we have $\sum_{j=1}^k \lambda_{i_j}(A + B) \leq \sum_{j=1}^k \lambda_{i_j}(A) + \sum_{i=1}^k \lambda_i(B)$, $k = 1, \dots, n$.

Theorem 2.2 (but not 2.1) directly leads to

COROLLARY 2.3. $|\Lambda(A) - \Lambda(B)| \prec_w S(A - B)$ for Hermitian A and B .

For general matrices A and B , it follows from Theorems 2.1 and 2.2 (since the top half of the spectrum of the Hermitian 2-by-2 block operator $\begin{bmatrix} 0 & A \\ A^* & 0 \end{bmatrix}$ is nothing but $S(A)$) that

COROLLARY 2.4. $S(A \pm B) \prec_w S(A) + S(B)$

and

COROLLARY 2.5. $|S(A) - S(B)| \prec_w S(A - B)$.

We finally need the so called ‘‘pinching’’ inequality,

THEOREM 2.6. [e.g. Bhatia [1], p. 97] *If P is an orthogonal projector then $S(PAP \pm (I - P)A(I - P)) \prec_w S(A)$.*

Proof. Indeed, $A = PAP + (I - P)A(I - P) + PA(I - P) + (I - P)AP$ so let $B = PAP + (I - P)A(I - P) - PA(I - P) - (I - P)AP$ then $(2P - I)A(2P - I) = B$, where $2P - I$ is unitary Hermitian, so A^*A and B^*B are similar and $S(A) = S(B)$. Evidently, $PAP + (I - P)A(I - P) = (A + B)/2$ so the pinching result with the plus follows from Corollary 2.4. The pinching result with the minus is equivalent to the pinching result with the plus since the sign does not change the singular values on the left-hand side. \square

2.2. Principal Angles Between Subspaces. Let $P_{\mathcal{X}}$ and $P_{\mathcal{Y}}$ be orthogonal projectors onto the subspaces \mathcal{X} and \mathcal{Y} , respectively, of the space \mathcal{H} . We define the set of cosines of principal angles between subspaces \mathcal{X} and \mathcal{Y} by

$$(2.1) \quad \cos \Theta(\mathcal{X}, \mathcal{Y}) = [s_1(P_{\mathcal{X}}P_{\mathcal{Y}}), \dots, s_m(P_{\mathcal{X}}P_{\mathcal{Y}})], \quad m = \min \{\dim \mathcal{X}; \dim \mathcal{Y}\}.$$

Our definition is evidently symmetric: $\Theta(\mathcal{X}, \mathcal{Y}) = \Theta(\mathcal{Y}, \mathcal{X})$. By definition, the cosines are arranged in the nonincreasing order, i.e. $\cos(\Theta(\mathcal{X}, \mathcal{Y})) = (\cos(\Theta(\mathcal{X}, \mathcal{Y})))^\downarrow$, while the angles $\theta_i(\mathcal{X}, \mathcal{Y}) \in [0, \pi/2]$, $i = 1, \dots, m$ and their sines are in nondecreasing order.

We need several simple but important statements about the angles that for completeness we prove here using ideas from Halmos [10]. Alternatively, they can be checked, e.g., using the CS decomposition Bhatia [1], Stewart and Sun [32], Stewart [33]. We refer the reader to the books referenced above for the history of principal angles and references to the original publications on the principal angles and the CS decomposition.

THEOREM 2.7. *When one of the two subspaces is replaced with its orthogonal complement, the corresponding pairs of angles sum up to $\pi/2$, specifically:*

$$(2.2) \quad \left[\frac{\pi}{2}, \dots, \frac{\pi}{2}, (\Theta(\mathcal{X}, \mathcal{Y}))^\downarrow \right] = \left[\frac{\pi}{2} - \Theta(\mathcal{X}, \mathcal{Y}^\perp), 0, \dots, 0 \right],$$

where there are $\max(\dim \mathcal{X} - \dim \mathcal{Y}, 0)$ values $\pi/2$ on the left, and possibly extra zeros on the right to match the sizes.

The angles between subspaces and between their orthogonal complements are essentially the same,

$$(2.3) \quad [(\Theta(\mathcal{X}, \mathcal{Y}))^\downarrow, 0, \dots, 0] = [(\Theta(\mathcal{X}^\perp, \mathcal{Y}^\perp))^\downarrow, 0, \dots, 0],$$

where extra 0s at the end may need to be added on either side to match the sizes.

Proof. Let $\mathfrak{M}_{00} = \mathcal{X} \cap \mathcal{Y}$, $\mathfrak{M}_{01} = \mathcal{X} \cap \mathcal{Y}^\perp$, $\mathfrak{M}_{10} = \mathcal{X}^\perp \cap \mathcal{Y}$, $\mathfrak{M}_{11} = \mathcal{X}^\perp \cap \mathcal{Y}^\perp$, as suggested in Halmos [10]. Each of the subspaces is invariant with respect to orthoprojectors $P_{\mathcal{X}}$ and $P_{\mathcal{Y}}$ and their products, and so each of the subspaces contributes independently to the set of singular values of $P_{\mathcal{X}}P_{\mathcal{Y}}$ in (2.1). Specifically, there are $\dim \mathfrak{M}_{00}$ ones, $\dim \mathfrak{M}_0$ singular values in the interval $(0, 1)$ equal to $\cos \Theta(\mathfrak{M}_0, \mathcal{Y})$, where $\mathfrak{M}_0 = \mathcal{X} \cap (\mathfrak{M}_{00} \oplus \mathfrak{M}_{01})^\perp$, and all other singular values are zeros; thus,

$$(2.4) \quad \Theta(\mathcal{X}, \mathcal{Y})^\downarrow = \left[\frac{\pi}{2}, \dots, \frac{\pi}{2}, (\Theta(\mathfrak{M}_0, \mathcal{Y}))^\downarrow, 0, \dots, 0 \right],$$

where there are $\min\{\dim(\mathfrak{M}_{01}); \dim(\mathfrak{M}_{10})\}$ values $\pi/2$ and $\dim(\mathfrak{M}_{00})$ zeros.

The subspace \mathfrak{M}_0 does not change if we substitute \mathcal{Y}^\perp for \mathcal{Y} in (2.4), so we have

$$\Theta(\mathcal{X}, \mathcal{Y}^\perp)^\downarrow = \left[\frac{\pi}{2}, \dots, \frac{\pi}{2}, (\Theta(\mathfrak{M}_0, \mathcal{Y}^\perp))^\downarrow, 0, \dots, 0 \right],$$

where there are $\min\{\dim(\mathfrak{M}_{00}); \dim(\mathfrak{M}_{11})\}$ values $\pi/2$ and $\dim(\mathfrak{M}_{01})$ zeros. Since λ is an eigenvalue of $(P_{\mathcal{X}}P_{\mathcal{Y}})|_{\mathfrak{M}_0}$ if and only if $1 - \lambda$ is an eigenvalue of $(P_{\mathcal{X}}P_{\mathcal{Y}^\perp})|_{\mathfrak{M}_0}$, we have $\frac{\pi}{2} - \Theta(\mathfrak{M}_0, \mathcal{Y}^\perp) = (\Theta(\mathfrak{M}_0, \mathcal{Y}))^\downarrow$, and the latter equality turns into

$$(2.5) \quad \frac{\pi}{2} - \Theta(\mathcal{X}, \mathcal{Y}^\perp) = \left[\frac{\pi}{2}, \dots, \frac{\pi}{2}, (\Theta(\mathfrak{M}_0, \mathcal{Y}))^\downarrow, 0, \dots, 0 \right],$$

where there are $\dim(\mathfrak{M}_{01})$ values $\pi/2$, and $\min\{\dim(\mathfrak{M}_{00}); \dim(\mathfrak{M}_{11})\}$ zeros. To obtain (2.2), we make (2.4) and (2.5) equal by adding $\max\{\dim\mathfrak{M}_{01} - \dim\mathfrak{M}_{10}; 0\}$ values $\pi/2$ to (2.4) and $\max\{\dim\mathfrak{M}_{00} - \dim\mathfrak{M}_{11}; 0\}$ zeros to (2.5), and noting that $\dim\mathfrak{M}_{01} - \dim\mathfrak{M}_{10} = \dim X - \dim Y$.

To prove (2.3) we simply substitute \mathcal{X}^\perp for \mathcal{X} and \mathcal{Y}^\perp for \mathcal{Y} in (2.2), add some zeroes on the right and then remove equal numbers of values $\pi/2$ on the left. \square

We also use the following simple, but crucial, statement in Section 4.

LEMMA 2.8. $\Lambda(P_{\mathcal{X}}P_{\mathcal{Y}}|_{\mathcal{X}}) = [\cos^2 \Theta(\mathcal{X}, \mathcal{Y}), 0, \dots, 0]$, with $\max\{\dim\mathcal{X} - \dim\mathcal{Y}, 0\}$ extra 0s.

Proof. The operator $P_{\mathcal{X}}P_{\mathcal{Y}}|_{\mathcal{X}}$ is Hermitian nonnegative, and its spectrum can be represented using the definition of angles (2.1). The number of extra 0s is exactly the difference between the number $\dim\mathcal{X}$ of Ritz values and the number $\min\{\dim\mathcal{X}, \dim\mathcal{Z}\}$ of principal angles. \square

Finally, we need the following characterization of singular values of the difference of projectors:

THEOREM 2.9.

$$[S(P_{\mathcal{X}} - P_{\mathcal{Y}}), 0, \dots, 0] = [1, \dots, 1, (\sin \Theta(\mathcal{X}, \mathcal{Y}), \sin \Theta(\mathcal{X}, \mathcal{Y}))^\downarrow, 0, \dots, 0],$$

where there are $|\dim\mathcal{X} - \dim\mathcal{Y}|$ extra 1s upfront, the set $\sin \Theta(\mathcal{X}, \mathcal{Y})$ is repeated twice and ordered, and extra 0s at the end may need to be added on either side to match the sizes.

Proof. The subspaces \mathcal{X} and \mathcal{X}^\perp are invariant complementary subspaces of the Hermitian operator $(P_{\mathcal{X}} - P_{\mathcal{Y}})^2 = P_{\mathcal{X}}P_{\mathcal{Y}^\perp} + P_{\mathcal{Y}}P_{\mathcal{X}^\perp} = P_{\mathcal{X}^\perp}P_{\mathcal{Y}} + P_{\mathcal{Y}^\perp}P_{\mathcal{X}}$, so

$$\Lambda((P_{\mathcal{X}} - P_{\mathcal{Y}})^2) = [\Lambda((P_{\mathcal{X}}P_{\mathcal{Y}^\perp})|_{\mathcal{X}}), \Lambda((P_{\mathcal{X}^\perp}P_{\mathcal{Y}})|_{\mathcal{X}^\perp})]^\downarrow.$$

Using Lemma 2.8 and statement (2.2) of Theorem 2.7,

$$\begin{aligned} [\Lambda((P_{\mathcal{X}}P_{\mathcal{Y}^\perp})|_{\mathcal{X}}), 0, \dots, 0] &= [\cos^2 \Theta(\mathcal{X}, \mathcal{Y}^\perp), 0, \dots, 0] \\ &= [1, \dots, 1, (\sin^2 \Theta(\mathcal{X}, \mathcal{Y}))^\downarrow, 0, \dots, 0], \end{aligned}$$

where there are $\max(\dim\mathcal{X} - \dim\mathcal{Y}, 0)$ leading 1s and possibly extra zeros to match the sizes, and

$$\begin{aligned} [\Lambda((P_{\mathcal{X}^\perp}P_{\mathcal{Y}})|_{\mathcal{X}^\perp}), 0, \dots, 0] &= [\cos^2 \Theta(\mathcal{X}^\perp, \mathcal{Y}), 0, \dots, 0] \\ &= [1, \dots, 1, (\sin^2 \Theta(\mathcal{X}, \mathcal{Y}))^\downarrow, 0, \dots, 0], \end{aligned}$$

where there are $\max(\dim\mathcal{Y} - \dim\mathcal{X}, 0)$ leading 1s and possibly extra zeros to match the sizes. Combining these two relations and taking the square root, completes the proof. \square

2.3. Extending Operators to Isometries and Projectors. In this subsection we present a simple and known technique, e.g., Halmos [9] and Riesz and Sz.-Nagy [30], p. 461, for extending a Hermitian operator to a projector. We give an alternative proof based on extending an arbitrary normalized operator B to an isometry \hat{B} (in matrix terms, a matrix with orthonormal columns). Bhatia [1] on p. 11 extends B to a block 2-by-2 unitary operator. Our technique is similar and results in a 1-by-2 isometry operator \hat{B} that coincides with the first column of the 2-by-2 unitary extension.

LEMMA 2.10. *Given an operator $B : \mathcal{H} \rightarrow \mathcal{H}$ with singular values less than or equal to one, there exists a block 1-by-2 isometry operator $\hat{B} : \mathcal{H} \rightarrow \mathcal{H}^2$, such that the upper block of \hat{B} coincides with B .*

Proof. B^*B is Hermitian nonnegative definite, and all its eigenvalues are bounded by one, since all singular values of B are bounded by one. Therefore, $I - B^*B$ is Hermitian and nonnegative definite, and thus possesses a Hermitian nonnegative square root. Let

$$\hat{B} = \begin{bmatrix} B \\ \sqrt{I - B^*B} \end{bmatrix}.$$

By direct calculation, $\hat{B}^*\hat{B} = B^*B + \sqrt{I - B^*B}\sqrt{I - B^*B} = I$, i.e. \hat{B} is an isometry. \square

As a side note, Lemma 2.10 shows that an arbitrary normalized operator B is unitary equivalent to a product of a (partial) isometry \hat{B} and an orthogonal projector in \mathcal{H}^2 (that selects the upper block in \hat{B}). This may serve as a useful canonical decomposition, enhancing the well known polar decomposition — the product of a partial isometry and a Hermitian nonnegative operator.

Now we use Lemma 2.10 to extend, in a similar sense, a shifted and normalized Hermitian operator to an orthogonal projector.

THEOREM 2.11 ([9] and [30], p. 461). *Given a Hermitian operator $A : \mathcal{H} \rightarrow \mathcal{H}$ with eigenvalues enclosed in the segment $[0, 1]$, there exists a block 2-by-2 orthogonal projector $\hat{A} : \mathcal{H}^2 \rightarrow \mathcal{H}^2$, such that its upper left block is equal to A .*

Proof. There exists \sqrt{A} , which is also Hermitian and has its eigenvalues enclosed in $[0, 1]$. Applying Lemma 2.10 to $B = \sqrt{A}$, we construct the isometry \hat{B} and set

$$\hat{A} = \hat{B}\hat{B}^* = \begin{bmatrix} \sqrt{A} \\ \sqrt{I - A} \end{bmatrix} \begin{bmatrix} \sqrt{A} & \sqrt{I - A} \end{bmatrix} = \begin{bmatrix} A & \sqrt{A(I - A)} \\ \sqrt{A(I - A)} & I - A \end{bmatrix}.$$

We see that indeed the upper left block is equal to A . We can use the fact that \hat{B} is an isometry to show that \hat{A} is an orthogonal projector, or that can be checked directly by calculating $\hat{A}^2 = \hat{A}$ and noticing that \hat{A} is evidently Hermitian. \square

Introducing $S = \sqrt{A}$ and $C = \sqrt{I - A}$, we obtain

$$\hat{A} = \begin{bmatrix} S^2 & SC \\ SC & C^2 \end{bmatrix},$$

which is a well known, e.g., Davis [5], Halmos [10], block form of an orthogonal projector that can alternatively be derived using the CS decomposition of unitary operators, e.g., Bhatia [1], Stewart and Sun [32], Stewart [33].

The importance of Theorem 2.11 can be better seen if we reformulate it as

THEOREM 2.12. *Given a Hermitian operator $A : \mathcal{H} \rightarrow \mathcal{H}$ with eigenvalues enclosed in a segment $[0, 1]$, there exist subspaces \mathcal{X} and \mathcal{Y} in \mathcal{H}^2 such that A is unitarily*

equivalent to $(P_{\mathcal{X}}P_{\mathcal{Y}})|_{\mathcal{X}}$, where $P_{\mathcal{X}}$ and $P_{\mathcal{Y}}$ are the corresponding orthogonal projectors in \mathcal{H}^2 and $|_{\mathcal{X}}$ denotes a restriction to the invariant subspace \mathcal{X} .

Proof. We use Theorem 2.11 and take $P_{\mathcal{Y}} = \hat{A}$ and $P_{\mathcal{X}} = \begin{bmatrix} I & 0 \\ 0 & 0 \end{bmatrix}$. \square

Using the definition of principal angles between the subspaces, Theorem 2.12 implies that *the spectrum of an arbitrary properly shifted and scaled Hermitian operator is nothing but a set of cosines squared of principal angles between some pair of subspaces*. This idea appears to be very powerful. It allows us, in Section 4, to obtain a novel result on proximity of Ritz values by reducing the investigation of the Rayleigh-Ritz method to the analysis of the principal angles between subspaces that we provide in the next section.

3. Majorization for Angles. In this section we prove the main results of the present paper involving sines and cosines and their squares of principal angles, but we start with a known statement that involves the principal angles themselves:

THEOREM 3.1 (Qiu et al. [29], Theorem 2, p. 8). *Let \mathcal{X} , \mathcal{Y} and \mathcal{Z} be subspaces of the same dimension. Then*

$$(3.1) \quad |\Theta(\mathcal{X}, \mathcal{Z}) - \Theta(\mathcal{Y}, \mathcal{Z})| \prec_w \Theta(\mathcal{X}, \mathcal{Y}).$$

Theorem 3.1 deals with the principal angles themselves, and the obvious question is: are there similar results for a function of these angles, in particular for sines and cosines and their squares? For one dimensional subspaces, estimate (3.1) turns into (1.1) that, as discussed in the Introduction, implies the estimate (1.2) for the sine. According to an anonymous referee, it appears to be known to some specialists that the same inference can be made for tuples of angles, but there is no good reference for this at present. Below we give easy direct proofs in a unified way for the sines and cosines and their squares.

We start with the simplest estimates for sine and cosine, which are straightforward generalizations of the 1D sine (1.2) and cosine (1.3) inequalities from the Introduction.

THEOREM 3.2. *Let $\dim \mathcal{X} = \dim \mathcal{Y}$ then*

$$(3.2) \quad |\sin \Theta(\mathcal{X}, \mathcal{Z}) - \sin \Theta(\mathcal{Y}, \mathcal{Z})| \prec_w \sin \Theta(\mathcal{X}, \mathcal{Y}),$$

$$(3.3) \quad |\cos \Theta(\mathcal{X}, \mathcal{Z}) - \cos \Theta(\mathcal{Y}, \mathcal{Z})| \prec_w \sin \Theta(\mathcal{X}, \mathcal{Y}).$$

Proof. Let $P_{\mathcal{X}}$, $P_{\mathcal{Y}}$ and $P_{\mathcal{Z}}$ be the corresponding orthogonal projectors onto the subspaces \mathcal{X} , \mathcal{Y} and \mathcal{Z} , respectively. We first prove the sine estimate (3.2), using the idea of Qiu and Zhang [28]. Starting with $(P_{\mathcal{X}} - P_{\mathcal{Z}}) - (P_{\mathcal{Y}} - P_{\mathcal{Z}}) = P_{\mathcal{X}} - P_{\mathcal{Y}}$, as in the proof of the 1D sine estimate (1.2), we use Corollary 2.5 to obtain

$$|S(P_{\mathcal{X}} - P_{\mathcal{Z}}) - S(P_{\mathcal{Y}} - P_{\mathcal{Z}})| \prec_w S(P_{\mathcal{X}} - P_{\mathcal{Y}}).$$

The singular values of the difference of two orthoprojectors are described by Theorem 2.9. Since $\dim \mathcal{X} = \dim \mathcal{Y}$ we have the same number of extra 1s upfront in $S(P_{\mathcal{X}} - P_{\mathcal{Z}})$ and in $S(P_{\mathcal{Y}} - P_{\mathcal{Z}})$ so that the extra 1's are canceled and the set of nonzero entries of $|S(P_{\mathcal{X}} - P_{\mathcal{Z}}) - S(P_{\mathcal{Y}} - P_{\mathcal{Z}})|$ consists of nonzero entries of $|\sin \Theta(\mathcal{X}, \mathcal{Z}) - \sin \Theta(\mathcal{Y}, \mathcal{Z})|$ repeated twice. The nonzero entries of $S(P_{\mathcal{X}} - P_{\mathcal{Y}})$ are by Theorem 2.9 the nonzero entries of $\sin \Theta(\mathcal{X}, \mathcal{Y})$ also repeated twice, thus we come to (3.2).

The cosine estimate (3.3) follows directly from the sine estimate (3.2) with \mathcal{Z}^\perp instead of \mathcal{Z} because of (2.2) utilizing the assumption $\dim\mathcal{X} = \dim\mathcal{Y}$. \square

In our earlier paper, Knyazev and Argentati [15], in Lemmas 5.1 and 5.2 we obtain a particular case of Theorem 3.2, only for the largest change in the sine and the cosine, but with improved constants. We are not presently able, however, to modify the proofs of [15] using weak majorization, in order to improve the estimates of Theorem 3.2 by introducing the same constants as in [15].

Our last, but not least, result in this series is the weak majorization estimate for the sines or cosines squared.

THEOREM 3.3. *Let $\dim\mathcal{X} = \dim\mathcal{Y}$, then*

$$|\cos^2 \Theta(\mathcal{X}, \mathcal{Z}) - \cos^2 \Theta(\mathcal{Y}, \mathcal{Z})| = |\sin^2 \Theta(\mathcal{X}, \mathcal{Z}) - \sin^2 \Theta(\mathcal{Y}, \mathcal{Z})| \prec_w \sin \Theta(\mathcal{X}, \mathcal{Y}).$$

Proof. The equality is evident. To prove the majorization result for the sines squared, we start with the identity

$$(P_{\mathcal{X}} - P_{\mathcal{Z}})^2 - (P_{\mathcal{Y}} - P_{\mathcal{Z}})^2 = P_{\mathcal{Z}^\perp}(P_{\mathcal{X}} - P_{\mathcal{Y}})P_{\mathcal{Z}^\perp} - P_{\mathcal{Z}}(P_{\mathcal{X}} - P_{\mathcal{Y}})P_{\mathcal{Z}}.$$

Applying Corollary 2.5 we obtain

$$|S((P_{\mathcal{X}} - P_{\mathcal{Z}})^2) - S((P_{\mathcal{Y}} - P_{\mathcal{Z}})^2)| \prec_w S(P_{\mathcal{Z}^\perp}(P_{\mathcal{X}} - P_{\mathcal{Y}})P_{\mathcal{Z}^\perp} - P_{\mathcal{Z}}(P_{\mathcal{X}} - P_{\mathcal{Y}})P_{\mathcal{Z}}).$$

For the left-hand side we use Theorem 2.9 similarly to that in the proof of Theorem 3.2, except that we are now working with the squares. For the right-hand side, the pinching Theorem 2.6 gives

$$S(P_{\mathcal{Z}^\perp}(P_{\mathcal{X}} - P_{\mathcal{Y}})P_{\mathcal{Z}^\perp} - P_{\mathcal{Z}}(P_{\mathcal{X}} - P_{\mathcal{Y}})P_{\mathcal{Z}}) \prec_w S(P_{\mathcal{X}} - P_{\mathcal{Y}})$$

and we use Theorem 2.9 again to characterize $S(P_{\mathcal{X}} - P_{\mathcal{Y}})$ the same way as in the proof of Theorem 3.2. \square

4. Changes in the Trial Subspace in the Rayleigh–Ritz Method. In this section, we explore a simple, but deep, connection between the principal angles and the Rayleigh–Ritz method that we discuss in the Introduction. We demonstrate that the analysis of the influence of changes in a trial subspace in the Rayleigh–Ritz method is a natural extension of the theory concerning principal angles and the proximity of two subspaces developed in the previous section.

We first give a brief definition of Ritz values. Let $A : \mathcal{H} \rightarrow \mathcal{H}$ be a Hermitian operator and let \mathcal{X} be a (so-called “trial”) subspace of \mathcal{H} . We define an operator $P_{\mathcal{X}}A|_{\mathcal{X}}$ on \mathcal{X} , where $P_{\mathcal{X}}$ is the orthogonal projector onto \mathcal{X} and $P_{\mathcal{X}}A|_{\mathcal{X}}$ denotes the restriction of operator $P_{\mathcal{X}}A$ to its invariant subspace \mathcal{X} , as discussed, e.g., in Parlett [27]. The eigenvalues $\Lambda(P_{\mathcal{X}}A|_{\mathcal{X}})$ are called Ritz values of operator A with respect to the trial subspace \mathcal{X} .

Before we formulate and prove the main result of the paper on the proximity of the Ritz values in terms of the proximity of the trial subspaces, we connect the Ritz values with extension Theorem 2.11 on the one hand and with the cosine squared of principal angles on the other hand. We have shown in Theorem 2.11 that a Hermitian nonnegative definite contraction operator can be extended to an orthogonal projector in a larger space. The extension has an extra nice property: it preserves the Ritz values.

COROLLARY 4.1. *Under the assumptions of Theorem 2.11, the Ritz values of operator $A : \mathcal{H} \rightarrow \mathcal{H}$ in the trial subspace $\mathcal{X} \subset H$ are the same as the Ritz values of operator $\hat{A} : \mathcal{H}^2 \rightarrow \mathcal{H}^2$ in the trial subspace*

$$\hat{\mathcal{X}} = \begin{bmatrix} \mathcal{X} \\ 0 \end{bmatrix} \subset \hat{\mathcal{H}} = \begin{bmatrix} \mathcal{H} \\ 0 \end{bmatrix} \subset \mathcal{H}^2.$$

Proof. Let $P_{\hat{\mathcal{H}}} : \mathcal{H}^2 \rightarrow \mathcal{H}^2$ be an orthogonal projector on the subspace $\hat{\mathcal{H}}$ and $P_{\hat{\mathcal{X}}} : \mathcal{H}^2 \rightarrow \mathcal{H}^2$ be an orthogonal projector on the subspace $\hat{\mathcal{X}}$. We use the equality sign to denote the trivial isomorphism between \mathcal{H} and $\hat{\mathcal{H}}$, i.e. we simply write $\mathcal{H} = \hat{\mathcal{H}}$ and $\mathcal{X} = \hat{\mathcal{X}}$.

In this notation, we first observe that $A = P_{\hat{\mathcal{H}}}\hat{A}|_{\hat{\mathcal{H}}}$, i.e. the operator A itself can be viewed as a result of the Rayleigh–Ritz method applied to the operator \hat{A} in the trial subspace $\hat{\mathcal{H}}$. Second, we use the fact that a recursive application of the Rayleigh–Ritz method on a system of enclosed trial subspaces is equivalent to a direct single application of the Rayleigh–Ritz method to the smallest trial subspace, indeed, in our notation, $P_{\hat{\mathcal{H}}}P_{\hat{\mathcal{X}}} = P_{\hat{\mathcal{X}}}P_{\hat{\mathcal{H}}} = P_{\hat{\mathcal{X}}}$, since $\hat{\mathcal{X}} \subset \hat{\mathcal{H}}$, thus

$$P_{\mathcal{X}}A|_{\mathcal{X}} = \left(P_{\hat{\mathcal{X}}}P_{\hat{\mathcal{H}}}\hat{A}|_{\hat{\mathcal{H}}} \right) \Big|_{\hat{\mathcal{X}}} = P_{\hat{\mathcal{X}}}\hat{A}|_{\hat{\mathcal{X}}}.$$

□

Next we note that Lemma 2.8, states that the Rayleigh–Ritz method applied to an orthogonal projector produces Ritz values, which are essentially the cosines squared of the principal angles between the range of the projector and the trial subspace. For the reader’s convenience we reformulate Lemma 2.8 here:

LEMMA 4.2. *Let the Rayleigh–Ritz method be applied to $A = P_{\mathcal{Z}}$, where $P_{\mathcal{Z}}$ is an orthogonal projector onto a subspace \mathcal{Z} , and let \mathcal{X} be the trial subspace in the Rayleigh–Ritz method. Then the set of the Ritz values is*

$$\Lambda(P_{\mathcal{X}}P_{\mathcal{Z}}|_{\mathcal{X}}) = [\cos^2 \Theta(\mathcal{X}, \mathcal{Z}), 0, \dots, 0],$$

where there are $\max\{\dim \mathcal{X} - \dim \mathcal{Z}, 0\}$ extra 0s.

Now we are ready to direct our attention to the main topic of this section: the influence of changes in a trial subspace in the Rayleigh–Ritz method on the Ritz values.

THEOREM 4.3. *Let $A : \mathcal{H} \rightarrow \mathcal{H}$ be Hermitian and let \mathcal{X} and \mathcal{Y} both be subspaces of \mathcal{H} and $\dim \mathcal{X} = \dim \mathcal{Y}$. Then*

$$(4.1) \quad |\Lambda(P_{\mathcal{X}}A|_{\mathcal{X}}) - \Lambda(P_{\mathcal{Y}}A|_{\mathcal{Y}})| \prec_w (\lambda_{\max} - \lambda_{\min}) \sin \Theta(\mathcal{X}, \mathcal{Y}),$$

where λ_{\min} and λ_{\max} are the smallest and largest eigenvalues of A , respectively.

Proof. We prove Theorem 4.3 in two steps. First we show that we can assume that A is a nonnegative definite contraction without losing generality. Second, under these assumptions, we extend the operator A to an orthogonal projector by Theorem 2.11 and use the facts that such an extension does not affect the Ritz values by Corollary 4.1 and that the Ritz values of an orthogonal projector can be interpreted as the cosines squared of principal angles between subspaces by Lemma 4.2, thus reducing the problem to the already established result on weak majorization of the cosine squared Theorem 3.3.

We observe that the statement of the theorem is invariant with respect to a shift and a scaling, indeed, for real α and β if the operator A is replaced with $\beta(A - \alpha)$ and

λ_{\min} and λ_{\max} are correspondingly updated, both sides of (4.1) are just multiplied by β and (4.1) is thus invariant with respect to α and β . Choosing $\alpha = \lambda_{\min}$ and $\beta = 1/(\lambda_{\max} - \lambda_{\min})$, the transformed operator $(A - \lambda_{\min})/(\lambda_{\max} - \lambda_{\min})$ is Hermitian with its eigenvalues enclosed in a segment $[0, 1]$, thus the statement (4.1) of the theorem can be equivalently rewritten as

$$(4.2) \quad |\Lambda(P_{\mathcal{X}}A|_{\mathcal{X}}) - \Lambda(P_{\mathcal{Y}}A|_{\mathcal{Y}})| \prec_w \sin \Theta(\mathcal{X}, \mathcal{Y}),$$

where we from now on assume that A is a nonnegative definite contraction without losing the generality.

The second step of the proof is to recast the problem into an equivalent problem for an orthogonal projector with the same Ritz values and principal angles. By Theorem 2.11 we can extend the nonnegative definite contraction A to an orthogonal projector $P_{\hat{\mathcal{Z}}}$, where $\hat{\mathcal{Z}}$ is a subspace of \mathcal{H}^2 . $P_{\hat{\mathcal{Z}}}$ has by Corollary 4.1 the same Ritz values with respect to trial subspaces

$$\hat{\mathcal{X}} = \begin{bmatrix} \mathcal{X} \\ 0 \end{bmatrix} \subset \hat{\mathcal{H}} = \begin{bmatrix} \mathcal{H} \\ 0 \end{bmatrix} \subset \mathcal{H}^2 \text{ and } \hat{\mathcal{Y}} = \begin{bmatrix} \mathcal{Y} \\ 0 \end{bmatrix} \subset \hat{\mathcal{H}} = \begin{bmatrix} \mathcal{H} \\ 0 \end{bmatrix} \subset \mathcal{H}^2$$

as A has with respect to the trial subspaces \mathcal{X} and \mathcal{Y} . By Lemma 4.2, these Ritz values are equal to the cosines squared of the principal angles between $\hat{\mathcal{Z}}$ and the trial subspace $\hat{\mathcal{X}}$ or $\hat{\mathcal{Y}}$ possibly with the same number of 0s being added. Moreover, the principal angles between $\hat{\mathcal{X}}$ and $\hat{\mathcal{Y}}$ in \mathcal{H}^2 are clearly the same as those between \mathcal{X} and \mathcal{Y} in \mathcal{H} and $\dim \hat{\mathcal{X}} = \dim \mathcal{X} = \dim \mathcal{Y} = \dim \hat{\mathcal{Y}}$. Thus, (4.2) can be equivalently reformulated as

$$(4.3) \quad |\cos^2 \Theta(\hat{\mathcal{X}}, \hat{\mathcal{Z}}) - \cos^2 \Theta(\hat{\mathcal{Y}}, \hat{\mathcal{Z}})| \prec_w \sin \Theta(\hat{\mathcal{X}}, \hat{\mathcal{Y}}).$$

Finally, we notice that (4.3) is already proved in Theorem 3.3. \square

REMARK 4.1. *Theorem 10 in Knyazev and Argentati [16] is a matrix version of Theorem 4.3, but with an extra factor $\sqrt{2}$ on the right-hand side. A conjecture in Knyazev and Argentati [16] states that this factor can be eliminated as we now prove in Theorem 4.3. The proof of Theorem 10 in Knyazev and Argentati [16] applies Corollary 2.3 to the matrices of $P_{\mathcal{X}}A|_{\mathcal{X}}$ and $P_{\mathcal{Y}}A|_{\mathcal{Y}}$.*

REMARK 4.2. *As in Remark 7 of Knyazev and Argentati [16], the constant $\lambda_{\max} - \lambda_{\min}$ in Theorem 4.3 can be replaced with*

$$\max_{x \in \mathcal{X} + \mathcal{Y}, \|x\|=1} (x, Ax) - \min_{x \in \mathcal{X} + \mathcal{Y}, \|x\|=1} (x, Ax),$$

which for some subspaces \mathcal{X} and \mathcal{Y} can provide a significant improvement.

REMARK 4.3. *The implications of the weak majorization inequality in Theorem 4.3 may not be obvious to every reader. To clarify, let $m = \dim \mathcal{X} = \dim \mathcal{Y}$ and let $\alpha_1 \geq \dots \geq \alpha_m$ be the Ritz values of A with respect to \mathcal{X} and $\beta_1 \geq \dots \geq \beta_m$ be the Ritz values of A with respect to \mathcal{Y} . The weak majorization inequality in Theorem 4.3 directly implies*

$$\sum_{i=1}^k |\alpha_i - \beta_i|^\downarrow \leq (\lambda_{\max} - \lambda_{\min}) \sum_{i=1}^k \sin(\Theta_i(\mathcal{X}, \mathcal{Y}))^\downarrow, \quad k = 1, \dots, m,$$

e.g., for $k = m$ we obtain

$$(4.4) \quad \sum_{i=1}^m |\alpha_i - \beta_i| \leq (\lambda_{\max} - \lambda_{\min}) \sum_{i=1}^m \sin(\Theta_i(\mathcal{X}, \mathcal{Y})),$$

and for $k = 1$ we have

$$(4.5) \quad \max_{j=1,\dots,m} |\alpha_j - \beta_j| \leq (\lambda_{\max} - \lambda_{\min}) \text{gap}(\mathcal{X}, \mathcal{Y}),$$

where the gap $\text{gap}(\mathcal{X}, \mathcal{Y})$ between equidimensional subspaces \mathcal{X} and \mathcal{Y} is the sine of the largest angle between \mathcal{X} and \mathcal{Y} . Inequality (4.5) is proved in Knyazev and Argentati [16].

For real vectors x and y the weak majorization $x \prec_w y$ is equivalent to the inequality $\sum \phi(x) \leq \sum \phi(y)$ for any continuous nondecreasing convex real valued function ϕ , e.g., Marshall and Olkin [21], Statement 4.B.2. Taking, e.g., $\phi(t) = t^p$ with $p \geq 1$, Theorem 4.3 also implies

$$\left(\sum_{i=1}^m |\alpha_i - \beta_i|^p \right)^{\frac{1}{p}} \leq (\lambda_{\max} - \lambda_{\min}) \left(\sum_{i=1}^m \sin(\Theta_i(\mathcal{X}, \mathcal{Y}))^p \right)^{\frac{1}{p}}, \quad 1 \leq p < \infty.$$

We finally note that the results of Theorem 4.3 are not intended for the case where one of the subspaces \mathcal{X} or \mathcal{Y} is invariant with respect to operator A . In such a case, it is natural to expect a much better bound that involves the square of the $\sin \Theta(\mathcal{X}, \mathcal{Y})$. Majorization results of this kind are not apparently known in the literature. Without majorization, estimates just for the largest change in the Ritz values are available, e.g., Knyazev and Argentati [16], Knyazev and Osborn [18].

5. Application of the Majorization Results to Graph Spectra Comparison. In this section, we show that our majorization results can be applied to compare graph spectra. The graph spectra comparison can be used for graphs matching and has applications in data mining, cf. Kosinov and Caelli [20].

The section is divided into three subsections. In Subsection 5.1, we give all necessary definitions and basic facts concerning Laplacian graph spectra. In Subsection 5.2, we connect the Laplacian graph spectrum and Ritz values, by introducing the graph edge Laplacian. Finally, in Subsection 5.3, we prove our main result on the Laplacian graph spectra comparison.

5.1. Incidence Matrices and Graph Laplacians. Here, we give mostly well known relevant definitions, e.g., Chung [3], Cvetković et al. [4], Merris [23, 24, 25], Mohar [26], just slightly tailored for our specific needs.

Let V be a finite ordered set (of vertices), with an individual element (vertex) denoted by $v_i \in V$. Let E_c be a finite ordered set (of all edges), with an individual element (edge) denoted by $e_k \in E_c$ such that every $e_k = [v_i, v_j]$ for all possible $i > j$. E_c can be viewed as the set of all edges of a complete simple graph with vertices V (without self-loops and/or multiple edges). The results of the present paper are invariant with respect to specific ordering of vertices and edges.

Let $w_c : E_c \rightarrow \mathbf{R}$ be a function describing edge weights, i.e. $w_c(e_k) \in \mathbf{R}$. If for some edge e_k the weight is positive, $w_c(e_k) > 0$, we call this edge present, if $w_c(e_k) = 0$ we say that the edge is absent. In this paper we do not allow negative edge weights. For a given weight function w_c , we define $E \subseteq E_c$ such that $e_k \in E$ if $w_c(e_k) \neq 0$ and we define w to be the restriction of w_c on all present edges E , i.e. w is made of all nonzero values of w_c . A pair of sets of vertices V and present edges E with weights w is called a graph (V, E) or a weighted graph (V, E, w) .

The vertex–edge incidence matrix Q_c of a complete graph (V, E_c) is a matrix which has a row for each vertex and a column for each edge, with column-wise entries determined as $q_{ik} = 1$, $q_{jk} = -1$ for every edge $e_k = [v_i, v_j]$, $i > j$ in E_c and with

all other entries of Q_c equal to zero. The vertex–edge incidence matrix Q of a graph (V, E) is determined in the same way, but only for the edges present in E . The vertex–edge incidence matrix can be viewed as a matrix representation of a graph analog of the divergence operator from partial differential equations (PDE).

Extending the analogy with PDE, the matrix $L = QQ^*$ is called the matrix of the graph (vertex) Laplacian. The operator form of the graph Laplacian Δ acting on real valued functions $f(v), v \in V$ is determined by $\Delta f(v_i) = \sum_{j:v_j \sim v_i} [f(v_i) - f(v_j)]$, where the sum runs over the vertices joined with v_i and no boundary conditions are imposed. In the PDE context, this definition corresponds to the negative Laplacian with the natural boundary conditions, cf. McDonald and Meyers [22].

If we want to take into account the weights, we can work with the matrix $Q \text{diag}(w(E))Q^*$, which is an analog of an isotropic diffusion operator, or we can introduce a more general edge matrix W and work with QWQ^* , which corresponds to a general anisotropic diffusion. It is interesting to notice the equality

$$(5.1) \quad Q_c \text{diag}(w_c(E_c))Q_c^* = Q \text{diag}(w(E))Q^*,$$

which shows two alternative equivalent formulas for the graph diffusion operator.

For simplicity of the presentation, we assume in the rest of the paper that the weights w_c take only the values zero and one. Under this assumption, we introduce matrix $P = \text{diag}(w_c(E_c))$ and notice that P is the matrix of an orthogonal projector on a subspace spanned by coordinate vectors with indices corresponding to the indices of edges present in E and that equality (5.1) turns into

$$(5.2) \quad Q_c P Q_c^* = Q Q^*.$$

Let us note that our results can be easily extended to a more general case of arbitrary nonnegative weights, or even to the case of the edge matrix W , assuming that it is nonnegative definite, $W \geq 0$.

Fiedler [6] pioneering work on using the eigenpairs of the graph Laplacian to determine some structural properties of the graph has attracted much attention in the past. Recent advances in large-scale eigenvalue computations using multilevel preconditioning, e.g., Knyazev [14], Knyazev and Neymeyr [17], Koren et al. [19], suggest novel efficient numerical methods to compute the Fiedler vector and may rejuvenate this classical approach, e.g., for graph partitioning. In this paper, we concentrate on the whole set of eigenvalues of L or Δ , which is called the Laplacian graph spectrum.

It is known that the Laplacian graph spectrum does not determine the graph uniquely, i.e. that there exist isospectral graphs, see, e.g., van Dam and Haemers [34] and references there. However, the intuition suggests that a small change in a large graph should not change the Laplacian graph spectrum very much; and attempts have been made to use the similarity of Laplacian graph spectra to judge the similarity of the graphs in applications; for alternative approaches, see Blondel et al. [2]. The goal of this section is to backup this intuition with rigorous estimates for proximity of the Laplacian graph spectra.

5.2. Laplacian graph spectrum and Ritz values. In the previous section, we obtain in Theorem 4.3 the weak majorization result for changes in the Ritz values depending on a change in the trial subspace, which we would like to apply to analyze the graph spectrum. In this subsection, we present an approach that allows us to interpret the Laplacian graph spectrum as a set of Ritz values obtained by the Rayleigh–Ritz method applied to the complete graph.

A graph (V, E) can evidently be obtained from the complete graph (V, E_c) by removing edges, moreover, as we already discussed, we can construct the (V, E) graph Laplacian by either of the terms in equality (5.2). The problem is that such a construction cannot be recast as an application of the Rayleigh–Ritz method, since the multiplication by the projector P takes place inside of the product, not outside, as required by the Rayleigh–Ritz method.

To resolve this difficulty, we use the matrix $K = Q^*Q$ that is sometimes called the matrix of the graph *edge* Laplacian, instead of the matrix of the graph *vertex* Laplacian $L = QQ^*$. Evidently, apart from zero, both matrices K and L share the same eigenvalues. The advantage of the edge Laplacian K is that it can be obtained from the edge Laplacian of the complete graph $Q_c^*Q_c$ by the Rayleigh–Ritz method:

THEOREM 5.1. *Let us remind the reader that the weights w_c take only the values zero and one and that $P = \text{diag}(w_c(E_c))$ is a matrix of an orthogonal projector on a subspace spanned by coordinate vectors with indices corresponding to the indices of edges present in E . Then $Q^*Q = (PQ_c^*Q_c)|_{\text{Range}(P)}$, in other words, the matrix Q^*Q is the result of the Rayleigh–Ritz method applied to the matrix $Q_c^*Q_c$ on the trial subspace $\text{Range}(P)$. The application of the Rayleigh–Ritz method in this case is reduced to simply crossing out rows and columns of the matrix $Q_c^*Q_c$ corresponding to absent edges, since P projects onto a span of coordinate vectors with the indices of the present edges.*

Theorem 5.1 is a standard tool in the spectral graph theory, e.g., Haemers [8], to prove the eigenvalues interlacing; however, the procedure is not apparently recognized in the spectral graph community as the classical Rayleigh–Ritz method. Theorem 5.1 provides us with the missing link in order to apply our Theorem 4.3 to Laplacian graph spectra comparison.

5.3. Majorization of Ritz Values for Laplacian Graph Spectra Comparison. Using the tools that we have presented in the previous subsections, we now can apply our weak majorization result of Section 4 to analyze the change in the graph spectrum when several edges are added to or removed from the graph.

THEOREM 5.2. *Let (V, E^1) and (V, E^2) be two graphs with the same set of n vertices V , with the same number of edges E^1 and E^2 , and with the number of differences in edges between E^1 and E^2 equal to l . Then*

$$(5.3) \quad \sum_k |\lambda_k^1 - \lambda_k^2| \leq nl,$$

where λ_k^1 and λ_k^2 are all elements of the Laplacian spectra of the graphs (V, E^1) and (V, E^2) in the nonincreasing order.

Proof. The spectra of the graph vertex and edge Laplacians QQ^* and Q^*Q are the same apart from zero, which does not affect the statement of the theorem, so we redefine λ_k^1 and λ_k^2 as elements of the spectra, counting the multiplicities, of the edge Laplacians of the graphs (V, E^1) and (V, E^2) . Then, by Theorem 5.1, λ_k^1 and λ_k^2 are the Ritz values of the edge Laplacian matrix $A = Q_c^*Q_c$ of the complete graph, corresponding to the trial subspaces $\mathcal{X} = \text{Range}(P_1)$ and $\mathcal{Y} = \text{Range}(P_2)$ spanned by coordinate vectors with indices of the edges present in E^1 and E^2 , respectively.

Let us apply Theorem 4.3, taking the sum over all available nonzero values in the weak majorization statement as in (4.4). This already gives us the left-hand side of (5.3). To obtain the right-hand side of (5.3) from Theorem 4.3, we now show in our case that, first, $\lambda_{\max} - \lambda_{\min} = n$ and, second, the sum of sines of all angles between the trial subspaces \mathcal{X} and \mathcal{Y} is equal to l .

The first claim follows from the fact, which is easy to check by direct calculation, that the spectrum of the vertex (and thus the edge) Laplacian of the complete graph with n vertices consists of only two eigenvalues $\lambda_{\max} = n$ and $\lambda_{\min} = 0$. Let us make a side note that we can interpret the Laplacian of the complete graph as a scaled projector, i.e. in this case we could have applied Theorem 3.3 directly, rather than Theorem 4.3, which would still result in (5.3).

The second claim, on the sum of sines of all angles, follows from the definition of \mathcal{X} and \mathcal{Y} and the assumption that the number of differences in edges between E^1 and E^2 is equal to l . Indeed, \mathcal{X} and \mathcal{Y} are spanned by coordinate vectors with indices of the edges present in E^1 and E^2 . The edges that are present both in E^1 and E^2 contribute zero angles into $\Theta(\mathcal{X}, \mathcal{Y})$, while the l edges that are different in E^1 and E^2 contribute l right angles into $\Theta(\mathcal{X}, \mathcal{Y})$, so that the sum of all terms in $\sin \Theta(\mathcal{X}, \mathcal{Y})$ is equal to l . \square

Remark 4.2 is also applicable for Theorem 5.2 — while the min term is always zero, since all graph Laplacians are degenerate, the max term can be made smaller by replacing n with the largest eigenvalue of the Laplacian of the graph $(V, E^1 \cup E^2)$.

It is clear from the proof that we do not use the full force of our weak majorization results in Theorem 5.2, because it concerns angles which are zero or $\pi/2$. Nevertheless, the results of Theorem 5.2 appear to be novel in graph theory. We note that these results can be easily extended on k -partite graphs, and possibly to mixed graphs.

Let us finally mention an alternative approach to compare Laplacian graph spectra, which we do not cover in the present paper, by applying Corollary 2.3 directly to graph Laplacians and estimating the right-hand side using the fact that the changes in l edges represents a low-rank perturbation of the graph Laplacian, cf. [31].

Conclusions.

- We prove that the absolute value of the change in the sines or cosines (squared) between two subspaces where one of them changes is weakly majorized by the sines of the angles between the original and the perturbed subspaces.
- We show that the result for the squares of the sines or cosines is equivalent to an inequality where the absolute values of the change in Ritz values with respect to the change in the trial subspace in the Rayleigh–Ritz method applied to an orthogonal projector are weakly majorized by the sines of the angles between the perturbed subspaces.
- We prove the general result for the Rayleigh–Ritz method applied to an arbitrary Hermitian operator, which confirms our previous conjecture that the square root of two factor that has been present in our earlier estimate can be eliminated. The proof is based on extending Hermitian operators to orthogonal projectors.
- An application of our Ritz values weak majorization result for Laplacian graph spectra comparison is suggested, based on a possibility to interpret eigenvalues of the edge Laplacian of a given graph as Ritz values of the edge Laplacian of the complete graph.

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