On Proximity of Rayleigh Quotients for Different Vectors and Ritz Values Generated by Different Trial Subspaces [⋆]

Andrew V. Knyazev [a,∗] Merico E. Argentati [a]

[a] *Department of Mathematics, University of Colorado at Denver, P.O. Box 173364, Campus Box 170, Denver, CO 80217-3364*

Abstract

The Rayleigh quotient is unarguably the most important function used in the analysis and computation of eigenvalues of symmetric matrices. The Rayleigh-Ritz method finds the stationary values of the Rayleigh quotient, called Ritz values, on a given trial subspace as optimal, in some sense, approximations to eigenvalues.

In the present paper, we derive upper bounds for proximity of the Ritz values in terms of the proximity of the trial subspaces without making an assumption that the trial subspace is close to an invariant subspace. The main result is that the absolute value of the perturbations in the Ritz values is bounded by a constant times the gap between the original trial subspace and its perturbation. The constant is the spread in the matrix spectrum, i.e. the difference between the largest and the smallest eigenvalues of the matrix. It's shown that the constant cannot be improved. We then generalize this result to arbitrary unitarily invariant norms, but we have to increase the constant by a factor of $\sqrt{2}$.

Our results demonstrate, in particular, the stability of the Ritz values with respect to a perturbation in the trial subspace.

Key words: Symmetric eigenvalue problem, Rayleigh, Ritz, perturbation, gap, subspace, trace, Euclidian, Frobenius, unitarily invariant norm, gauge function, angles between subspaces
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∗ Corresponding author.
Email addresses: andrew.knyazev@cudenver.edu (Andrew V. Knyazev), rargenta@math.cudenver.edu (Merico E. Argentati).
URL: http://www-math.cudenver.edu/~aknyazev/ (Andrew V. Knyazev).

1 Introduction

Let $A \in \mathbf{R^{n\times n}}$ be a symmetric real-valued matrix and x be a real vector in $\mathbf{R^n}$. Let $\lambda_{\min} \leq \cdots \leq \lambda_{\max}$ be the eigenvalues of A. The Rayleigh quotient $\lambda(x)$ is defined for $x \in \mathbf{R^n}$ with $x \neq 0$ as

$$\lambda(x) = \frac{(x, Ax)}{(x, x)},$$

where $(x, x) = x^T x = \|x\|^2$. In Sections 2 and 3, the norm $\|A\|$ of a matrix A denotes the spectral norm, while in Section 4 we start using general unitary invariant norms of matrices.

The acute angle between two non–zero vectors x and $y \in \mathbf{R^n}$ is denoted by

$$\angle\{x, y\} = \arccos \frac{|(x, y)|}{\|x\|\|y\|}.$$

It is important to emphasize that $0 \leq \angle\{x, y\} \leq \pi/2$, by definition.

The following result is proved in [5] in order to analyze the convergence rate of preconditioned iterative methods for large scale symmetric eigenvalue problems: Let $A \in \mathbf{R^{n\times n}}$ be in addition positive definite, then

$$\frac{|\lambda(x) - \lambda(y)|}{\lambda(x)} \leq \left(\frac{\lambda_{\max}}{\lambda_{\min}} - 1\right) \sin(\angle\{x, y\}). \tag{1}$$

The proof of this bound in [5] is rather involved.

The first result of the present paper is the following estimate:

$$|\lambda(x) - \lambda(y)| \leq (\lambda_{\max} - \lambda_{\min}) \sin(\angle\{x, y\}), \tag{2}$$

with a simple proof, which takes only a few lines. Since $\lambda(x) \geq \lambda_{\min}$, the previous result (1) follows from (2) trivially.

The main result of the present paper is a generalization of (2), where the Rayleigh quotients are replaced with Ritz values, and the angle between vectors is replaced with the angle between the trial subspaces (of the same dimension) in the Rayleigh–Ritz method. This result, therefore, bounds the absolute value of the difference of the Ritz values from above by a constant $\lambda_{\max} - \lambda_{\min}$ times the gap between the trial subspaces. It is shown that the constant $\lambda_{\max} - \lambda_{\min}$ cannot be improved. We then generalize this result to unitarily invariant norms.

Let us note that with trivial modifications our results can be reformulated for the case of a Hermitian matrix in a complex vector space. It also seems feasible to extend our results to the case of a selfadjoint operator A in a Hilbert space and to allow the trial subspaces to be infinite dimensional.

Several potential applications of the results of the present paper can already be foreseen. While applications are outside of the scope of the present paper, we provide possible examples in the next two paragraphs.

Inequality (1) is used in [5] to analyze the convergence rate of preconditioned single vector iterative methods. Our new results and the proof technique used to cover the case of unitarily invariant norms can be helpful in attempts to generalize the analysis of [5] to preconditioned block methods, where several approximate eigenvectors are iterated simultaneously.

Another potential application is for analysis of the influence of changes in the trial subspace in the Rayleigh–Ritz method. There are several situations, where the trial subspace is modified: round off errors in finite-precision computations, intentional inexact representation of the basis of the trial subspace, and trial functions of changing shapes in finite element methods.

Let us finally highlight that we do not assume that any of our trail subspaces is invariant with respect to the matrix A itself or contains an invariant subspace. Under such an assumption, our estimates are not intended to be used, since they do not capture a possible error improvement.

The rest of the paper is organized as follows. We prove (2) in Section 2 and show that the constant is sharp. Our main result is in Section 3, where we also combine it with estimates of [6] to show how Ritz values may vary with the change of a basis of the trial subspace. In Section 4, we generalize our estimate from the spectral norm to other unitarily invariant norms, but we are unable to preserve the constant which becomes $\sqrt{2}$ larger. Finally, in Section 5, we discuss the results of our numerical tests.

Some preliminary results of the present paper have appeared in [1].

2 Bounds on Changes in the Rayleigh Quotient

In this section we present an upper bound for the change in the Rayleigh quotient with respect to the change of the vector in order to extend this result to the Ritz values in the next section.

Theorem 1 *Let $x, y \in \mathbf{R^n}$ with $x, y \neq 0$. Then estimate (2), which we repeat* *here for the reader's convenience,*

$$|\lambda(x) - \lambda(y)| \le (\lambda_{\max} - \lambda_{\min}) \sin(\angle\{x, y\}),$$

holds.

PROOF. Without loss of generality, we assume that $\|x\| = \|y\| = 1$. Let

$$A_s = A - \left(\frac{\lambda_{\min} + \lambda_{\max}}{2}\right) I. \tag{3}$$

Using the fact that the difference $|\lambda(x) - \lambda(y)|$ is independent of a shift to the matrix A by any constant times the identity, we have

$$\begin{aligned} |\lambda(x) - \lambda(y)| &= |(x, Ax) - (y, Ay)| \\ &= |(x, A_s x) - (y, A_s y)| \\ &= |(A_s(x - y), x + y)|. \end{aligned}$$

Then by the Cauchy–Schwarz inequality

$$\begin{aligned} &|(A_s(x - y), x + y)| \\ &\qquad \le 2\,\|A_s\|\, \frac{\|x - y\|\|x + y\|}{2} \\ &\qquad = (\lambda_{\max} - \lambda_{\min}) \sin(\angle\{x, y\}). \end{aligned}$$

□

An alternative proof of Theorem 1 can be found in [1].

The constant in estimate (2) is sharp in the following sense:

Theorem 2 *For any value $s \in (0, 1]$, we have*

$$\max_{x, y \,:\, \sin(\angle\{x, y\}) = s} \frac{|\lambda(x) - \lambda(y)|}{\sin(\angle\{x, y\})} = \lambda_{\max} - \lambda_{\min}. \tag{4}$$

PROOF. Let $\mathcal{Z}$ be a two-dimensional subspace of $\mathbf{R^n}$ spanned by two normalized and mutually orthogonal eigenvectors u and v of A corresponding to the smallest $\lambda_{\min}$ and largest $\lambda_{\max}$, respectively, eigenvalues of A. For the given $s \in (0, 1]$, we can find vectors x and y in $\mathcal{Z}$ such that $\sin(\angle\{x, y\}) = s$ and that the Cauchy–Schwarz inequality in the previous proof turns into equality:

$$|(A_s(x - y), x + y)| = \|A_s\|\, \|x - y\|\|x + y\|.$$

Namely, to satisfy both requirements, we choose

$$x = \sqrt{\frac{1-s}{2}}\, u + \sqrt{\frac{1+s}{2}}\, v \text{ and } y = \sqrt{\frac{1+s}{2}}\, u + \sqrt{\frac{1-s}{2}}\, v.$$

Direct calculations show that $\sin(\angle\{x, y\}) = s$ and that

$$|\lambda(x) - \lambda(y)| = (\lambda_{\max} - \lambda_{\min}) \sin(\angle\{x, y\})$$

for these two vectors. □

It is easy to see that when we have equality in (2), the vectors x and y must be of the form (modulo an exchange of x and y)

$$x = \delta_1\sqrt{\frac{1-s}{2}}u + \delta_2\sqrt{\frac{1+s}{2}}v \text{ and } y = \delta_3\sqrt{\frac{1+s}{2}}u + \delta_4\sqrt{\frac{1-s}{2}}v,$$

with $\delta_j = \pm 1$ and $\delta_1\delta_2\delta_3\delta_4$=1.

Remark 3 *The constant in estimate (2) can be improved if more information about vectors x and y is available. Namely, let us observe that in the proof of Theorem 1 matrix A appears only within scalar products of vectors x and y and their linear combinations. Thus, we can replace matrix A in the proof of Theorem 1 with the projection of A on the two-dimensional subspace* $\operatorname{span}\{x, y\}$ *restricted to* $\operatorname{span}\{x, y\}$. *This allows replacing the constant $\lambda_{\max} - \lambda_{\min}$ in estimate (2) with the following constant:*

$$\max_{z \in \operatorname{span}\{x,y\}, \|z\|=1} (z, Az) - \min_{z \in \operatorname{span}\{x,y\}, \|z\|=1} (z, Az),$$

which may in some cases be significantly smaller.

If it is known in addition that one of the vectors x or y is an eigenvector of A, estimate (2) can be greatly improved. Following [2], we provide for completeness the corresponding estimate in the next theorem even though such improved estimates are outside of the scope of the present paper.

Theorem 4 *Let x or y is an eigenvector of A, then*

$$|\lambda(x) - \lambda(y)| \le C \sin^2(\angle\{x, y\}),$$

where

$$C = \max_{z \in \operatorname{span}\{x,y\}, \|z\|=1} (z, Az) - \min_{z \in \operatorname{span}\{x,y\}, \|z\|=1} (z, Az) \le \lambda_{\max} - \lambda_{\min}.$$

PROOF. Suppose that y is an eigenvector of A, let P_y denotes the orthogonal projector on $\operatorname{span}\{y\}$, then $AP_y = \lambda(y)P_y$, so $A - \lambda(y) = (A - \lambda(y))(I - P_y)$. Assuming vector x being normalized, we get

$$
\begin{aligned}
|\lambda(x) - \lambda(y)| &= |(x, (A - \lambda(y)I)x)| \\
&= |((I - P_y)x, (A - \lambda(y)I)(I - P_y)x)| \\
&\le \|A - \lambda(y)I\| \|(I - P_y)x)\|^2 \\
&\le (\lambda_{\max} - \lambda_{\min}) \sin^2(\angle\{x, y\}).
\end{aligned}
$$

In order to obtain the same estimate with a better constant C, we use the approach suggested in Remark 3, namely, we introduce the new operator A_{xy} as the projection of A on the two-dimensional subspace span$\{x, y\}$ restricted to span$\{x, y\}$. Vector y is also an eigenvector of A_{xy} corresponding to the eigenvalue $\lambda(y)$, so we can repeat the arguments above, replacing A with A_{xy}. Finally, $\|A_{xy} - \lambda(y)I\| \le C$, since C is the difference of the largest and the smallest eigenvalues of A_{xy} and $\lambda(y)$ coincides with one of them. $\square$

3 Ritz Value Proximities

To formulate and prove a generalization of (2) to Ritz values, we need to introduce the concepts involving principal angles between subspaces that are discussed, e.g., in [6] and in most advanced textbooks on linear algebra. In the present paper, we need just the definition and one of the basic results, e.g., [6], formulated in the next paragraph.

Let $\mathcal{X}$ and $\mathcal{Y}$ both be m–dimensional subspaces of $\mathbf{R^n}$ and let $Q_{\mathcal{X}},\ Q_{\mathcal{Y}} \in \mathbf{R^{n\times m}}$ be matrices with orthonormal columns spanning respectively the subspaces $\mathcal{X}$ and $\mathcal{Y}$. Angles between the subspaces $\mathcal{X}$ and $\mathcal{Y}$ are defined by

$$
\cos(\angle_j\{\mathcal{X}, \mathcal{Y}\}) = \sigma_j,\ j = 1, \ldots, m,
$$

where $1 \ge \sigma_1 \ge \cdots \ge \sigma_m \ge 0$ and σ's are the m singular values of $Q_{\mathcal{X}}^T Q_{\mathcal{Y}}$. This definition of angles does not depend on the particular choice of matrices $Q_{\mathcal{X}}$ and $Q_{\mathcal{Y}}$, moreover, there exist matrices $Q_{\mathcal{X}}$ and $Q_{\mathcal{Y}}$ such that $Q_{\mathcal{X}}^T Q_{\mathcal{Y}} = \text{diag}\ (\sigma_1, \ldots, \sigma_m)$, which will be used later in the paper in the proofs of Theorems 5 and 10.

The largest principal angle $\angle_m\{\mathcal{X}, \mathcal{Y}\}$ is also commonly denoted by $\angle\{\mathcal{X}, \mathcal{Y}\}$. The value $\sin(\angle\{\mathcal{X}, \mathcal{Y}\})$ is called the *gap* between subspaces and can be used to measure how close the subspaces $\mathcal{X}$ and $\mathcal{Y}$ are to each other.

The main result of the paper is the following theorem.

Theorem 5 *Let $\mathcal{X}$ and $\mathcal{Y}$ both be m–dimensional subspaces of $\mathbf{R^n}$, and $\alpha_1 \le \cdots \le \alpha_m$ and $\beta_1 \le \cdots \le \beta_m$ denote the Ritz values for A with respect to $\mathcal{X}$ and $\mathcal{Y}$, i.e. α's and β's are the stationary values of the the Rayleigh quotient* *on subspaces $\mathcal{X}$ and $\mathcal{Y}$, correspondingly. Then*

$$\max_{j=1,\ldots,m} |\alpha_j - \beta_j| \leq (\lambda_{\max} - \lambda_{\min}) \sin(\angle\{\mathcal{X}, \mathcal{Y}\}). \tag{5}$$

PROOF. Let $Q_{\mathcal{X}},\ Q_{\mathcal{Y}} \in \mathbf{R}^{\mathbf{n}\times\mathbf{m}}$ be matrices with orthonormal columns spanning respectively the subspaces $\mathcal{X}$ and $\mathcal{Y}$ such that $Q_{\mathcal{X}}^T Q_{\mathcal{Y}} = \text{diag}\ (\sigma_1, \ldots, \sigma_m)$. By Weyl's theorem, we have

$$|\alpha_j - \beta_j| \leq \rho(Q_{\mathcal{X}}^T A Q_{\mathcal{X}} - Q_{\mathcal{Y}}^T A Q_{\mathcal{Y}}), \qquad j = 1, \ldots, m, \tag{6}$$

where $\rho(\cdot)$ denotes the spectral radius. Since the matrix $Q_{\mathcal{X}}^T A Q_{\mathcal{X}} - Q_{\mathcal{Y}}^T A Q_{\mathcal{Y}}$ is symmetric, there exists a unit vector $v \in \mathbf{R}^{\mathbf{m}}$, which is an eigenvector of $Q_{\mathcal{X}}^T A Q_{\mathcal{X}} - Q_{\mathcal{Y}}^T A Q_{\mathcal{Y}}$, such that

$$\begin{aligned}\rho(Q_{\mathcal{X}}^T A Q_{\mathcal{X}} - Q_{\mathcal{Y}}^T A Q_{\mathcal{Y}}) &= |(v, (Q_{\mathcal{X}}^T A Q_{\mathcal{X}} - Q_{\mathcal{Y}}^T A Q_{\mathcal{Y}})v)| \\ &= |(v, Q_{\mathcal{X}}^T A Q_{\mathcal{X}} v) - (v, Q_{\mathcal{Y}}^T A Q_{\mathcal{Y}} v)| \\ &= |\lambda(Q_{\mathcal{X}} v) - \lambda(Q_{\mathcal{Y}} v)|.\end{aligned} \tag{7}$$

By Theorem 1,

$$\begin{aligned}|\lambda(Q_{\mathcal{X}} v) - \lambda(Q_{\mathcal{Y}} v)| &\leq (\lambda_{\max} - \lambda_{\min}) \sin(\angle\{Q_{\mathcal{X}} v, Q_{\mathcal{Y}} v\}) \\ &\leq (\lambda_{\max} - \lambda_{\min}) \sin(\angle\{\mathcal{X}, \mathcal{Y}\}).\end{aligned} \tag{8}$$

The last inequality in (8) holds since

$$\begin{aligned}\cos(\angle\{Q_{\mathcal{X}} v, Q_{\mathcal{Y}} v\}) &= \frac{(Q_{\mathcal{X}}^T Q_{\mathcal{Y}} v, v)}{\|Q_{\mathcal{X}} v\| \|Q_{\mathcal{Y}} v\|} \\ &= (Q_{\mathcal{X}}^T Q_{\mathcal{Y}} v, v) \\ &= (\text{diag}\ (\sigma_1, \ldots, \sigma_m) v, v) \\ &\geq \sigma_m \\ &= \cos(\angle\{\mathcal{X}, \mathcal{Y}\}).\end{aligned}$$

Combining (6), (7) and (8), we obtain (5). $\square$

If $m = n$, both parts of inequality (5) vanish. If $m < n$, the constant in the estimate (5) is sharp in the following somewhat weak sense, not necessarily for a fixed single matrix, but rather for the whole class of symmetric matrices with given largest and smallest eigenvalues:

Theorem 6 *Under the assumptions of Theorem 5, let $m < n$. Then for any value $s \in (0, 1]$, we have*

$$\max_{\substack{A = A^T \\ \lambda_{\max}(A) = \lambda_{\max} \\ \lambda_{\min}(A) = \lambda_{\min}}} \max_{\substack{\mathcal{X}, \mathcal{Y} : \\ \sin(\angle\{\mathcal{X}, \mathcal{Y}\}) = s}} \frac{\max_{j=1,\ldots,m} |\alpha_j - \beta_j|}{\sin(\angle\{\mathcal{X}, \mathcal{Y}\})} = \lambda_{\max} - \lambda_{\min}.$$

PROOF. For the given $s \in (0, 1]$, we construct the matrix A and subspaces $\mathcal{X}$ and $\mathcal{Y}$ such that $\sin(\angle\{\mathcal{X}, \mathcal{Y}\}) = s$ and that the inequality (5) turns into an equality. We start with a construction for A. For a arbitrary fixed nontrivial orthoprojector P we set $A = (\lambda_{\max} - \lambda_{\min})P + \lambda_{\min} I$, so that $\lambda_{\max}$ and $\lambda_{\min}$ are the only distinct eigenvalues of A.

To construct $\mathcal{X}$ and $\mathcal{Y}$, we again (as in the proof of Theorem 2) consider the two-dimensional subspace $\mathcal{Z}$ spanned by two eigenvectors of A corresponding to the smallest $\lambda_{\min}$ and largest $\lambda_{\max}$ eigenvalues of A and choose vectors $x \in \mathcal{X}$ and $y \in \mathcal{Y}$ the same way that they were chosen in the proof of Theorem 2, i.e., such that vectors x and y in $\mathcal{Z}$ satisfy $\sin(\angle\{x, y\}) = s$ and

$$|\lambda(x) - \lambda(y)| = (\lambda_{\max} - \lambda_{\min}) \sin(\angle\{x, y\}).$$

To complete the construction of m-dimensional subspaces $\mathcal{X}$ and $\mathcal{Y}$, we choose $\mathcal{X}$ and $\mathcal{Y}$ such that they have a $m-1$ dimensional intersection, which is an invariant subspace of A and is orthogonal to $\mathcal{Z}$. In other words, we construct $\mathcal{X}$ and $\mathcal{Y}$ by choosing the first $m-1$ columns of matrices $Q_{\mathcal{X}}$ and $Q_{\mathcal{Y}}$ to be the same and to coincide with some eigenvectors of A orthogonal to $\mathcal{Z}$, and we put x and y as the last columns of $Q_{\mathcal{X}}$ and $Q_{\mathcal{Y}}$.

Such choice makes $m-1$ Ritz values α_j and β_j to be the same and to coincide with either $\lambda_{\max}$ or $\lambda_{\min}$, taking into account that α_j and β_j must be in the ascending order. Then, on the one hand, the only nonzero term under the $\max_{j=1,\ldots,m} |\alpha_j - \beta_j|$ is $|\lambda(x) - \lambda(y)|$. On the other hand, by construction of $\mathcal{X}$ and $\mathcal{Y}$ we have $\sigma_1 = \ldots = \sigma_{m-1} = 1$ and $\sigma_m = \cos(\angle\{x, y\})$ as vectors x and y are chosen to be in $\mathcal{Z}$, which is orthogonal to the $m-1$ dimensional intersection of subspaces $\mathcal{X}$ and $\mathcal{Y}$. This leads to the equalities $s = \sin(\angle\{x, y\}) = \sin(\angle\{\mathcal{X}, \mathcal{Y}\})$. □

We note that the restriction on A in the proof of Theorem 6 is essential: the proof may break if A has intermediate eigenvalues. We would still have $m-1$ Ritz identical values α_i and β_j, but because of the ordering they might have different indexes, breaking the pairs needed to claim that the only nonzero term under the $\max_{j=1,\ldots,m} |\alpha_j - \beta_j|$ is $|\lambda(x) - \lambda(y)|$.

Remark 7 *The constant in estimate (5) can be improved in the same manner as in Remark 3 the constant in estimate (2) is improved. Namely, we can* *replace the constant $\lambda_{\max} - \lambda_{\min}$ in estimate (5) with the following constant:*

$$\max_{z \in \mathcal{X}+\mathcal{Y}, \|z\|=1} (z, Az) - \min_{z \in \mathcal{X}+\mathcal{Y}, \|z\|=1} (z, Az).$$

Remark 8 *The results of the present paper are evidently applicable to a particular case, when one of the trial subspaces is an invariant subspace of A, thus producing bounds for the absolute error between eigenvalues of A and approximating them by Ritz values. However, our results are not intended to be used and do not provide sharp estimates in this situation. Indeed, let $\mathcal{Y}$ be an invariant subspace of A corresponding to the smallest eigenvalues $\beta_1 \leq \cdots \leq \beta_m$, which will also be in this case the Ritz values for A with respect to $\mathcal{Y}$. Let us repeat here estimate (5) for the reader's convenience:*

$$|\alpha_j - \beta_j| \leq (\lambda_{\max} - \lambda_{\min}) \sin(\angle\{\mathcal{X}, \mathcal{Y}\}), j = 1, \ldots, m.$$

The following better estimate is well known, e.g., [5],

$$0 \leq \alpha_j - \beta_j \leq (\lambda_{\max} - \lambda_{\min}) \sin^2(\angle\{\mathcal{X}, \mathcal{Y}\}), j = 1, \ldots, m.$$

Let us finally combine estimate (5) with the simplified version of the statement of [6, Lemma 5.5] to obtain the following theorem, showing the level of sensitivity of Ritz values with the respect to changes in the basis of the trial subspace.

Theorem 9 *Let $\mathcal{X}$ and $\mathcal{Y}$ both be m–dimensional subspaces of $\mathbf{R}^{\mathbf{n}}$, which are column spaces of full rank matrices X and Y, and $\alpha_1 \leq \cdots \leq \alpha_m$ and $\beta_1 \leq \cdots \leq \beta_m$ denote the Ritz values for A with respect to $\mathcal{X}$ and $\mathcal{Y}$, i.e. α's and beta's are the stationary values of the the Rayleigh quotient on subspaces $\mathcal{X}$ and $\mathcal{Y}$, correspondingly. Then*

$$\max_{j=1,\ldots,m} |\alpha_j - \beta_j| \leq (\lambda_{\max} - \lambda_{\min}) \operatorname{cond}(X) \frac{\|X - Y\|}{\|X\|},$$

where $\operatorname{cond}(X)$ is the spectral condition number of X.

Theorem 9 highlights the importance of having a well conditioned, preferably orthonormal, basis of the trial subspace for stability of the Rayleigh-Ritz procedure. We note that Theorem 9 cannot be easily applied to analyze the stability of the Lanczos method without reorthogonalization, since the constructed basis of the Krylov subspace is known to be ill-conditioned in this case, so $\operatorname{cond}(X)$ is large.

In Theorem 5, only the largest principal angle $\angle\{\mathcal{X},\mathcal{Y}\} = \angle_m\{\mathcal{X},\mathcal{Y}\}$ between the subspaces $\mathcal{X}$ and $\mathcal{Y}$ is used. But we also have other angles at our disposal. Let us replace max with min on the left and the largest principal angle $\angle\{\mathcal{X},\mathcal{Y}\}$ between the subspaces $\mathcal{X}$ and $\mathcal{Y}$ with the smallest $\angle_1\{\mathcal{X},\mathcal{Y}\}$ on the right in inequality (5) to formulate

$$\min_{j=1,\ldots,m} |\alpha_j - \beta_j| \le (\lambda_{\max} - \lambda_{\min}) \sin(\angle_1\{\mathcal{X},\mathcal{Y}\}). \tag{9}$$

Let us state right away that the estimate (9) does not hold in general. Indeed, let two-dimensional subspaces $\mathcal{X}$ and $\mathcal{Y}$ have a one-dimensional intersection, then evidently $\angle_1\{\mathcal{X},\mathcal{Y}\} = 0$ and (9) would imply that at least one Ritz value $\alpha_j = \beta_j$ is shared. This is not the case in general, an exception is when the intersection is an invariant subspace of A.

Again, estimate (9) is wrong. However, it raises an interesting possibility to formulate a generalization of (5) that would involve all, not just the largest, angles between the subspaces $\mathcal{X}$ and $\mathcal{Y}$. To cover a general case, let $\|\cdot\|$ be a unitarily invariant norm associated with a symmetric gauge function $g(\cdot)$, e.g., [3, 7], so that

$$\|T\| = g([s_1(T), \ldots, s_m(T)]),$$

where different $s(T)$ represent all singular values of the matrix T. We can prove the following theorem, which is a generalization of Theorem 5, with the exception of the constant that is larger by a factor $\sqrt{2}$.

Theorem 10 *Under the assumptions of Theorem 5, we have*

$$\|\text{diag}\,(\alpha_1,\ldots,\alpha_m) - \text{diag}\,(\beta_1,\ldots,\beta_m)\| \le \\ \sqrt{2}(\lambda_{\max} - \lambda_{\min})\|\text{diag}\,(\sin(\angle_1\{\mathcal{X},\mathcal{Y}\}),\ldots,\sin(\angle_m\{\mathcal{X},\mathcal{Y}\}))\|, \tag{10}$$

in an arbitrary unitarily invariant norm or, equivalently, in terms of the corresponding gauge function,

$$g([\alpha_1 - \beta_1, \ldots, \alpha_m - \beta_m]) \le \\ \sqrt{2}(\lambda_{\max} - \lambda_{\min})\, g([\sin(\angle_1\{\mathcal{X},\mathcal{Y}\}),\ldots,\sin(\angle_m\{\mathcal{X},\mathcal{Y}\})]). \tag{11}$$

PROOF. A straightforward generalization of the proof of Theorem 5 does not allow us to prove (11) for any general unitarily invariant norm other than the spectral norm, already covered by Theorem 5. We need to use more advanced arguments involving unitarily invariant norms and singular value inequalities.

Let again, as in (3),

$$A_s = A - \left(\frac{\lambda_{\min} + \lambda_{\max}}{2}\right) I.$$

As in the proof of Theorem 5, let $Q_{\mathcal{X}},\ Q_{\mathcal{Y}} \in \mathbf{R^{n\times m}}$ be matrices with orthonormal columns spanning respectively, the subspaces $\mathcal{X}$ and $\mathcal{Y}$ such that $Q_{\mathcal{X}}^T Q_{\mathcal{Y}} = \text{diag}\ (\sigma_1, \ldots, \sigma_m)$, where

$$\sigma_j = \cos(\angle_j\{\mathcal{X}, \mathcal{Y}\}),\ j = 1, \ldots, m$$

are the cosines of the principal angles between the subspaces $\mathcal{X}$ and $\mathcal{Y}$.

By a Corollary of Mirsky's theorem [8, Corollary IV.4.12]

$$\|\text{diag}\ (\alpha_1, \ldots, \alpha_m) - \text{diag}\ (\beta_1, \ldots, \beta_m)\| \leq \|Q_{\mathcal{X}}^T A_s Q_{\mathcal{X}} - Q_{\mathcal{Y}}^T A_s Q_{\mathcal{Y}}\|.$$

Using the triangle inequality and [8, Theorem II.3.9] we have

$$\begin{aligned}
&\|Q_{\mathcal{X}}^T A_s Q_{\mathcal{X}} - Q_{\mathcal{Y}}^T A_s Q_{\mathcal{Y}}\| = \|Q_{\mathcal{X}}^T A_s Q_{\mathcal{X}} - Q_{\mathcal{X}}^T A_s Q_{\mathcal{Y}} + Q_{\mathcal{X}}^T A_s Q_{\mathcal{Y}} - Q_{\mathcal{Y}}^T A_s Q_{\mathcal{Y}}\| \\
&\leq \|Q_{\mathcal{X}}^T A_s Q_{\mathcal{X}} - Q_{\mathcal{X}}^T A_s Q_{\mathcal{Y}}\| + \|Q_{\mathcal{X}}^T A_s Q_{\mathcal{Y}} - Q_{\mathcal{Y}}^T A_s Q_{\mathcal{Y}}\| \\
&= \|Q_{\mathcal{X}}^T A_s (Q_{\mathcal{X}} - Q_{\mathcal{Y}})\| + \|(Q_{\mathcal{X}} - Q_{\mathcal{Y}})^T A_s Q_{\mathcal{Y}}\| \\
&\leq \|Q_{\mathcal{X}}^T A_s\|_2 \|(Q_{\mathcal{X}} - Q_{\mathcal{Y}})\| + \|(Q_{\mathcal{X}} - Q_{\mathcal{Y}})^T\| \|A_s Q_{\mathcal{Y}}\|_2 \\
&\leq 2\|A_s\|_2 \|Q_{\mathcal{X}} - Q_{\mathcal{Y}}\| \\
&= (\lambda_{\max} - \lambda_{\min}) \|Q_{\mathcal{X}} - Q_{\mathcal{Y}}\|,
\end{aligned}$$

where $\|\cdot\|_2$ denotes the spectral matrix norm. Let us introduce notation $\theta_j = \angle_j\{\mathcal{X}, \mathcal{Y}\}$, $j = 1, \ldots, m$ for the angles. Since $Q_{\mathcal{X}}^T Q_{\mathcal{Y}} = \text{diag}\ (\sigma_1, \ldots, \sigma_m)$, where $\sigma_j = \cos\theta_j$, $j = 1, \ldots, m$, we have

$$\begin{aligned}
(Q_{\mathcal{X}} - Q_{\mathcal{Y}})^T (Q_{\mathcal{X}} - Q_{\mathcal{Y}}) &= 2(I - \text{diag}\ (\sigma_1, \ldots, \sigma_m)) \\
&= 2(I - \text{diag}\ (\cos\theta_1, \ldots, \cos\theta_m)),
\end{aligned}$$

so the singular values of $Q_{\mathcal{X}} - Q_{\mathcal{Y}}$ are $\sqrt{2(1 - \cos\theta_j)} = 2\sin(\theta_j/2)$, $j = 1, \ldots, m$ and for an arbitrary unitary invariant norm,

$$\|Q_{\mathcal{X}} - Q_{\mathcal{Y}}\| = \left\|\text{diag}\ \left(\sin\left(\frac{\theta_1}{2}\right), \ldots, \sin\left(\frac{\theta_m}{2}\right)\right)\right\|.$$

Thus

$$\begin{aligned}
&\|\text{diag}\ (\alpha_1, \ldots, \alpha_m) - \text{diag}\ (\beta_1, \ldots, \beta_m)\| \\
&\leq 2\ (\lambda_{\max} - \lambda_{\min}) \left\|\text{diag}\ \left(\sin\left(\frac{\theta_1}{2}\right), \ldots, \sin\left(\frac{\theta_m}{2}\right)\right)\right\|.
\end{aligned} \tag{12}$$

We have

$$\sin(\theta) = 2\cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right),$$

and since $\theta \in [0, \pi/2]$,

$$2\sin\left(\frac{\theta}{2}\right) \le \sqrt{2}\sin(\theta).$$

Unitarily invariant norms are monotone [3, Theorem 5.5.10, Theorem 7.4.24], so

$$2\left\|\mathrm{diag}\left(\sin\left(\frac{\theta_1}{2}\right), \ldots, \sin\left(\frac{\theta_m}{2}\right)\right)\right\| \le \sqrt{2}\|\mathrm{diag}\left(\sin(\theta_1), \ldots, \sin(\theta_m)\right)\|.$$

Combining (12) with the latter inequality completes the proof. □

Our numerical tests in Section 5 suggest that the constant in (10) and (11) can be improved.

Conjecture 11 *The multiplier $\sqrt{2}$ in the constant in (10) and (11) can be removed.*

Without the $\sqrt{2}$, Theorem 10 would be a direct generalization of Theorem 5. We are not able to prove it, except for the asymptotic case, where the angles are small, i.e. when the subspaces $\mathcal{X}$ and $\mathcal{Y}$ are close. In this particular case, the statement of Conjecture 11 follows from (12), since $2\sin(\theta/2) \to \sin(\theta)$ as $\theta \to 0$.

It is instructive to repeat here the inequality in Theorem 5 in terms of orthogonal projectors. We have

$$\max_{j=1,\ldots,m} |\alpha_j - \beta_j| \le (\lambda_{\max} - \lambda_{\min})\|P_{\mathcal{X}} - P_{\mathcal{Y}}\|_2. \tag{13}$$

We can derive an analogous result, using the Frobenius norm in (11), as

$$\sqrt{\sum_{j=1}^{m}(\alpha_j - \beta_j)^2} \le (\lambda_{\max} - \lambda_{\min})\|P_{\mathcal{X}} - P_{\mathcal{Y}}\|_F, \tag{14}$$

since the Frobenius norm is unitarily invariant and [8, Theorem I.5.5] implies that

$$\|P_{\mathcal{X}} - P_{\mathcal{Y}}\|_F = \sqrt{2\sum_{j=1}^{m}\sin^2(\angle_j\{\mathcal{X}, \mathcal{Y}\})}.$$

We know from Theorem 6 that (13) is sharp. If our Conjecture 11 holds, the constant in (14) would be $(\lambda_{\max} - \lambda_{\min})/\sqrt{2}$ instead of $(\lambda_{\max} - \lambda_{\min})$.

Using the 1-norm in (11) we have

$$\sum_{j=1}^{m} |\alpha_j - \beta_j| \leq \sqrt{2}(\lambda_{max} - \lambda_{min}) \sum_{j=1}^{m} \sin(\angle_j\{\mathcal{X}, \mathcal{Y}\}). \tag{15}$$

Again, if our Conjecture 11 holds, there would be no multiplier $\sqrt{2}$ in (15), which we cannot prove. However, it is easy to derive the following weaker estimate without $\sqrt{2}$.

Lemma 12 *Under the assumptions of Theorem 5, we have*

$$|\sum_{j=1}^{m}(\alpha_j - \beta_j)| \leq (\lambda_{max} - \lambda_{min}) \sum_{j=1}^{m} \sin(\angle_j\{\mathcal{X}, \mathcal{Y}\}). \tag{16}$$

PROOF. Indeed, we have

$$\begin{aligned}
|\sum_{j=1}^{m}(\alpha_j - \beta_j)| &= |\text{tr } (Q_{\mathcal{X}}^T A Q_{\mathcal{X}}) - \text{tr } (Q_{\mathcal{Y}}^T A Q_{\mathcal{Y}})| \\
&= |\text{tr } (Q_{\mathcal{X}}^T A_s Q_{\mathcal{X}}) - \text{tr } (Q_{\mathcal{Y}}^T A_s Q_{\mathcal{Y}})| \\
&= |\text{tr } (A_s Q_{\mathcal{X}} Q_{\mathcal{X}}^T) - \text{tr } (A_s Q_{\mathcal{Y}} Q_{\mathcal{Y}}^T)| \\
&= |\text{tr } (A_s P_{\mathcal{X}}) - \text{tr } (A_s P_{\mathcal{Y}})| \\
&= |\text{tr } (A_s (P_{\mathcal{X}} - P_{\mathcal{Y}}))|.
\end{aligned}$$

By [4, Theorem 3.3.13]

$$\begin{aligned}
|\text{tr } (A_s (P_{\mathcal{X}} - P_{\mathcal{Y}}))| &\leq \sum_{j=1}^{n} s_j(A_s(P_{\mathcal{X}} - P_{\mathcal{Y}})) \\
&\leq \|A_s\|_2 \sum_{j=1}^{n} s_j(P_{\mathcal{X}} - P_{\mathcal{Y}}) \\
&= (\lambda_{\max} - \lambda_{\min}) \sum_{j=1}^{m} \sin(\angle_j\{\mathcal{X}, \mathcal{Y}\}).
\end{aligned}$$

□

Notice that (15) estimates a sum of absolute values, while (16) deals with the absolute value of the sum.

Remark 13 *If $2m > n$ in Theorem 10, then the gauge function on the right hand side is only a function of $n - m$ of the largest angles (here $n - m < m$), e.g., in the case $n - m = 1$ the gauge function would only be a function of* *the largest angle since the other angles vanish. For example, if $n-m=1$, the Frobenius norm yields*

$$\sqrt{\sum_{j=1}^{n-1}(\alpha_j-\beta_j)^2} \leq \sqrt{2}(\lambda_{\max}-\lambda_{\min})\sin\angle\{X,Y\}.$$

5 Numerical Tests

In this section we provide some numerical results. We use a 4-dimensional vector space and 2-dimensional subspaces. There are two principal angles between each pair of subspaces. We compute the Ky–Fan N_k norms for $k=1,2$ and form the N_1 ratio

$$\frac{\max\{|\alpha_1-\beta_1|,|\alpha_2-\beta_2|\}}{(\lambda_{\max}-\lambda_{\min})\sin(\angle_2\{\mathcal{X},\mathcal{Y}\})},$$

and the N_2 ratio

$$\frac{|\alpha_1-\beta_1|+|\alpha_2-\beta_2|}{(\lambda_{\max}-\lambda_{\min})(\sin(\angle_1\{\mathcal{X},\mathcal{Y}\})+\sin(\angle_2\{\mathcal{X},\mathcal{Y}\}))}.$$

In Figure 1, we plot the largest N_1 (left) and N_2 (right) ratios for 400,000 trials, each trial involving a different random symmetric 4×4 matrix. For each trial (matrix), we vary the two principal angles from 0 to 90 degrees by 2 degree increments. For each pair of angles we generate random matrices $X,\ Y\in\mathbf{R^{4\times 2}}$ with orthonormal columns with the specified pair of principal angles between them. We then compute the Ritz values and the N_1 and N_2 ratios for this matrix and the two given angles. We accumulate the maximum ratios over all the trials for each pair of angles.

The graph of the N_1 ratio, Figure 1 (left), supports Theorem 5 since this ratio is always less than or equal to one. It also demonstrates the weak sense of sharpness used in Theorem 6, as the N_1 ratio is close to one, but does not reach one for all angles, since we test all possible symmetric 4×4 matrices, not just those without intermediate eigenvalues, and apparently do not run enough trials to reach 1 everywhere.

The graph of the N_2 ratio, Figure 1 (right), illustrates Theorem 10, since this ratio is less than or equal to $\sqrt{2}$. In fact, this ratio is less than or equal to one, which supports our Conjecture 11 and suggests that estimates (10) and (11) without $\sqrt{2}$ would be sharp, if they were true. A careful look at the construction of the subspaces in the proof of Theorem 6 reveals that the N_2 ratio for such subspaces must be one even for arbitrary symmetric matrices with intermediate eigenvalues. In other words, if estimate (15) without $\sqrt{2}$ holds, as suggested by Conjecture 11, it would be sharp in a stronger sense compared to that of Theorem 6, i.e. for every fixed symmetric matrix with extreme eigenvalues $\lambda_{\max}$ and $\lambda_{\min}$.

In Figure 1 (right), we also observe that the maximum value occurs where one of the angles is zero. This observation may be helpful in a future attempt to prove Conjecture 11. We note that when one of the angles is zero the N_2 ratio is always greater than or equal to the N_1 ratio, since the denominator remains the same and the numerator can only increase.

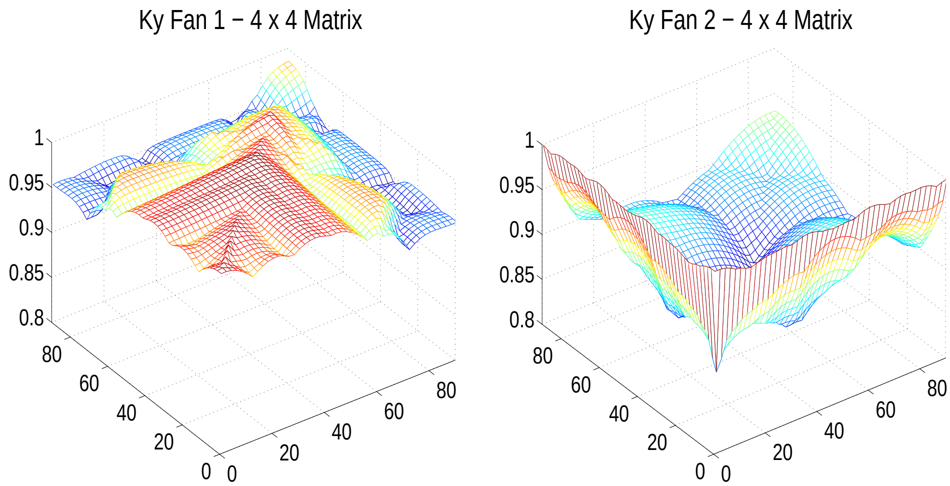

Fig. 1. Ky–Fan N_1 (left) and N_2 (right) Ratios

6 Conclusions

- A new simple proof of a sharp bound on the difference of the Rayleigh quotient with respect to a change in the vector is provided.
- We prove that the absolute value of the perturbations in the Ritz values is bounded by a constant times the gap between the original trial subspace and its perturbation, and we show that the constant is sharp.
- We generalize this result to unitarily invariant norms, but we have to increase the constant by a factor $\sqrt{2}$.
- Numerical results are consistent with our theorems and support our hypothesis that the $\sqrt{2}$ factor is artificial.

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