Open Mathematics

Research Article

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Rayleigh-Ritz Majorization Error Bounds for the Linear Response Eigenvalue Problem

Abstract: In the linear response eigenvalue problem arising from computational quantum chemistry and physics, one needs to compute a few of smallest positive eigenvalues together with the corresponding eigenvectors. For such a task, most of efficient algorithms are based on an important notion that is the so-called pair of deflating subspaces. If a pair of deflating subspaces is at hand, the computed approximated eigenvalues are partial eigenvalues of the linear response eigenvalue problem. In the case the pair of deflating subspaces is not available, only approximate one, in a recent paper [SIAM J. Matrix Anal. Appl., 35(2), pp.765-782, 2014], Zhang, Xue and Li obtained the relationships between the accuracy in eigenvalue approximations and the distances from the exact deflating subspaces to their approximate ones. In this paper, we establish majorization type results for these relationships. From our majorization results, various bounds are readily available to estimate how accurate the approximate eigenvalues based on information on the approximate accuracy of a pair of approximate deflating subspaces. These results will provide theoretical foundations for assessing the relative performance of certain iterative methods in the linear response eigenvalue problem.

Keywords: linear response eigenvalue problem, Rayleigh-Ritz approximation, canonical angles, majorization, error bounds

MSC: 65F15, 65L15

1 Introduction

In computational quantum chemistry and physics, the excitation states and absorption spectra for molecules or surface of solids are described by the random phase approximation (RPA) or the Bethe-Salpeter (BS) equation [1, 2]. One important question in RPA or BS equation is to compute a few eigenpairs associated with the smallest positive eigenvalues of the following eigenvalue problem:

$$\mathcal{H}w = \begin{bmatrix} A & B \\ -B & -A \end{bmatrix} \begin{bmatrix} u \\ v \end{bmatrix} = \lambda \begin{bmatrix} u \\ v \end{bmatrix} = \lambda w, \tag{1.1}$$

where $A, B \in \mathbb{R}^{n \times n}$ are both symmetric matrices and $\begin{bmatrix} A & B \\ B & A \end{bmatrix}$ is positive definite [3–5]. The matrix $\mathcal{H}$ in (1.1) is a special Hamiltonian matrix whose eigenvalues are real and in pairs $\{\lambda, -\lambda\}$. Therefore, we can order the $2n$ eigenvalues of $\mathcal{H}$ as

$$-\lambda_n \le \cdots \le -\lambda_1 < \lambda_1 \le \cdots \le \lambda_n. \tag{1.2}$$

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Through a similarity transformation, the eigenvalue problem (1.1) can be equivalently transformed into

$$Hz = \begin{bmatrix} 0 & K \\ M & 0 \end{bmatrix} \begin{bmatrix} y \\ x \end{bmatrix} = \lambda \begin{bmatrix} y \\ x \end{bmatrix} = \lambda z, \tag{1.3}$$

where $K = A - B$ and $M = A + B$ are both $n \times n$ real symmetric positive definite matrices. But, in consistent with [3], throughout the rest of paper, we relax the condition on K and M to that they are symmetric positive semi-definite and one of them is definite, unless explicitly stated differently. This means that possibly $\lambda_1 = 0$. This eigenvalue problem was still referred to as the linear response eigenvalue problem (LREP) [3, 6] and will be so in this paper, too. There are immense recent interest in developing new theories, efficient numerical algorithms of LREP and the associated excitation response calculations of molecules for materials design in energy science [7–10].

As the dimension n is usually very large, LREP (1.3) is generally solved by iterative methods, such as the Locally Optimal Block Preconditioned 4D Conjugate Gradient Method (LOBP4DCG) [6] and its space-extended variation [11], the block Chebyshev-Davidson method [12], and the generalized Lanczos type methods [13, 14]. These efficient numerical algorithms are all based on the concept of the so-called pair of deflating subspaces which is a generation of the invariant subspace in the standard eigenvalue problem. For given k-dimensional subspaces $\mathcal{X} \subseteq \mathbb{R}^n$ and $\mathcal{Y} \subseteq \mathbb{R}^n$, $\{\mathcal{X}, \mathcal{Y}\}$ is called a pair of deflating subspaces if they satisfy

$$K\mathcal{X} \subseteq \mathcal{Y} \quad \text{and} \quad M\mathcal{Y} \subseteq \mathcal{X}.$$

Whenever such a pair of deflating subspaces is available, LREP (1.3) can be projected into a much smaller problem in the form of (1.3) whose spectrum is part of that of H. That means a pair of deflating subspaces can be used to extract the eigenvalues corresponding to the deflating subspace pair. In practice, such a pair of exact deflating subspaces is usually not available, only approximate one, then the projection method computes good the approximate eigenvalues of LREP (1.3). Quantifying how good the approximate eigenvalues is the objective of this paper.

For the standard symmetric eigenvalue problem, there are existing results to estimate how well of such approximate eigenvalues may be; see [15–19]. For LREP (1.3), in [20], residual-based error bounds for approximate eigenvalues computed through the pair of approximated deflating subspaces are obtained. These results bound eigenvalue approximations characterized by the certain residuals. Another set of results also bound the eigenvalue errors in [21] but in terms of the canonical angles between the approximate deflating subspace pair and the exact pair. In this paper, we put forward two improvements to the Rayleigh-Ritz approximation theories in [21] by using weak majorization. The Rayleigh-Ritz majorization type eigenvalue error bounds have been well established in the symmetric eigenvalue problem; see [15, 17]. Compared with typical inequality results, majorization type bounds provide a succinct way to express numerous useful inequalities involving two vectors. The major goals of this paper are two-fold: to establish Rayleigh-Ritz majorization error bounds for LREP, and to extend our results by considering the unequal dimension between the exact and approximate pair of deflating subspaces. These improvements are helpful to understand how approximate eigenvalues move towards the associated exact eigenvalues in iterative methods of LREP.

The rest of the paper is organized as follows. In Section 2, some notations and preliminaries including the concept of majorization and the canonical angles of two subspaces are collected for use later. Section 3 contains our main results on how the vector of differences between the exact eigenvalues and their approximations is weakly majorized by the canonical angles from the exact to approximate pair of deflating subspaces. In Section 4, some numerical examples are presented to support our analysis. Finally, Conclusions are given in Section 5.

2 Preliminaries

2.1 Basic definitions

$\mathbb{R}^{m \times n}$ is the set of all $m \times n$ real matrices, $\mathbb{R}^n = \mathbb{R}^{n \times 1}$, and $\mathbb{R} = \mathbb{R}^1$. For $\mathcal{X} \subseteq \mathbb{R}^n$, $\dim(\mathcal{X})$ is the dimension of $\mathcal{X}$. For $X \in \mathbb{R}^{m \times n}$, X^T is its transpose, $\mathcal{R}(X)$ is the column space of X, and the submatrix $X_{(:,i:j)}$ of X consists of column i to column j. I_n is the $n \times n$ identity matrix or simply I if its dimension is clear from the context. For $x \in \mathbb{R}^n$ and $y \in \mathbb{R}^n$,

$$x_{(k:\ell)} = \begin{cases} [x_k, \ldots, x_n, \underbrace{0, \ldots, 0}_{\ell-n}]^T, & \text{for } k \le n < \ell, \\ [x_k, \ldots, x_\ell]^T, & \text{for } k \le \ell \le n, \end{cases}$$

the notation $x \le y$ is used to compare x with y componentwise, and $x \circ y = [x_1 y_1, \ldots, x_n y_n]^T$ denotes the Hadamard product of x and y, in particular, $x^{\circ 2} = x \circ x$. For scalars α_i, $\mathrm{diag}(\alpha_1, \alpha_2, \ldots, \alpha_k) \in \mathbb{R}^{k \times k}$ is a diagonal matrix with diagonal entries $\alpha_1, \alpha_2, \ldots, \alpha_k$.

For $x = [x_1, x_2, \ldots, x_n]^T \in \mathbb{R}^n$, $x^\downarrow = [x_1^\downarrow, x_2^\downarrow, \ldots, x_n^\downarrow]^T$ is the rearrangement of x_i in descending order, i.e., $x_1^\downarrow \ge x_2^\downarrow \ge \cdots \ge x_n^\downarrow$, and $x^\uparrow = [x_1^\uparrow, x_2^\uparrow, \ldots, x_n^\uparrow]^T$ represents x with its elements rearranged in ascending order. We use $\lambda(A) = \lambda^\downarrow(A)$ to denote the vector of eigenvalues of a symmetric matrix A arranged in descending order. $\sigma(B) = \sigma^\downarrow(B) = [\sigma_1(B), \sigma_2(B), \ldots, \sigma_n(B)]^T$ is denoted as the vector of singular values of $B \in \mathbb{R}^{m \times n}$ arranged in descending order, where $\sigma_i(B) \ge 0$ and $m \ge n$.

For vectors $x, y \in \mathbb{R}^n$, the usually inner product and its induced norm are defined by

$$\langle x, y \rangle = x^T y, \quad \|x\|_2 = \sqrt{\langle x, x \rangle}.$$

Consider two subspaces $\mathcal{X}$ and $\mathcal{Y}$ in $\mathbb{R}^n$, and suppose

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

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

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

The vector of cosines of canonical angels from[1] the subspace $\mathcal{X}$ to the subspace $\mathcal{Y}$ is defined by $\cos \Theta(\mathcal{X}, \mathcal{Y}) = \sigma^\uparrow(X^T Y)$ with

$$\Theta(\mathcal{X}, \mathcal{Y}) = \Theta^\downarrow(\mathcal{X}, \mathcal{Y}) = [\theta_1(\mathcal{X}, \mathcal{Y}), \ldots, \theta_k(\mathcal{X}, \mathcal{Y})]^T, \tag{2.2}$$

i.e., $\theta_1(\mathcal{X}, \mathcal{Y}) \ge \cdots \ge \theta_k(\mathcal{X}, \mathcal{Y})$. It is clear that $\Theta(\mathcal{X}, \mathcal{Y})$ so defined is invariant with respect to the different choice of the orthonormal basis matrices X and Y. Therefore, in what follows we sometimes place a matrix in one of or both arguments of $\theta_i(\cdot, \cdot)$ and $\Theta(\cdot, \cdot)$, with the understanding that it refers to the subspace spanned by the columns of the matrix argument.

Lemma 2.1 ([22, Proposition 2.1 and Proposition 2.4]). *Let $\mathcal{X}$ and $\mathcal{Y}$ be two subspaces in $\mathbb{R}^n$.*

(a) If $\dim(\mathcal{X}) = k \le \dim(\mathcal{Y}) = \ell$, for any $\widehat{\mathcal{Y}} \subseteq \mathcal{Y}$ with $\dim(\widehat{\mathcal{Y}}) = \dim(\mathcal{X}) = k$, we have $\Theta(\mathcal{X}, \widehat{\mathcal{Y}}) \ge \Theta(\mathcal{X}, \mathcal{Y})$. In addition, there exists a k-dimensional subspace $\widehat{\mathcal{Y}}_1 \subseteq \mathcal{Y}$ such that $\Theta(\mathcal{X}, \widehat{\mathcal{Y}}_1) = \Theta(\mathcal{X}, \mathcal{Y})$.
(b) If $\dim(\mathcal{X}) = \dim(\mathcal{Y}) = \ell$, for any $\widehat{\mathcal{X}} \subseteq \mathcal{X}$ with $\dim(\widehat{\mathcal{X}}) = k \le \ell$, we have $\Theta(\mathcal{X}, \mathcal{Y})_{(1:k)} \ge \Theta(\widehat{\mathcal{X}}, \mathcal{Y}) \ge \Theta(\mathcal{X}, \mathcal{Y})_{(\ell-k+1:\ell)}$.

Lemma 2.2 ([23, Proposition 2.2]). *Let $\mathcal{X}$ and $\mathcal{Y}$ be two subspaces in $\mathbb{R}^n$ satisfying* (2.1). *Then*

$$\theta_i(\mathcal{X}, \mathcal{Y}) = 0, \quad \text{for } k - m_0 + 1 \le i \le k,$$

where $m_0 = \dim(\mathcal{X} \cap \mathcal{Y})$.

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[1] If $k = \ell$, we say that the angles between subspaces $\mathcal{X}$ and $\mathcal{Y}$ [22].

Lemma 2.3 ([17, Theorem 4.7]). *Let $\mathcal{X}$ and $\mathcal{Y}$ be two subspaces in $\mathbb{R}^n$ with $\dim(\mathcal{X}) = \dim(\mathcal{Y}) = k$. Then,*
$\lambda\left(\Pi_{\mathcal{X}} - \Pi_{\mathcal{Y}}\right)_{(1:k)} = \sin\Theta(\mathcal{X}, \mathcal{Y})$, *where $\Pi_{\mathcal{X}}$ and $\Pi_{\mathcal{Y}}$ are orthogonal projectors onto subspaces $\mathcal{X}$ and $\mathcal{Y}$, respectively.*

For any given symmetric and positive definite matrix $W \in \mathbb{R}^{n \times n}$, the W-inner product and its induced W-norm are defined by

$$\langle x, y \rangle_W = y^\mathrm{T} W x, \quad \|x\|_W = \sqrt{\langle x, x \rangle_W}.$$

For two subspaces $\mathcal{X}$, $\mathcal{Y} \subseteq \mathbb{R}^n$ satisfying (2.1), let X and Y be the W-orthonormal basis matrices of subspaces $\mathcal{X}$ and $\mathcal{Y}$, respectively, i.e.,

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

Similarly to the standard canonical angles (2.2), we define

$$\cos\Theta_W(\mathcal{X}, \mathcal{Y}) = \sigma^\uparrow(X^\mathrm{T} W Y),$$

where

$$\Theta_W(\mathcal{X}, \mathcal{Y}) = \Theta_W^\downarrow(\mathcal{X}, \mathcal{Y}) = [\theta_W^{(1)}(\mathcal{X}, \mathcal{Y}), \dots, \theta_W^{(k)}(\mathcal{X}, \mathcal{Y})]^\mathrm{T}.$$

denotes the vector of the W-canonical angles from $\mathcal{X}$ to $\mathcal{Y}$ in descending order. Let $W = CC^\mathrm{T}$ with nonsingular $C \in \mathbb{R}^{n \times n}$. Then, by [24, Theorem 4.2],

$$\Theta_W(\mathcal{X}, \mathcal{Y}) = \Theta(C^\mathrm{T}\mathcal{X}, C^\mathrm{T}\mathcal{Y}). \tag{2.3}$$

Therefore, Lemmas 2.1 and 2.2 in which the standard canonical angles are simply replaced by W-canonical angles still hold.

2.2 Majorization and weak majorization

For $x, y \in \mathbb{R}^n$, we say that x is weakly majorized by y, in symbols $x \prec_w y$, if

$$\sum_{i=1}^k x_i^\downarrow \leq \sum_{i=1}^k y_i^\downarrow, \quad \text{for } 1 \leq k \leq n.$$

If in addition,

$$\sum_{i=1}^n x_i^\downarrow = \sum_{i=1}^n y_i^\downarrow,$$

we say that the vector x is (strongly) majorized by y, written $x \prec y$.

To facilitate our discussion, we collect several simple and general properties of the majorization and weak majorization in Lemma 2.4, and the reader is referred to [25] for proofs and more.

Lemma 2.4. *Let $x, y \in \mathbb{R}^n$ and $x \prec_w y$.*

(a) *If $y \leq z$, then $x \prec_w z$.*
(b) *If $u \prec_w v$, then $x + u \prec x^\downarrow + u^\downarrow \prec_w y + v$. This also holds with all $\prec_w$ replaced by $\prec$.*
(c) *If $u \in \mathbb{R}_+^n$, then $x^\downarrow \circ u^\downarrow \prec_w y^\downarrow \circ u^\downarrow$. In particular, if α is a positive real number, then $x \prec_w y$ implies $\alpha x \prec_w \alpha y$.*

The following lemmas on the majorization or weak majorization relations of eigenvalues and singular values are critical to our main results.

Lemma 2.5 ([25, Theorem II.3.6]). *Let A be an $n \times n$ matrix. We have $|\lambda(A)| \prec_w \sigma(A)$. In particular, if $A^\mathrm{T} = A$, we have $|\lambda(A)| = \sigma(A)$.*

Lemma 2.6 ([25, Exercise II.1.14])**.** *Let A and B be symmetric matrices. The eigenvalues of A, B and A+B satisfy $\lambda(A + B) \prec_w \lambda(A) + \lambda(B)$.*

Lemma 2.7 ([25, Corollary III.4.2])**.** *Let A and B be symmetric matrices. The eigenvalues of A, B and A − B satisfy $\lambda(A) - \lambda(B) \prec \lambda(A - B)$.*

Lemma 2.8 ([26, Theorem 1])**.** *For $B, D, E \in \mathbb{R}^{n \times n}$, we have*

$$\sigma(DBE^{\mathrm{T}}) \prec_w \sigma(B) \circ \delta^{\downarrow},$$

where δ is any vector which weakly majorizes $\sigma(D) \circ \sigma(E)$.

Lemma 2.8 implies that if $B \in \mathbb{R}^{n \times m}$, $D \in \mathbb{R}^{k \times n}$ and $E \in \mathbb{R}^{\ell \times m}$ where $k \le \ell \le m \le n$, then

$$\sigma(DBE^{\mathrm{T}}) \prec_w \sigma(B)_{(1:k)} \circ \sigma(D)_{(1:k)} \circ \sigma(E)_{(1:k)}. \tag{2.4}$$

The weakly majorization relationship (2.4) is obtained by extending B, D and E with zero blocks to $n \times n$ matrices. The extension with zero blocks only appends zero singular values and does not change the ranks.

3 Main results

Many theoretical properties of LREP (1.3) have been established in [3]. In particular, the following theorem presents decompositions on K and M, which is necessary for our later developments.

Lemma 3.1 ([3, Theorem 2.3])**.** *The following statements hold for any symmetric matrices K, $M \in \mathbb{R}^{n \times n}$ with M being positive definite.*

(a) There exists a nonsingular $\Psi \in \mathbb{R}^{n \times n}$ such that

$$K = \Psi \Lambda^2 \Psi^{\mathrm{T}} \quad and \quad M = \Phi \Phi^{\mathrm{T}}, \tag{3.1}$$

where $\Lambda = \mathrm{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$, $\lambda_1^2 \le \lambda_2^2 \le \cdots \le \lambda_n^2$ and $\Phi = \Psi^{-\mathrm{T}}$.
(b) If K is also definite, then all $\lambda_i > 0$ and H is diagonalizable:

$$H \begin{bmatrix} \Psi\Lambda & \Psi\Lambda \\ \Phi & -\Phi \end{bmatrix} = \begin{bmatrix} \Psi\Lambda & \Psi\Lambda \\ \Phi & -\Phi \end{bmatrix} \begin{bmatrix} \Lambda & \\ & \Lambda \end{bmatrix}.$$

(c) The eigen-decomposition of KM and MK are

$$(KM)\Psi = \Psi\Lambda^2 \quad and \quad (MK)\Phi = \Phi\Lambda^2,$$

respectively.

As we have introduced in Section 1, for two k-dimensional subspaces $\mathcal{X}$ and $\mathcal{Y}$ in $\mathbb{R}^n$, we call $\{\mathcal{X}, \mathcal{Y}\}$ a pair of deflating subspaces if

$$K\mathcal{X} \subseteq \mathcal{Y} \quad and \quad M\mathcal{Y} \subseteq \mathcal{X}. \tag{3.2}$$

Let $X, Y \in \mathbb{R}^{n \times k}$ be the basis matrices for $\mathcal{X}$ and $\mathcal{Y}$, respectively. Then (3.2) implies that there exist $K_{\mathrm{R}} \in \mathbb{R}^{k \times k}$ and $M_{\mathrm{R}} \in \mathbb{R}^{k \times k}$ such that

$$KX = YK_{\mathrm{R}} \quad and \quad MY = XM_{\mathrm{R}},$$

or equivalently,

$$H \begin{bmatrix} Y \\ & X \end{bmatrix} = \begin{bmatrix} Y \\ & X \end{bmatrix} H_{\mathrm{R}} \quad with \quad H_{\mathrm{R}} = \begin{bmatrix} & K_{\mathrm{R}} \\ M_{\mathrm{R}} & \end{bmatrix}.$$

Furthermore, if

$$H_{\mathrm{R}}\hat{z} = \begin{bmatrix} & K_{\mathrm{R}} \\ M_{\mathrm{R}} & \end{bmatrix} \begin{bmatrix} \hat{y} \\ \hat{x} \end{bmatrix} = \hat{\lambda} \begin{bmatrix} \hat{y} \\ \hat{x} \end{bmatrix} = \hat{\lambda}\hat{z},$$

then $(\hat{\lambda}, \begin{bmatrix} Y\hat{y} \\ X\hat{x} \end{bmatrix})$ is an eigenpair of H.

Roughly speaking, most of efficient algorithms for LREP usually generate a sequence of approximate deflating subspace pairs that hopefully converge to or contain subspaces near the pair of deflating subspaces associated with the first few smallest λ_i. Therefore, in the rest of the paper, we focus on the pair of deflating subspaces $\{\mathcal{R}(\Phi_1), \mathcal{R}(\Psi_1)\}$ where $\Phi_1 = \Phi_{(:,1:k)}$ and $\Psi_1 = \Psi_{(:,1:k)}$, and let $\{\mathcal{U}, \mathcal{V}\}$ satisfying

$$\dim(\mathcal{U}) = \dim(\mathcal{V}) = \ell \geq k \quad \text{and} \quad \theta_1(\mathcal{U}, \mathcal{V}) < \frac{\pi}{2} \tag{3.3}$$

be a pair of approximate deflating subspaces of $\{\mathcal{R}(\Phi_1), \mathcal{R}(\Psi_1)\}$ if $\ell = k$, or, if $\ell > k$, contain a k-dimensional subspace pair approximating $\{\mathcal{R}(\Phi_1), \mathcal{R}(\Psi_1)\}$. Let $U, V \in \mathbb{R}^{n \times \ell}$ be any basis matrices for $\mathcal{U}$ and $\mathcal{V}$, respectively. Then, the condition $\theta_1(\mathcal{U}, \mathcal{V}) < \pi/2$ implies $U^{\mathrm{T}}V$ being nonsingular. By [6], the best approximation eigenpairs in sense of the trace minimization principle are obtained via computing the eigenpairs of

$$H_{\mathrm{SR}} = \begin{bmatrix} & K_{\mathrm{SR}} \\ M_{\mathrm{SR}} & \end{bmatrix},$$

where $K_{\mathrm{SR}} = W_1^{-\mathrm{T}}U^{\mathrm{T}}KUW_1^{-1}$, $M_{\mathrm{SR}} = W_2^{-\mathrm{T}}V^{\mathrm{T}}MVW_2^{-1}$, and $W_1, W_2 \in \mathbb{R}^{\ell \times \ell}$ are from factorizing $U^{\mathrm{T}}V = W_1^{\mathrm{T}}W_2$ and nonsingular. In particular, if $U^{\mathrm{T}}V = I_\ell$, then H_{SR} becomes

$$H_{\mathrm{SR}} = \begin{bmatrix} & U^{\mathrm{T}}KU \\ V^{\mathrm{T}}MV & \end{bmatrix}.$$

Notice that H_{SR} so defined is of LREP type since both K_{SR} and M_{SR} are symmetric and have the same definiteness property as their corresponding K and M. Therefore, we can denote its eigenvalues by

$$-\mu_\ell \leq \cdots \leq -\mu_1 \leq \mu_1 \leq \cdots \leq \mu_\ell,$$

in which some of μ_i should be good approximate eigenvalues of H. Moreover, by [3, Theorem 2.9], these eigenvalues of H_{SR} are independence of the basis matrices U and V, and factorization $U^{\mathrm{T}}V = W_1^{\mathrm{T}}W_2$ which is not unique. Now, we would like to bound the errors in μ_i as approximations to λ_i for $1 \leq i \leq k$ in terms of the distances from $\{\mathcal{R}(\Phi_1), \mathcal{R}(\Psi_1)\}$ to $\{\mathcal{U}, \mathcal{V}\}$. For the purpose, Zhang, Xue and Li in [21] established an inequality in the case $\ell = k$, i.e.,

$$\sum_{i=1}^{k}(\mu_i^2 - \lambda_i^2) \leq \tan^2 \theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V}) \sum_{i=1}^{k} \lambda_i^2 + \frac{\lambda_n^2 - \lambda_1^2}{\cos^2 \theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V})} \| \sin \Theta_{M^{-1}}(\mathcal{U}, \Phi_1)\|_2^2. \tag{3.4}$$

We first continue the effort to extend the result by using the weak majorization replacing the traditional inequality in (3.4). To prove our main results, we also need the following lemma to provide special basis matrices for the pair $\{\mathcal{U}, \mathcal{V}\}$ which are used in the proof of [21, Theorem 3.1].

Lemma 3.2. *Let $\mathcal{U}, \mathcal{V} \subseteq \mathbb{R}^n$ satisfy (3.3) and $\ell = k$. These exist basis matrices $U, V \in \mathbb{R}^{n \times k}$ of $\mathcal{U}$ and $\mathcal{V}$, respectively, and an orthonormal matrix $P \in \mathbb{R}^{n \times n}$ such that*

$$U^{\mathrm{T}}V = I_k, \quad \widetilde{U} = \Psi^{\mathrm{T}}U = P^{\mathrm{T}} \begin{bmatrix} \Gamma^{-1} \\ 0 \end{bmatrix}, \quad \widetilde{V} = \Phi^{\mathrm{T}}V = P^{\mathrm{T}} \begin{bmatrix} \Gamma \\ \Sigma \end{bmatrix}, \tag{3.5}$$

where $\Gamma = \mathrm{diag}(\gamma_1, \ldots, \gamma_k)$ with $\gamma_i = \cos \theta_{M^{-1}}^{(i)}(\mathcal{U}, M\mathcal{V})$ for $1 \leq i \leq k$ and
– for $2k \leq n$,

$$\Sigma = \begin{matrix} k \\ n-2k \end{matrix} \begin{bmatrix} \overset{k}{\widetilde{\Sigma}} \\ 0 \end{bmatrix}, \quad \widetilde{\Sigma} = \mathrm{diag}\left(\sin \theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V}), \ldots, \sin \theta_{M^{-1}}^{(k)}(\mathcal{U}, M\mathcal{V})\right),$$

- *for $2k > n$,*

$$\Sigma = {}_{n-k}\left[\overset{n-k\;\;2k-n}{\begin{array}{cc}\widetilde{\Sigma} & 0\end{array}}\right], \quad \widetilde{\Sigma} = \mathrm{diag}\left(\sin\theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V}), \ldots, \sin\theta_{M^{-1}}^{(n-k)}(\mathcal{U}, M\mathcal{V})\right).$$

Theorem 3.1. *Let $\{\mathcal{U}, \mathcal{V}\}$ satisfying (3.3) with $\ell = k$ be an approximation to $\{\mathcal{R}(\Phi_1), \mathcal{R}(\Psi_1)\}$, $\mu = [\mu_k, \ldots, \mu_1]^T$ and $\lambda = [\lambda_k, \ldots, \lambda_1]^T$. Assume that M is definite. We have*

$$0 \le \mu^{\circ 2} - \lambda^{\circ 2} \prec_w \delta \circ \sin^{\circ 2}\Theta_{M^{-1}}(\mathcal{U}, \Phi_1) + \tan^2\theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V})\,\lambda^{\circ 2}, \tag{3.6}$$

where $\delta = \left[\left(\dfrac{\lambda_n^2}{\cos^2\theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V})} - \dfrac{\lambda_1^2}{\cos^2\theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V})}\right), \ldots, \left(\dfrac{\lambda_{n-k+1}^2}{\cos^2\theta_{M^{-1}}^{(k)}(\mathcal{U}, M\mathcal{V})} - \dfrac{\lambda_1^2}{\cos^2\theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V})}\right)\right]^T.$

Proof. Since the eigenvalues of H_{SR} are unchanged with different choices of the basis matrices for $\mathcal{U}$ and $\mathcal{V}$, we choose the basis matrices U and V as mentioned in Lemma 3.2. Let $\widetilde{U}, \widetilde{V}, P,$ and Γ be defined in Lemma 3.2. Partition $P, \widetilde{U}$ and Λ as

$$P = \begin{array}{c}k \\ n-k\end{array}\left[\overset{k\quad\;\;n-k}{\begin{array}{cc}P_{11} & P_{12} \\ P_{21} & P_{22}\end{array}}\right], \quad \widetilde{U} = \begin{array}{c}k \\ n-k\end{array}\left[\overset{k}{\begin{array}{c}\widetilde{U}_1 \\ \widetilde{U}_2\end{array}}\right], \quad \Lambda = \begin{array}{c}k \\ n-k\end{array}\left[\overset{k\quad n-k}{\begin{array}{cc}\Lambda_1 & \\ & \Lambda_2\end{array}}\right]. \tag{3.7}$$

Then, it follows by (3.5) that,

$$\widetilde{U}_1 = P_{11}^T\Gamma^{-1}, \quad \widetilde{U}_2 = P_{12}^T\Gamma^{-1}, \quad \widetilde{U}^T\widetilde{V} = I_k, \quad \widetilde{V}^T\widetilde{V} = I_k. \tag{3.8}$$

If $2k > n$, we caution the reader that here $\gamma_i = \cos\theta_{M^{-1}}^{(i)}(\mathcal{U}, M\mathcal{V}) = 1$ for $n - k + 1 \le i \le k$ by Lemma 2.2 are used to prove $\widetilde{V}^T\widetilde{V} = I_k$. Notice that $M^{-1} = \Psi\Psi^T$, $\mathcal{R}\left(\widetilde{U}\right) = \mathcal{R}\left(\begin{bmatrix}P_{11}^T \\ P_{12}^T\end{bmatrix}\right)$ and $P_{12}P_{12}^T = I_k - P_{11}P_{11}^T$. Thus, by (2.3), we have

$$\cos\Theta_{M^{-1}}(U, \Phi_1) = \cos\Theta(\widetilde{U}, I_{(:,1:k)}) = \cos\Theta\left(\begin{bmatrix}P_{11}^T \\ P_{12}^T\end{bmatrix}, \begin{bmatrix}I_k \\ 0\end{bmatrix}\right) = \sigma^\uparrow(P_{11}), \tag{3.9}$$

$$\sin\Theta_{M^{-1}}(U, \Phi_1) = \sqrt{e - \sigma^\uparrow(P_{11}P_{11}^T)} = \sqrt{\lambda(I_k - P_{11}P_{11}^T)} = \sqrt{\lambda(P_{12}P_{12}^T)}, \tag{3.10}$$

where $e = [\underbrace{1, \ldots, 1}_{k}]^T$.

By Lemma 3.1, $K = \Psi\Lambda^2\Psi^T$, $M = \Phi\Phi^T$, $\mu^{\circ 2} = \lambda\left((U^TKU)(V^TMV)\right)$ and $\lambda^{\circ 2} = \lambda(\Lambda_1^2)$. Therefore, by $\lambda \le \mu$ known in [3, Theorem 4.1], we have

$$\begin{aligned}0 \le \mu^{\circ 2} - \lambda^{\circ 2} &= \lambda\left((U^TKU)(V^TMV)\right) - \lambda(\Lambda_1^2) \\ &= \lambda\left(\widetilde{U}^T\Lambda^2\widetilde{U}\widetilde{V}^T\widetilde{V}\right) - \lambda(\Lambda_1^2) = \lambda\left(\widetilde{U}^T\Lambda^2\widetilde{U}\right) - \lambda(\Lambda_1^2) \quad\quad \text{(by (3.8))} \\ &= \lambda\left(\widetilde{U}_1^T\Lambda_1^2\widetilde{U}_1 + \widetilde{U}_2^T\Lambda_2^2\widetilde{U}_2\right) - \lambda(\Lambda_1^2) \\ &= \lambda\left(\widetilde{U}_1^T\Lambda_1^2\widetilde{U}_1 + \widetilde{U}_2^T\Lambda_2^2\widetilde{U}_2\right) - \lambda(\widetilde{U}_1^T\Lambda_1^2\widetilde{U}_1) + \lambda(\widetilde{U}_1^T\Lambda_1^2\widetilde{U}_1) - \lambda(\Lambda_1^2) \\ &\prec \lambda(\widetilde{U}_2^T\Lambda_2^2\widetilde{U}_2) + \left(\lambda(\widetilde{U}_1^T\Lambda_1^2\widetilde{U}_1) - \lambda(\Lambda_1^2)\right)^\downarrow. \end{aligned} \tag{3.11}$$

The last line holds because of Lemmas 2.4(b) and 2.7. Now, we bound separately the two terms in the sum on the right-hand side of the last line. We start with the first term. By (3.10), and Lemmas 2.4(c), 2.5 and 2.8, we get

$$\begin{aligned}\lambda(\widetilde{U}_2^T\Lambda_2^2\widetilde{U}_2) = \lambda(\Lambda_2^2\widetilde{U}_2\widetilde{U}_2^T)_{(1:k)} &\prec_w \sigma(\Lambda_2^2\widetilde{U}_2\widetilde{U}_2^T)_{(1:k)} \\ &\prec_w \sigma(\Lambda_2^2)_{(1:k)} \circ \sigma(\widetilde{U}_2\widetilde{U}_2^T)_{(1:k)}\end{aligned}$$

$$
\begin{aligned}
&= \sigma(\Lambda_2^2)_{(1:k)} \circ \sigma(P_{12}^{\mathrm{T}} \Gamma^{-1} \Gamma^{-\mathrm{T}} P_{12})_{(1:k)} \\
&\prec_w \sigma(\Lambda_2^2)_{(1:k)} \circ \sigma(P_{12}^{\mathrm{T}})_{(1:k)} \circ \sigma(\Gamma^{-1}\Gamma^{-\mathrm{T}}) \circ \sigma(P_{12})_{(1:k)} \\
&= \sigma(\Lambda_2^2)_{(1:k)} \circ \sigma(\Gamma^{-2}) \circ \sin^{\circ 2} \Theta_{M^{-1}}(U, \Phi_1).
\end{aligned} \tag{3.12}
$$

Considering the second term, by (3.8), and Lemmas 2.4 and 2.7, we have

$$
\begin{aligned}
\lambda(\widetilde{U}_1^{\mathrm{T}} \Lambda_1^2 \widetilde{U}_1) - \lambda(\Lambda_1^2) &= \lambda(\Lambda_1 \widetilde{U}_1 \widetilde{U}_1^{\mathrm{T}} \Lambda_1) - \lambda(\Lambda_1^2) = \lambda(\Lambda_1 P_{11}^{\mathrm{T}} \Gamma^{-1} \Gamma^{-\mathrm{T}} P_{11} \Lambda_1) - \lambda(\Lambda_1^2) \\
&\leq \frac{1}{\gamma_1^2} \lambda(\Lambda_1 P_{11}^{\mathrm{T}} P_{11} \Lambda_1) - \lambda(\Lambda_1^2) \\
&= \frac{1}{\gamma_1^2} \lambda(\Lambda_1 P_{11}^{\mathrm{T}} P_{11} \Lambda_1) - \frac{1}{\gamma_1^2} \lambda(\Lambda_1^2) + \frac{1-\gamma_1^2}{\gamma_1^2} \lambda(\Lambda_1^2) \\
&\prec \frac{1}{\gamma_1^2} \lambda\left(\Lambda_1(P_{11}^{\mathrm{T}} P_{11} - I_k)\Lambda_1\right) + \frac{1-\gamma_1^2}{\gamma_1^2} \lambda(\Lambda_1^2) \\
&= \frac{1}{\gamma_1^2} \lambda\left((I_k - P_{11}^{\mathrm{T}} P_{11})^{1/2}(-\Lambda_1^2)(I_k - P_{11}^{\mathrm{T}} P_{11})^{1/2}\right) + \frac{1-\gamma_1^2}{\gamma_1^2} \lambda(\Lambda_1^2) \\
&\leq \frac{-\lambda_1^2}{\gamma_1^2} \lambda(I_k - P_{11}^{\mathrm{T}} P_{11}) + \frac{1-\gamma_1^2}{\gamma_1^2} \lambda(\Lambda_1^2) \\
&= \frac{-\lambda_1^2}{\gamma_1^2} \left(e - \lambda^{\uparrow}(P_{11}^{\mathrm{T}} P_{11})\right) + \frac{1-\gamma_1^2}{\gamma_1^2} \lambda(\Lambda_1^2) \\
&= \frac{-\lambda_1^2}{\gamma_1^2} \left(e - \cos^{\circ 2} \Theta_{M^{-1}}(U, \Phi_1)\right) + \frac{1-\gamma_1^2}{\gamma_1^2} \lambda(\Lambda_1^2) \\
&= \frac{-\lambda_1^2}{\gamma_1^2} \sin^{\circ 2} \Theta_{M^{-1}}(U, \Phi_1) + \frac{1-\gamma_1^2}{\gamma_1^2} \lambda(\Lambda_1^2).
\end{aligned} \tag{3.13}
$$

At last, (3.11), (3.12) and (3.13) together give

$$
\begin{aligned}
\mu^2 - \lambda^2 &= \lambda\left((U^{\mathrm{T}} K U)(V^{\mathrm{T}} M V)\right) - \lambda(\Lambda_1^2) \\
&\prec_w \sigma(\Lambda_2^2)_{(1:k)} \circ \sigma(\Gamma^{-2}) \circ \sin^{\circ 2} \Theta_{M^{-1}}(U, \Phi_1) - \frac{\lambda_1^2}{\gamma_1^2} \sin^{\circ 2} \Theta_{M^{-1}}(U, \Phi_1) + \frac{1-\gamma_1^2}{\gamma_1^2} \lambda(\Lambda_1^2) \\
&= \left(\sigma(\Lambda_2^2)_{(1:k)} \circ \sigma(\Gamma^{-2}) - \frac{\lambda_1^2}{\gamma_1^2} e\right) \sin^{\circ 2} \Theta_{M^{-1}}(U, \Phi_1) + \tan^2 \theta_{M^{-1}}^{(1)}(U, MV)\lambda(\Lambda_1^2),
\end{aligned} \tag{3.14}
$$

which leads to (3.6). □

Remark 3.1. Listed below are some comments for Theorem 3.1.

(a) Recall (3.6) and (3.14). It is noted that, if $2k > n$, $\sigma(\Lambda_2^2)_{(1:k)} = [\lambda_n^2, \ldots, \lambda_{k+1}^2, \underbrace{0, \ldots, 0}_{2k-n}]^{\mathrm{T}}$ in (3.14) is not equal

to $[\lambda_n^2, \ldots, \lambda_{k+1}^2, \underbrace{\lambda_k^2, \ldots, \lambda_{n-k+1}^2}_{2k-n}]^{\mathrm{T}}$ in δ of (3.6). In fact, in such a case, the last $2k - n$ entries of $\Theta_{M^{-1}}(\mathcal{U}, \Phi_1)$

are all zero by Lemma 2.2. Thus, the weak majorization relationship (3.6) still holds for the case $2k > n$.

(b) The weak majorization bound (3.6) directly implies that, for $j = 1, \ldots, k$,

$$
\begin{aligned}
\sum_{i=1}^{j}(\mu_i^2 - \lambda_i^2)^{\downarrow} &\leq \sum_{i=1}^{j} \left(\frac{\lambda_{n-i+1}^2}{\cos^2 \theta_{M^{-1}}^{(i)}(\mathcal{U}, M\mathcal{V})} - \frac{\lambda_1^2}{\cos^2 \theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V})}\right) \sin^2 \theta_{M^{-1}}^{(i)}(\mathcal{U}, \Phi_1) \\
&\quad + \tan^2 \theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V}) \sum_{i=1}^{j} \lambda_i^2 \\
&\leq \frac{\lambda_n^2 - \lambda_1^2}{\cos^2 \theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V})} \sum_{i=1}^{j} \sin^2 \theta_{M^{-1}}^{(i)}(\mathcal{U}, \Phi_1) + \tan^2 \theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V}) \sum_{i=1}^{j} \lambda_i^2.
\end{aligned} \tag{3.15}
$$

Two implied inequalities by (3.15) that are often sufficient for numerical purposes are (3.4) and

$$\max_{1\le i\le k}(u_i^2 - \lambda_i^2) \le \frac{\lambda_n^2 - \lambda_1^2}{\cos^2\theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V})}\sin^2\theta_{M^{-1}}^{(1)}(\mathcal{U}, \Phi_1) + \lambda_1^2\tan^2\theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V}).$$

(c) In some numerical methods for LREP, such as the first Lanczos method [13, 27] and Chebyshev-Davidson method [12], the subspace $\mathcal{U}$ is chosen such that $\mathcal{U} = M\mathcal{V}$, which leads to $\cos\theta_{M^{-1}}^{(i)}(\mathcal{U}, M\mathcal{V}) = 1$ for $1 \le i \le k$ and $\tan\theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V}) = 0$. Then, the majorization relationship (3.6) reduces to

$$0 \le \mu^{\circ 2} - \lambda^{\circ 2} \prec_w [(\lambda_n^2 - \lambda_1^2), \dots, (\lambda_{n-k+1}^2 - \lambda_1^2)]^{\mathsf{T}} \circ \sin^{\circ 2}\Theta_{M^{-1}}(\mathcal{U}, \Phi_1).$$

(d) Suppose that K is definite. Then, a simple modification by exchanging the roles of K and M in the above proof leads to the following majorization relationship

$$0 \le \mu^{\circ 2} - \lambda^{\circ 2} \prec_w \delta_K \circ \sin^{\circ 2}\Theta_{K^{-1}}(\mathcal{V}, \widehat{\Psi}_1) + \tan^2\theta_{K^{-1}}^{(1)}(\mathcal{V}, K\mathcal{U})\lambda^{\circ 2}, \tag{3.16}$$

where $\delta_K = \left[\left(\frac{\lambda_n^2}{\cos^2\theta_{K^{-1}}^{(1)}(\mathcal{V}, K\mathcal{U})} - \frac{\lambda_1^2}{\cos^2\theta_{K^{-1}}^{(1)}(\mathcal{V}, K\mathcal{U})}\right), \dots, \left(\frac{\lambda_{n-k+1}^2}{\cos^2\theta_{K^{-1}}^{(k)}(\mathcal{V}, K\mathcal{U})} - \frac{\lambda_1^2}{\cos^2\theta_{K^{-1}}^{(1)}(\mathcal{V}, K\mathcal{U})}\right)\right]^{\mathsf{T}}$ and $\widehat{\Psi}_1 = \widehat{\Psi}_{(:,1:k)}$ coming from the new decompositions $M = \widehat{\Phi}\Lambda^2\widehat{\Phi}^{\mathsf{T}}$ and $K = \widehat{\Psi}\widehat{\Psi}^{\mathsf{T}}$ instead of (3.1). In particular, if M is also definite, there is no need to distinguish Ψ from $\widehat{\Psi}$ in (3.16) because of $\mathcal{R}(\Psi) = \mathcal{R}(\widehat{\Psi})$.

As stated in [21, Example 3.1], if $\Theta_{M^{-1}}(\mathcal{U}, \Phi_1) = 0$, then $\mu^2 - \lambda^2 = 0$. However, $\Theta_{M^{-1}}(\mathcal{U}, M\mathcal{V})$ is not necessary being 0 because of the indefiniteness of K. This phenomenon is overcome under the assumption that K and M are both definite, and in the following theorem, we will establish the associated majorization upper bounds for $\sin\Theta_{M^{-1}}(\mathcal{U}, M\mathcal{V})$ and $\sin\Theta_{K^{-1}}(\mathcal{V}, K\mathcal{U})$, respectively, by using $\sin\Theta_{M^{-1}}(\mathcal{U}, \Phi_1)$ and $\sin\Theta_{K^{-1}}(\mathcal{V}, \Psi_1)$.

Theorem 3.2. *Let $\{\mathcal{U}, \mathcal{V}\}$ satisfy (3.3) and $\ell = k$. Suppose both K and M being definite. We have*

$$\sin\Theta_{M^{-1}}(\mathcal{U}, M\mathcal{V}) \prec_w \sin\Theta_{M^{-1}}(\mathcal{U}, \Phi_1) + \kappa \circ \sin\Theta_{K^{-1}}(\mathcal{V}, \Psi_1), \tag{3.17}$$
$$\sin\Theta_{K^{-1}}(\mathcal{V}, K\mathcal{U}) \prec_w \sin\Theta_{K^{-1}}(\mathcal{V}, \Psi_1) + \kappa \circ \sin\Theta_{M^{-1}}(\mathcal{U}, \Phi_1), \tag{3.18}$$

where $\kappa = \left[\frac{\lambda_n}{\lambda_1}, \dots, \frac{\lambda_{n-k+1}}{\lambda_k}\right]^{\mathsf{T}}$.

Proof. Use the same notations and basis matrices U and V for $\mathcal{U}$ and $\mathcal{V}$, respectively, as the proof of Theorem 3.1. Partition $\widetilde{U}$, P and Λ as in (3.7) and $\widetilde{V}$ as

$$\widetilde{V} = \begin{matrix} k \\ n-k \end{matrix}\begin{bmatrix} \overset{k}{\widetilde{V}_1} \\ \widetilde{V}_2 \end{bmatrix}.$$

Thus, by (2.3) and (3.9),

$$\sin\Theta_{M^{-1}}(U, \Phi_1) = \sin\Theta(\widetilde{U}, I_{(:,1:k)}) = \sin\Theta\left(\begin{bmatrix} P_{11}^{\mathsf{T}} \\ P_{12}^{\mathsf{T}} \end{bmatrix}, \begin{bmatrix} I_k \\ 0 \end{bmatrix}\right) = \sigma(P_{12})_{(1:k)}, \tag{3.19}$$

$$\sin\Theta_{K^{-1}}(V, \Psi_1) = \sin\Theta(\Lambda^{-1}\widetilde{V}, I_{(:,1:k)}) = \sigma\left(\Lambda_2^{-1}\widetilde{V}_2(\widetilde{V}^{\mathsf{T}}\Lambda^{-2}\widetilde{V})^{-1/2}\right)_{(1:k)}. \tag{3.20}$$

The first equality in (3.20) holds because $\mathcal{R}(I_{(:,1:k)}) = \mathcal{R}(\Lambda^{-1}I_{(:,1:k)})$. By Lemmas 2.3 and 2.6,

$$\sin\Theta_{M^{-1}}(U, MV) = \sin\Theta(\widetilde{U}, \widetilde{V}) = \lambda(\Pi_{\mathcal{R}(\widetilde{U})} - \Pi_{\mathcal{R}(\widetilde{V})})_{(1:k)}$$
$$= \lambda\left(\Pi_{\mathcal{R}(\widetilde{U})} - I_{(:,1:k)}I_{(:,1:k)}^{\mathsf{T}} + I_{(:,1:k)}I_{(:,1:k)}^{\mathsf{T}} - \Pi_{\mathcal{R}(\widetilde{V})}\right)_{(1:k)}$$
$$\prec_w \lambda\left(\Pi_{\mathcal{R}(\widetilde{U})} - I_{(:,1:k)}I_{(:,1:k)}^{\mathsf{T}}\right)_{(1:k)} + \lambda\left(I_{(:,1:k)}I_{(:,1:k)}^{\mathsf{T}} - \Pi_{\mathcal{R}(\widetilde{V})}\right)_{(1:k)}$$

$$= \sin \Theta(\widetilde{U}, I_{(:,1:k)}) + \sin \Theta(I_{(:,1:k)}, \widetilde{V}). \tag{3.21}$$

Now, we need to relate $\sin \Theta(I_{(:,1:k)}, \widetilde{V})$ to $\sin \Theta(\Lambda^{-1}\widetilde{V}, I_{(:,1:k)})$. It follows by $\widetilde{V}^{\mathrm{T}}\widetilde{V} = I_k$ and Lemma 2.8 that

$$
\begin{aligned}
\sin \Theta(I_{(:,1:k)}, \widetilde{V}) = \sigma(\widetilde{V}_2)_{(1:k)} &= \sigma \left(\Lambda_2 \Lambda_2^{-1} \widetilde{V}_2 (\widetilde{V}^{\mathrm{T}} \Lambda^{-2} \widetilde{V})^{-1/2} (\widetilde{V}^{\mathrm{T}} \Lambda^{-2} \widetilde{V})^{1/2} \right)_{(1:k)} \\
&\prec_w \sigma(\Lambda_2)_{(1:k)} \circ \sigma \left(\Lambda_2^{-1} \widetilde{V}_2 (\widetilde{V}^{\mathrm{T}} \Lambda^{-2} \widetilde{V})^{-1/2} \right)_{(1:k)} \circ \sigma \left((\widetilde{V}^{\mathrm{T}} \Lambda^{-2} \widetilde{V})^{1/2} \right) \\
&\le \sigma(\Lambda_2)_{(1:k)} \circ \sigma \left(\Lambda_2^{-1} \widetilde{V}_2 (\widetilde{V}^{\mathrm{T}} \Lambda^{-2} \widetilde{V})^{-1/2} \right)_{(1:k)} \circ \sigma(\Lambda^{-1})_{(1:k)} \\
&= \kappa \circ \sin \Theta(\Lambda^{-1}\widetilde{V}, I_{(:,1:k)}).
\end{aligned} \tag{3.22}
$$

Then, (3.19), (3.20), (3.21) and (3.22) together yield (3.17). Similarly, to prove (3.18), we consider

$$
\begin{aligned}
\sin \Theta_{K^{-1}}(V, KU) = \sin \Theta(\Lambda^{-1}\Phi^{\mathrm{T}}V, \Lambda^{-1}\Phi^{\mathrm{T}}KU) &= \sin \Theta(\Lambda^{-1}\widetilde{V}, \Lambda\widetilde{U}) \\
&= \lambda(\Pi_{\mathcal{R}(\Lambda^{-1}\widetilde{V})} - \Pi_{\mathcal{R}(\Lambda\widetilde{U})})_{(1:k)} \\
&= \lambda \left(\Pi_{\mathcal{R}(\Lambda^{-1}\widetilde{V})} - I_{(:,1:k)}I_{(:,1:k)}^{\mathrm{T}} + I_{(:,1:k)}I_{(:,1:k)}^{\mathrm{T}} - \Pi_{\mathcal{R}(\Lambda\widetilde{U})} \right)_{(1:k)} \\
&\prec_w \lambda \left(\Pi_{\mathcal{R}(\Lambda^{-1}\widetilde{V})} - I_{(:,1:k)}I_{(:,1:k)}^{\mathrm{T}} \right)_{(1:k)} + \lambda \left(I_{(:,1:k)}I_{(:,1:k)}^{\mathrm{T}} - \Pi_{\mathcal{R}(\Lambda\widetilde{U})} \right)_{(1:k)} \\
&= \sin \Theta(\Lambda^{-1}\widetilde{V}, I_{(:,1:k)}) + \sin \Theta(I_{(:,1:k)}, \Lambda\widetilde{U}),
\end{aligned} \tag{3.23}
$$

and clarify the majorization relationship between $\sin \Theta(I_{(:,1:k)}, \Lambda\widetilde{U})$ with $\sin \Theta(\widetilde{U}, I_{(:,1:k)})$, i.e.,

$$
\begin{aligned}
\sin \Theta(I_{(:,1:k)}, \Lambda\widetilde{U}) = \sin \Theta(I_{(:,1:k)}, \Lambda P_1) &= \sigma \left(\Lambda_2 P_{12}^{\mathrm{T}} (P_1^{\mathrm{T}} \Lambda^2 P_1)^{-1/2} \right)_{(1:k)} \\
&\prec_w \sigma(\Lambda_2)_{(1:k)} \circ \sigma(P_{12}^{\mathrm{T}})_{(1:k)} \circ \sigma \left((P_1^{\mathrm{T}} \Lambda^2 P_1)^{-1/2} \right) \\
&\le \sigma(\Lambda_2)_{(1:k)} \circ \sigma(P_{12})_{(1:k)} \circ \sigma(\Lambda^{-1})_{(1:k)} \\
&= \kappa \circ \sin \Theta_{M^{-1}}(U, \Phi_1),
\end{aligned} \tag{3.24}
$$

where $P_1 = [P_{11}, P_{12}]^{\mathrm{T}}$. At last, (3.18) is obtained by combining (3.19), (3.20), (3.23) and (3.24). $\square$

Theorems 3.1 and 3.2 are established in assuming $\ell = k$. But, the case $\ell > k$ is more common in practical eigenvalue computations of LREP, e.g., in the first Lanczos type method for LREP, the subspaces $\mathcal{U}$ and $\mathcal{V}$ are the Krylov subspaces generated by initial vectors $v_0 \in \mathbb{R}^n$ and $u_0 = Mv_0$, i.e., $\mathcal{U} = \mathcal{K}_\ell(MK, u_0)$ and $\mathcal{V} = \mathcal{K}_\ell(KM, v_0)$, and usually the pair of Krylov subspaces $\{\mathcal{U}, \mathcal{V}\}$ as a whole is not close to any pair of deflating subspaces but more likely it contains a subspace pair of lower dimension being a good approximation of $\{\mathcal{R}(\Phi_1), \mathcal{R}(\Psi_1)\}$. Thus, it is natural to generalize Theorems 3.1 and 3.2 for the case $\ell > k$. This gives Theorem 3.3 and 3.4 below. Similar comments we made in Remark 3.1 are also valid for Theorem 3.3.

Theorem 3.3. *Let $\{\mathcal{U}, \mathcal{V}\}$ satisfying (3.3) contain a pair of k-dimensional subspaces approximating $\{\mathcal{R}(\Phi_1), \mathcal{R}(\Psi_1)\}$. Assume that M is definite. Using the notations of Theorem 3.1, we have*

$$0 \le \mu^2 - \lambda^2 \prec_w \frac{\omega}{\cos^2 \theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V})} \circ \sin^{\circ 2} \Theta_{M^{-1}}(\mathcal{U}, \Phi_1) + \tan^2 \theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V}) \lambda^{\circ 2}, \tag{3.25}$$

where $\omega = \left[(\lambda_n^2 - \lambda_1^2), \dots, (\lambda_{n-k+1}^2 - \lambda_1^2) \right]^{\mathrm{T}}$.

Proof. By Lemma 2.1(a), we choose k-dimensional subspaces $\mathcal{U}_1 \subset \mathcal{U}$ satisfying

$$\Theta_{M^{-1}}(\mathcal{U}_1, \Phi_1) = \Theta_{M^{-1}}(\mathcal{U}, \Phi_1), \tag{3.26}$$

and $\mathcal{V}_1 \subset \mathcal{V}$ such that $\Theta_{M^{-1}}(\mathcal{U}_1, M\mathcal{V}_1) = \Theta_{M^{-1}}(\mathcal{U}_1, M\mathcal{V})$. Since $\theta_1(\mathcal{U}, \mathcal{V}) < \pi/2$, by Lemma 2.1(b), we have

$$\Theta_{M^{-1}}(\mathcal{U}_1, M\mathcal{V}_1) = \Theta_{M^{-1}}(\mathcal{U}_1, M\mathcal{V}) \le \Theta_{M^{-1}}(\mathcal{U}, M\mathcal{V})_{(1:k)} < \frac{\pi}{2}. \tag{3.27}$$

Let U_1, $V_1 \in \mathbb{R}^{n \times k}$ be basis matrices of $\mathcal{U}_1$ and $\mathcal{V}_1$, respectively. Then, (3.27) means $U_1^T V_1$ being nonsingular. We consider the matrix

$$\widetilde{H}_{SR} = \begin{bmatrix} 0 & \widetilde{K}_{SR} \\ \widetilde{M}_{SR} & 0 \end{bmatrix},$$

where $\widetilde{K}_{SR} = (V_1^T U_1)^{-T} U_1^T K U_1 (V_1^T U_1)^{-1}$ and $\widetilde{M}_{SR} = V_1^T M V_1$. Since $\mathcal{U}_1 \subset \mathcal{U}$ and $\mathcal{V}_1 \subset \mathcal{V}$, we have $\lambda(\widetilde{K}_{SR} \widetilde{M}_{SR}) \geq \mu^{\circ 2}$ by [3, Theorem 4.1]. By Theorem 3.1,

$$\begin{aligned} 0 \leq \mu^{\circ 2} - \lambda^{\circ 2} &\leq \lambda(\widetilde{K}_{SR} \widetilde{M}_{SR}) - \lambda^{\circ 2} \\ &\prec_w \frac{\omega}{\cos^2 \theta_{M^{-1}}^{(1)}(\mathcal{U}_1, M\mathcal{V}_1)} \circ \sin^{\circ 2} \Theta_{M^{-1}}(\mathcal{U}_1, \Phi_1) + \tan^2 \theta_{M^{-1}}^{(1)}(\mathcal{U}_1, M\mathcal{V}_1) \lambda^{\circ 2}. \end{aligned} \tag{3.28}$$

At last, combine (3.26), (3.27) and (3.28) to give (3.25). □

Theorem 3.4. *Let* $\{\mathcal{U}, \mathcal{V}\}$ *satisfy* (3.3)*, and both K and M be definite. Using the notations of Theorem 3.2, we have*

$$\sin \Theta_{M^{-1}}(\mathcal{U}, M\mathcal{V})_{(\ell-k+1:\ell)} \prec_w \sin \Theta_{M^{-1}}(\mathcal{U}, \Phi_1) + \kappa \circ \sin \Theta_{K^{-1}}(\mathcal{V}, \Psi_1), \tag{3.29}$$

$$\sin \Theta_{K^{-1}}(\mathcal{V}, K\mathcal{U})_{(\ell-k+1:\ell)} \prec_w \sin \Theta_{K^{-1}}(\mathcal{V}, \Psi_1) + \kappa \circ \sin \Theta_{M^{-1}}(\mathcal{U}, \Phi_1). \tag{3.30}$$

Proof. Similarly to the proof of Theorem 3.3, let k-dimensional subspaces $\mathcal{U}_2 \subset \mathcal{U}$ and $\mathcal{V}_2 \subset \mathcal{V}$ be chosen such that

$$\Theta_{M^{-1}}(\mathcal{U}_2, \Phi_1) = \Theta_{M^{-1}}(\mathcal{U}, \Phi_1) \quad \text{and} \quad \Theta_{K^{-1}}(\mathcal{V}_2, \Psi_1) = \Theta_{K^{-1}}(\mathcal{V}, \Psi_1).$$

Based on the results in Lemma 2.1 and Theorem 3.2, we have

$$\begin{aligned} \sin \Theta_{M^{-1}}(\mathcal{U}, M\mathcal{V})_{(\ell-k+1:\ell)} &\leq \sin \Theta_{M^{-1}}(\mathcal{U}_2, M\mathcal{V}) \leq \sin \Theta_{M^{-1}}(\mathcal{U}_2, M\mathcal{V}_2) \\ &\prec_w \sin \Theta_{M^{-1}}(\mathcal{U}_2, \Phi_1) + \kappa \circ \sin \Theta_{K^{-1}}(\mathcal{V}_2, \Psi_1) \\ &= \sin \Theta_{M^{-1}}(\mathcal{U}, \Phi_1) + \kappa \circ \sin \Theta_{K^{-1}}(\mathcal{V}, \Psi_1), \end{aligned}$$

which gives (3.29). Similarly we can prove (3.30). □

Theorems 3.2 and 3.4 can be regarded as an extension of [21, Lemma 3.3] in which κ is a scalar λ_n/λ_1. Comparing to the results of Theorem 3.2, one may argue that an unsatisfactory part in Theorem 3.4 is the majorization upper bounds on the first smallest k components of the vectors $\sin \Theta_{M^{-1}}(\mathcal{U}, M\mathcal{V})$ and $\sin \Theta_{K^{-1}}(\mathcal{V}, K\mathcal{U})$, not for the first largest k components. In fact, if $\ell > k$, $\sin \Theta_{M^{-1}}(\mathcal{U}, \Phi_1) = \sin \Theta_{K^{-1}}(\mathcal{V}, \Psi_1) = 0$ fails to yield $\sin \Theta_{M^{-1}}(\mathcal{U}, M\mathcal{V})_{(1:\ell-k)} = 0$ or $\sin \Theta_{K^{-1}}(\mathcal{V}, K\mathcal{U})_{(1:\ell-k)} = 0$ even if both K and M are definite. For example, we consider an LREP with $K = M^{-1} = \Psi\Psi^T$, and let $\mathcal{U}$ and $\mathcal{V}$ be spanned by the columns of M^{-1}-orthonormal and K^{-1}-orthonormal basis matrices $U = [\Phi_1, u_\ell] \in \mathbb{R}^{n \times \ell}$ and $V = [\Psi_1, v_\ell] \in \mathbb{R}^{n \times \ell}$, respectively, where $\ell = k + 1$,

$$u_\ell = \Phi_{(:,k+1:k+2)} \times \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{and} \quad v_\ell = \Psi_{(:,k+1:k+2)} \times \begin{bmatrix} \frac{\sqrt{2}}{2} \\ \frac{\sqrt{2}}{2} \end{bmatrix}.$$

Notice that $\sigma(U^T V) = \sigma\left(\begin{bmatrix} I_k & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{bmatrix} \right)$ satisfies the condition of Theorem 3.4, and

$$\cos \Theta_{M^{-1}}(\mathcal{U}, \Phi_1) = \sigma^\uparrow(\Phi_1^T M^{-1} U) = \sigma^\uparrow([I_k, 0]).$$

Therefore, $\sin \Theta_{M^{-1}}(\mathcal{U}, \Phi_1) = 0$. Similarly, we can check $\sin \Theta_{K^{-1}}(\mathcal{V}, \Psi_1) = 0$. However, in this example,

$$\cos \Theta_{M^{-1}}(\mathcal{U}, M\mathcal{V}) = \cos \Theta_{K^{-1}}(\mathcal{V}, K\mathcal{U}) = \sigma^\uparrow(U^T V) = \sigma^\uparrow\left(\begin{bmatrix} I_k & 0 \\ 0 & \frac{\sqrt{2}}{2} \end{bmatrix} \right),$$

which leads to $\sin \theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V}) = \sin \theta_{K^{-1}}^{(1)}(\mathcal{V}, K\mathcal{U}) = \sqrt{2}/2$.

4 Numerical examples

In this section, we present some numerical examples to illustrate our results in Theorems 3.1 and 3.3. In particular, we will demonstrate the terms associated with $\Theta_{M^{-1}}(\mathcal{U}, M\mathcal{V})$ in majorization upper bounds of (3.6) and (3.25) are not able to be neglected.

Example 4.1. We first examine majorization upper bounds of Theorem 3.1. For simplicity, we consider diagonal matrices for K and M in this example. Take $K = M = \text{diag}(\lambda_1, \ldots, \lambda_n)$ with $n = 100$ and $\lambda_i = i/n$ for $1 \le i \le n$. In such a case, $\Phi = M^{1/2}$ and $\Psi = M^{-1/2}$. Let $k = \ell = 3$ and

$$
E = \begin{bmatrix}
1 & 0 & 0 \\
0 & 1 & 0 \\
0 & 0 & 1 \\
\frac{4}{n} + 4 & \sin 4 & \tan 4 \\
\vdots & \vdots & \vdots \\
\frac{n}{n} + n & \sin(n) & \tan(n)
\end{bmatrix} .
$$

Consider two pairs of approximate deflating subspaces $\{\mathcal{U}_1, \mathcal{V}_1\}$ and $\{\mathcal{U}_2, \mathcal{V}_2\}$ which are spanned by the basis matrices $U_1 = \Phi_1 + \eta \times E$ with $\eta = 10^{-5}$, $V_1 = U_1$, and $U_2 = U_1$, $V_2 = M^{-1}U_2$, respectively. In such a way, the pairs $\{\mathcal{U}_1, \mathcal{V}_1\}$ and $\{\mathcal{U}_2, \mathcal{V}_2\}$ satisfy the condition (3.3). We are interested in bounding the differences between the eigenvalues λ_i for $1 \le i \le k$ and their approximations μ_i by (3.6). We measure the following errors, for $1 \le j \le k$,

$$
\varepsilon_{1,j} = \sum_{i=1}^{j} (\mu_i^2 - \lambda_i^2)^{\downarrow}, \tag{4.1}
$$

$$
\varepsilon_{2,j} = \sum_{i=1}^{j} \left(\frac{\lambda_{n-i+1}^2}{\cos^2 \theta_{M^{-1}}^{(i)}(\mathcal{U}, M\mathcal{V})} - \frac{\lambda_1^2}{\cos^2 \theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V})} \right) \sin^2 \theta_{M^{-1}}^{(i)}(\mathcal{U}, \Phi_1)
$$

$$
+ \tan^2 \theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V}) \sum_{i=1}^{j} \lambda_i^2, \tag{4.2}
$$

$$
\varepsilon_{3,j} = \sum_{i=1}^{j} (\lambda_{n-i+1}^2 - \lambda_1^2) \sin^2 \theta_{M^{-1}}^{(i)}(\mathcal{U}, \Phi_1). \tag{4.3}
$$

Since $\mathcal{U}_2 = M\mathcal{V}_2$, by Remark 3.1(c), then $\varepsilon_{2,j} = \varepsilon_{3,j}$ for $1 \le j \le k$ are the upper bounds on the approximate eigenvalue errors $\varepsilon_{1,j}$ associated with $\{\mathcal{U}_2, \mathcal{V}_2\}$.

Table 4.1 reports the errors $\varepsilon_{2,j}$ and $\varepsilon_{3,j}$ as defined in (4.2) and (4.3) on the eigenvalue approximations $\varepsilon_{1,j}$ as defined in (4.1) corresponding to $\{\mathcal{U}_1, \mathcal{V}_1\}$ and $\{\mathcal{U}_2, \mathcal{V}_2\}$, respectively. It follows from Table 4.1 that our upper bounds provided by Theorem 3.1 are rather sharp in this example, and they are comparable to the observed errors $\varepsilon_{1,j}$. In particular, for the pair of approximate deflating subspaces $\{\mathcal{U}_1, \mathcal{V}_1\}$, though $\varepsilon_{3,2} > \varepsilon_{1,2}$ and $\varepsilon_{3,3} > \varepsilon_{1,3}$, $\varepsilon_{3,1}$ in absence of the terms $\cos^2 \theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V})$ and $\tan^2 \theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V})$ is a little smaller than $\varepsilon_{1,1}$ in this example. However, for the pair $\{\mathcal{U}_2, \mathcal{V}_2\}$, $\varepsilon_{3,j}$ for $1 \le j \le k$ are always available to bound $\varepsilon_{1,j}$.

Example 4.2. In this example, we use a pair of matrices K and M from the linear response analysis of sodium dimer Na$_2$ [12] with order $n = 1862$. Let $k = 3 < \ell = 6$, $U_1 = [\phi_1, E] + \eta \times F$, $V_1 = U_1$, $U_2 = U_1$ and $V_2 = M^{-1}U_2$

Table 4.1: Eigenvalue approximations $\varepsilon_{1,j}$ corresponding to the approximate deflating subspace pairs $\{\mathcal{U}_1, \mathcal{V}_1\}$ and $\{\mathcal{U}_2, \mathcal{V}_2\}$ together with their associated $\varepsilon_{2,j}$ and $\varepsilon_{3,j}$ in Example 4.1.

	Results of $\{\mathcal{U}_1, \mathcal{V}_1\}$			Results of $\{\mathcal{U}_2, \mathcal{V}_2\}$	
j	$\varepsilon_{1,j}$	$\varepsilon_{2,j}$	$\varepsilon_{3,j}$	$\varepsilon_{1,j}$	$\varepsilon_{2,j} = \varepsilon_{3,j}$
1	5.7693×10^{-5}	2.9445×10^{-4}	5.4394×10^{-5}	2.6003×10^{-5}	5.4394×10^{-5}
2	5.9402×10^{-5}	4.4015×10^{-4}	9.9443×10^{-5}	2.6995×10^{-5}	9.9443×10^{-5}
3	5.9407×10^{-5}	4.6531×10^{-4}	9.9459×10^{-5}	2.6997×10^{-5}	9.9459×10^{-5}

where η and E as defined in Example 4.1, and

$$F = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & 0 & 1 \\ \frac{6}{n} & \frac{6}{n}+6 & \sin 6 & \cos 6 & \tan 6 & \cot 6 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \frac{n}{n} & \frac{n}{n}+n & \sin(n) & \cos(n) & \tan(n) & \cot(n) \end{bmatrix}.$$

As Example 4.1, we also consider to bound the eigenvalue approximations based on the approximate deflating subspace pairs $\{\mathcal{U}_1, \mathcal{V}_1\}$ and $\{\mathcal{U}_2, \mathcal{V}_2\}$, respectively, where $\mathcal{U}_1 = \mathcal{R}(U_1)$, $\mathcal{V}_1 = \mathcal{R}(V_1)$, $\mathcal{U}_2 = \mathcal{R}(U_2)$ and $\mathcal{V}_2 = \mathcal{R}(V_2)$. Since $\ell > k$ here, by Theorem 3.3, we compute $\varepsilon_{1,j}$, $\tilde{\varepsilon}_{2,j}$ and $\varepsilon_{3,j}$ for $1 \le j \le k$ in Table 4.2 where

$$\tilde{\varepsilon}_{2,j} = \sum_{i=1}^{j} \frac{\lambda_{n-i+1}^2 - \lambda_1^2}{\cos^2 \theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V})} \sin^2 \theta_{M^{-1}}^{(i)}(\mathcal{U}, \Phi_1) + \tan^2 \theta_{M^{-1}}^{(1)}(\mathcal{U}, M\mathcal{V}) \sum_{i=1}^{j} \lambda_i^2,$$

and $\varepsilon_{1,j}$, $\varepsilon_{3,j}$ as defined in (4.1) and (4.3), respectively. Table 4.2 suggests that our bounds $\tilde{\varepsilon}_{2,j}$ for $1 \le j \le k$ are also very sharp in the case $\ell > k$, while $\varepsilon_{3,j}$ for $1 \le j \le k$ in the numerical results of $\{\mathcal{U}_1, \mathcal{V}_1\}$ underestimate $\varepsilon_{1,j}$ too much in this example.

Table 4.2: Approximate eigenvalue errors $\varepsilon_{1,j}$ associated with the pairs $\{\mathcal{U}_1, \mathcal{V}_1\}$ and $\{\mathcal{U}_2, \mathcal{V}_2\}$ together with their corresponding $\tilde{\varepsilon}_{2,j}$ and $\varepsilon_{3,j}$ of Example 4.2.

	Results of $\{\mathcal{U}_1, \mathcal{V}_1\}$			Results of $\{\mathcal{U}_2, \mathcal{V}_2\}$	
j	$\varepsilon_{1,j}$	$\tilde{\varepsilon}_{2,j}$ (bound for $\varepsilon_{1,j}$)	$\varepsilon_{3,j}$	$\varepsilon_{1,j}$	$\tilde{\varepsilon}_{2,j} = \varepsilon_{3,j}$
1	0.7247	0.7799	1.0741×10^{-7}	2.0972×10^{-9}	1.0741×10^{-7}
2	1.2544	1.5431	1.1451×10^{-7}	3.0659×10^{-9}	1.1451×10^{-7}
3	1.5944	2.1888	1.1892×10^{-7}	3.5445×10^{-9}	1.1892×10^{-7}

5 Conclusion

The pair of k-dimensional deflating subspaces $\{\mathcal{R}(\Phi_1), \mathcal{R}(\Psi_1)\}$ due to its ability in recovering the eigenvalues of interest plays a vital role in some efficient numerical methods of LREP. Given a pair of ℓ-dimensional subspaces $\{\mathcal{U}, \mathcal{V}\}$ with $\ell \ge k$ which approximates or contains a pair of k-dimensional subspaces approximating $\{\mathcal{R}(\Phi_1), \mathcal{R}(\Psi_1)\}$, Zhang, Xue and Li [21] established the Rayleigh-Ritz error bounds of LREP on the differences between the approximate eigenvalues and the eigenvalues of interest by the canonical angles between the exact and approximate pair of deflating subspaces in the case $\ell = k$. There are two major contributions in this

paper to improve the exist results in [21]. One is to obtain the Rayleigh-Ritz majorization type upper bounds for the approximate eigenvalue errors of LREP, i.e., Theorem 3.1. The other one is to extend Theorem 3.1 to Theorem 3.3 by considering $\ell > k$. Numerical examples are presented to confirm the sharpness of these upper bounds, and to demonstrate the necessity of the terms on $\Theta_{M^{-1}}(\mathcal{U}, M\mathcal{V})$ in Theorems 3.1 and 3.3.

From the point of view that the generalized linear response eigenvalue problem

$$Hz = \begin{bmatrix} 0 & K \\ M & 0 \end{bmatrix} \begin{bmatrix} y \\ x \end{bmatrix} = \lambda \begin{bmatrix} E_+ & \\ & E_- \end{bmatrix} \begin{bmatrix} y \\ x \end{bmatrix} = \lambda Ez$$

where K and M are $n \times n$ symmetric positive semi-definite and one of them is definite, $E_\pm$ are $n \times n$ nonsingular matrices and $E_+^{\mathrm{T}} = E_-$, can be equivalently transformed to the standard LREP by decomposing $E_+ = CD^{\mathrm{T}}$ [11, 28]. The development of Theorems 3.1, 3.2, 3.3 and 3.4 can be made to work for the generalized linear response eigenvalue problem by simple modifications: replacing $\Theta_{M^{-1}}(\mathcal{U}, M\mathcal{V})$ by $\Theta_{M^{-1}}(E_-\mathcal{U}, M\mathcal{V})$, $\Theta_{M^{-1}}(\mathcal{U}, \Phi_1)$ by $\Theta_{M^{-1}}(E_-\mathcal{U}, E_-\Phi_1)$, $\Theta_{K^{-1}}(\mathcal{V}, K\mathcal{U})$ by $\Theta_{K^{-1}}(E_+\mathcal{V}, K\mathcal{U})$ and $\Theta_{K^{-1}}(\mathcal{V}, \Psi_1)$ by $\Theta_{K^{-1}}(E_+\mathcal{V}, E_+\Psi_1)$. We omit the details.

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