Relative Perturbation Bound for Invariant Subspaces of Graded Indefinite Hermitian Matrices

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Abstract

We give a bound for the perturbations of invariant subspaces of graded indefinite Hermitian matrix $H = D^*AD$ which is perturbed into $H+\delta H = D^*(A+\delta A)D$. Such relative perturbations include important case where H is given with an element-wise relative error. Application of our bounds requires only the knowledge of the size of relative perturbation $\|\delta A\|$, and not the perturbation δA itself. This typically occurs when data are given with relative uncertainties, when the matrix is being stored into computer memory, and when analyzing some numerical algorithms. Subspace perturbations are measured in terms of perturbations of angles between subspaces, and our bound is therefore relative variant of the well-known Davis–Kahan $\sin\Theta$ theorem. Our bounds generalize some of the recent relative perturbation results.

1 Introduction and preliminaries

We are considering the Hermitian eigenvalue problem

$$Hu_i = \lambda_i u_i,$$

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or

$$H = U\Lambda U^* = \sum_{i=1}^{n} \lambda_i u_i u_i^*,$$

where H is a non-singular Hermitian matrix of order n, $\Lambda = \mathrm{diag}(\lambda_i)$ is a diagonal matrix whose diagonal elements are the eigenvalues of H, and $U = [\, u_1 \quad u_2 \quad \cdots \quad u_n \,]$ is unitary matrix whose i-th column is an eigenvector which corresponds to λ_i. Subspace $\mathcal{X}$ is an invariant subspace of a general matrix H if $H\mathcal{X} \subseteq \mathcal{X}$. If H is Hermitian and the set of eigenvalues $\{\lambda_{i_1}, \lambda_{i_2}, \cdots, \lambda_{i_k}\}$ does not intersect the rest of the spectrum of H, then the corresponding k-dimensional invariant subspace is spanned by the eigenvectors $u_{i_1}, u_{i_2}, \cdots, u_{i_k}$. Throughout the paper $\|\cdot\|$ and $\|\cdot\|_F$ will denote the 2-norm and the Frobenius norm, respectively.

Our aim is to give bound for perturbations of invariant subspaces for the case when H is a graded Hermitian matrix, that is,

$$H = D^* A D, \tag{1}$$

where D is some non-singular grading matrix, under Hermitian relative perturbation of the form

$$H + \delta H \equiv \widetilde{H} = D^*(A + \delta A)D.$$

Our bound is a relative variant of the well-known $\sin\Theta$ theorems by Davis and Kahan [2], [24, Section V.3.3].

The development of relative perturbation results for eigenvalue and singular value problems has been very active area of research in the past years [3,1,4,29,21,6,5,15,16,7,13] (see also the review article [12]). We shall first describe the relative perturbation and state the existing eigenvalue perturbation results. Let δH be the Hermitian relative perturbation which satisfies

$$|x^* \delta H x| \leq \eta x^* \left| H \right| x, \quad \forall x, \; \eta < 1, \tag{2}$$

where $\left| H \right| = \sqrt{H^2} = U|\Lambda|U^*$ is a spectral absolute value of H (that is, $\left| H \right|$ is the positive definite polar factor of H). Under such perturbations the relative change in eigenvalues is bounded by [29]

$$1 - \eta \leq \frac{\widetilde{\lambda}_j}{\lambda_j} \leq 1 + \eta. \tag{3}$$

This inequality implies that the perturbations which satisfy (2) are inertia preserving. This result is very general and includes important classes of perturbations. If H is a graded matrix defined by (1) and

$$\widehat{A} = D^{-*}\boldsymbol{|}H\boldsymbol{|}D^{-1}, \tag{4}$$

then (3) holds with [2]

$$\eta = \|\delta A\|\|\widehat{A}^{-1}\|. \tag{5}$$

Indeed,

$$\begin{aligned} |x^*\delta H x| = |x^* D^* \delta A D x| &= \|x^* D^* \delta A D x\| \leq \|x^* D^*\|\|\delta A\|\|Dx\| \\ &\leq \|\delta A\|\|\widehat{A}^{-1}\|\, x^* \boldsymbol{|}H\boldsymbol{|} x, \end{aligned} \tag{6}$$

as desired. Another important class of perturbations is when H is perturbed element-wise in the relative sense,

$$|\delta H_{ij}| \leq \varepsilon |H_{ij}|. \tag{7}$$

By setting

$$D = \operatorname{diag}(\sqrt{\boldsymbol{|}H\boldsymbol{|}_{ii}}), \tag{8}$$

since $|\delta A_{ij}| \leq \varepsilon |A_{ij}|$, the relation (6) implies that (3) holds with

$$\eta = \varepsilon \|\,|A|\,\|\|\widehat{A}^{-1}\|. \tag{9}$$

Since $\widehat{A}_{ii} = 1$, we have $\|\widehat{A}^{-1}\| \leq \kappa(\widehat{A}) \leq n\|\widehat{A}^{-1}\|$, where $\kappa(A) \equiv \|A\|\|A^{-1}\|$ is the spectral condition number. Also, $\|\,|A|\,\| \leq n$ (see [29, Proof of Theorem 2.16]). The diagonal grading matrix D from (8) is almost optimal in the sense that [23]

$$\kappa(\widehat{A}) \leq n \min_{\bar{D}} \kappa(\bar{D}^* \boldsymbol{|}H\boldsymbol{|} \bar{D}) \leq n\kappa(\boldsymbol{|}H\boldsymbol{|}) = n\kappa(H),$$

where the minimum is taken over all non-singular diagonal matrices. Similarly, for more general perturbations of the type

$$|\delta H_{ij}| \leq \varepsilon D_{ii} D_{jj}, \tag{10}$$

[2] In [29] no attention was paid to scalings with non-diagonal matrix D, so this result is new. Also notice that any perturbation $H + \delta H$ can clearly be interpreted as the perturbation of a graded matrix, and vice versa.

(3) holds with

$$\eta = \varepsilon n \|\widehat{A}^{-1}\| \leq \varepsilon n \kappa(\widehat{A}). \tag{11}$$

Remark 1 Application of the bounds (5), (9) and (11) requires only the knowledge of the size of relative perturbation $\|\delta A\|$, and not the perturbation δA itself. Such situation occurs in several cases which are very important in applications. When the data are determined to some relative accuracy or when the matrix is being stored in computer memory, the only available information about δH is that it satisfies (7). Similarly, in error analysis of various numerical algorithms (matrix factorizations, eigenvalue or singular value computations), the the only available information is that δH satisfies more general condition (10).

If H is positive definite, then $|H| = H$, and (9) and (11) reduce to the corresponding results from [4]. We would like to point out a major difference between positive definite and indefinite case.

Remark 2 If H is positive definite, then small perturbations of the type (7) and (10) cause small relative changes in eigenvalues if and only if $\kappa(\widehat{A}) \equiv \kappa(A)$ is small [4]. If H is indefinite, then from (9) and (11) it follows that small $\kappa(\widehat{A})$ implies small relative changes in eigenvalues. However, these changes can be small even if $\kappa(\widehat{A})$ is large [29,18]. Although such examples can be successfully analyzed by perturbations through factors as in [29,28], this shows that the graded indefinite case is essentially more difficult than the positive definite one.

Perturbation bounds for eigenvectors of simple eigenvalues were given for scaled diagonally dominant matrices in [1], and for positive definite matrices in [4]. The bound for invariant subspace which corresponds to single, possibly multiple, eigenvalue of an indefinite Hermitian matrix was given in [29, Theorem 2.48]. This bound, given in terms of projections which are defined by Dunford integral as in [14, Section II.1.4], is generalized to invariant subspaces which correspond to a set of neighboring eigenvalues in [25]. In [16, Theorems 3.3 and 3.4] two bounds for invariant subspaces of a graded positive definite matrix were given. We generalize the result of [16, Theorem 3.3] and give the bound for $\|\sin\Theta\|_F$ for a graded non-singular indefinite matrix. Our results are, therefore, relative variants of the well-known $\sin\Theta$ theorems [2, Section 2], [24, Theorem V.3.4]. Our results also generalize the ones from [29,25] to subspaces which correspond to arbitrary set of eigenvalues. Our results and the related results from [1,4,29,21] and other works, are also useful in estimating the accuracy of highly accurate algorithms for computing eigenvalue decompositions [1,4,27,18].

The paper is organized as follows: in Section 2 we prove our main theorem. In Section 3 we show how to efficiently apply that theorem, in particular for the important types of relative perturbations (7) and (10) (c.f. Remarks 1 and 2). We also describe some classes of well-behaved indefinite matrices. In Section 4 we give some concluding remarks.

2 Bound for invariant subspaces

Let the eigenvalue decomposition of the graded matrix H be given by

$$H \equiv D^* A D = U \Lambda U^* = \begin{bmatrix} U_1 & U_2 \end{bmatrix} \begin{bmatrix} \Lambda_1 & 0 \\ 0 & \Lambda_2 \end{bmatrix} \begin{bmatrix} U_1^* \\ U_2^* \end{bmatrix}, \tag{12}$$

where

$$\Lambda_1 = \mathrm{diag}(\lambda_{i_1}, \lambda_{i_2}, \cdots, \lambda_{i_k}), \quad \Lambda_2 = \mathrm{diag}(\lambda_{j_1}, \lambda_{j_2}, \cdots, \lambda_{j_l}),$$

and $k + l = n$. We assume that Λ_1 and Λ_2 have no common eigenvalues, thus, U_1 and U_2 both span simple invariant subspaces according to [24, Definition V.1.2]. Similarly, let the eigenvalue decomposition of $\widetilde{H}$ be

$$\widetilde{H} \equiv D^*(A + \delta A) D = \widetilde{U} \widetilde{\Lambda} \widetilde{U}^* = \begin{bmatrix} \widetilde{U}_1 & \widetilde{U}_2 \end{bmatrix} \begin{bmatrix} \widetilde{\Lambda}_1 & 0 \\ 0 & \widetilde{\Lambda}_2 \end{bmatrix} \begin{bmatrix} \widetilde{U}_1^* \\ \widetilde{U}_2^* \end{bmatrix}, \tag{13}$$

where $\widetilde{\Lambda}_1 = \mathrm{diag}(\widetilde{\lambda}_{i_1}, \cdots, \widetilde{\lambda}_{i_k})$ and $\widetilde{\Lambda}_2 = \mathrm{diag}(\widetilde{\lambda}_{j_1}, \cdots, \widetilde{\lambda}_{j_l})$.

Let $X \Sigma Y^*$ be a singular value decomposition of the matrix $\widetilde{U}_2^* U_1$. The diagonal entries of the matrix $\sin\Theta \equiv \Sigma$, are the sines of canonical angles between subspaces which are spanned by the columns of U_1 and $\widetilde{U}_1$ [24, Corollary I.5.4].

Before stating the theorem, we need some additional definitions. Let

$$A = Q \Delta Q^* = Q |\Delta|^{1/2} J |\Delta|^{1/2} Q^*, \tag{14}$$

be an eigenvalue decomposition of A. Here J is diagonal matrix of signs whose diagonal elements define the inertia of A and, by Sylvester's theorem [10, Theorem 4.5.8], of H, as well. Set

$$G = D^* Q |\Delta|^{1/2}, \tag{15}$$

such that $H = GJG^*$. Further, set

$$N = |\Delta|^{-1/2} Q^* \delta A Q |\Delta|^{-1/2}, \tag{16}$$

such that $\widetilde{H} = G(J+N)G^*$.

Finally, the hyperbolic eigenvector matrix of a matrix pair (M, J), where M is a Hermitian positive definite matrix, and $J = \mathrm{diag}(\pm 1)$, is the matrix X which simultaneously diagonalizes the pair such that $X^*MX = \Lambda_M$ and $X^*JX = J$, where Λ_M is a positive definite diagonal matrix. Some properties of hyperbolic eigenvector matrices will be discussed in the next section.

Theorem 3 *Let H and $\widetilde{H}$ be given as above, and let $\|A^{-1}\|\|\delta A\| < 1$. Then H and $\widetilde{H}$ have the same inertia, thus $\widetilde{U}_1$ and $\widetilde{U}_2$ from (13) span simple invariant subspaces, as well, and the canonical angles between the subspaces spanned by U_1 and $\widetilde{U}_1$ are bounded by*

$$\|\sin\Theta\|_F \equiv \|\widetilde{U}_2^* U_1\|_F \leq \frac{\|A^{-1}\|\,\|\delta A\|_F}{\sqrt{1-\|A^{-1}\|\,\|\delta A\|}} \cdot \frac{\|V_1\|\,\|\widetilde{V}_2\|}{\displaystyle\min_{\substack{1\leq p\leq k\\ 1\leq q\leq l}} \frac{|\lambda_{i_p} - \widetilde{\lambda}_{j_q}|}{\sqrt{|\lambda_{i_p}\widetilde{\lambda}_{j_q}|}}}, \tag{17}$$

provided that the above minimum is greater than zero. Here $V = [\,V_1 \quad V_2\,]$ is the hyperbolic eigenvector matrix of the pair (G^*G, J), where G is defined by (14) and (15), and $\widetilde{V} = [\,\widetilde{V}_1 \quad \widetilde{V}_2\,]$ is the hyperbolic eigenvector matrix of the pair

$$([(I+NJ)^{1/2}]^* G^* G (I+NJ)^{1/2}, J),$$

where N is defined by (16). V and $\widetilde{V}$ are partitioned accordingly to (12) and (13). Note that the matrix square root exists since by the assumption $\|N\| \leq \|A^{-1}\|\,\|\delta A\| < 1$ (see [11, Theorem 6.4.12]).

Proof. The proof is similar to the proof of [16, Theorem 3.3]. From $\|N\| < 1$ we conclude that the matrices $H = GJG^*$, $J+N$ and $\widetilde{H} = G(J+N)G^*$ all have the same inertia defined by J. Therefore, (12) and (13) can be written as

$$H = U\Lambda JU^*, \qquad \widetilde{H} = \widetilde{U}\widetilde{\Lambda}J\widetilde{U}^*, \tag{18}$$

with the same $J = \mathrm{diag}(\pm 1)$ as in (14), respectively. Also, $J+N$ can be decomposed as

$$J+N = (I+NJ)^{1/2} J [(I+NJ)^{1/2}]^*, \tag{19}$$

which follows from $(I+NJ)^{1/2} = J[(I+NJ)^{1/2}]^*J$. Thus, we can write $\widetilde{H}$ as

$$\widetilde{H} = G(I+NJ)^{1/2} J [(I+NJ)^{1/2}]^* G^*. \tag{20}$$

From (18) and $H = GJG^*$ we conclude that the matrix G has the hyperbolic singular value decomposition [17] given by

$$G = U|\Lambda|^{1/2} JV^* J, \qquad V^* JV = J. \tag{21}$$

Similarly, from (18) and (20) we conclude that the matrix $G(I + JN)^{1/2}$ has the hyperbolic singular value decomposition given by

$$G(I + NJ)^{1/2} = \widetilde{U}|\widetilde{\Lambda}|^{1/2} J\widetilde{V}^* J, \qquad \widetilde{V}^* J\widetilde{V} = J. \tag{22}$$

Now (20) and (19) imply that

$$\begin{aligned}\widetilde{H} - H &= G(I + NJ)^{1/2} J[(I + NJ)^{1/2}]^* G^* - GJG^* \\ &= G(I + NJ)^{1/2}\, \Xi\, G^*,\end{aligned} \tag{23}$$

where

$$\Xi = J[(I + NJ)^{1/2}]^* - (I + NJ)^{-1/2} J = (I + NJ)^{-1/2} N. \tag{24}$$

Pre- and post-multiplication of (23) by $\widetilde{U}$ and U, respectively, together with (12), (13), (21) and (22), gives

$$\widetilde{\Lambda}\widetilde{U}^* U - \widetilde{U}^* U\Lambda = |\widetilde{\Lambda}|^{1/2} J\widetilde{V}^* J\, \Xi\, JVJ|\Lambda|^{1/2}.$$

This, in turn, implies

$$\widetilde{\Lambda}_2\widetilde{U}_2^* U_1 - \widetilde{U}_2^* U_1\Lambda_1 = |\widetilde{\Lambda}_2|^{1/2} J_2\widetilde{V}_2^* J\, \Xi\, JV_1 J_1|\Lambda_1|^{1/2},$$

where $J = J_1 \oplus J_2$ is partitioned accordingly to (12) and (13). By interpreting this equality component-wise we have

$$[\widetilde{U}_2^* U_1]_{qp} = [J_2\widetilde{V}_2^* J\, \Xi\, JV_1 J_1]_{qp} \frac{\sqrt{|\widetilde{\Lambda}_{2,qq}||\Lambda_{1,pp}|}}{\widetilde{\Lambda}_{2,qq} - \Lambda_{1,pp}},$$

for all $p \in \{1, \ldots, k\}$ and $q \in \{1, \ldots, l\}$. By taking the Frobenius norm we have

$$\|\widetilde{U}_2^* U_1\|_F \leq \|J_2\widetilde{V}_2^* J\, \Xi\, JV_1 J_1\|_F \cdot \max_{p,q} \frac{\sqrt{|\widetilde{\Lambda}_{2,qq}||\Lambda_{1,pp}|}}{\widetilde{\Lambda}_{2,qq} - \Lambda_{1,pp}}.$$

Further,

$$\|J_2\widetilde{V}_2^* J\,\Xi\,JV_1J_1\|_F \leq \|\widetilde{V}_2\|\,\|V_1\|\,\|\Xi\|_F.$$

The relations (24), (16) and the assumption imply

$$\begin{aligned}\|\Xi\|_F &\leq \|(I+JN)^{-1/2}\|\,\|N\|_F \leq \frac{1}{\sqrt{1-\|N\|}}\|N\|_F \\ &\leq \frac{\|A^{-1}\|\,\|\delta A\|_F}{\sqrt{1-\|A^{-1}\|\,\|\delta A\|}},\end{aligned}$$

and the theorem follows by combining the last three relations. □

For positive definite H the matrices $\widetilde{V}$ and V are unitary. Thus $\|V_1\| = \|\widetilde{V}_2\| = 1$, and Theorem 3 reduces to [16, Theorem 3.3]. Thus, the difference from the positive definite and indefinite case is existence of the additional factor $\|V_1\|\,\|\widetilde{V}_2\|$ in the indefinite case. This again shows that the indefinite case is essentially more difficult (c.f. Remark 2). The minimum in (17) plays the role of the relative gap, although the function $|\lambda - \widetilde{\lambda}|/\sqrt{|\lambda\widetilde{\lambda}|}$ does not necessarily increase with the distance between λ and $\widetilde{\lambda}$ if they have different signs. For example, if $\Lambda_1 = \{1\}$ and $\widetilde{\Lambda}_2 = \{-1, 0.1\}$, then the minimum is attained between 1 and -1 and not between 1 and 0.1. Some other results for positive definite matrices and singular value decomposition from [15,16] can be generalized to indefinite case and hyperbolic singular value decomposition, respectively, by using the techniques similar to those used in the proof of Theorem 3 and Section 3. As already mentioned in Section 1, Theorem 3 generalizes some other relative bounds from [1,4,29,21], as well.

The bound (17) involves unperturbed and the perturbed quantities (λ and $\widetilde{\lambda}$, V_1 and $\widetilde{V}_2$), and can, therefore be computed only if δA is known. The existing bounds for graded indefinite Hermitian matrices from [29,21,25], depend neither upon perturbed vectors nor eigenvalues, and are therfore simpler to compute, and can be applied to some important problems where only the size of the relative perturbation is known (c.f. Remark 1). Our next aim is to remove the dependence on the perturbed quantities from (17), and to explain when is the factor $\|V_1\|\,\|\widetilde{V}_2\|$ in (17) expected to be small. We do this in the next section.

3 Applying the bound

We show how to remove the perturbed quantities from the bound of Theorem 3. In particular, we show how to efficiently compute η and the upper bound for the factor $\|V_1\|\,\|\widetilde{V}_2\|$. In Section 3.1 we show that this factor will be small if, for the chosen grading D, the matrix $\widehat{A}$ which is defined by (4) is well conditioned. We also describe some easily recognisable classes of matrices which fulfill this condition for any diagonal grading D.

First note that the perturbed eigenvalues can be expressed in terms of the unperturbed one by using (3) and (5), that is, the minimum in (17) is bounded by

$$\min_{\substack{1\leq p\leq k\\ 1\leq q\leq l}} \frac{|\lambda_{i_p}-\widetilde{\lambda}_{j_q}|}{\sqrt{|\lambda_{i_p}\widetilde{\lambda}_{j_q}|}} \geq \min_{\substack{1\leq p\leq k\\ 1\leq q\leq l}} \frac{|\lambda_{i_p}-\lambda_{j_q}(1+\operatorname{sign}(\lambda_i-\lambda_j)\operatorname{sign}(\lambda_j)\eta)|}{\sqrt{|\lambda_{i_p}\lambda_{j_q}(1+\eta)|}}. \tag{25}$$

We now proceed as follows: we first bound $\|\widetilde{V}\|$ in terms of $\|V\|$; we then bound $\|V\|$ in terms of $\|A^{-1}\|$ and $\|\widehat{A}\|$; and, finally, we show how to efficiently compute $\|\widehat{A}\|$ and η from (5), (9) or (11).

The matrices for which $X^*JX=J$, where $J=\operatorname{diag}(\pm 1)$ are called J-unitary. Such matrices have the following properties:

- $XJX^*=J$.
- $\|X\|=\|X^{-1}\|$. Moreover, the singular values of X come in pairs of reciprocals, $\{\sigma,1/\sigma\}$.
- Let

  $$J=I_l\oplus(-I_{n-l}) \tag{26}$$

  and let X be partitioned accordingly,

  $$X=\begin{bmatrix} X_{11} & X_{12}\\ X_{21} & X_{22}\end{bmatrix}.$$

  Then $\|X_{11}\|=\|X_{22}\|$, $\|X_{12}\|=\|X_{21}\|$, and

  $$\|X\|=\|X_{21}\|+\sqrt{1+\|X_{21}\|^2}=\|X_{21}\|+\|X_{11}\|. \tag{27}$$

  These equalities follow from the CS decomposition of X [20].

Lemma 4 *Let J be given by (26) and let X and $\widetilde{X}$ be two J-unitary matrices which are partitioned accordingly in block columns as*

$$X=[\,X_p\quad X_n\,] \qquad \textit{and} \qquad \widetilde{X}=[\,\widetilde{X}_p\quad \widetilde{X}_n\,].$$

X_p spans the so called positive subspace with respect to J since $X_p^* J X_p = I_l$. Similarly, X_n spans the negative subspace. Then the matrix $X^* J \widetilde{X}$ is also J-unitary, and

$$\|X^* J \widetilde{X}\| = \|X_n^* J \widetilde{X}_p\| + \sqrt{1 + \|X_n^* J \widetilde{X}_p\|}.$$

Also,

$$\|\widetilde{X}\| \leq \left(\|X_n^* J \widetilde{X}_p\| + \sqrt{1 + \|X_n^* J \widetilde{X}_p\|} \right) \|X\|. \tag{28}$$

Proof. The equality follows from (27), and the inequality follows since $\|\widetilde{X}\| = \|X^{-*} X^* J \widetilde{X}\| \leq \|X^{-*}\| \, \|X^* J \widetilde{X}\| = \|X\| \, \|X^* J \widetilde{X}\|$. $\square$

Lemma 5 *Let X and $\widetilde{X}$ be the hyperbolic eigenvector matrices of the pairs (M, J) and $(\widetilde{M}, J)$ where M and $\widetilde{M}$ are positive definite, $\widetilde{M} = (I + \Gamma)^* M (I + \Gamma)$, and J is given by (26). Let X and $\widetilde{X}$ be partitioned as in Lemma 4. Define $\gamma = \|\Gamma\|_F / (1 - \|\Gamma\|)$. If*

$$\gamma \|X\|^2 < \frac{1}{4}, \tag{29}$$

then

$$\|\widetilde{X}\| \leq \frac{\|X\|}{\sqrt{1 - 4\gamma \|X\|^2}}.$$

Proof. The fact that X diagonalizes the pair (M, J) can be written as

$$X^* M X = \Lambda \equiv \begin{bmatrix} \Lambda_p & \\ & \Lambda_n \end{bmatrix}, \tag{30}$$

where Λ is diagonal positive definite matrix which is partitioned according to J and X. J-unitarity of X and (30) imply $MX = X^{-*} \Lambda = J X J \Lambda$, thus

$$M X_p = J X_p \Lambda_p \qquad \text{and} \qquad M X_n = -J X_n \Lambda_n. \tag{31}$$

Relations analogous to (30) and (31) hold for $\widetilde{M}$, $\widetilde{X}$ and $\widetilde{\Lambda}$, as well. By pre-multiplying $\widetilde{M} \widetilde{X}_p = J \widetilde{X}_p \widetilde{\Lambda}_p$ by X_n^* we have, after using (31) and rearranging,

$$\Lambda_n X_n^* J \widetilde{X}_p + X_n^* J \widetilde{X}_p \widetilde{\Lambda}_p = X_n^* (\widetilde{M} - M) \widetilde{X}_p.$$

Set $\widehat{\Gamma} = I - (I + \Gamma)^{-*}$ (the inverse exists since (29) implies $\|\Gamma\| < 1$). By using the identity $\widetilde{M} - M = \widehat{\Gamma}\widetilde{M} + M\Gamma$, the above equality can be written component-wise as

$$\begin{aligned}
[X_n^* J\widetilde{X}_p]_{ij}([\Lambda_n]_{ii} + [\widetilde{\Lambda}_p]_{jj}) &= [X_n]_{:i}^* \{\widehat{\Gamma}\widetilde{M} + M\Gamma\}[\widetilde{X}_p]_{:j} \\
&= [X_n]_{:i}^* \widehat{\Gamma} J [\widetilde{X}_p]_{:j} [\widetilde{\Lambda}_p]_{jj} - [\Lambda_n]_{ii} [X_n]_{:i}^* J\Gamma [\widetilde{X}_p]_{:j}.
\end{aligned}$$

Here $[X]_{:k}$ denotes the k-th column of the matrix X. By dividing this equality by $[\Lambda_n]_{ii} + [\widetilde{\Lambda}_p]_{jj}$ and by using the fact that

$$\frac{\max\{[\Lambda_n]_{ii}, [\widetilde{\Lambda}_p]_{jj}\}}{[\Lambda_n]_{ii} + [\widetilde{\Lambda}_p]_{jj}} < 1,$$

we have

$$|[X_n^* J\widetilde{X}_p]_{ij}| \le |[X_n]_{:i}^* \widehat{\Gamma} J [\widetilde{X}_p]_{:j}| + |[X_n]_{:i}^* J\Gamma [\widetilde{X}_p]_{:j}|.$$

Since $\|\widehat{\Gamma}\|_F \le \gamma$, by taking Frobenius norm we have

$$\|X_n^* J\widetilde{X}_p\|_F \le \|X_n\|\,\|\widetilde{X}_p\|(\|\widehat{\Gamma}\|_F + \|\Gamma\|_F) \le 2\gamma\|X\|\,\|\widetilde{X}\|.$$

By inserting this inequality in (28), we have

$$\|\widetilde{X}\| \le \left(2\gamma\|X\|\,\|\widetilde{X}\| + \sqrt{1 + (2\gamma\|X\|\,\|\widetilde{X}\|)^2}\right) \|X\|.$$

After a simple manipulation we obtain

$$\|\widetilde{X}\|^2 \le \frac{\|X\|^2}{1 - 4\gamma\|X\|^2}.$$

as desired. □

Now we can use Lemma 5 to bound $\|\widetilde{V}\|$ by $\|V\|$ in Theorem 3. V diagonalizes the pair (G^*G, J) where G is defined by (15), and $\widetilde{V}$ diagonalizes the pair $([(I + NJ)^{1/2}]^* G^* G (I + NJ)^{1/2}, J)$, where N is defined by (16). In order to apply Lemma 5 with $M = G^*G$ and $I + \Gamma = (I + NJ)^{1/2}$ we need to bound $\|\Gamma\|$ in terms of $\|N\|$. Since $\|NJ\| < 1$, we can apply Taylor series of the function $(1 + x)^{1/2}$ to the matrix $(I + NJ)^{1/2}$ [11, Theorem 6.2.8], which gives

$$(I + NJ)^{1/2} = I + \sum_{n=1}^{\infty} (-1)^{n-1} \frac{(2n-3)!!}{2^n n!} (NJ)^n \equiv I + \Gamma.$$

Here $(2n-3)!! = 1 \cdot 1 \cdot 3 \cdot 5 \cdots (2n-3)$. By taking norms we have

$$\begin{aligned}\|\Gamma\| &\leq \sum_{n=1}^{\infty} \frac{(2n-3)!!}{2^n n!} \|N\|^n = \frac{1}{2}\|N\| \sum_{n=1}^{\infty} \frac{(2n-3)!!}{2^{n-1} n!} \|N\|^{n-1} \\ &\leq \frac{1}{2}\|N\| \sum_{n=1}^{\infty} \|N\|^{n-1} \leq \frac{1}{2} \cdot \frac{\|N\|}{1-\|N\|}.\end{aligned}$$

Similarly, for the Frobenius norm we have

$$\|\Gamma\|_F \leq \frac{1}{2} \cdot \frac{\|N\|_F}{1-\|N\|}.$$

From the above two inequalities we see that γ from Lemma 5 is bounded by

$$\gamma \leq \frac{\|N\|_F}{2-3\|N\|} \leq \frac{\|A^{-1}\| \, \|\delta A\|_F}{2-3\|A^{-1}\| \, \|\delta A\|} \equiv \alpha. \tag{32}$$

If

$$\|A^{-1}\| \, \|\delta A\|_F < \frac{2}{4\|V\|^2+3}, \tag{33}$$

then $\alpha < 1/(4\|V\|^2)$, that is, (29) holds and Lemma 5 gives

$$\|\widetilde{V}\| \leq \frac{\|V\|}{\sqrt{1-4\alpha\|V\|^2}}. \tag{34}$$

We can further bound $\|V\|$ in terms of A and $\widehat{A}$ from (4). By definition, V diagonalizes the pair (G^*G, J) where $H = GJG^*$, that is, $V^*G^*GV = |\Lambda|$, where Λ is the eigenvalue matrix of H. Then, the eigenvalue decomposition of H is given by $H = U\Lambda U^*$ where $U = GV|\Lambda|^{-1/2}$. Then

$$\boldsymbol{|} H \boldsymbol{|} = U|\Lambda|U^* = GVV^*G^*. \tag{35}$$

Therefore $\|V\|^2 = \|VV^*\| = \|G^{-1} \boldsymbol{|} H \boldsymbol{|} G^{-*}\|$. In our case, from (4) and (15), we have

$$\|V\|^2 = \||\Delta|^{-1/2} Q^* D^{-*} D^* \widehat{A} D D^{-1} Q |\Delta|^{-1/2}\| \leq \|A^{-1}\| \, \|\widehat{A}\|. \tag{36}$$

We can now prove the following theorem.

Theorem 6 *Let the assumptions of Theorem 3 hold and let, in addition,* $\|A^{-1}\|\,\|\delta A\|_F < 2/(4\|A^{-1}\|\,\|\widehat{A}\|+3)$. *Then*

$$\|\sin\Theta\|_F \leq \frac{\|A^{-1}\|\,\|\delta A\|_F}{\sqrt{1-\|A^{-1}\|\,\|\delta A\|}} \cdot \frac{1}{\min\limits_{\substack{1\leq p\leq k\\ 1\leq q\leq l}} \frac{|\lambda_{i_p}-\widetilde{\lambda}_{j_q}|}{\sqrt{|\lambda_{i_p}\widetilde{\lambda}_{j_q}|}}} \cdot \frac{\|V\|^2}{\sqrt{1-4\alpha\|V\|^2}} \tag{37}$$

$$\leq \frac{\|A^{-1}\|\,\|\delta A\|_F}{\sqrt{1-\|A^{-1}\|\,\|\delta A\|}} \cdot \frac{1}{\min\limits_{\substack{1\leq p\leq k\\ 1\leq q\leq l}} \frac{|\lambda_{i_p}-\widetilde{\lambda}_{j_q}|}{\sqrt{|\lambda_{i_p}\widetilde{\lambda}_{j_q}|}}} \cdot \frac{\|A^{-1}\|\,\|\widehat{A}\|}{\sqrt{1-4\alpha\|A^{-1}\|\,\|\widehat{A}\|}} \tag{38}$$

where α *is defined by (32).*

Proof. The assumption and (36) imply (33), which in turn implies (34). Now (37) follows by inserting (34) in Theorem 3, and (38) follows by inserting (36) in (37). □

Note that the assumption of the theorem implies the positivity of the second square root in (38), and is therefore not too restrictive provided that $\|A^{-1}\|$ and $\|\widehat{A}\|$ are not too large. Some classes of matrices which fulfill this condition are described in Section 3.1. Also, instead of (36) we can use an alternative bound

$$\|V\|^2 = \|V^{-1}\|^2 \leq \|A\|\,\|\widehat{A}^{-1}\|. \tag{39}$$

In order to apply (38), besides $\|A^{-1}\|$, $\|\delta A\|_F$ and $\|\delta A\|$, we also need to know $\|\widehat{A}\|$. For the special case (8) when D is diagonal, we simply have $\|\widehat{A}\| \leq \operatorname{trace}(\widehat{A}) = n$. Such D appears naturally when we consider perturbations of the type (7) and (10) which occur in numerical computation (see Remark 1).

We now show that, for any D, $\|\widehat{A}\|$ from (38) and η from (25) can be computed by highly accurate eigenreduction algorithm from [27,18] at little extra cost [3]. This algorithm first factorizes H as $H = FJF^*$ by symmetric indefinite factorization [19]. This factorization is followed by one-sided J-orthogonal Jacobi method on the pair F, J. This method forms the sequence of matrices

$$F_{k+1} = F_k X_k, \qquad \text{where} \qquad X_k^* J X_k = J.$$

[3] In [18] only the algorithm for the real symmetric case was analyzed, but a version for the Hermtian case is possible, as well.

This sequence converges to some matrix FX which has numerically orthogonal columns, and F is J orthogonal, that is, $F^*JF = J$. The eigenvalues of H are approximated by $\Lambda = J\,\mathrm{diag}(X^*F^*FX)$, and the eigenvectors are approximated by $U = FX|\Lambda|^{-1/2}$. Therefore, $\lvert H \rvert = FXX^*F^*$. Note that X also diagonalizes the pair (F^*F, J). Since the matrix FX is readily available in the computer, we can compute $\widehat{A}$ as

$$\widehat{A} = D^{-*}FXX^*F^*D^{-1}, \tag{40}$$

or, even simpler, just its factor $D^{-*}FX$. Finally, after computing $\widehat{A}$, η can be computed directly from the definitions (5), (9), or (11), respectively.

3.1 "Well-behaved" matrices

Our bounds differ from the bounds for the positive definite case [16, Theorem 3.3] by additional factors, namely the last quotients in (37) and (38). From (36) and (39) we also have $\|V\|^2 \leq (\kappa(A)\kappa(\widehat{A}))^{1/2}$. From (1) and (4) and the definitions of H and $\lvert H \rvert$ from Section 1, we have

$$A = D^{-*}U|\Lambda|^{1/2}J|\Lambda|^{1/2}U^*D^{-1}, \quad \widehat{A} = D^{-*}U|\Lambda|^{1/2}|\Lambda|^{1/2}U^*D^{-1}.$$

This implies that (see also [29, Proof of Theorem 2.16])

$$|A_{ij}|^2 \leq \widehat{A}_{ii}\widehat{A}_{jj}, \quad |A^{-1}_{ij}|^2 \leq \widehat{A}^{-1}_{ii}\widehat{A}^{-1}_{jj},$$

and hence

$$\|\,|A|\,\| \leq \mathrm{trace}(\widehat{A}), \quad \|\,|A^{-1}|\,\| \leq \mathrm{trace}(\widehat{A}^{-1}).$$

This implies that A is well conditioned if so is $\widehat{A}$.

We conclude that the additional factors will be small if, for the chosen grading D, any of the right hand sides in (36) or (39) are small, or (which is a more restrictive condition) simply if $\widehat{A}$ is well conditioned. We call such matrices "well-behaved". We also conclude that an invariant subspace is stable under small relative perturbations for the chosen grading D, if $\|A^{-1}\|$ is small, any of the three above conditions is fulfilled, and the eigenvalues which define the subspace are well relatively separated from the rest of the spectrum.

Although $\widehat{A}$ can be easily computed as described in the comments of Theorem 6, we are interested in identifying classes of "well-behaved" matrices in advance. In the positive definite case the answer is simple – such are the well graded matrices, that is the matrices of the form $H = DAD$, where D is diagonal positive definite such that $A_{ii} = 1$, and A is well conditioned. In the indefinite case we have two easily recognisable classes of "well-behaved" matrices, namely *scaled diagonally dominant matrices* [1] and *Hermitian quasidefinite matrices* [26,8]. Moreover, for the same A such matrices are well-behaved for any diagonal grading D.

Scaled diagonally dominant matrices have the form $H = D(J + \Psi)D$, where D is diagonal positive definite, $J = \mathrm{diag}(\pm 1)$ and $\|\Psi\| < 1$. For these matrices $A = J + \Psi$ and $\|A\|\,\|\widehat{A}^{-1}\| \leq n(1 + \|\Psi\|)/(1 - \|\Psi\|)$ [29, Theorem 2.29]. Thus, (39) implies that the last quotient in (37) is small when $\|\Psi\|$ is not too close to one. Also, $\|\delta A\|$ which is used in the definition of α in (32) has to be sufficiently small.

Hermitian matrix H is quasidefinite if there exists a permutation P such that

$$P^T H P = \bar{H} = \begin{bmatrix} \bar{H}_{11} & \bar{H}_{12} \\ \bar{H}_{12}^* & -\bar{H}_{22} \end{bmatrix},$$

where H_{11} and H_{22} are positive definite. The proof that such matrix is "well-behaved" is rather involved. Quasidefinite matrix always has a triangular factorization $H = FJF^*$, where F is lower triangular with real diagonal and J is diagonal with $J_{ii} = \mathrm{sign}(H_{ii})$ [26] [4]. Set $H = DAD$ where $D = \mathrm{diag}(|H_{ii}|)$. Then

$$\bar{H} = \bar{D}\bar{A}\bar{D} = \bar{D} \begin{bmatrix} \bar{A}_{11} & \bar{A}_{12} \\ \bar{A}_{12}^* & -\bar{A}_{22} \end{bmatrix} \bar{D}, \quad \bar{D} = P^T D P, \ \bar{A} = P^T A P. \tag{41}$$

Note that A is also quasidefinite, and its triangular factorization is given by $A = BJB^*$ where $B = D^{-1}F$. Let us now bound $\kappa(\widehat{A})$. Assume without loss of generality that the diagonal elements of D are nonincreasing which can be easily attained by permutation. From (40) we have

$$\kappa(\widehat{A}) \leq \kappa(B)^2 \kappa(X)^2, \tag{42}$$

where, as already mentioned, X diagonalizes the pair (F^*F, J). In [22] it was shown that

$$\kappa(X) \leq \min_{\Delta} \sqrt{\kappa(\Delta^* F^* F \Delta)},$$

[4] The proof in [26] is for the real symmetric case, but it is easily seen that it holds for the Hermitian case, as well.

where the minimum is over all matrices which commute with J. In our case this clearly implies

$$\|X\|^2 \leq \kappa(FD^{-1}) = \kappa(DBD^{-1}).$$

Since B is lower triangular and D has nondecreasing diagonal elements, we have $|DBD^{-1}| \leq |B|$ and $|DB^{-1}D^{-1}| \leq |B^{-1}|$, so that

$$\kappa(X) \leq \| \, |B| \, \| \, \| \, |B^{-1}| \, \| \leq \|B\|_F \|B^{-1}\|_F \equiv \kappa_F(B). \tag{43}$$

The matrix JA is positive definite according to [9]. By appropriately modifying the proof of [9, Theorem], we have

$$\| \, |B| \, |B|^T \|_F \leq n(\|T\| + \|ST^{-1}S\|),$$

where $T = [JA + (JA)^T]/2$ and $S = [JA - (JA)^T]/2$. Note that the proof in [9] is for the real case, but it readily holds in the complex case as is recently shown in [28]. From (41) we have

$$\begin{aligned} \| \, |B| \, |B|^T \|_F &\leq n(\|P^T T P\| + \|P^T S P P^T T^{-1} P P^T S P\|) \\ &\leq n \max\{\|\bar{A}_{11}\| + \|\bar{A}_{12}\bar{A}_{22}^{-1}\bar{A}_{12}^*\|, \|\bar{A}_{22}\| + \|\bar{A}_{12}^*\bar{A}_{11}^{-1}\bar{A}_{12}\|. \end{aligned} \tag{44}$$

Now note that the inverse of a quasidefinite matrix is also quasidefinite [26, Theorem 1.1]. By modifying the proof of [9, Theorem] we obtain a bound similar to (44) for $\| \, |B^{-T}| \, |B^{-1}| \|_F$ (for details see [28]). By combining this discussion with (43), from (42) we conclude that essentially $\kappa(\widehat{A})$ will be small if in (41) $\bar{A}_{11}$ and $\bar{A}_{22}$ are well conditioned and $\|\bar{A}_{12}\|$ is not too large.

4 Conclusion

We derived new perturbation bounds for invariant subspaces of non-singular Hermitian matrices. Our bounds improve the existing bounds in the following aspects. Our bounds extend the bounds for scaled diagonally dominant matrices from [1] to general indefinite matrices. Our bounds also extend the bound of [16, Theorem 3.3] for positive definite matrices to indefinite case. Finally, our bounds extend the bounds for indefinite matrices from [29,25] to subspaces which correspond to any set of possibly nonadjacent eigenvalues (numerical experiments also indicate that our bounds tend to be sharper). For graded matrices of the form (1) which are well-behaved according to Section 3.1, our bounds are sharper that the general bound for diagonalizable matrices from [13],

$$\|\sin\Theta\|_F \leq \frac{\|H^{-1}\delta H\|_F}{\min\limits_{\substack{1\leq p\leq k\\ 1\leq q\leq l}} \frac{|\lambda_{i_p}-\widetilde{\lambda}_{j_q}|}{|\lambda_{i_p}|}}. \tag{45}$$

This bound makes no preference for positive definite matrices over indefinite ones, and is easier to interpret than our bound. However, since in (45) δH is multiplied by H^{-1} from the left, this bound does not accommodate two sided grading well. Finally, our bounds are computable from unperturbed quantities and can be efficiently used in analyzing numerical algorithms in which graded perturbations naturally occur.

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