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Weyl-type relative perturbation bounds for eigensystems of Hermitian matrices

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Abstract

We present a Weyl-type relative bound for eigenvalues of Hermitian perturbations $A + E$ of (not necessarily definite) Hermitian matrices A . This bound, given in function of the quantity $\eta = \|A^{-1/2}EA^{-1/2}\|_2$, that was already known in the definite case, is shown to be valid as well in the indefinite case. We also extend to the indefinite case relative eigenvector bounds which depend on the same quantity η . As a consequence, new relative perturbation bounds for singular values and vectors are also obtained. Using matrix differential calculus techniques we obtain for eigenvalues a sharper, first-order bound involving the logarithm matrix function, which is smaller than η not only for small E , as expected, but for any perturbation. © 2000 Published by Elsevier Science Inc. All rights reserved.

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1. Introduction

Relative perturbation theory of eigensystems has become of late a remarkably active area of research (see [9,10,13,14] and the references therein) as a consequence of its applications in developing high accuracy numerical methods for spectral and singular value problems [1–3,16,19].

In this paper we focus first on relative perturbation bounds for eigenvalues of additive Hermitian perturbations of Hermitian matrices. The main motivation for this

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is that, while the study of multiplicative perturbations preserving the inertia is quite satisfactory [9, Section 5], additive perturbation theory suffers from several drawbacks in the relative setting. The underlying reason is that eigenvalues of Hermitian matrices are naturally ordered due to their real character. Thus, when comparing the eigenvalues of two Hermitian matrices, it is desirable to keep this order, as in the classical absolute Weyl bound [21, Corollary IV.4.10], or the Hermitian version of the Hoffman–Wielandt theorem [21, Corollary IV.4.13]. However, no relative bounds with this natural order are available for additive perturbations of general Hermitian matrices: either a permutation of the perturbed eigenvalues is introduced [9, Section 2.3], or the bounds are written in terms of quantities which are not explicitly identified as a function of the matrices involved [22]. So far, the only case in which the relative bounds preserve the natural order and are given explicitly in terms of the unperturbed and perturbation matrices is the positive definite case [2,5,12,13,17,20]. To be more precise, let A and $A + E$ be Hermitian matrices with eigenvalues $\lambda_1 \geq \dots \geq \lambda_n$ and $\widehat{\lambda}_1 \geq \dots \geq \widehat{\lambda}_n$, respectively. It has been shown in [17] that if *both* A and $A + E$ are positive definite, then

$$\frac{|\widehat{\lambda}_i - \lambda_i|}{|\lambda_i|} \leq \|A^{-1/2}EA^{-1/2}\|_2 \quad \text{for } i = 1, \dots, n, \quad (1)$$

where $\|\cdot\|_2$ stands for the spectral norm. We show in Section 2 (Theorem 2.1) that the same bound holds for *arbitrary* Hermitian matrices A and E , provided A is nonsingular, $A^{1/2}$ is any normal square root of A and

$$\|A^{-1/2}EA^{-1/2}\|_2 \leq 1. \quad (2)$$

Although the bound (1) is, essentially, a particular case of [22, Theorem 2.1], we include an elementary proof whose main point is drawing the attention to the previously unnoticed fact that (1) is valid for both the definite and indefinite cases. This seems to support the idea that there are no essential differences between definite and indefinite matrices from the point of view of relative eigenvalue perturbation theory, much in the same way as in the classical absolute perturbation theory. As to the restriction (2), some examples are provided which show that it cannot be removed without additional assumptions on the matrices A or E . Furthermore we show in Lemma 2.2 that (1) is sharper than other usual relative perturbation bounds in the literature¹ for the Hermitian case, namely $\|A^{-1}E\|_2$ or $\|EA^{-1}\|_2$, and we also discuss in Corollary 2.3 how the diagonal elements of a Hermitian matrix approximate its eigenvalues.

Section 2 concludes by extending to indefinite matrices the general results for eigenvectors of positive definite matrices given in [17, Section 2.2]. Using structured Sylvester equations [14] we get nonasymptotic simple bounds for invariant subspace variations. From them we easily get first-order bounds in terms of $\|A^{-1/2}EA^{-1/2}\|_F$

¹ All these quantities, $\|A^{-1}E\|_2$, $\|EA^{-1}\|_2$ and $\|A^{-1/2}EA^{-1/2}\|_2$, are used in [5] in Bauer–Fike type bounds for diagonalizable matrices. In [5] the bounds of Weyl type are only developed in the case of Hermitian positive definite matrices using $\|A^{-1/2}EA^{-1/2}\|_2$.

in the case of subspaces, or $\|A^{-1/2}EA^{-1/2}\|_2$ for individual eigenvectors. Our approach extends the one in [17] in two ways: it is valid for general nonsingular indefinite Hermitian matrices and for general invariant subspaces.

In Section 3 we apply the results of Section 2 to Jordan–Wielandt matrices to obtain previously unknown bounds on the variation of singular values and singular subspaces, that in some cases can improve the existing results.

Section 4 is devoted to comparing the bound in Theorem 2.1 with a sharper, first-order bound. Using matrix differential calculus techniques we obtain in Theorem 4.1 a differential quantity which collectively bounds the first-order terms of the perturbation expansions of all relative eigenvalue variations. Furthermore we show that $\|A^{-1/2}EA^{-1/2}\|_2$ is larger than this first-order differential bound not only for small E , as expected, but for any perturbation E . To be precise, the extent to which $\|A^{-1/2}EA^{-1/2}\|_2$ exceeds the first order bound is given by a Löwner-like matrix which depends exclusively on the size of the eigenvalues of A relative to each other. It turns out that both bounds are roughly of the same size unless the eigenvalues of A differ greatly in modulus.

Notation. Both the unperturbed matrix A and the perturbed matrix $\widehat{A} = A + E$ are complex n by n Hermitian (eventually indefinite) matrices. Hermitian matrices are ordered in Section 2 according to the positive semidefinite ordering: we say that $A \leq B$ if $B - A$ is positive semidefinite. The conjugate transpose of a matrix A is denoted by A^* , its spectral norm (or 2-norm) by $\|A\|_2$ and its Frobenius norm by $\|A\|_F$. Any square root $A^{1/2}$ of a Hermitian matrix A should be taken to be a *normal* matrix such that $(A^{1/2})^2 = A$. This distinction is not vacuous, since Hermitian matrices have nonnormal square roots, even if they are positive definite [8, Section 6.4]. $\mathcal{L}(A)$ will denote the set of eigenvalues of any Hermitian matrix A , which should be taken to be indexed in decreasing order, i.e.

$$\lambda_1(A) \geq \dots \geq \lambda_n(A). \tag{3}$$

The logarithm, as well as any other function of the Hermitian matrix A , is to be understood in the usual way: if $f : \Omega \subset \mathbb{R} \mapsto \mathbb{C}$ is any function whose domain Ω contains the spectrum of the matrix A , we define f on A by

$$f(A) = V \operatorname{diag}[f(\lambda_1), \dots, f(\lambda_n)] V^*, \tag{4}$$

where V is any unitary matrix such that $A = V \Lambda V^*$ and $\Lambda = \operatorname{diag}[\lambda_1, \dots, \lambda_n]$. Finally, for any matrix B , $\sigma(B)$ denotes the set of its singular values and $\mathcal{R}(B)$ denotes the column space of B .

2. Relative perturbation bounds for eigensystems of Hermitian matrices

2.1. Eigenvalue bounds

Our starting point is, as announced in the Introduction, the following Weyl-type relative perturbation bound for eigenvalues of Hermitian matrices. In the proof we first

derive the simple, but previously unnoticed, equality (7). From there our discussion is identical to that of [22, Theorem 2.1], we include it for the sake of completeness.

Theorem 2.1. *Let A be Hermitian and nonsingular with eigenvalues $\lambda_1 \geq \dots \geq \lambda_n$ and $A + E$ Hermitian with eigenvalues $\widehat{\lambda}_1 \geq \dots \geq \widehat{\lambda}_n$. If $\eta = \|A^{-1/2}EA^{-1/2}\|_2 \leq 1$, with $A^{1/2}$ any normal square root of A , then*

$$\frac{|\widehat{\lambda}_i - \lambda_i|}{|\lambda_i|} \leq \eta \quad \text{for } i = 1, \dots, n. \quad (5)$$

Proof. We begin by rewriting η in a more convenient way. Let $A = V|A|V^*$ be a unitary diagonalization of A , i.e. V is unitary and $|A| = \text{diag}[\lambda_1, \dots, \lambda_n]$. Then,

$$A = V|A|V^* V\Phi V^*, \quad (6)$$

where $|A|$ and Φ are diagonal matrices with diagonal elements $|\lambda_i|$ and $\text{sign}(\lambda_i)$, respectively. Thus, Eq. (6) is in fact the unique polar decomposition $A = PU$ of A , where $P = V|A|V^*$ is the positive definite square root of AA^* and $U = V\Phi V^*$ is unitary. We now write $P^{1/2}$ in terms of $A^{1/2} = VA^{1/2}V^*$, with $A^{1/2} = \text{diag}[\lambda_1^{1/2}, \dots, \lambda_n^{1/2}]$ any diagonal square root of A so that $A^{1/2}$ is any normal square root of A ,

$$P^{1/2} = V|A|^{1/2}V^* = VA^{1/2}V^* V\Phi^{-1/2}V^* = A^{1/2}U^{-1/2}.$$

Also, using now that $|A|^{1/2} = \Phi^{-1/2}A^{1/2}$, we may write $P^{1/2}$ as

$$P^{1/2} = U^{-1/2}A^{1/2}.$$

Therefore η can be written as

$$\begin{aligned} \eta &= \|A^{-1/2}EA^{-1/2}\|_2 = \|U^{1/2}A^{-1/2}EA^{-1/2}U^{1/2}\|_2 \\ &= \|P^{-1/2}EP^{-1/2}\|_2 \end{aligned} \quad (7)$$

since $U^{1/2}$ is unitary². Hence, η satisfies the inequalities

$$-\eta I \leq P^{-1/2}EP^{-1/2} \leq \eta I,$$

which remain valid if both sides are multiplied by the Hermitian matrix $P^{1/2}$

$$-\eta P \leq E \leq \eta P \quad (8)$$

or the matrix A is added

$$A - \eta P \leq A + E \leq A + \eta P. \quad (9)$$

Now, we apply the monotonicity theorem [7, Corollary 4.3.3] to obtain that

$$\lambda_i(A - \eta P) \leq \lambda_i(A + E) \leq \lambda_i(A + \eta P), \quad (10)$$

² In fact it is easy to prove that η can be written still in more general forms, e.g. $\eta = \|G^{-1}EG^{-*}\|_2$ for any decomposition $P = GG^*$.

where $\lambda_i(A \pm \eta P)$ denotes the i th largest eigenvalue of $A \pm \eta P$. That is, the eigenvalues $\{\lambda_i \pm \eta|\lambda_i|\}_{i=1}^n$ of $A \pm \eta P$ are upper/lower bounds for the set of perturbed eigenvalues $\{\widehat{\lambda}_i\}_{i=1}^n$. The order of these bounds depends on η , and it is not difficult to show that if $\eta \leq 1$ then

$$\lambda_i(A \pm \eta P) = \lambda_i \pm \eta|\lambda_i| \quad \text{for } i = 1, \dots, n. \tag{11}$$

Bringing together (10) and (11) we get the final result

$$\lambda_i - \eta|\lambda_i| \leq \widehat{\lambda}_i \leq \lambda_i + \eta|\lambda_i|. \quad \square \tag{12}$$

As we mentioned in the Introduction this result is mostly contained in [22, Theorem 2.1] as a particular case. To be precise, Theorem 2.1 can be obtained from [22, Theorem 2.1] (setting $K = I$), once it is established that the quantity η is the best possible η_H in [22]. The main difference in our approach is to identify explicitly the bound in terms of the perturbed and unperturbed matrices, and drawing the attention to the previously unnoticed fact that the same quantity appears in both the definite and the indefinite case.

The proof of Theorem 2.1 also follows closely the one given in [17] for the case in which both A and $A + E$ are positive definite. However, under this hypothesis it is not necessary to restrict the size of the perturbation to $\eta \leq 1$ (we will see below that this is absolutely necessary in the general indefinite case, including the case in which only A is positive definite). The reason is that when $\lambda_i \geq 0$ the order of the upper bounds is kept: $\lambda_i + \eta\lambda_i \geq \lambda_{i+1} + \eta\lambda_{i+1}$ for $i = 1, \dots, n - 1$ and arbitrary η . Moreover, since the perturbed eigenvalues are also required to be positive, we have

$$\lambda_i - \eta\lambda_i < 0 < \widehat{\lambda}_i \leq \lambda_i + \eta\lambda_i \quad \forall \eta > 1.$$

As the result for $\eta \leq 1$ is still valid, we have that (5) is valid for any value of η if both A and $A + E$ are positive definite. Observe that to extend the validity of the result beyond $\eta = 1$ it has been necessary to use something else than Eq. (9) and the monotonicity theorem.

This said, one may ask what happens in the indefinite case if η is allowed to be bigger than one. We present two simple examples in which the relative change of the eigenvalues is larger than η .

1. We first consider the case in which only A is positive definite. The following example shows that the result (5) does not hold for any value of η if only A is required to be positive definite. Consider the following matrices:

$$A = \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix} \quad \text{and} \quad A + E = \begin{bmatrix} .1 & 10 \\ 10 & 1.5 \end{bmatrix}. \tag{13}$$

The perturbed eigenvalues are $\widehat{\lambda}_1 = 10.82447$ and $\widehat{\lambda}_2 = -9.22447$, that gives, even allowing permutations π of the indices,

$$\min_{\pi} \max_{i=1,2} \frac{|\widehat{\lambda}_{\pi(i)} - \lambda_i|}{|\lambda_i|} = 9.82447,$$

while $\eta = 7.33314$.

2. One might think that if the perturbation does not change the inertia Theorem 2.1 might be extended beyond $\eta = 1$ as in the case when both A and $A + E$ are positive definite. One reason for this is that it is known [4] that for any size of a (multiplicative) perturbation keeping the inertia there are relative bounds of the type (5), although expressed in terms of a different quantity. If $A + E$ is written as DAD^* then

$$|\widehat{\lambda}_i - \lambda_i| \leq |\lambda_i| \|DD^* - I\|_2. \quad (14)$$

Consider now

$$A = \begin{bmatrix} 2 & 0 \\ 0 & -1 \end{bmatrix} \quad (15)$$

with $A + E$ the same as in (13). The relative perturbation of the eigenvalues

$$\min_{\pi} \max_{i=1,2} \frac{|\widehat{\lambda}_{\pi(i)} - \lambda_i|}{|\lambda_i|} = 8.22447$$

is larger than $\eta = 8.05344$, while the bound (14) holds: if we use

$$D = \begin{bmatrix} 0.223607 & 0 \\ 22.36068 & 31.59905 \end{bmatrix}$$

then $\|DD^* - I\|_2 = 1496.51$.

The relative perturbation to A is given in Theorem 2.1 in terms of the spectral norm of the matrix $A^{-1/2}EA^{-1/2}$. This is not the only way to measure the size of a relative perturbation. Among many possible choices, probably the two other most usual in the diagonalizable case are the 2-norms of either $A^{-1}E$ or EA^{-1} (see [5], for instance, where all three kinds of bound are used). The following lemma shows that η is the best bound among these three possibilities.

Lemma 2.2. *Let A be normal and B Hermitian. Then*

$$\|A^{1/2}BA^{1/2}\|_2 \leq \|AB\|_2 = \|BA\|_2$$

Proof. Let $A = P_A U_A = U_A P_A$ and $B = P_B U_B = U_B P_B$ be the polar decompositions of A and B , respectively. Since the 2-norm is unitarily invariant

$$\begin{aligned} \|AB\|_2 &= \|P_A P_B\|_2 = \|(P_A P_B)^*\|_2 \\ &= \|P_B P_A\|_2 = \|U_B P_B P_A U_A\|_2 = \|BA\|_2. \end{aligned}$$

On the other hand

$$\begin{aligned} \|BA\|_2 &= \|B P_A\|_2 \geq \max_i |\lambda_i(B P_A)| \\ &= \max_i |\lambda_i(P_A^{1/2} B P_A^{1/2})| = \|P_A^{1/2} B P_A^{1/2}\|_2 = \|A^{1/2} B A^{1/2}\|_2. \quad \square \end{aligned}$$

As an immediate consequence we obtain that

$$\eta = \|A^{-1/2}EA^{-1/2}\|_2 \leq \|A^{-1}E\|_2 = \|EA^{-1}\|_2.$$

This result allows to use Theorem 2.1 choosing for the bound in (5) any of the previous quantities, depending on which is more convenient. For instance one may be interested in introducing left (resp. right) scalings. In that case, $\|A^{-1}E\|_2$ (resp. $\|EA^{-1}\|_2$) may be chosen since it is invariant under such transformations, unlike $\|A^{-1/2}EA^{-1/2}\|_2$ which is invariant under congruence transformations of the polar factor in the sense of Corollary 3.4 in [5].

We conclude this section by drawing one direct consequence of Theorem 2.1: we discuss how the diagonal elements of a Hermitian matrix approximate its eigenvalues. This is a crucial question for numerical eigenvalue methods, like two-sided Jacobi, which converge to an almost diagonal matrix. As a straightforward consequence of Theorem 2.1 we obtain the following result.

Corollary 2.3. *Let $A = [a_{ij}]$ be a Hermitian matrix such that $D = \text{diag}[a_{ii}]$ is invertible and $\alpha_1 \geq \dots \geq \alpha_n$ its diagonal entries in decreasing order. Let $\lambda_1 \geq \dots \geq \lambda_n$ be the eigenvalues of A . If $\|D^{-1/2}(A - D)D^{-1/2}\|_2 \leq 1$, with $D^{1/2}$ any normal square root of D , then*

$$\frac{|\lambda_i - \alpha_i|}{|\alpha_i|} \leq \|D^{-1/2}(A - D)D^{-1/2}\|_2, \quad i = 1, \dots, n. \tag{16}$$

Proof. Apply Theorem 2.1 to $A = D + N$ with D as unperturbed matrix, N as perturbation, and A as perturbed matrix. \square

Note that if A is positive definite, then D is positive definite too and the restriction $\|D^{-1/2}(A - D)D^{-1/2}\|_2 \leq 1$ is not needed, as noted after Theorem 2.1.³ The positive definite case is well known in the literature [17], and can be traced back to [2, Proposition 2.7]. The indefinite case is also known. In fact, Corollary 2.3 is the Proposition 2 of [1], because the condition $\|D^{-1/2}(A - D)D^{-1/2}\|_2 \leq 1$ means, in the notation of [1], that A is γ -scaled diagonally dominant with respect to $\|\cdot\|_2$ with $\gamma = \|D^{-1/2}(A - D)D^{-1/2}\|_2$. The proof presented here is simpler than the one in [1], and besides it provides a nice connection between the relative perturbation theory of scaled diagonally dominant matrices and Hermitian matrices. Another way to look at Theorem 2.1 is as a generalization of Corollary 2.3 to general perturbations.

From Corollary 2.3 is easy to justify a stopping criterion for the Jacobi method which has been used in [2,16] for positive definite matrices and in [19] for indefinite matrices. To be precise, let A be an $n \times n$ invertible Hermitian matrix with nonzero diagonal entries, and tol a real number such that

$$n \, tol < 1 \quad \text{and} \quad |a_{ij}| \leq tol \sqrt{|a_{ii}a_{jj}|} \quad \text{for all } i \neq j. \tag{17}$$

Then, a straightforward consequence of Corollary 2.3 is that

³ However the properties of positive definite matrices imply that $\|D^{-1/2}(A - D)D^{-1/2}\|_2 \leq \sqrt{n(n-1)}$.

$$\frac{|\lambda_i - \alpha_i|}{|\lambda_i|} \leq \frac{n \text{ tol}}{1 - n \text{ tol}}, \quad i = 1, \dots, n. \tag{18}$$

2.2. Eigenvector bounds

Some of the results for eigenvectors of positive definite matrices given in [17] can be extended to indefinite matrices. Nevertheless, the techniques used here are different from the ones in [17]. First we use the theory for structured Sylvester equations appearing in [14, Section 2.4] to get nonasymptotic bounds for invariant subspace variations and for simple eigenvectors. From them we easily get first-order bounds using classical analyticity results.

Theorem 2.4. *Let A and $\widehat{A} = A + E$ be two Hermitian and nonsingular matrices with unitary eigendecompositions*

$$A = \begin{bmatrix} X_1 & X_2 \end{bmatrix} \begin{bmatrix} A_1 & 0 \\ 0 & A_2 \end{bmatrix} \begin{bmatrix} X_1^* \\ X_2^* \end{bmatrix},$$

$$\widehat{A} = \begin{bmatrix} \widehat{X}_1 & \widehat{X}_2 \end{bmatrix} \begin{bmatrix} \widehat{A}_1 & 0 \\ 0 & \widehat{A}_2 \end{bmatrix} \begin{bmatrix} \widehat{X}_1^* \\ \widehat{X}_2^* \end{bmatrix}. \tag{19}$$

Define

$$\rho = \min_{\widehat{\lambda} \in \mathcal{L}(\widehat{A}_1), \lambda \in \mathcal{L}(A_2)} \frac{|\lambda - \widehat{\lambda}|}{\sqrt{|\lambda \widehat{\lambda}|}} \quad \text{and} \quad \rho_i = \min_{j \neq i} \frac{|\lambda_j - \widehat{\lambda}_i|}{\sqrt{|\lambda_j \widehat{\lambda}_i|}}. \tag{20}$$

Let Θ be the matrix of the canonical angles between $\mathcal{R}(X_1)$ and $\mathcal{R}(\widehat{X}_1)$. If $\rho > 0$ then

$$\|\sin \Theta\|_F \leq \frac{1}{\rho} \|A^{-1/2} E \widehat{A}^{-1/2}\|_F. \tag{21}$$

Furthermore, let θ_i be the acute angle between an eigenvector x_i of A corresponding to λ_i and an eigenvector \widehat{x}_i of \widehat{A} corresponding to $\widehat{\lambda}_i$. If $\rho_i > 0$ then

$$\sin \theta_i \leq \frac{1}{\rho_i} \|A^{-1/2} E \widehat{A}^{-1/2}\|_2. \tag{22}$$

Proof. Define the residual

$$R = A \widehat{X}_1 - \widehat{X}_1 \widehat{A}_1 = (A - \widehat{A}) \widehat{X}_1.$$

Multiply on the left by X_2^* and define $S = X_2^* \widehat{X}_1$, thus

$$A_2 S - S \widehat{A}_1 = X_2^* (A - \widehat{A}) \widehat{X}_1 = X_2^* A^{1/2} A^{-1/2} (A - \widehat{A}) \widehat{A}^{-1/2} \widehat{A}^{1/2} \widehat{X}_1.$$

Using the eigendecompositions (19) we obtain the following Sylvester equation for the matrix S , whose singular values are the sines of the canonical angles between $\mathcal{R}(X_1)$ and $\mathcal{R}(\widehat{X}_1)$ [21]:

$$A_2 S - S \widehat{A}_1 = A_2^{1/2} X_2^* A^{-1/2} (A - \widehat{A}) \widehat{A}^{-1/2} \widehat{X}_1 \widehat{A}_1^{1/2}. \tag{23}$$

Setting

$$G = X_2^* A^{-1/2} (A - \widehat{A}) \widehat{A}^{-1/2} \widehat{X}_1, \tag{24}$$

Eq. (23) reads entrywise

$$[(A_2)_{kk} - (\widehat{A}_1)_{ll}] S_{kl} = (A_2)_{kk}^{1/2} G_{kl} (\widehat{A}_1)_{ll}^{1/2},$$

which implies

$$\|S\|_F \leq \frac{1}{\rho} \|G\|_F \leq \frac{1}{\rho} \|A^{-1/2} E \widehat{A}^{-1/2}\|_F.$$

We finish the proof applying the previous inequality to bound the sine of the angle between x_i and \widehat{x}_i . In this case, if we identify x_i with X_1 and \widehat{x}_i with \widehat{X}_1 , the matrices S and G become $(n - 1) \times 1$ column vectors, thus $\|G\|_F = \|G\|_2$, and $\|S\|_F = \sin \theta_i$. \square

The bounds in Theorem 2.4 do not impose any restriction on the size of the perturbation, but, unlike the bound η in Theorem 2.1, they involve A , E and also \widehat{A} . However, using well-known results of Kato [11, Section II 6.2], one can get:

$$A^{-1/2} E \widehat{A}^{-1/2} = A^{-1/2} E A^{-1/2} + O(\|E\|_F^2),$$

and

$$\rho = \rho^\circ + O(\|E\|_F),$$

where the relative gap ρ° only involves eigenvalues of A :

$$\rho^\circ = \min_{\mu \in \mathcal{L}(A_1), \lambda \in \mathcal{L}(A_2)} \frac{|\lambda - \mu|}{\sqrt{|\lambda \mu|}}.$$

Hence, we can easily get first-order bounds in terms of η :

$$\|\sin \Theta\|_F \leq \frac{1}{\rho^\circ} \|A^{-1/2} E A^{-1/2}\|_F + O(\|E\|_F^2) \quad \text{as} \quad \|E\|_F \longrightarrow 0. \tag{25}$$

It is also possible to obtain a first-order bound in the spectral norm from (22) but only for one eigenvector. The bound (25) extends [17, Theorem 2.7], as announced, in two ways: it is valid for general indefinite Hermitian matrices and for general invariant subspaces.

3. Relative perturbation bounds for singular value decompositions

3.1. Singular value bounds

Theorem 2.1 can also be used to obtain relative perturbation bounds for singular values of nonsingular square matrices. To be precise, let B be an $n \times n$ nonsingular

matrix and $B + F$ an $n \times n$ matrix. It is well known [7, Chapter 7] that there exist two standard ways of transforming the singular value problem of B into a Hermitian eigenvalue problem. The first one is to study the positive definite eigenvalue problem of B^*B (or BB^*), and the second one the indefinite eigenvalue problem for the Jordan–Wielandt matrix

$$\begin{bmatrix} 0 & B^* \\ B & 0 \end{bmatrix}. \tag{26}$$

A bound for the singular values can be immediately obtained by applying Theorem 2.1 to the relative difference between the eigenvalues of B^*B (resp. BB^*) and the eigenvalues of $(B + F)^*(B + F)$ using the remark in footnote 2. The result so obtained is equivalent, up to second-order terms in F , to the one proved by Demmel and Veselić [2] and is valid for any size of F because B^*B is positive definite. Instead, in this section, we focus on applying Theorem 2.1 to the eigenvalue variation of matrix (26) under perturbations to prove the following theorem:

Theorem 3.1. *Let B be a nonsingular $n \times n$ matrix with singular values $\sigma_1 \geq \dots \geq \sigma_n$ and $B = P_1 Q = Q P_2$ its left and right polar decompositions, where Q is unitary. Let $B + F$ be a square matrix with singular values $\widehat{\sigma}_1 \geq \dots \geq \widehat{\sigma}_n$. If*

$$\|P_1^{-1/2} F P_2^{-1/2}\|_2 \leq 1 \tag{27}$$

then

$$\frac{|\widehat{\sigma}_i - \sigma_i|}{\sigma_i} \leq \|P_1^{-1/2} F P_2^{-1/2}\|_2 \quad i = 1, \dots, n. \tag{28}$$

Furthermore, let $B = U \Sigma V^*$ be a singular value decomposition of B and $S = V \Sigma^{-1/2} U^*$. Then

$$\|S F S\|_2 = \|P_1^{-1/2} F P_2^{-1/2}\|_2. \tag{29}$$

Proof. The theorem is easily proven applying Theorem 2.2 to the matrices

$$\tilde{B} = \begin{bmatrix} 0 & B^* \\ B & 0 \end{bmatrix}, \quad \tilde{B} + \tilde{F} = \begin{bmatrix} 0 & (B + F)^* \\ B + F & 0 \end{bmatrix}, \tag{30}$$

and taking into account that the positive definite polar factor of \tilde{B} is

$$\begin{bmatrix} P_2 & 0 \\ 0 & P_1 \end{bmatrix} = \frac{1}{\sqrt{2}} \begin{bmatrix} V & V \\ U & -U \end{bmatrix} \begin{bmatrix} \Sigma & 0 \\ 0 & \Sigma \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} V^* & U^* \\ V^* & -U^* \end{bmatrix}. \tag{31}$$

Eq. (29) follows from the fact that the spectral norm is unitarily invariant. \square

Previous additive Weyl-type relative perturbation bounds for singular values have been obtained either without any reference to relative perturbation bounds for eigenvalues [2,9] or using relative bounds for eigenvalues of the positive definite matrices B^*B or BB^* [13]. Theorem 2.1 allows us to deal with the indefinite eigenvalue problem of the Hermitian matrix (26) to obtain a new bound (28) for the singular value problem.

We continue by comparing the bound (28) with the following one obtained in [2], which we state as in [9, Corollary 3.2]:

Theorem 3.2. *Let B be a nonsingular $n \times n$ matrix with singular values $\sigma_1 \geq \dots \geq \sigma_n$. Let $B + F$ be a square matrix with singular values $\hat{\sigma}_1 \geq \dots \geq \hat{\sigma}_n$. Then*

$$\left| \frac{\hat{\sigma}_i - \sigma_i}{\sigma_i} \right| \leq \min \left\{ \|B^{-1}F\|_2, \|FB^{-1}\|_2 \right\}, \quad i = 1, \dots, n. \tag{32}$$

The relation between the bounds in Theorems 3.1 and 3.2 is not straightforward. Lemma 2.2 can be applied to the matrices \tilde{B}^{-1} and \tilde{F} defined in (30) to show that

$$\|SFS\|_2 = \|P_1^{-1/2}FP_2^{-1/2}\|_2 \leq \max \left\{ \|B^{-1}F\|_2, \|FB^{-1}\|_2 \right\} \tag{33}$$

with the notation of Theorem 3.1, but it is not possible to decide if $\|SFS\|_2$ is smaller than $\min \left\{ \|B^{-1}F\|_2, \|FB^{-1}\|_2 \right\}$ or vice versa, because their relation depends on how the matrices B and F are chosen. Numerical simulations of random matrices B and F , with entries chosen from a normal distribution with mean zero and different variances, show that usually $\|SFS\|_2$ is smaller than $\min \left\{ \|B^{-1}F\|_2, \|FB^{-1}\|_2 \right\}$. This happens almost always for matrices of dimension 20 or larger, although it becomes less frequent as the dimension decreases. For 2×2 matrices it is observed only in about half of the cases. However, examples of arbitrary dimension can be easily constructed in which either of the two quantities is much smaller than the other. This is the case, for instance, in a situation that appears frequently in the analysis of high accuracy numerical methods for singular values [2]: if $B = B_0D$ and $F = F_0D$ with D being an ill-conditioned diagonal nonsingular matrix, B_0 is a well-conditioned matrix and F_0 is sufficiently small, then it usually happens that $\min \left\{ \|B^{-1}F\|_2, \|FB^{-1}\|_2 \right\} \ll \|SFS\|_2$.

As in the case of Corollary 2.3 for eigenvalues, the bounds given in Theorems 3.1 and 3.2 can be easily computed when approximating the singular values of a matrix by the absolute values of its diagonal elements. This is an important question for some numerical singular value methods, like two-sided Jacobi [6, Section 8.6.3], which converge to an almost diagonal matrix. A straightforward consequence of Theorems 3.1 and 3.2 is the following corollary (see [9, Section 4] for more on these questions):

Corollary 3.3. *Let $B = [b_{ij}]$ be a nonsingular square matrix such that $D = \text{diag}[b_{ii}]$ is invertible and let $s_1 \geq \dots \geq s_n$ be the absolute values of its diagonal entries in decreasing order. Let $\sigma_1 \geq \dots \geq \sigma_n$ be the singular values of B . If $\|D^{-1/2}(B - D)D^{-1/2}\|_2 \leq 1$, with $D^{1/2}$ any normal square root of D , then*

$$\frac{|\sigma_i - s_i|}{s_i} \leq \|D^{-1/2}(B - D)D^{-1/2}\|_2, \quad i = 1, \dots, n, \tag{34}$$

and, for any B ,

$$\frac{|\sigma_i - s_i|}{s_i} \leq \min \left\{ \|D^{-1}(B - D)\|_2, \|(B - D)D^{-1}\|_2 \right\}, \quad i = 1, \dots, n. \quad (35)$$

To use these results to approximate the singular values of a matrix by the absolute values of its diagonal elements one should check carefully which bound is best, because the differences can be quite large. For example, consider the matrix

$$B = \begin{bmatrix} 10^{20} & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 10^{20} & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

The bound (34) applied to this matrix yields 10^{-10} , however the bound (35) yields 1.

To end this part it is interesting to observe that (34) allows the use of the same stopping criterion for singular value algorithms, converging to an almost diagonal matrix, as the one used for eigenvalues (17).

3.2. Singular vector bounds

The approach followed in the proof of Theorem 3.1, using the Jordan–Wielandt matrix, can also be used to apply Theorem 2.4 for obtaining bounds on the sines of the canonical angles between singular subspaces of square nonsingular matrices. The notation in Theorem 3.1 is used.

Theorem 3.4. *Let B and $\widehat{B} = B + F$ be two $n \times n$ nonsingular matrices with singular value decompositions*

$$\begin{aligned} B &= [U_1 \quad U_2] \begin{bmatrix} \Sigma_1 & 0 \\ 0 & \Sigma_2 \end{bmatrix} \begin{bmatrix} V_1^* \\ V_2^* \end{bmatrix}, \\ \widehat{B} &= [\widehat{U}_1 \quad \widehat{U}_2] \begin{bmatrix} \widehat{\Sigma}_1 & 0 \\ 0 & \widehat{\Sigma}_2 \end{bmatrix} \begin{bmatrix} \widehat{V}_1^* \\ \widehat{V}_2^* \end{bmatrix} \end{aligned} \quad (36)$$

with no particular order assumed on the singular values. Define

$$\rho_s = \min_{\widehat{\mu} \in \sigma(\widehat{\Sigma}_1), \mu \in \sigma(\Sigma_2)} \frac{|\mu - \widehat{\mu}|}{\sqrt{\mu \widehat{\mu}}} \quad \text{and} \quad \rho_{si} = \min_{j \neq i} \frac{|\sigma_j - \widehat{\sigma}_i|}{\sqrt{\sigma_j \widehat{\sigma}_i}}. \quad (37)$$

Let Φ be the matrix of the canonical angles between $\mathcal{R}(U_1)$ and $\mathcal{R}(\widehat{U}_1)$ and Θ the matrix of the canonical angles between $\mathcal{R}(V_1)$ and $\mathcal{R}(\widehat{V}_1)$. If $\rho_s > 0$ then

$$\sqrt{\|\sin \Phi\|_F^2 + \|\sin \Theta\|_F^2} \leq \frac{1}{\rho_s} \sqrt{\|P_1^{-1/2} F \widehat{P}_2^{-1/2}\|_F^2 + \|\widehat{P}_1^{-1/2} F P_2^{-1/2}\|_F^2}. \quad (38)$$

Furthermore, let ϕ_i be the acute angle between u_i and \widehat{u}_i , left singular vectors of respectively, B and \widehat{B} , and let θ_i be the corresponding angle between right singular vectors. If $\rho_{si} > 0$ then

$$\max\{\sin \phi_i, \sin \theta_i\} \leq \frac{\sqrt{2}}{\rho_{si}} \max\{\|P_1^{-1/2} F \widehat{P}_2^{-1/2}\|_2, \|\widehat{P}_1^{-1/2} F P_2^{-1/2}\|_2\} \quad (39)$$

Proof. Consider the Jordan–Wielandt matrices \tilde{B} and $\tilde{B} + \tilde{F}$ defined in (30). The theorem is easily proven applying Theorem 2.4 to their respective matrices of orthonormal eigenvectors

$$X_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} V_1 & V_1 \\ U_1 & -U_1 \end{bmatrix} \quad \text{and} \quad \widehat{X}_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} \widehat{V}_1 & \widehat{V}_1 \\ \widehat{U}_1 & -\widehat{U}_1 \end{bmatrix}.$$

corresponding, respectively, to the eigenvalues of $\text{diag}(\Sigma_1, -\Sigma_1)$ and $\text{diag}(\widehat{\Sigma}_1, -\widehat{\Sigma}_1)$. The rest of the proof is similar to that in [21, Theorem V.4.1] for the classical absolute theorem of Wedin [23]. \square

As in the case of invariant subspaces of Hermitian matrices it is also possible to get first-order bounds

$$\sqrt{\|\sin \Phi\|_F^2 + \|\sin \Theta\|_F^2} \leq \frac{\sqrt{2}}{\rho_s^\circ} \|P_1^{-1/2} F P_2^{-1/2}\|_F + O(\|F\|_F^2) \text{ as } \|F\|_F \rightarrow 0,$$

where the relative gap ρ_s° only involves singular values of B

$$\rho_s^\circ = \min_{\mu \in \sigma(\Sigma_1), \alpha \in \sigma(\Sigma_2)} \frac{|\alpha - \mu|}{\sqrt{\alpha\mu}}.$$

4. Relative bounds for eigenvalues and differential calculus

In this final section, the quantity $\eta = \|A^{-1/2} E A^{-1/2}\|_2$ appearing in Theorem 2.1 is compared with a first-order relative bound. This will be done in two steps. First we obtain a differential first-order collective bound for all relative eigenvalue variations. Then we show that this bound is smaller than η irrespective of the size of the perturbation. Finally, the difference between the two bounds is shown to depend exclusively on how separated in size are the eigenvalues of A .

Each eigenvalue λ of the Hermitian matrix A is considered as a function $\lambda = \lambda(A)$ of the matrix itself. If λ has multiplicity k , one can show [15,18] that the eigenvalue $\lambda(A)$ is *directionally* (or *Gateaux-*) *differentiable*, that is, each copy $\lambda_i(A)$, $i = 1, \dots, k$, of the multiple eigenvalue λ has an expansion

$$\lambda_i(A + E) = \lambda_i(A) + \xi_i + O(\|E\|^2), \quad (40)$$

where each of the k *directional derivatives* $\xi_i = d \lambda_i(A, E)$ is an eigenvalue of the $k \times k$ matrix $X^* E X$, and the columns of X constitute an orthonormal basis of the invariant subspace associated with λ . Note that, since the ξ_i are, as a rule, *nonlinear* functions of the perturbation matrix E , multiple eigenvalues need no longer be totally differentiable in the usual sense. We are now ready to state the main result of this section.

Theorem 4.1. *Let A be a nonsingular Hermitian matrix with eigenvalues $\lambda_1 \geq \dots \geq \lambda_n$ and $A + E$ Hermitian with eigenvalues $\widehat{\lambda}_1 \geq \dots \geq \widehat{\lambda}_n$. Then*

$$\frac{|\widehat{\lambda}_i - \lambda_i|}{|\lambda_i|} \leq \|d \log(P, E)\|_2 + O(\|E\|_2^2), \quad i = 1, \dots, n, \tag{41}$$

and

$$\|d \log(P, E)\|_2 \leq \|A^{-1/2} E A^{-1/2}\|_2, \tag{42}$$

where P is the unique positive definite polar factor of A and $d \log(P, E)$ stands for the derivative of the logarithm at P in the direction of E (see (43) below for an explicit expression of $d \log$).

Proof. The proof of (41) is, except for some technical details, the result of applying standard differential calculus arguments to the result of dividing Eq. (40) by $\lambda_i(A)$. The essential tool is the chain rule for directionally differentiable functions, which can be applied in this case since both $d\lambda(\log(P), \cdot)$, and $d \log(\lambda(P), \cdot)$ are continuous functions of their second argument.

In order to prove (42), consider a unitary matrix V such that $A = VAV^*$ with $A = \text{diag}[\lambda_1, \dots, \lambda_n]$. Then (see [8, § 6.6.28]), the derivative of the logarithm at P in the direction of E is given by

$$d \log(P, E) = V(K \circ \widetilde{E})V^*, \tag{43}$$

where \circ stands for the Hadamard product, $\widetilde{E} = V^*EV$ and K is the Löwner matrix whose (i, j) th element is

$$k_{ij} = \begin{cases} 1/|\lambda_i| & \text{if } |\lambda_i| = |\lambda_j|, \\ \frac{\log |\lambda_i| - \log |\lambda_j|}{|\lambda_i| - |\lambda_j|} & \text{if } |\lambda_i| \neq |\lambda_j|. \end{cases}$$

The matrix K is symmetric by construction, and positive semidefinite (see [8, § 6.6.36]), since the real logarithm is a monotone matrix function on the set of positive definite matrices [8, Section 6.6, p. 554]. On the other hand, due to the unitary invariance of the 2-norm, we have $\|P^{-1/2} E P^{-1/2}\|_2 = \|F\|_2$ for

$$F = |A|^{-1/2} \widetilde{E} |A|^{-1/2}.$$

Since conventional multiplication by a diagonal matrix commutes with Hadamard multiplication, we may rewrite

$$K \circ \widetilde{E} = (|A|^{1/2} K |A|^{1/2}) \circ F = L \circ F,$$

where the matrix $L = |A|^{1/2} K |A|^{1/2}$ has all diagonal entries equal to 1, and is still semidefinite, being congruent with K . Hence,

$$\|d \log(P, E)\|_2 = \|V(L \circ F)V^*\|_2 = \|L \circ F\|_2. \tag{44}$$

Now, we use the fact that the largest singular value of a Hadamard product $L \circ F$ with L positive semidefinite is less than or equal to the product of the largest diagonal entry of L and the largest singular value of F [8, § 5.5.18]. Thus,

$$\|L \circ F\|_2 \leq (\max_i l_{ii}) \|F\|_2 = \|F\|_2 = \|P^{-1/2} E P^{-1/2}\|_2. \tag{45}$$

Using (7) the proof is completed. \square

Some remarks are in order. First, note that we have used $\|d \log(P, E)\|_2$, which is not the directional derivative of the eigenvalue function, but a different, larger differential quantity which collectively bounds all eigenvalue relative variations for sufficiently small perturbations. Notice also that this differential quantity $\|d \log(P, E)\|_2$ can be computed through (43) once the eigenvalues and eigenvectors of A are known.

Finally, Theorem 4.1 not only shows that, as expected, the quantity $\|d \log(P, E)\|_2$ is a better bound than η to first-order, but that the inequality holds for any size of E . Furthermore it allows us to measure how far off is one bound from the other. This information is contained in the Löwner-like matrix L (see (44) and (45)), which depends only on the eigenvalues of A . The bounds are equal, for example, in the special case in which all the eigenvalues of A have the same modulus, since then all the elements of L are equal to 1 and

$$\|d \log(P, E)\|_2 = \|L \circ F\|_2 = \|F\|_2 = \eta.$$

In the other extreme case, if the eigenvalues of A differ greatly in modulus then some off-diagonal elements of L are very small and it is possible to get

$$\|L \circ F\|_2 \ll \|F\|_2.$$

In this case the differential bound will be much better than η . Consider for example the matrices

$$A = \begin{bmatrix} 10^4 & 0 \\ 0 & 10^{-2} \end{bmatrix} \quad \text{and} \quad E = \begin{bmatrix} 10^{-2} & 10^{-2} \\ 10^{-2} & 10^{-8} \end{bmatrix}. \tag{46}$$

The maximum relative variation of the eigenvalues is

$$\frac{|\widehat{\lambda}_1 - \lambda_1|}{|\lambda_1|} = 1.000001 \times 10^{-6}.$$

In this case

$$F = P^{-1/2} E P^{-1/2} = \begin{bmatrix} 10^{-6} & 10^{-3} \\ 10^{-3} & 10^{-6} \end{bmatrix}$$

and $\eta = \|F\|_2 = 1.001 \times 10^{-3}$, while

$$L = \begin{bmatrix} 1 & l \\ l & 1 \end{bmatrix}$$

with $l = 1.381552 \times 10^{-2}$, and $\|L \circ F\|_2 = \|d \log(P, E)\|_2 = 1.481552 \times 10^{-5}$, which is a better bound than η .

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