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Floating-point perturbations of Hermitian matrices

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Abstract

We consider the perturbation properties of the eigensolution of Hermitian matrices. For the matrix entries and the eigenvalues we use the realistic "floating-point" error measure $|\delta a/a|$. Recently, Demmel and Veselić considered the same problem for a positive definite matrix H showing that the floating-point perturbation theory holds with constants depending on the condition number of the matrix $A = DHD$, where $A_{ii} = 1$ and D is a diagonal scaling. We study the general Hermitian case along the same lines thus obtaining new classes of well-behaved matrices and matrix pairs. Our theory is applicable to the already known class of scaled diagonally dominant matrices as well as to matrices given by factors - like those in symmetric indefinite decompositions. We also obtain norm-estimates for the perturbations of the eigenprojections, and show that some of our techniques extend to non-hermitian matrices. However, unlike in the positive definite case, we are still unable to simply describe the set of all well behaved Hermitian matrices.

Key words. Hermitian matrix, perturbation theory.

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1 Introduction and preliminaries

The standard perturbation result for the eigenvalue problem of a Hermitian matrix H of order n , $Hx = \lambda x$, reads [5]

$$|\delta \lambda_i| \leq \|\delta H\|_2, \quad (1.1)$$

where

$$\begin{aligned} \lambda_1 &\leq \lambda_2 \leq \dots \leq \lambda_n, \\ \lambda'_1 &= \lambda_1 + \delta \lambda_1 \leq \dots \leq \lambda'_n = \lambda_n + \delta \lambda_n, \end{aligned}$$

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are the eigenvalues of H and $H + \delta H$, respectively. The perturbation matrix δH is again Hermitian, and $\|\cdot\|_2$ is the spectral norm. The backward error analysis of various eigenvalue algorithms initiated by Wilkinson [11] follows the same pattern, i.e. the round-off error estimates are given in terms of norms. A more realistic perturbation theory starts from the fact that both the input entries of the matrix H and the output eigenvalues are given in the floating point form. Thus, a desirable estimate would read

$$\max_i \left| \frac{\delta \lambda_i}{\lambda_i} \right| \leq C \max_{i,j} \left| \frac{\delta H_{ij}}{H_{ij}} \right|, \quad (1.2)$$

where we define $0/0 = 0$. Colloquially, "floating-point" perturbations are those with $|\delta H_{ij}| \leq \varepsilon |H_{ij}|$, ε small. Similarly, we call a matrix "well-behaved" if (1.2) holds with a "reasonable" C , i.e. if the small relative changes in the matrix elements cause small relative changes in the eigenvalues. Now (1.1) implies (1.2) with $C = n \cdot \kappa(H) \equiv n \cdot \|H\|_2 \|H^{-1}\|_2$, and this bound is nearly attainable. This is illustrated by the positive definite matrix

$$H = \begin{bmatrix} 1 & 1 \\ 1 & 1 + \varepsilon \end{bmatrix}, \quad 0 < \varepsilon \ll 1.$$

The small eigenvalue of H is very sensitive to small relative changes in the matrix elements.

Our results generalize the results obtained in [3, 1, 4]. Demmel and Veselić [4] showed that for a positive definite matrix H (1.2) holds with

$$C = \frac{n}{\lambda_{\min}(A)},$$

where

$$A = (\text{diag}(H))^{-1/2} H (\text{diag}(H))^{-1/2} \quad (1.3)$$

is the *standard scaled matrix*. The condition of A can be much smaller and is never much larger than that of H . Indeed, since $A_{ii} = 1$ it follows

$$\frac{1}{\lambda_{\min}(A)} \leq \kappa(A) \leq \frac{n}{\lambda_{\min}(A)},$$

whereas van der Sluis [10] proved that

$$\kappa(A) \leq n \cdot \kappa(H). \quad (1.4)$$

Similar results hold for the singular value problem [4].

The aim of this paper is to extend the above result to general non-singular Hermitian matrices. The nature of the estimate (1.2) shows that the non-singularity is a natural condition to require. We show (Th. 2.13) that (1.2) holds for a non-singular Hermitian matrix H with

$$C = \| \|A\|_2 \| \hat{A}^{-1} \|_2,$$

where

$$H = DAD, \quad \hat{A} = D^{-1}\mathbf{H}D^{-1}.$$

Here D is *any scaling matrix*, i.e. a positive definite diagonal matrix, and $|\cdot|, \mathbf{|\cdot|}$ denote the two kinds of absolute value functions, "pointwise" and "spectral":

$$|A|_{ij} = |A_{ij}|, \quad \mathbf{H} = \sqrt{H^2},$$

respectively. Note that $\|A\|_2 \leq \|\mathbf{H}\|_2 \leq \sqrt{n}\|A\|_2$ holds for any matrix A . The scaling D is typically, but not necessarily of the standard form $D = (\text{diag } \mathbf{H})^{1/2}$. This result is stated and proved in a more general setting, namely that of a matrix pair H, K with K positive definite, thus properly generalizing corresponding results of [1, 4]. Our eigenvector result, stated in Subsect. 2.1, concerns the case of a single non-singular Hermitian matrix and it essentially generalizes the norm-estimates from [1, 4]. An unpleasant point of our theory is that the matrix \mathbf{H} , which has to be scaled, is not easy to compute. Moreover, the set of well-behaved indefinite Hermitian matrices *is not scaling-invariant*.

Barlow and Demmel [1] showed that for matrices of the type

$$H = D(E + N)D, \quad (1.5)$$

where D, E are diagonal, $E^2 = I$, $\text{diag}(N) = 0$ and $\|N\|_2 < 1$, (1.2) holds with

$$C = \frac{n}{1 - \|N\|_2}. \quad (1.6)$$

The matrices (1.5) are called *scaled diagonally dominant* (s.d.d.). We show that for a s.d.d. matrix

$$\|\mathbf{H}\|_2 \|\hat{A}^{-1}\|_2 \leq n \frac{1 + \|\mathbf{H}\|_2}{1 - \|N\|_2}.$$

Although this does not reproduce the constant C in (1.6) (there is an extra factor $1 + \|\mathbf{H}\|_2 \leq 1 + \sqrt{n}$), we see that s.d.d. matrices are included in our theory.

In the positive definite case the only well-behaved matrices are those which can be well scaled, i.e. for which the scaled matrix A from (1.3) is "reasonably" conditioned. More precisely, if (1.2) holds for sufficiently small δH , then $\lambda_{\min}(A) \geq 2/(1 + C)$ for A from (1.3). This, rather sharp result is proved in Lemma 2.20 and Cor. 2.23 below. It improves a related result of [4] and also yields a slight improvement of the van der Sluis estimate (1.4).

In contrast to this, the choice of well-behaved indefinite matrices is, in a sense, richer. Writing

$$H = GJG^*$$

with G^*G positive definite (G need not be square) and J non-singular, the eigenvalue problem $Hx = \lambda x$ converts into the problem

$$\hat{H}y = \lambda J^{-1}y, \quad \hat{H} = G^*G. \quad (1.7)$$

In Sect. 3 we prove the estimate of the type (1.2) for the problem (1.7) under the perturbations of the factor $|\delta G_{ij}| \leq \varepsilon |G_{ij}|$. The latter is a generalization of the singular value problem known as *hyperbolic singular value problem* [8]. The estimates again depend on the condition number of the matrix obtained by scaling G^*G . As an amazing application we obtain floating-point perturbation estimates for matrices of the type

$$H = \begin{bmatrix} H_{11} & H_{12} \\ H_{12}^* & 0 \end{bmatrix}, \quad (1.8)$$

where $H_{12}H_{12}^*$ is positive definite. Note that this H may be singular. As could be expected, the only well-behaved singular matrices are those where the rank defect can be read-off from the zero pattern.

Although our paper deals with Hermitian matrices, some of our techniques can be used to investigate the eigenvalues of general matrices. As an example we prove a floating-point version of the known Bauer–Fike theorem.

Another approach to the matrices of the type (1.8) is to convert the problem $Hx = \lambda x$ into the quadratic eigenvalue problem

$$(\lambda^2 I - \lambda H_{11} - H_{12}H_{12}^*)x = 0$$

for which a good minimax theory is available [6]. As a consequence, in Sect. 4 we obtain a perturbation result which is different from that of Sect. 3. All this shows that we are still not in a position to give a simple description of the set of all "well-behaved" Hermitian matrices.

Similarly as in [1], [4] we note the remarkable fact that our eigenvalue estimates are independent of the condition number of the corresponding eigenvector matrices - in generalized Hermitian eigenvalue problems they are not unitary and there is no upper bound for their condition. This phenomenon seems to be typical for the "floating-point" perturbation theory.

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2 Well-conditioned scalings

In this section we present perturbation results which are natural extensions of those from [1] and [4]. We first give a general perturbation result for the eigenvalues of the pair H, K with K positive definite. (An eigenvalue of the pair H, K is a scalar λ for which $\det(H - \lambda K) = 0$.) For this purpose we introduce a new *absolute value of H relative to K* denoted by $\|H\|_K$. We then apply our general perturbation result to the floating-point perturbations of the matrices H and K . Theorems 2.13 and 2.16 give two simplifications of the perturbation bounds and Th. 2.17 gives bounds for another, more

general, type of perturbation where perturbing the zero elements is also allowed. Our theory applied to a single positive definite matrix slightly improves the corresponding results of [4]. It also improves the van der Sluis estimate (1.4) in some cases. Then we apply our theory to a single non-singular indefinite matrix. We prove that our theory includes scaled diagonally dominant matrices [1]. We also characterize the class of matrices with the best perturbation bounds. At the end we give some examples, and also consider some singular matrices. In Subsect. 2.1 we consider the perturbation of the eigenvectors of a single non-singular matrix H .

Theorem 2.1 *Let H, K be Hermitian and K positive definite. Set $K = ZZ^*$ and*

$$\mathbf{H}\mathbf{K} = Z|Z^{-1}HZ^{-*}|Z^* . \quad (2.2)$$

$\mathbf{H}\mathbf{K}$ is independent of the freedom of choice in Z .¹ Let $\delta H, \delta K$ be Hermitian perturbations such that for all $x \in \mathbf{C}^n$

$$|x^*\delta Hx| \leq \eta_H x^*\mathbf{H}\mathbf{K}x , \quad |x^*\delta Kx| \leq \eta_K x^*Kx , \quad \eta_H, \eta_K < 1 \quad (2.3)$$

holds. Let λ_i and λ'_i be the increasingly ordered eigenvalues of the matrix pairs H, K and $H' \equiv H + \delta H, K' \equiv K + \delta K$, respectively. Then $\lambda'_i = 0$ if and only if $\lambda_i = 0$, and for non-vanishing λ_i 's we have

$$\frac{1 - \eta_H}{1 + \eta_K} \leq \frac{\lambda'_i}{\lambda_i} \leq \frac{1 + \eta_H}{1 - \eta_K} . \quad (2.4)$$

PROOF. Let $K = ZZ^* = FF^*$. Then $Z = FU$, where U is a unitary matrix, and

$$Z|Z^{-1}HZ^{-*}|Z^* = FU|U^*F^{-1}HF^{-*}U|U^*F^* = F|F^{-1}HF^{-*}|F^* .$$

Thus, $\mathbf{H}\mathbf{K}$ is independent of the freedom of choice in Z . From (2.3) it follows

$$x^*(H - \eta_H\mathbf{H}\mathbf{K})x \leq x^*(H + \delta H)x \leq x^*(H + \eta_H\mathbf{H}\mathbf{K})x , \quad (2.5)$$

$$(1 - \eta_K)x^*Kx \leq x^*(K + \delta K)x \leq (1 + \eta_K)x^*Kx . \quad (2.6)$$

Now note that the pair $H \pm \eta_H\mathbf{H}\mathbf{K}, K$ has the same eigenvectors as the pair H, K with the (again increasingly ordered) eigenvalues $\lambda_i \pm \eta_H|\lambda_i|$. Let $\hat{\lambda}_i$ be the increasingly ordered eigenvalues of the pair H', K . The monotonicity property of the eigenvalues together with (2.5) yields immediately

$$1 - \eta_H \leq \frac{\hat{\lambda}_i}{\lambda_i} \leq 1 + \eta_H . \quad (2.7)$$

¹For H positive definite we obviously have $\mathbf{H}\mathbf{K} = H$.

It is also clear that H and H' have the same inertia.² The transition from H', K to H', K' is similar. Note that both pairs have again the same inertia. If e.g. $\hat{\lambda}_i \leq 0$, then $\lambda'_i \leq 0$ and (2.6) implies

$$\min_{S_i} \max_{x \in S_i} \frac{x^* H' x}{(1 - \eta_K) x^* K x} \leq \min_{S_i} \max_{x \in S_i} \frac{x^* H' x}{x^* K' x} \leq \min_{S_i} \max_{x \in S_i} \frac{x^* H' x}{(1 + \eta_K) x^* K x},$$

where S_i is any i -dimensional subspace of \mathbf{C}^n . In other words,

$$\frac{\hat{\lambda}_i}{1 - \eta_K} \leq \lambda'_i \leq \frac{\hat{\lambda}_i}{1 + \eta_K}. \quad (2.8)$$

Similarly, if $\hat{\lambda}_i \geq 0$, then $\lambda'_i \geq 0$, and we obtain

$$\frac{\hat{\lambda}_i}{1 + \eta_K} \leq \lambda'_i \leq \frac{\hat{\lambda}_i}{1 - \eta_K}. \quad (2.9)$$

Now (2.8) and (2.9) combined with (2.7) give (2.4). Q.E.D.

We now apply this result to the floating-point perturbations of matrix entries. Set

$$\tilde{C}(H, K) = \sup_{x \neq 0} \frac{|x|^T |H| |x|}{x^* \mathbf{H} \mathbf{K} x}$$

and

$$\tilde{C}(H) = \tilde{C}(H, I).$$

Obviously, $\tilde{C}(H, K)$ is defined and finite if and only if H is non-singular. For every H, K with K positive definite, we have

$$\tilde{C}(H, K) \geq 1. \quad (2.10)$$

Indeed, if $\tilde{C}(H, K)$ were less than one, then the matrices $H, K, \delta H = -H$ and $\delta K = 0$ would satisfy the assumptions of Th. 2.1 and this would, in turn, imply that $H + \delta H$ is non-singular — a contradiction.

Theorem 2.11 *Let H, K be Hermitian matrices with H non-singular and K positive definite. Let Hermitian perturbations δH and δK satisfy*

$$|\delta H_{ij}| \leq \varepsilon |H_{ij}|, \quad |\delta K_{ij}| \leq \varepsilon |K_{ij}|, \quad (2.12)$$

such that

$$\eta_H = \varepsilon \tilde{C}(H, K) < 1, \quad \eta_K = \varepsilon \tilde{C}(K) < 1.$$

Then the assumption (2.3) of Th. 2.1 is fulfilled, hence its assertion holds.

PROOF. We have

$$|x^* \delta H x| \leq |x|^T |\delta H| |x| \leq \varepsilon |x|^T |H| |x| \leq \varepsilon \tilde{C}(H, K) x^* \mathbf{H} \mathbf{K} x,$$

²In fact, H and H' have the same null-spaces.

and similarly

$$|x^* \delta K x| \leq \varepsilon \tilde{C}(K) x^* K x .$$

Q.E.D.

Th. 2.1 is a significant improvement over Lemma 1 and Th. 4 from [1] which require a more restrictive condition

$$|x^* \delta H x| \leq \eta_H |x^* H x|$$

which has non-trivial applications only for positive definite H .

The values $\tilde{C}(H, K)$ and $\tilde{C}(K)$ are not readily computable and we now exhibit a chain of simpler upper bounds for them.

Theorem 2.13 *Let H, K be as in Th. 2.11, and let A, \hat{A} and B be defined by*

$$H = DAD , \quad \mathbf{H} \mathbf{I}_K = D\hat{A}D , \quad K = D_1 B D_1 , \quad (2.14)$$

where D and D_1 are scaling matrices. Then

$$\begin{aligned} \tilde{C}(H, K) &\leq \|A\|_2 \|\hat{A}^{-1}\|_2 \equiv C(A, \hat{A}) , \\ \tilde{C}(K) &\leq \|B\|_2 \|B^{-1}\|_2 \equiv C(B) , \end{aligned} \quad (2.15)$$

and $\eta_H = \varepsilon C(A, \hat{A}) < 1$, $\eta_K = \varepsilon C(B) < 1$ implies the assertion of Th. 2.1.

PROOF. We have

$$\begin{aligned} |x|^T |H| |x| &= |x|^T D |A| D |x| \leq \|A\|_2 x^* D^2 x \\ &\leq C(A, \hat{A}) x^* D \hat{A} D x = C(A, \hat{A}) x^* \mathbf{H} \mathbf{I}_K x , \end{aligned}$$

and similarly

$$|x|^T |K| |x| \leq C(B) x^* D_1 B D_1 x = C(B) x^* K x .$$

Q.E.D.

The constant $C(A, \hat{A})$ cannot be uniformly improved. Indeed, take H as diagonal with $H^2 = I$ and let $H' = H + \delta H$ be obtained by setting to zero any of the diagonal elements of H . Then the assertion of the above theorem, applied to the pair $H, K = I$ with $\delta K = 0$, is obviously not true and we have $\eta_H = 1$, $\eta_K = 0$.

Of course, all this does not mean that Th. 2.13 covers all well behaved matrices. Next sections will show the contrary.

The constants $C(A, \hat{A})$, $C(B)$ are further estimated as follows:

Theorem 2.16 *Let H, K be as in Th. 2.11, and let A, \hat{A} and B be defined by (2.14), where D, D_1 are scalings. Then*

$$C(A, \hat{A}) \leq \text{Tr } \hat{A} \|\hat{A}^{-1}\|_2 , \quad C(B) \leq \text{Tr } B \|B^{-1}\|_2 ,$$

and $\eta_H = \varepsilon \text{Tr } \hat{A} \|\hat{A}^{-1}\|_2 < 1$, $\eta_K = \varepsilon \text{Tr } B \|B^{-1}\|_2 < 1$ implies the assertion of Th. 2.1.

PROOF. Let

$$Z^{-1}HZ^{-*} = U\Lambda U^*$$

be an eigenvalue decomposition of $Z^{-1}HZ^{-*}$ with U unitary and Λ diagonal. Then $\mathbf{[}Z^{-1}HZ^{-*}\mathbf{]} = U|\Lambda|U^*$ and from (2.2) it follows

$$\mathbf{[}H\mathbf{]}_K = ZU|\Lambda|U^*Z^* = GG^* ,$$

where $G = ZU\sqrt{|\Lambda|}$. Furthermore,

$$H = Z(Z^{-1}HZ^{-*})Z^* = ZU\Lambda U^*Z^* = GJG^* ,$$

where J is diagonal with ± 1 's on the diagonal. Setting $F = D^{-1}G$ for some positive definite diagonal D and using the obvious estimate

$$|(FJF^*)_{ij}| \leq \sqrt{(FF^*)_{ii}(FF^*)_{jj}} ,$$

we obtain $|A_{ij}|^2 \leq \hat{A}_{ii}\hat{A}_{jj}$, and hence $\|A\|_2 \leq \text{Tr } \hat{A}$. Similarly, $\|B\|_2 \leq \text{Tr } B$, and the theorem now follows from the definitions of $C(A, \hat{A})$ and $C(B)$. Q.E.D.

For the standard scalings $D = (\text{diag } \mathbf{[}H\mathbf{]}_K)^{1/2}$, $D_1 = (\text{diag } K)^{1/2}$, Th. 2.16 yields

$$C(A, \hat{A}) \leq n\|\hat{A}^{-1}\|_2 , \quad C(B) \leq n\|B^{-1}\|_2 .$$

In addition, the above upper bounds can accomodate another class of perturbations where perturbing the zero elements is also allowed.

Theorem 2.17 *Let H, K be Hermitian matrices with H non-singular and K positive definite. Let Hermitian perturbations δH and δK satisfy*

$$|\delta H_{ij}| \leq \varepsilon D_{ii}D_{jj} , \quad |\delta K_{ij}| \leq \varepsilon D_{1,ii}D_{1,jj} , \quad (2.18)$$

such that

$$\eta_H = \varepsilon n\|\hat{A}^{-1}\|_2 < 1 , \quad \eta_K = \varepsilon n\|B^{-1}\|_2 < 1 .$$

Then the assumption (2.3) of Th. 2.1 is fulfilled, hence its assertion holds.

PROOF. Let us define the matrix E with $E_{ij} = 1$. We have

$$|x^*\delta Hx| \leq |x|^T|\delta H|x \leq \varepsilon|x|^TDED|x| \leq \varepsilon\|E\|_2x^*D^2x \leq \varepsilon n\|\hat{A}^{-1}\|_2x^*\mathbf{[}H\mathbf{]}_Kx ,$$

and similarly

$$|x^*\delta Kx| \leq \varepsilon n\|B^{-1}\|_2x^*Kx .$$

Q.E.D.

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Remark 2.1 Note that for the standard scaling the bounds of Theorems 2.13 and 2.17 differ by at most a factor n . Therefore, the relative error bounds which use $C(A, \hat{A})$ and $C(B)$ actually allow both kinds of perturbations, (2.12) and (2.18), which makes them inappropriate in some cases (see Rem. 2.2 below).

We now apply our general theory to a single positive definite matrix H ($K = I$). Th. 2.16 reproduces the main floating-point perturbation result of Th. 2.3 from [4], while Th. 2.11 is even sharper. The perturbations allowed by Th. 2.17 are of the form

$$|\delta H_{ij}| \leq \varepsilon \sqrt{H_{ii}H_{jj}} . \quad (2.19)$$

The following lemma and its corollary tell us that the only well-behaved positive definite matrices are those which are well-scaled. A similar result was proved in [4], but our constants are better.

Lemma 2.20 *Let H be positive definite, and let $\mu > 0$ be such that for every Hermitian perturbation δH with $|\delta H_{ij}| \leq \mu |H_{ij}|$ the matrix $H + \delta H$ is positive definite. Then $\mu < 1$ and for*

$$A = D^{-1}HD^{-1} , \quad D = (\text{diag } H)^{1/2} \quad (2.21)$$

we have

$$\|A^{-1}\|_2 < \frac{\mu + 1}{2\mu} . \quad (2.22)$$

PROOF. Set

$$A_\mu = (1 + \mu)A - 2\mu I , \quad H_\mu = DA_\mu D = H + \delta H .$$

Then $\delta H = \mu(H - 2D^2)$, which implies $|\delta H_{ij}| = \mu |H_{ij}|$. By the assumption on $H + \delta H$ we have $\mu < 1$ and A_μ is positive definite for every μ . Hence

$$\lambda_{\min}(A_\mu) = (1 + \mu)\lambda_{\min}(A) - 2\mu > 0 ,$$

and (2.22) follows. Q.E.D.

Corollary 2.23 *Let H be positive definite, and let $M > 0$ be such that for every $\varepsilon < 1/M$ and every Hermitian perturbation δH with $|\delta H_{ij}| \leq \varepsilon |H_{ij}|$ the eigenvalues λ_i and λ'_i of H and $H + \delta H$, respectively, satisfy*

$$1 - \varepsilon M \leq \frac{\lambda'_i}{\lambda_i} \leq 1 + \varepsilon M . \quad (2.24)$$

Then the matrix A from (2.21) satisfies

$$\|A^{-1}\|_2 < \frac{1 + M}{2} . \quad (2.25)$$

Lemma 2.20 and Cor. 2.23 hold for the perturbations of the type (2.12), so they also hold for the more general perturbations of the type (2.19).

In Th. 2.11 we can take M as $\tilde{C}(H)$ and obtain a lower bound

$$\tilde{C}(H) \geq 2\|A^{-1}\|_2 - 1 . \quad (2.26)$$

Taking any positive definite diagonal matrix D_1 and setting $H_1 = D_1 A_1 D_1$ and $D = D_1^{-1} D$, the estimates (2.26) and (2.15) yield

$$\frac{\kappa(A)}{n} \leq \|A^{-1}\|_2 \leq \frac{1 + \|D|A|D\|_2 \|D^{-1} A^{-1} D^{-1}\|_2}{2} . \quad (2.27)$$

This is an estimate of the same type as the van der Sluis' estimate (1.4). These two estimates are generally incomparable. So, for A with non-negative elements ($A = |A|$) we obtain

$$\kappa(A) \leq n\|A^{-1}\|_2 \leq n \frac{1 + \kappa(DAD)}{2} , \quad (2.28)$$

which is slightly sharper than (1.4).

We now turn to the case of the single non-singular indefinite matrix H . We first prove that the class of matrices H with well-behaved $C(A, \hat{A})$ includes the already known class of scaled diagonally dominant matrices. We have

Theorem 2.29 *Let*

$$H = DAD , \quad A = E + N ,$$

with $E = E^* = E^{-1}$, $ED = DE$, and $\|N\|_2 < 1$. If \hat{A} is defined by $\mathbf{H} = D\hat{A}D$, then

$$C(A, \hat{A}) \leq n \frac{1 + \|N\|_2}{1 - \|N\|_2} . \quad (2.30)$$

PROOF. Since D commutes with E , there exists a unitary matrix U which simultaneously diagonalizes D and E , i.e.

$$U^* D U = \Delta , \quad U^* E U = \text{diag}(\pm 1) .$$

Since Δ is only a permuted version of the matrix D , there exists a permutation matrix P such that $\Delta = P D P^T$. Setting $V = U P$, we have

$$V^* D V = D , \quad V^* E V = E_1 ,$$

where E_1 is diagonal with ± 1 's on the diagonal. Now perform the unitary transformation

$$H_1 = V^* H V = D(V^* E V + V^* N V) D = D(E_1 + N_1) D .$$

Here we used the fact that D and V commute, and $\|N_1\|_2 = \|N\|_2$.

By Lemma 3 of [1] for any eigenpair λ, y of H_1 we have

$$(1 - \|N_1\|_2)\|Dy\|_2^2 \leq |\lambda|\|y\|_2^2 \leq (1 + \|N_1\|_2)\|Dy\|_2^2. \quad (2.31)$$

Note that formally [1] needs that N_1 have a zero diagonal. It is easily seen that this condition is not necessary. For any eigenpair λ, y of H , (2.31) implies

$$(1 - \|N\|_2)\|Dy\|_2^2 \leq |\lambda|\|y\|_2^2 \leq (1 + \|N\|_2)\|Dy\|_2^2. \quad (2.32)$$

Now let $H = Y\Lambda Y^*$, $Y^*Y = I$, $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$, be an eigenvalue decomposition of H . Then $\mathbf{H} = Y|\Lambda|Y^*$ and

$$\hat{A}^{-1} = D\mathbf{H}^{-1}D = DY|\Lambda|^{-1/2}|\Lambda|^{-1/2}Y^*D.$$

Therefore,

$$\|\hat{A}^{-1}\|_2 = \|DY|\Lambda|^{-1/2}\|_2^2 \leq n \max_i \|Dy_i\|_2^2 \frac{1}{|\lambda_i|} \leq \frac{n}{1 - \|N\|_2}.$$

Here we have set $Y = [y_1, \dots, y_n]$ and used (2.32) for every pair λ_i, y_i . The theorem now follows from³

$$\|A\|_2 \leq \|I + |N|\|_2 \leq 1 + \|N\|_2.$$

Q.E.D.

The s.d.d. matrices are a special case of the matrices considered in Th. 2.29, i.e. we do not require the diagonality of E . Note that the argument of [1] leading to the estimate (1.6) can be easily modified to hold under the conditions of Th. 2.29 as well.

Even though we could only bound our measure $C(A, \hat{A})$ by (2.30) which is somewhat weaker than (1.6), we expect that $C(A, \hat{A})$ is actually much better. The following example illustrates the power of our theory. Set

$$\hat{A} = \begin{bmatrix} 1 & 0.9 & 0.9 \\ 0.9 & 1 & 0.9 \\ 0.9 & 0.9 & 1 \end{bmatrix}, \quad D = \begin{bmatrix} 1 & & \\ & d & \\ & & d^2 \end{bmatrix}, \quad d \geq 1.$$

Then $\|\hat{A}^{-1}\|_2 = 10$. For $d = 10^2$ the spectrum of $\mathbf{H} = D\hat{A}D$ is, properly rounded, $1.47 \cdot 10^{-1}$, $1.90 \cdot 10^3$, $1.00 \cdot 10^8$. Now H is obtained from \mathbf{H} by just turning the smallest eigenvalue into its negative. We obtain

$$H = \begin{bmatrix} 0.705 & 9.00 \cdot 10^1 & 9.00 \cdot 10^3 \\ 9.00 \cdot 10^1 & 1.00 \cdot 10^4 & 9.00 \cdot 10^5 \\ 9.00 \cdot 10^3 & 9.00 \cdot 10^5 & 1.00 \cdot 10^8 \end{bmatrix}$$

³The case of the pair H, K of s.d.d. matrices is not covered by this result (cf. a similar claim in [1]), although it seems highly probable that such a generalization holds.

with

$$A = \begin{bmatrix} 0.705 & 0.9 & 0.9 \\ 0.9 & 1 & 0.9 \\ 0.9 & 0.9 & 1 \end{bmatrix}, \quad \|A\| \leq 3.$$

Thus, $C(A, \hat{A}) \leq 30$ and H is far from being s.d.d.

A natural question is to ask which matrix pairs or single non-singular matrices have the smallest η_H, η_K in Th. 2.13. Obviously, $C(B) \geq 1$ and the equality is attained, if and only if K is diagonal. In this case we can take $K = I$ and the whole problem reduces to the case of the single matrix H .

We first derive some useful inequalities. Set $x = K^{-1/2}y = D^{-1}z$. Then

$$|x^* H x| = |y^* K^{-1/2} H K^{-1/2} y| \leq y^* \mathbf{[} K^{-1/2} H K^{-1/2} \mathbf{]} y = x^* \mathbf{[} H \mathbf{]}_K x, \quad (2.33)$$

and thus

$$|z^* A z| \leq z^* \hat{A} z. \quad (2.34)$$

Similarly, $|x^* H^{-1} x| \leq x^* \mathbf{[} H \mathbf{]}_K^{-1} x$, and

$$|z^* A^{-1} z| \leq z^* \hat{A}^{-1} z. \quad (2.35)$$

Now we have $\|A^{-1}\|_2 \leq \|\hat{A}^{-1}\|_2$, and

$$C(A, \hat{A}) \geq \|A\|_2 \|\hat{A}^{-1}\|_2 \geq \|A\|_2 \|A^{-1}\|_2 \geq 1. \quad (2.36)$$

Theorem 2.37 *Let $H = DAD$ be Hermitian and non-singular and let $\mathbf{[} H \mathbf{]} = D\hat{A}D$. Then*

$$C(A, \hat{A}) = \| \|A\|_2 \|\hat{A}^{-1}\|_2 = 1 \quad (2.38)$$

if and only if A is proportional to $P \text{diag}(A_1, \dots, A_p) P^T$, where each of the blocks A_i has one of the forms

$$1, \quad -1, \quad \begin{bmatrix} 0 & e^{i\varphi} \\ e^{-i\varphi} & 0 \end{bmatrix},$$

A and D commute, and P is a permutation matrix.

PROOF. If H has the form described above, then $\mathbf{[} H \mathbf{]} = D^2 \mathbf{[} A \mathbf{]} = D^2$, i.e. $\hat{A} = I$ and (2.38) holds.

Conversely, if (2.38) holds, then all inequalities in (2.36) go into equalities. Without loss of generality we can assume that

$$\hat{A}_{11} = 1. \quad (2.39)$$

Now the equality $\|A\|_2 \|A^{-1}\|_2 = 1$ means that

$$A = cV, \quad c > 0, \quad V = V^{-1} = V^*. \quad (2.40)$$

From $\mathbf{H}^2 = H^2$ it follows that

$$c^2 V D^2 V = \widehat{A} D^2 \widehat{A} . \quad (2.41)$$

This is equivalent to the unitarity of the matrix

$$W = c D^{-1} \widehat{A}^{-1} V D .$$

This, in turn, implies that W is similar to $c \widehat{A}^{-1/2} V \widehat{A}^{-1/2}$. Since the latter matrix is also Hermitian, it must be unitary, i.e.

$$c^2 \widehat{A}^{-1/2} V \widehat{A}^{-1} V \widehat{A}^{-1/2} = I .$$

This is equivalent to

$$V \left(\frac{\widehat{A}}{c} \right)^{-1} V = \frac{\widehat{A}}{c} . \quad (2.42)$$

We now use $\|A\|_2 \|\widehat{A}^{-1}\|_2 = \|(\widehat{A}/c)^{-1}\|_2 = 1$ which, together with (2.42), implies $\|\widehat{A}/c\|_2 = 1$. We conclude that \widehat{A}/c is unitary, which, together with its hermiticity and positive definiteness, implies $\widehat{A}/c = I$. Hence, (2.39) implies $\widehat{A} = I$ and $c = 1$. Now we can write (2.41) as $D^2 A = A D^2$, i.e. A and D commute. Finally, we use $\|A\|_2 \|\widehat{A}^{-1}\|_2 = \|A\|_2 = 1$. By $c = 1$, the relation (2.40) gives

$$A = A^{-1} = A^* .$$

Here we need the following

Lemma 2.43 *Let $U^* U = I$ and $\|U\|_2 = 1$. Then $|U|^T |U| = I$, i.e. each row of U contains at most one non-vanishing element. If, in addition, U is square, then U is a (one sided) permutation of a diagonal matrix. Conversely, $|U|^T |U| = I$ implies $U^* U = I$ and $\|U\|_2 = 1$.*

PROOF. From $U^* U = I$ it follows $(|U|^T |U|)_{ii} \equiv 1$. If $a_{ij} = (|U|^T |U|)_{ij} \neq 0$ for some pair $i \neq j$, then the submatrix

$$\begin{bmatrix} 1 & a_{ij} \\ a_{ij} & 1 \end{bmatrix}$$

of $|U|^T |U|$ has an eigenvalue greater than one – a contradiction to the assumption $\|U\|_2 = 1$. The rest of the assertion is trivial. Q.E.D.

To finish the proof of the theorem just use the lemma above and the hermiticity of A . Thus, up to a simultaneous permutation of rows and columns, A is a direct sum of

$$A_i \in \left\{ 1, -1, \begin{bmatrix} 0 & e^{i\varphi} \\ e^{-i\varphi} & 0 \end{bmatrix} \right\} , \quad i = 1, \dots, p .$$

Q.E.D.

\varkappa The simple upper bounds in Th. 2.16 take their minimum n on a much larger class of matrices, namely those with A unitary and commuting with D . Indeed, from the proof of Th. 2.37 we immediately obtain

Corollary 2.44 *Let H , D , A , and \hat{A} be as in Th. 2.37 such that $\hat{A}_{11} = 1$. Then the following assertions are equivalent:*

(i) $\text{Tr } \hat{A} \|\hat{A}^{-1}\|_2 = n$,

(ii) $\hat{A} = I$,

(iii) A is unitary and commutes with D .

An example of such matrix is given by

$$A = \begin{bmatrix} c & s & 0 \\ s & -c & 0 \\ 0 & 0 & 1 \end{bmatrix}, \quad D = \begin{bmatrix} d_1 & & \\ & d_1 & \\ & & d_3 \end{bmatrix},$$

where $s^2 + c^2 = 1$ and $d_1, d_3 > 0$. Note that Th. 2.29 concerns a certain sort of small perturbations of such matrices. Also note that the only positive definite matrices satisfying Cor. 2.44 are again diagonal ones.

The next natural question is: how good are the matrices $H = DAD$ with A unitary, but not necessarily commuting with D ? As an example take the matrix $H = DAD$ with

$$A = \frac{1}{2} \begin{bmatrix} 1 & -1 & -1 & -1 \\ -1 & 1 & -1 & -1 \\ -1 & -1 & 1 & -1 \\ -1 & -1 & -1 & 1 \end{bmatrix}, \quad D = \begin{bmatrix} d & & & \\ & 1 & & \\ & & 1 & \\ & & & d \end{bmatrix}, \quad (2.45)$$

where $d > 0$. Here A is unitary, but it does not commute with D . The eigenvalues of H are $\lambda_1 = d^2$, $\lambda_2 = d$, $\lambda_3 = -d$, $\lambda_4 = 1$, and the corresponding eigenvectors are

$$U = \begin{bmatrix} 1/\sqrt{2} & 1/2 & 1/2 & 0 \\ 0 & -1/2 & 1/2 & 1/\sqrt{2} \\ 0 & -1/2 & 1/2 & -1/\sqrt{2} \\ -1/\sqrt{2} & 1/2 & 1/2 & 0 \end{bmatrix}.$$

If we choose a relative perturbation of the form

$$\delta H = \varepsilon d^2 w w^T, \quad w = \begin{bmatrix} 1 & 0 & 0 & 1 \end{bmatrix}^T,$$

and set $H' = H + \delta H$, we have $|\delta H_{ij}| \leq 2\varepsilon |H_{ij}|$ and

$$U^T H' U = \text{diag}(d^2, d, -d, 1) + \varepsilon d^2 U^T w w^T U = \begin{bmatrix} d^2 & 0 & 0 & 0 \\ 0 & d + \varepsilon d^2 & \varepsilon d^2 & 0 \\ 0 & \varepsilon d^2 & -d + \varepsilon d^2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}.$$

Therefore, $\lambda'_2 = d(\varepsilon d + \sqrt{1 + \varepsilon^2 d^2})$ and $|\delta\lambda_2|/|\lambda_2| > \varepsilon d$, so H is not well-behaved for large d . Since the matrix

$$HA = \frac{1}{2} \begin{bmatrix} d^2 + d & 0 & 0 & -d^2 + d \\ 0 & d + 1 & d - 1 & 0 \\ 0 & d - 1 & d + 1 & 0 \\ -d^2 + d & 0 & 0 & d^2 + d \end{bmatrix}$$

is symmetric and positive definite, we conclude that $\mathbf{H} = HA$. For $x = [1 \ 0 \ 0 \ 1]^T$ we have

$$\frac{|x|^T |H| |x|}{x^* \mathbf{H} x} = d,$$

and thus $\tilde{C}(H) \rightarrow \infty$ as $d \rightarrow \infty$. This example shows that the properties of the matrix A alone are in general not enough for the good behaviour of the indefinite matrix $H = DAD$. In other words, *contrary to the positive definite case*, an additional scaling $H_1 = D_1 H D_1$ of a well-behaved H need not produce a well-behaved H_1 .

Remark 2.2 For the indefinite matrices we do not have the equivalent of Lemma 2.20 telling us that the matrix behaves well under the perturbations of the type (2.12) if and only if $\tilde{C}(H)$ is small. Moreover, estimating $\tilde{C}(H)$ with $C(A, \hat{A})$ is in some cases not appropriate. For example, matrices of the type (1.8) behave well under the perturbations of the type (2.12) (see the following sections), but are very sensitive to the perturbations of the type (2.18) for the standard scaling. Therefore, η_H from Th. 2.17 and then, in turn, η_H from Th. 2.16 must necessarily be large and some other kind of analysis is required.

Remark 2.3 (*Some singular matrices*). Although Th. 2.1 does not require the non-singularity of the unperturbed matrix H , the subsequent theory, as it stands, cannot handle singular matrices. However, for a single matrix of the type

$$H = \begin{bmatrix} \tilde{H} & 0 \\ 0 & 0 \end{bmatrix}, \quad \tilde{H} \text{ non-singular}, \quad (2.46)$$

the condition $|\delta H_{ij}| \leq \varepsilon |H_{ij}|$ obviously preserves the zero structure and the problem trivially reduces to the perturbation of \tilde{H} to which our theory can be applied. For a pair H, K with H as above and K positive definite of the form

$$K = \begin{bmatrix} K_{11} & K_{12}^* \\ K_{12} & K_{22} \end{bmatrix}$$

we proceed as follows: from the proof of Th. 2.11 we see that the perturbation on K does not need the non-singularity of H . Furthermore, the non-zero eigenvalues of the pair H, K coincide with the eigenvalues of the pair \tilde{H}, \tilde{K} , where $\tilde{K} = K_{11} - K_{12} K_{22}^{-1} K_{12}^*$. Thus, in perturbing H the zero

eigenvalues do not change and we can apply Th. 2.11 to the pair \tilde{H}, \tilde{K} . We obtain the full assertion of Th. 2.11 with $\tilde{C}(\tilde{H}, \tilde{K})$ instead of $\tilde{C}(H, K)$.

Similarly, Th. 2.13 holds where A, \hat{A} and B are obtained by scaling $\tilde{H}, \mathbb{H}_{\tilde{K}}$ and K , respectively. If, in addition, H is positive semidefinite, then $\mathbb{H}_{\tilde{K}} = \tilde{H}$ and Th. 2.13 and the subsequent theory hold with $A = \hat{A}$ and B obtained by scaling \tilde{H} and K , respectively.

It is readily seen that (2.46) is the only form (up to a permutation) of a positive semidefinite matrix whose eigenvalues behave well under the floating-point perturbations. As we shall see later, the indefinite case is more complicated in this aspect.

æ

2.1 Perturbation of the eigenvectors

In this subsection we consider the behaviour of the eigenvectors under the perturbations as in Th. 2.1. We consider the case of a single non-singular Hermitian matrix H (i.e. $K = I, \delta K = 0$). Like in [1, 4], this behaviour is influenced by a relative gap between the neighbouring eigenvalues. Our definition of relative gap is similar but not identical with the ones from [1, 4] which makes an exact comparison of (actually similar) results difficult. Our approach – in contrast to the one from [1, 4] – is that of [7] which deals with the norm-estimates of the spectral projections and thus allows the treatment of multiple and clustered eigenvalues. We also expect our bounds to be better than those of [1, 4], since they do not depend on n .

We now define *the relative gap*, $rg(\lambda)$, for the possibly multiple eigenvalue λ of H . To simplify the notation, as well as the statement and the proof of the following theorem, we shall assume that λ is positive. Negative eigenvalues of H are considered as the positive eigenvalues of the matrix $-H$. By λ_L and λ_R we denote the left and the right neighbour of λ in the spectrum $\sigma(H)$ of H , respectively. We set

$$rg(\lambda) = \begin{cases} \min \left\{ \frac{\sqrt{\lambda} - \sqrt{\lambda_L}}{\sqrt{\lambda}}, \frac{\sqrt{\lambda_R} - \sqrt{\lambda}}{\sqrt{\lambda_R}} \right\} & \text{if } \lambda_L > 0, \\ \min \left\{ 2(\sqrt{2} - 1), \frac{\lambda_R - \lambda}{\lambda_R + \lambda} \right\} & \text{otherwise.} \end{cases} \quad (2.47)$$

Theorem 2.48 *Let λ be a positive (possibly multiple) eigenvalue of a non-singular Hermitian matrix H , and let*

$$P = \frac{1}{2\pi i} \int_{\Gamma} R_{\mu} d\mu, \quad R_{\mu} = (\mu I - H)^{-1}, \quad (2.49)$$

be the corresponding eigenprojection. Here Γ is a curve around λ which separates λ from the rest of the spectrum. Let $P + \delta P$ be the corresponding

spectral projection of the matrix $H + \delta H$ with $|x^* \delta H x| \leq \eta x^* \mathbf{[H]} x$. Then

$$\|\delta P\|_2 \leq \begin{cases} \frac{\eta}{rg(\lambda)} \cdot \frac{1}{1 - (1 + \frac{1}{rg(\lambda)})\eta} & \text{for } \lambda_L > 0, 2\sqrt{\lambda} - \sqrt{\lambda_L} < \sqrt{\lambda_R}, \\ \frac{\eta}{rg(\lambda)} \cdot \frac{1}{1 - \frac{\eta}{rg(\lambda)}} & \text{otherwise,} \end{cases} \quad (2.50)$$

provided that the right hand side is positive.

PROOF. By setting

$$\Delta = \mathbf{[H]}^{-1/2} \delta H \mathbf{[H]}^{-1/2}, \quad z_\mu = R_\mu \mathbf{[H]}^{1/2}, \quad w_\mu = \mathbf{[H]}^{1/2} R_\mu \mathbf{[H]}^{1/2},$$

we obtain $\|\Delta\|_2 \leq \eta$ and

$$\delta P = \frac{1}{2\pi i} \int_\Gamma z_\mu \Delta \sum_{k=0}^{\infty} (w_\mu \Delta)^k z_\mu d\mu.$$

Choosing Γ as a circle around λ with the radius r , we obtain

$$\|\delta P\|_2 \leq rz^2 \eta \frac{1}{1 - w\eta}$$

with

$$z^2 = \max_{\mu \in \Gamma} \|z_\mu\|_2^2 = \max_{\mu \in \Gamma} \max_{\nu \in \sigma(H)} \frac{|\nu|}{|\mu - \nu|^2}$$

$$w = \max_{\mu \in \Gamma} \|w_\mu\|_2 = \max_{\mu \in \Gamma} \max_{\nu \in \sigma(H)} \frac{|\nu|}{|\mu - \nu|},$$

provided that $\eta < 1/w$. We obviously have

$$z^2 = \max \left\{ \frac{|\lambda_L|}{(\lambda - r - \lambda_L)^2}, \frac{\lambda}{r^2}, \frac{\lambda_R}{(\lambda_R - \lambda - r)^2} \right\}$$

$$w = \max \left\{ \frac{|\lambda_L|}{\lambda - r - \lambda_L}, \frac{\lambda}{r}, \frac{\lambda_R}{\lambda_R - \lambda - r} \right\}. \quad (2.51)$$

We first consider the case $\lambda_L > 0$. If $2\sqrt{\lambda} - \sqrt{\lambda_L} < \sqrt{\lambda_R}$, then by setting

$$r = \sqrt{\lambda}(\sqrt{\lambda} - \sqrt{\lambda_L}) \quad (2.52)$$

we obtain

$$z^2 = \frac{1}{(\sqrt{\lambda} - \sqrt{\lambda_L})^2}, \quad w \leq \frac{\sqrt{\lambda}}{\sqrt{\lambda} - \sqrt{\lambda_L}} + 1.$$

Here we used our assumption and the fact that both rightmost terms in (2.51) are decreasing functions of λ_R . Therefore,

$$\|\delta P\|_2 \leq \frac{\sqrt{\lambda}}{\sqrt{\lambda} - \sqrt{\lambda_L}} \eta \frac{1}{1 - \left(1 + \frac{\sqrt{\lambda}}{\sqrt{\lambda} - \sqrt{\lambda_L}}\right) \eta},$$

and (2.50) holds. Positivity of the right hand side of (2.50) justifies, in turn, our choice of the same η in the definitions of P and $P + \delta P$ as follows: the perturbation theorem for the eigenvalues implies that λ_L can increase to at most $\lambda_L(1 + \eta)$, λ_R can decrease to at least $\lambda_R(1 - \eta)$, and the eigenvalues of $H + \delta H$ which correspond to λ remain in the interval $[\lambda(1 - \eta), \lambda(1 + \eta)]$. Positivity of the right hand side of (2.50) always implies $rg(\lambda) > \eta$. This, together with our choice of r , implies that η contains no points of the spectrum of $H + \delta H$ and that the interior of η contains exactly those eigenvalues of $H + \delta H$ which correspond to λ . This remark holds for the subsequent cases, as well.

If $2\sqrt{\lambda} - \sqrt{\lambda_L} \geq \sqrt{\lambda_R}$, then by setting

$$r = \sqrt{\lambda}(\sqrt{\lambda_R} - \sqrt{\lambda})$$

we obtain

$$z^2 = \frac{1}{(\sqrt{\lambda_R} - \sqrt{\lambda})^2}, \quad w = \frac{\sqrt{\lambda_R}}{\sqrt{\lambda_R} - \sqrt{\lambda}}.$$

Here we used our assumption and the fact that both leftmost terms in the right hand side of (2.51) are increasing functions of $\lambda_L > 0$. Therefore,

$$\|\delta P\|_2 \leq \frac{\sqrt{\lambda}}{\sqrt{\lambda_R} - \sqrt{\lambda}} \eta \frac{1}{1 - \frac{\sqrt{\lambda_R}}{\sqrt{\lambda_R} - \sqrt{\lambda}} \eta},$$

and (2.50) holds. If λ is the largest positive eigenvalue (i.e. λ_R does not exist), then by setting r as in (2.52) we obtain

$$z^2 = \frac{1}{(\sqrt{\lambda} - \sqrt{\lambda_L})^2}, \quad w = \frac{\sqrt{\lambda}}{\sqrt{\lambda} - \sqrt{\lambda_L}},$$

and (2.50) holds again.

If $\lambda_L < 0$ or if λ_L does not exist, we proceed as follows: if $rg(\lambda) = 2(\sqrt{2} - 1)$ (if λ_R exists, this implies $\lambda(4\sqrt{2} + 5) \leq \lambda_R$), then by setting

$$r = 2(\sqrt{2} - 1)\lambda$$

we obtain

$$z^2 = \frac{1}{4(\sqrt{2} - 1)^2\lambda}, \quad w = \frac{1}{2(\sqrt{2} - 1)},$$

so (2.50) holds. Finally, if $rg(\lambda) = (\lambda_R - \lambda)/(\lambda_R + \lambda)$, then by setting

$$r = \lambda \frac{\lambda_R - \lambda}{\lambda_R + \lambda}$$

we obtain

$$z^2 = \frac{1}{\lambda} \left(\frac{\lambda_R + \lambda}{\lambda_R - \lambda} \right)^2, \quad w = \frac{\lambda_R + \lambda}{\lambda_R - \lambda},$$

and (2.50) holds again. Q.E.D.

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3 Perturbations by factors

In this section we consider perturbations of the eigenvalues of a single Hermitian matrix H given in a factorized form

$$H = GJG^* , \quad (3.1)$$

where G need not to be square but must have full column rank, whereas J is Hermitian and non-singular. A typical J is

$$J_1 = \begin{bmatrix} I & 0 \\ 0 & -I \end{bmatrix} . \quad (3.2)$$

Here the unit blocks need not have the same dimension and one of them may be void. Such factorization is obtained e.g. by the indefinite symmetric decomposition of H [2, 9]. We consider the change of the eigenvalues of H under perturbation of G while J remains unchanged. Here it is natural to use the one-sided scaling $G = BD$. The behaviour of the eigenvectors does not seem to be as easy to follow as in Subsect. 2.1, and we have no corresponding results as yet.

For $J = I$ the problem reduces to considering singular values of G . We reproduce the result of [4] with somewhat better constants. The same technique allows an interesting floating-point estimate for the eigenvalues of G (which is non-Hermitian).

The section is organized as follows. Th. 3.3 gives a general perturbation theory, while Th. 3.9 applies this theory to the floating-point perturbations. In the following discussion we simplify the perturbation bounds analogously to the previous section. As an application we derive floating-point perturbation estimates for some classes of matrices not covered by Sect. 2. Finally, Th. 3.16 and 3.17 show that good behaviour of the singular values often implies the same for the eigenvalues, if the matrix is not positive definite, or even non-hermitian. Th. 3.17 is in fact a "floating-point version" of the known Bauer-Fike result.

Theorem 3.3 *Let $H = GJG^*$ be as above and let $H' = G'JG'^*$ with*

$$G' = G + \delta G , \quad \|\delta Gx\|_2 \leq \eta \|Gx\|_2 , \quad (3.4)$$

for all $x \in \mathbf{C}^n$ and some $\eta < 1$. Then H and H' have the same inertia and their non-vanishing eigenvalues λ_k, λ'_k , respectively, satisfy the inequalities

$$(1 - \eta)^2 \leq \frac{\lambda'_k}{\lambda_k} \leq (1 + \eta)^2 . \quad (3.5)$$

PROOF. We first show that the non-vanishing eigenvalues of H coincide with the eigenvalues of the pair G^*G, J^{-1} . Indeed, since G^*G is positive definite, there exists a non-singular F such that

$$F^*G^*GF = \gamma \quad (3.6)$$

and

$$F^* J^{-1} F = J_1 \quad (3.7)$$

are diagonal matrices, and J_1 is from (3.2). Then the eigenvalues of the pair G^*G, J^{-1} are found on the diagonal of $\gamma J_1 = J_1 \gamma$. Set $U = GF\gamma^{-1/2}$. By (3.6) we have $U^*U = I$ (but not necessarily $UU^* = I$). Using (3.6) and (3.7) we obtain

$$\begin{aligned} HU &= GJG^*GF\gamma^{-1/2} = GJF^{-*}F^*G^*GF\gamma^{-1/2} \\ &= GJF^{-*}\gamma^{1/2} = GFF^{-1}JF^{-*}\gamma^{1/2} \\ &= GF(F^*J^{-1}F)^{-1}\gamma^{1/2} = UJ_1\gamma . \end{aligned}$$

Thus, the columns of U are eigenvectors of H and the eigenvalues of H coincide with those of G^*G, J^{-1} . Furthermore, $U^*x = 0$ implies $Hx = 0$, so the eigenvalues of G^*G, J^{-1} are exactly all non-vanishing eigenvalues of H . By (3.4) we have

$$(1 - \eta)\|Gx\|_2 \leq \|G'x\|_2 \leq (1 + \eta)\|Gx\|_2 , \quad (3.8)$$

so that everything said for H holds for H' as well. In particular, H and H' have the same inertia. Now square (3.8), use the monotonicity property from the proof of Th. 2.1 for the pairs J^{-1}, G^*G and J^{-1}, G'^*G' , and take reciprocals in (2.8) and (2.9).

Q.E.D.

We now consider floating-point perturbations and scalings.

Theorem 3.9 *Let $H = GJG^*$ be as in (3.1) and (3.2). Let $H' = G'JG'^*$ where $G' = G + \delta G$, and for all i, j and some $\varepsilon > 0$ holds*

$$|\delta G_{ij}| \leq \varepsilon |G_{ij}| . \quad (3.10)$$

Set

$$\eta \equiv \frac{\varepsilon \|B\|_2}{\sigma_{\min}(B)} ,$$

where $B = GD^{-1}$, D is diagonal and positive definite, and $\sigma_{\min}(B)$ is the smallest singular value of B . If $\eta < 1$ then the assumptions of Th. 3.3 are fulfilled, hence its assertion holds.

PROOF. For $x \in \mathbf{C}^n$ we have

$$\begin{aligned} \|\delta Gx\|_2 &\leq \varepsilon \|B\|_2 \|Dx\|_2 \leq \varepsilon \|B\|_2 \|Dx\|_2 \\ &\leq \frac{\varepsilon \|B\|_2 \|BDx\|_2}{\sigma_{\min}(B)} = \frac{\varepsilon \|B\|_2 \|Gx\|_2}{\sigma_{\min}(B)} . \end{aligned}$$

Q.E.D.

By $\|B\|_2 \geq \|B\|_2$ we have

$$\frac{\|B\|_2}{\sigma_{\min}(B)} \geq \frac{\sigma_{\max}(B)}{\sigma_{\min}(B)} \geq 1 .$$

Here both inequalities go over into equalities, if and only if B has the property

$$B^*B = \gamma^2 I, \quad \gamma > 0, \quad \|B\|_2 = \gamma,$$

or, equivalently (Lemma 2.43), if and only if $|B|^T|B| = \gamma^2 I$. Similarly as in Sect. 2 we can make a simplifying estimate

$$\frac{\|B\|_2}{\sigma_{\min}(B)} \leq \frac{(\operatorname{Tr}(B^*B))^{1/2}}{\sigma_{\min}(B)},$$

so that

$$\eta = \frac{\varepsilon(\operatorname{Tr}(B^*B))^{1/2}}{\sigma_{\min}(B)} < 1 \quad (3.11)$$

again implies (3.4) and therefore (3.5). This yields a new "condition number"

$$\frac{(\operatorname{Tr}(B^*B))^{1/2}}{\sigma_{\min}(B)} \geq \sqrt{n},$$

where the equality is attained if and only if $B^*B = \gamma^2 I$. For the standard scaling where $(B^*B)_{ii} = 1$ the relation (3.5) is implied by

$$\eta = \frac{\varepsilon\sqrt{n}}{\sigma_{\min}(B)} < 1. \quad (3.12)$$

This is a slight improvement over [4] (our constant is \sqrt{n} times better).

æ For $J = I$ (or $J = -I$) we can handle the matrix $H = GG^*$ in two ways. If G has full column rank, then we apply our theory as described in Theorems 3.3 and 3.9. If G^* has full column rank, then we apply our theory to the matrix $\hat{H} = G^*G$, whose non-vanishing eigenvalues are the eigenvalues of H . In the indefinite case ($J \neq \pm I$) the situation is different. The following simple example illustrates this important asymmetry. Take

$$G = [a, b], \quad \delta G = [\delta a, \delta b].$$

Our theory cannot be applied to

$$H = GG^* = |a|^2 + |b|^2,$$

but it works on

$$H = G^*G,$$

where $G^* = \tilde{B}\tilde{D}$, $\tilde{B} = \begin{bmatrix} 1/\sqrt{2} & 1/\sqrt{2} \end{bmatrix}^T$, $\tilde{D} = (|a|^2 + |b|^2)^{1/2}$, thus giving $\eta = \varepsilon$ independently of a and b . On the contrary, no theory can "save" the matrix

$$H = G \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} G^* = |a|^2 - |b|^2$$

since

$$\frac{|a + \delta a|^2 - |b + \delta b|^2}{|a|^2 - |b|^2}$$

cannot be made small uniformly in a, b if $|\delta a/a|$ and $|\delta b/b|$ are sufficiently small.⁴

Similarly as in Th. 2.17 we can show that a perturbation result holds under perturbations δG defined by

$$|\delta G_{ij}| \leq \varepsilon D_j \quad \text{for all } i, j,$$

where D is a scaling. The above type of perturbation is less restrictive than (3.10), e.g. it allows us to change zero elements. We have

$$\begin{aligned} \|\delta Gx\|_2^2 &= \sum_{i,j,k} \bar{x}_i \delta \bar{G}_{ji} \delta G_{jk} x_k \leq n \left(\varepsilon \sum_j |D_j x_j| \right)^2 \\ &\leq n^2 \varepsilon^2 \|Dx\|_2^2 \leq \frac{n^2 \varepsilon^2 \|Gx\|_2^2}{\lambda_{\min}(B^*B)}, \end{aligned}$$

hence (3.5) is implied by

$$\eta = \frac{n\varepsilon}{\sigma_{\min}(B)} < 1. \quad (3.13)$$

Similarly one shows that the estimate (3.5) is obtained under the perturbation

$$\delta G = \delta B D, \quad \eta = \frac{\|\delta B\|_2}{\sigma_{\min}(B)} < 1. \quad (3.14)$$

The following two examples show how Th. 3.9 can accommodate floating-point perturbations of some matrices which, in spite of Rem. 2.1, cannot be handled by the theory from Sect. 2. For the first example set

$$H = \begin{bmatrix} A & F^* \\ F & 0 \end{bmatrix},$$

where A is of order m and $m \leq n - m$. Then $H = GJG^*$ with

$$G = \begin{bmatrix} \frac{1}{2}A & I \\ F & 0 \end{bmatrix}, \quad J = \begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix},$$

where the unit blocks have the order m . Now the perturbation δH of H with $|H_{ij}| \leq \varepsilon |H_{ij}|$ gives rise to a perturbation δG of G with $|\delta G_{ij}| \leq \varepsilon |G_{ij}|$, and Th. 3.9 holds e.g. with

$$B = \begin{bmatrix} \frac{1}{2}A & I \\ F & 0 \end{bmatrix} \begin{bmatrix} D^{-1} & 0 \\ 0 & I \end{bmatrix},$$

where D is the standard scaling

$$D_{ii}^2 = \left(\frac{1}{4}A^2 + F^*F \right)_{ii}.$$

⁴In the indefinite case the values $\mu_k = \sqrt{|\lambda_k|} \text{sign } \lambda_k$ are called the *hyperbolic singular values* [8].

The requirement that G have full column rank is equivalent to the same requirement on F . Note that this allows singular matrices H .

An even simpler case is the one with $A = 0$. Then we can apply the theory to

$$H = \begin{bmatrix} 0 & F^* \\ F & 0 \end{bmatrix} = \begin{bmatrix} 0 & I \\ F & 0 \end{bmatrix} \begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix} \begin{bmatrix} 0 & F^* \\ I & 0 \end{bmatrix}, \quad (3.15)$$

as well as to

$$H = \begin{bmatrix} 0 & F \\ F^* & 0 \end{bmatrix} = \begin{bmatrix} 0 & F \\ I & 0 \end{bmatrix} \begin{bmatrix} 0 & I \\ I & 0 \end{bmatrix} \begin{bmatrix} 0 & I \\ F^* & 0 \end{bmatrix}.$$

In any case, the non-vanishing eigenvalues of H coincide with the singular values of F taken with both signs. Now $|\delta G_{ij}| \leq \varepsilon |G_{ij}|$ means $|\delta F_{ij}| \leq \varepsilon |F_{ij}|$ and we can apply our theory in two ways:

(i) take e.g. (3.15) and use Th. 3.9 to obtain (3.5) with

$$\eta = \frac{\|B\|_2}{\sigma_{\min}(B)},$$

where $B = FD^{-1}$, $(B^*B)_{ii} = 1$, or

(ii) apply Th. 3.9 to the factorized matrix FF^* (with the same B) which yields a slightly better estimate

$$(1 - \eta)^2 \leq \frac{\lambda_k'^2}{\lambda_k^2} \leq (1 + \eta)^2.$$

In both cases the theory from Sect. 2 would require both BB^* and B^*B to scale well, which is certainly a further unnecessary restriction.

As a second example set

$$H = \begin{bmatrix} a & b & c \\ b & 0 & 0 \\ c & 0 & \alpha^2 \end{bmatrix}.$$

We can e.g. decompose H as

$$H = \begin{bmatrix} a/2 & 1 & 0 \\ b & 0 & 0 \\ c & 0 & \alpha \end{bmatrix} \begin{bmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a/2 & b & c \\ 1 & 0 & 0 \\ 0 & 0 & \alpha \end{bmatrix}.$$

Now $|\delta H_{ij}| \leq \varepsilon |H_{ij}|$ again implies $|\delta G_{ij}| \leq \varepsilon |G_{ij}|$ and we can apply our theory as in the previous example. For e.g. $a = b = c = 1$ we obtain $\|B\|_2 \|B^{-1}\|_2 = 2 + \sqrt{3}$, independently of α . Especially, if α is small then even the absolutely smallest eigenvalue $\alpha^2/2 + O(\alpha^4)$ is well defined by the

matrix elements of H . On the other side, the theory from Sect. 2 applied to H, I gives nothing useful here. Indeed, as $\alpha \rightarrow 0$ we have

$$\mathbf{H} = \frac{1}{3} \begin{bmatrix} 5 & 1 & 1 \\ 1 & 2 & 2 \\ 1 & 2 & 2 \end{bmatrix} + O(\alpha^2) ,$$

so that $C(A, \hat{A}) = O(1/\alpha^2)$. Moreover, numerical experiments show that $\tilde{C}(H) > 1/|\alpha|$.

The eigenvalues of a general Hermitian matrix coincide with the singular values up to the signs. Thus, if H has well-behaved singular values the same is expected for the eigenvalues. We have⁵

Theorem 3.16 *Let H be Hermitian and non-singular and $H = BD$ a scaling. Let δH be a Hermitian perturbation with $|\delta H_{ij}| \leq \varepsilon |H_{ij}|$ and*

$$\eta = \varepsilon C(B) < 1 .$$

Then the eigenvalues λ_k, λ'_k of $H, H' = H + \delta H$ satisfy

$$1 - \eta < \frac{\lambda'_k}{\lambda_k} < 1 + \eta .$$

PROOF. As in the proof of Th. 3.9 we obtain

$$|x^* \delta H^* \delta H x| \leq \eta^2 x^* H^2 x .$$

By the Löwner's theorem ([7], Ch. V, §4.3) we have

$$|x^* \delta H x| \leq x^* \mathbf{H} x \leq \eta x^* \mathbf{H} x .$$

Now apply Th. 2.1 with $K = I, \delta K = 0$.

Q.E.D.

The rule "well-behaved singular values, well-behaved eigenvalues" extends to many non-hermitian matrices. We present a simple floating-point version of the known Bauer-Fike theorem.

Theorem 3.17 *Let G, S be non-singular matrices with*

$$S^{-1}GS = \text{diag} (\lambda_1, \dots, \lambda_n) ,$$

and let δG be a perturbation with $\|\delta Gx\|_2 \leq \eta \|Gx\|_2$. Then the eigenvalues of $G + \delta G$ lie in the union of disks

$$\{\lambda; |\lambda - \lambda_i| \leq r_i\} , \quad r_i = \eta |\lambda_i| \kappa(S) , \quad i = 1, \dots, n .$$

⁵Although the two following theorems do not concern matrices in factorized form, we present them here since they use results of this section.

PROOF. Let $(G + \delta G - \lambda I)x = 0$. If λ is an eigenvalue of G , then the theorem is proved. Otherwise set $z = (G - \lambda I)^{-1}x$. Then $z \neq 0$ and

$$z = \delta G G^{-1} G (\lambda I - G)^{-1} z .$$

Hence

$$\|z\|_2 \leq \eta \left\| S \operatorname{diag} \left(\frac{\lambda_i}{\lambda - \lambda_i} \right) S^{-1} \right\|_2 \|z\|_2 \leq \eta \kappa(S) \frac{|\lambda_{i_0}|}{|\lambda - \lambda_{i_0}|} \|z\|_2$$

for some i_0 , and

$$|\lambda - \lambda_{i_0}| \leq \eta \kappa(S) |\lambda_{i_0}| .$$

Q.E.D.

Here, too, the number of the eigenvalues in any component of the union equals to the number of disks in it.

Taking the perturbation $|\delta G_{ij}| \leq \varepsilon |G_{ij}|$ Th. 3.9 gives the radii

$$r_i = \varepsilon |\lambda_i| C(B) \kappa(S)$$

with two condition numbers: $C(B)$ and $\kappa(S)$. An eigenprojection estimate similar to that in Subsect. 2.1 is possible here as well.

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4 Quadratic pencil approach

In this section we consider once more Hermitian matrices of the type

$$H = \begin{bmatrix} A & B^* \\ B & 0 \end{bmatrix} . \quad (4.1)$$

Here we assume A , B^*B as positive definite of order m with

$$m \leq n - m . \quad (4.2)$$

We develop a perturbation theory by reducing the eigenproblem for H to a quadratic eigenvalue problem.

Proposition 4.3 *A non-vanishing number λ is an eigenvalue of H if and only if*

$$\det(\lambda^2 - \lambda A - B^*B) = 0 .$$

PROOF. Let $Hx = \lambda x$, $x \neq 0$. With the corresponding partitioning $x = (x_1^T, x_2^T)^T$ this can be written as

$$\begin{aligned} Ax_1 + B^*x_2 &= \lambda x_1 \\ Bx_1 &= \lambda x_2 . \end{aligned}$$

If $\lambda \neq 0$, we have $x_2 = Bx_1/\lambda$ and

$$(\lambda^2 I - \lambda A - B^*B)x_1 = 0 , \quad (4.4)$$

where $\lambda \neq 0$ implies $x_1 \neq 0$. Conversely, if (4.4) holds for some $x_1 \neq 0$, then $\lambda \neq 0$, and $Hx = \lambda x$ with $x = (x_1^T, x_1^T B^*/\lambda)^T$. Q.E.D.

Thus, the perturbations of H which have the same zero structure can be reduced to the perturbations of the quadratic eigenvalue problem (4.4) for which a satisfactory minimax theory is available. Set $C = B^*B$. Then the eigenvalues of the problem

$$(\lambda^2 I - \lambda A - C)x = 0$$

can be written as

$$\lambda_1^- \leq \dots \leq \lambda_m^- < 0 < \lambda_m^+ \leq \dots \leq \lambda_1^+ . \quad (4.5)$$

Theorem 4.6 *Let H be defined with (4.1) and (4.2). Let*

$$\delta H = \begin{bmatrix} \delta A & \delta B^* \\ \delta B & 0 \end{bmatrix}$$

be a Hermitian perturbation with the same structure as H such that

$$|x^* \delta A x| \leq \eta x^* A x , \quad \|\delta B x\|_2 \leq \eta \|B x\|_2 \quad (4.7)$$

holds for all $x \in \mathbf{C}^m$ and some $\eta < 1$. Let $\lambda_k'^{\pm}$ be the non-vanishing eigenvalues of H' ordered as in (4.5). Then H and $H' = H + \delta H$ have the same inertia and for the non-vanishing eigenvalues of H' we have

$$\frac{1 - \eta}{1 + \eta} \leq \frac{\lambda_k'^{\pm}}{\lambda_k^{\pm}} \leq \frac{1 + \eta}{1 - \eta} .$$

PROOF. Set $A' = A + \delta A$, $B' = B + \delta B$. Then (4.7) implies

$$\begin{aligned} (1 - \eta)x^* A x &\leq x^* A' x \leq (1 + \eta)x^* A x , \\ (1 - \eta)^2 x^* B^* B x &\leq x^* B'^T B' x \leq (1 + \eta)^2 x^* B^* B x . \end{aligned}$$

According to [6] the following minimax formula holds

$$|\lambda_k^{\pm}| = \max_{S_k} \min_{\substack{x \in S_k \\ \|x\|_2=1}} |p_{\pm}(A, C, x)| , \quad (4.8)$$

where

$$p_{\pm}(A, C, x) = \frac{x^* A x \pm \sqrt{(x^* A x)^2 + 4x^* C x}}{2} . \quad (4.9)$$

Here S_k is any k -dimensional subspace of \mathbf{C}^m and the maximum in (4.8) is taken over all such subspaces. Note that

$$p_-(A, C, x) = -\frac{2x^* C x}{x^* A x + \sqrt{(x^* A x)^2 + 4x^* C x}} . \quad (4.10)$$

From (4.9) we have

$$(1 - \eta)p_+(A, C, x) \leq p_+(A', C', x) \leq (1 + \eta)p_+(A, C, x) .$$

Now (4.8) implies

$$(1 - \eta)\lambda_k^+ \leq \lambda_k'^+ \leq (1 + \eta)\lambda_k^+ . \quad (4.11)$$

For p_- we have from (4.10)

$$\frac{1 - \eta}{1 + \eta}|p_-(A, C, x)| \leq |p_-(A', C', x)| \leq \frac{1 + \eta}{1 - \eta}|p_-(A, C, x)| ,$$

which implies

$$\frac{1 - \eta}{1 + \eta}|\lambda_k^-| \leq |\lambda_k'^-| \leq \frac{1 + \eta}{1 - \eta}|\lambda_k^-| . \quad (4.12)$$

The assertion of the theorem now follows from (4.11) and (4.12). Q.E.D.

Note that the positive eigenvalues enjoy better bounds. If A is negative definite, then the roles of λ_k^\pm 's change and λ_k^- 's behave better. We can now apply the estimates from Sections 2, 3. So, Th. 4.6 holds, if e.g. we take the standard scalings $A = DA_S D$, $B = B_S D_1$, and require

$$\varepsilon n \|A_S^{-1}\|_2 \leq \eta < 1 , \quad \frac{\varepsilon \sqrt{n}}{\sigma_{\min}(B_S)} \leq \eta < 1 .$$

These conditions seem to be incomparable with the ones obtained in Sect. 3 for the same type of matrices.

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