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RELATIVE PERTURBATION BOUND FOR INVARIANT SUBSPACES OF HERMITIAN MATRIX

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Abstract. We give a bound for the perturbations of invariant subspaces of a non-singular Hermitian matrix H under relative additive perturbations of H. Such perturbations include the case when the elements of H are known up to some relative tolerance. Our bound is, in appropriate cases, sharper than the classical bounds, and it generalizes some of the recent relative perturbation results.

1. Introduction and preliminaries

We consider the Hermitian eigenvalue problem

$$H = Q\Lambda Q^* = \sum_{i=1}^{n} \lambda_i q_i q_i^*,$$

where H is a non-singular Hermitian matrix of order n, $\Lambda = \mathrm{diag}(\lambda_i)$ is a diagonal matrix whose diagonal elements are the eigenvalues of H, and $Q = \begin{bmatrix} q_1 & q_2 & \cdots & q_n \end{bmatrix}$ is an unitary matrix whose i-th column is the eigenvector which corresponds to λ_i. We denote the set of all eigenvalues of H by $\sigma(H) = \{\lambda_1, \cdots, \lambda_n\}$. We also assume that the eigenvalues are ordered, $\lambda_1 \leq \lambda_2 \leq \cdots \leq \lambda_n$.

Subspace $\mathcal{X}$ is an invariant subspace of a general matrix H if $H\mathcal{X} \subseteq \mathcal{X}$. We consider invariant subspaces which correspond to the set of k neighboring eigenvalues

$$\mathcal{T} = \{\lambda_i, \lambda_{i+1}, \cdots, \lambda_{i+k-1}\}, \tag{1.1}$$

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such that the intersection of $\mathcal{T}$ with the rest of the spectrum of H is empty. That is, if $i > 1$, then $\lambda_{i-1} < \lambda_i$, and if $i + k - 1 < n$ then $\lambda_{i+k-1} < \lambda_{i+k}$. Then the corresponding invariant subspace is spanned by the columns of the matrix

$$Q_{\mathcal{T}} = \left[\begin{array}{cccc} q_i & q_{i+1} & \cdots & q_{i+k-1} \end{array} \right],$$

and the spectral projection onto that subspace is defined by $P = Q_{\mathcal{T}} Q_{\mathcal{T}}^*$. Furthermore, let $\widetilde{H} = H + \delta H$ be a perturbed matrix for some Hermitian perturbation δH. Let $\sigma(\widetilde{H}) = \{\widetilde{\lambda}_1, \cdots, \widetilde{\lambda}_n\}$, and let $\widetilde{\lambda}_1 \leq \widetilde{\lambda}_2 \leq \cdots \leq \widetilde{\lambda}_n$.

If

$$\widetilde{\mathcal{T}} = \{\widetilde{\lambda}_i, \widetilde{\lambda}_{i+1}, \cdots, \widetilde{\lambda}_{i+k-1}\}$$

is separated from the rest of $\sigma(\widetilde{H})$, then $\widetilde{P} \equiv P + \delta P$ is the spectral projection onto the invariant subspace which is spanned by the columns of the matrix $\widetilde{Q}_{\mathcal{T}} = \left[\begin{array}{cccc} \widetilde{q}_i & \cdots & \widetilde{q}_{i+k-1} \end{array} \right]$. Also, $\widetilde{P} = \widetilde{Q}_{\mathcal{T}} \widetilde{Q}_{\mathcal{T}}^*$.

Aim of this paper is to bound $\|\delta P\|$ for certain types of relative matrix perturbations, where $\|A\| = \max_{x \neq 0} \sqrt{x^* A^* A x} / \sqrt{x^* x}$. $\|\delta P\|$ is also the sine of the largest canonical angle between subspaces spanned by the columns of $Q_{\mathcal{T}}$ and $\widetilde{Q}_{\mathcal{T}}$. More precisely, the sines of the canonical angles between these subspaces are diagonal entries of the matrix $\sin\Theta \equiv \Sigma$, where $U\Sigma V^*$ is a singular value decomposition of the matrix $(Q_{\mathcal{T}}^{\perp})^* \widetilde{Q}_{\mathcal{T}}$ [18, Definition I.5.3]. Since $\|\delta P\| = \|\sin\Theta\|$ [18, Theorem I.5.5], the classical bound for $\|\delta P\|$ is given by the well-known $\sin\Theta$ theorem [2, Section 2], [18, Theorem V.3.6],

$$\|\delta P\| \leq \frac{\|R\|}{\min\{\lambda_i - \widetilde{\lambda}_{i-1}, \widetilde{\lambda}_{i+k} - \lambda_{i+k-1}\}} \tag{1.2}$$

$$\leq \frac{\|\delta H\|}{\min\{\lambda_i - \widetilde{\lambda}_{i-1}, \widetilde{\lambda}_{i+k} - \lambda_{i+k-1}\}}, \tag{1.3}$$

provided that both terms in the denominators are positive. Here, $R = \widetilde{H} Q_{\mathcal{T}} - Q_{\mathcal{T}} \operatorname{diag}(\lambda_i, \cdots, \lambda_{i+k-1})$. The upper bound (1.3) is applicable to cases where the perturbation δH is not known exactly, but just the upper bound for $\|\delta H\|$. The above bounds are, like other classical norm-based perturbation bounds such as those from [12, Sections 11.5 and 11.7] and [18, Section V.3.3], proportional to the norm of the perturbation or residual, and are inversely proportional to some sort of the absolute distance between the eigenvalues which define the observed subspace and the rest of the spectrum. In this paper we derive a relative bound for $\|\delta P\|$. Our bound is proportional to parameter η which determines the size of relative perturbation of H as described below, and inversely proportional to a relative distance between the eigenvalues from $\mathcal{T}$ and the rest of the spectrum of H.

Relative perturbation bounds for eigenvalue and singular value problems have been actively researched in the past years [3, 1, 4, 21, 16, 6, 5, 10, 11, 7, 8].

We consider perturbations δH which satisfy

$$|x^*\delta H x| \le \eta x^* \left|H\right| x, \tag{1.4}$$

for all x and some $\eta \in [0,1)$. Here

$$\left|H\right| = \sqrt{H^2} = Q|\Lambda|Q^*, \tag{1.5}$$

is a spectral absolute value of H, that is, a positive definite polar factor of H. This inequality implies that the perturbations which satisfy (1.4) are inertia preserving. Such perturbations are very general. If H is a graded matrix of the form

$$H = D^*AD, \tag{1.6}$$

then we can write $\widetilde{H} = D^*(A+\delta A)D$, and (1.4) holds with

$$\eta = \|\delta A\|\,\|\widehat{A}^{-1}\|, \tag{1.7}$$

where

$$\widehat{A} = D^{-*}\left|H\right|D^{-1}. \tag{1.8}$$

Indeed,

$$\begin{aligned} |x^*\delta H x| &\le |x^*D^*\delta A D x| = \|x^*D^*\delta A D x\| \le \|x^*D^*\|\,\|\delta A\|\,\|Dx\| \\ &\le \|\delta A\|\,\|\widehat{A}^{-1}\|\,x^*\left|H\right|x. \end{aligned}$$

Note that any perturbation $H+\delta H$ can clearly be interpreted as the perturbation of a graded matrix, and vice versa. Another important class of perturbations is when H is perturbed element-wise in the relative sense,

$$|\delta H_{ij}| \le \varepsilon |H_{ij}|. \tag{1.9}$$

By setting

$$D = \mathrm{diag}(\sqrt{\left|H\right|_{ii}}) \tag{1.10}$$

and using $|\delta A_{ij}| \le \varepsilon |A_{ij}|$, the relation (1.7) implies that (1.4) holds with

$$\eta = \varepsilon \|\,|A|\,\|\,\|\widehat{A}^{-1}\|. \tag{1.11}$$

Since $\widehat{A}_{ii} = 1$, we have $\|\widehat{A}^{-1}\| \le \kappa(\widehat{A}) \le n\|\widehat{A}^{-1}\|$, where $\kappa(A) \equiv \|A\|\,\|A^{-1}\|$ denotes the spectral condition number. Also, $\|\,|A|\,\| \le n$ [14]. The diagonal grading matrix D from (1.10), which is also called the scaling matrix, is almost optimal in the sense that [17]

$$\kappa(\widehat{A}) \le n \min_{\bar{D}} \kappa(\bar{D}\left|H\right|\bar{D}) \le n\kappa(\left|H\right|) = n\kappa(H),$$

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

$$|\delta H_{ij}| \le \varepsilon D_{ii}D_{jj}, \tag{1.12}$$

(1.4) holds with

$$\eta = \varepsilon n \|\widehat{A}^{-1}\| \leq \varepsilon n \kappa(\widehat{A}). \tag{1.13}$$

Perturbations of the form (1.9) typically occur when the matrix is stored into computer with machine precision ε. Such perturbations are also caused by measurements since data are often determined to some relative accuracy. Perturbations of the form (1.12) occur during various numerical algorithms (matrix factorizations, eigenvalue or singular value computations).

Another important class of matrices are scaled diagonally dominant matrices. Such matrix has the form $H = D(J+N)D$, where D is a diagonal positive definite, $J = J^* = J^{-1}$, and $\|N\| < 1$ [1, 21]. Under perturbations of type (1.9) we have $\eta = n(1 + \| \, |N| \, \|)/(1 - \|N\|)$ [21, Theorem 2.29].

Note that η also bounds relative changes in eigenvalues [21], that is,

$$1 - \eta \leq \frac{\widetilde{\lambda}_j}{\lambda_j} \leq 1 + \eta. \tag{1.14}$$

Perturbation bounds for eigenvectors of simple eigenvalues were given for scaled diagonally dominant matrices in [1], and for positive definite matrices in [4][1]. The bound for perturbation of the spectral projection onto invariant subspace which corresponds to single, possibly multiple, eigenvalue of an indefinite Hermitian matrix was given in [21, Theorem 2.48]. We generalize this bound to spectral projections onto invariant subspaces which correspond to a set of neighboring eigenvalues. Our result and the related results from [1, 4, 21, 16] and other works, are also useful in estimating the accuracy of highly accurate algorithms for computing eigenvalue decompositions [1, 4, 20, 14].

The rest of the paper is organized as follows. In Section 2 we prove our bound. In Section 3 we show how to effectively compute our bound in the case of graded matrices, and give an example which illustrates our bound and compares it with the classical bounds (1.2) and (1.3).

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2. The bound

In this section we use the notation of Section 1. To simplify the notation set

$$\begin{aligned} &a = \lambda_{i-1}, \quad \alpha = \lambda_i, \quad \beta = \lambda_{i+k-1}, \quad b = \lambda_{i+k}, \\ &\widetilde{a} = \widetilde{\lambda}_{i-1}, \quad \widetilde{\alpha} = \widetilde{\lambda}_i, \quad \widetilde{\beta} = \widetilde{\lambda}_{i+k-1}, \quad \widetilde{b} = \widetilde{\lambda}_{i+k}. \end{aligned} \tag{2.15}$$

Without loss of generality we assume that $\beta > 0$; otherwise one should consider the matrix $-H$. The relative gap (or relative distance) between the set

[1] If H is positive definite, then $\left|H\right| = H$.

$\mathcal{T}$ and the rest of the spectrum of H is defined by

$$\mathrm{rg}_{\mathcal{T}} = \min\{\mathrm{rg}_\alpha, \mathrm{rg}_\beta\}, \tag{2.16}$$

where

$$\mathrm{rg}_\beta = \frac{b-\beta}{b+\beta}, \quad \mathrm{rg}_\alpha = \begin{cases} \dfrac{\alpha - a}{\alpha + \sqrt{\alpha|a|}}, & \text{if } \alpha > 0, \\ \dfrac{\alpha - a}{|\alpha| + |a|}, & \text{if } \alpha < 0. \end{cases}$$

Here the quotients are defined if all the values they contain are defined as well. More precisely, if b does not exist, then rg_β is not defined and $\mathrm{rg}_{\mathcal{T}} = \mathrm{rg}_\alpha$. Thus, relative gap is always defined, except when neither a nor b exist, in which case trivially $\|\delta P\| = 0$. This relative gap is similar to relative gaps used in [21, 13, 1, 4].

We now state our theorem.

THEOREM 2.1. *Let H be a non-singular Hermitian matrix of order n. Let $\mathcal{T} = \{\lambda_i, \ldots, \lambda_{i+k-1}\}$, where $\beta \equiv \lambda_{i+k-1} > 0$, and let P be the spectral projection onto the invariant subspace which corresponds to the eigenvalues from the set $\mathcal{T}$. Let the relative gap between $\mathcal{T}$ and the rest of the spectrum of H, $\mathrm{rg}_{\mathcal{T}}$, be defined by (2.16) and (2.15). Let $\widetilde{H} = H + \delta H$ be the perturbed matrix, where δH is Hermitian perturbation such that $|x^*\delta H x| \leq \eta x^* |H| x$, for all x and some $\eta \in [0, 1)$. Let $\widetilde{\mathcal{T}} = \{\widetilde{\lambda}_i, \ldots, \widetilde{\lambda}_{i+k-1}\}$, and let $\widetilde{P} = P + \delta P$ be the spectral projection onto invariant subspace which corresponds to the eigenvalues from the set $\widetilde{\mathcal{T}}$. If $\eta < \mathrm{rg}_{\mathcal{T}}$, then*

$$\|\delta P\| \leq \frac{1}{2}\left(\frac{\beta - \alpha}{\min\{|\alpha|, \beta\}} \cdot \frac{1}{\mathrm{rg}_{\mathcal{T}}} + \frac{|\alpha| + \beta}{\min\{|\alpha|, \beta\}}\right) \frac{\eta}{\mathrm{rg}_{\mathcal{T}}} \cdot \frac{1}{1 - \dfrac{\eta}{\mathrm{rg}_{\mathcal{T}}}}.$$

Proof. The proof is similar to the proof of [21, Theorem 2.48]. The projection P is defined by the Dunford integral [9, Section II.1.4],

$$P = \frac{1}{2\pi i} \int_\Gamma (\mu I - H)^{-1} d\mu. \tag{2.17}$$

Here Γ is a curve around $\mathcal{T}$ which separates $\mathcal{T}$ from the rest of the spectrum of H. We choose Γ as the circle with the center C and the radius r defined by

$$C = \left(\frac{1}{2}(\alpha + \beta + r_\beta - r_\alpha), 0\right), \quad r = \frac{1}{2}(\beta - \alpha + r_\beta + r_\alpha), \tag{2.18}$$

where $r_\alpha = |\alpha|\mathrm{rg}_{\mathcal{T}}$ and $r_\beta = \beta \mathrm{rg}_{\mathcal{T}}$. Therefore, Γ passes through the points $(\alpha - r_\alpha, 0)$ and $(\beta + r_\beta, 0)$. Let us show that $\widetilde{\mathcal{T}}$ is also in the interior of Γ while the rest of the spectrum of $\widetilde{H}$ remains outside Γ. By using (1.14), the

definition of $\mathrm{rg}_{\mathcal{T}}$, and the assumption of the theorem $\eta < \mathrm{rg}_{\mathcal{T}}$, we have

$$\begin{aligned}\widetilde{\beta} &\leq \beta + \eta\beta < \beta + \mathrm{rg}_{\mathcal{T}}\beta = \beta + r_\beta \leq \beta + \mathrm{rg}_\beta \beta \\ &= b - \mathrm{rg}_\beta b \leq b - \mathrm{rg}_{\mathcal{T}} b < b - \eta b \leq \widetilde{b}.\end{aligned}$$

Similarly,

$$\widetilde{a} \leq a + \eta\,\mathrm{sign}(a)a < \alpha - r_\alpha < \alpha - \eta\,\mathrm{sign}(\alpha)\alpha \leq \widetilde{\alpha}.$$

In the last relation the three cases *(i)* $a > 0$, *(ii)* $a < 0$ and $\alpha > 0$, and *(iii)* $\alpha < 0$, have to be verified separately. We conclude that the same Γ can be used to define $\widetilde{P}$, as well. Therefore,

$$\widetilde{P} = \frac{1}{2\pi i}\int_\Gamma (\mu I - (H + \delta H))^{-1} d\,\mu. \tag{2.19}$$

Set $R_\mu = (\mu I - H)^{-1}$. From (2.17) and (2.19) it follows that

$$\delta P = \frac{1}{2\pi i}\int_\Gamma R_\mu \delta H \left[\sum_{k=0}^{\infty} (R_\mu \delta H)^k\right] R_\mu d\,\mu,$$

provided that $\rho(R_\mu \delta H) < 1$, where ρ denotes the spectral radius. This condition is verified later. Set

$$\Delta = |H|^{-1/2}\delta H |H|^{-1/2}, \quad z_\mu = R_\mu |H|^{1/2}, \quad \omega_\mu = |H|^{1/2} R_\mu |H|^{1/2}.$$

Note that (1.4) implies $\|\Delta\|_2 \leq \eta$. Since R_μ and $|H|^{1/2}$ commute, we have

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

Also, since $R_\mu \delta H$ and $\omega_\mu \Delta$ are similar, we have

$$\rho(R_\mu \delta H) = \rho(\omega_\mu \Delta) < \|\omega_\mu\|\eta. \tag{2.20}$$

Our choice of Γ implies that

$$\|\delta P\| \leq r\zeta\eta \frac{1}{1 - \omega\eta}, \tag{2.21}$$

where

$$\begin{aligned}\zeta &= \max_{\mu\in\Gamma} \|z_\mu\|^2 = \max_{\mu\in\Gamma} \max_{\nu\in\sigma(H)} \frac{|\nu|}{|\mu - \nu|^2}, \\ \omega &= \max_{\mu\in\Gamma} \|\omega_\mu\| = \max_{\mu\in\Gamma} \max_{\nu\in\sigma(H)} \frac{|\nu|}{|\mu - \nu|}.\end{aligned}$$

Minimal distance between a variable point which lies on the circle with the center on the real axis and some fixed point on the real axis is attained in one of the two points where the circle intersects the real axes. Thus, the maxima over μ in the above equalities are attained at those μ which lie on the real

axis. Consequently, maxima over $\nu \in \sigma(H)$ are attained for eigenvalues which are closest to the circle Γ, and we have

$$\begin{aligned}\zeta &= \max\left\{\frac{|a|}{(\alpha - r_\alpha - a)^2}, \frac{|\alpha|}{r_\alpha^2}, \frac{\beta}{r_\beta^2}, \frac{b}{(b-\beta-r_\beta)^2}\right\} \equiv \max\{\zeta_a, \zeta_\alpha, \zeta_\beta, \zeta_b\},\\ \omega &= \max\left\{\frac{|a|}{\alpha - r_\alpha - a}, \frac{|\alpha|}{r_\alpha}, \frac{\beta}{r_\beta}, \frac{b}{b-\beta-r_\beta}\right\} \equiv \max\{\omega_a, \omega_\alpha, \omega_\beta, \omega_b\}.\end{aligned}$$

Now

$$\omega_\beta = \frac{1}{\mathrm{rg}_{\mathcal{T}}} \geq \frac{1}{\mathrm{rg}_\beta} = \frac{b}{b - \beta - \mathrm{rg}_\beta \beta} \geq \omega_b. \tag{2.22}$$

Since $\beta < b$, squaring (2.22) and dividing by β gives $\zeta_\beta > \zeta_b$. We split the rest of the proof in two cases, $\alpha > 0$ and $\alpha < 0$.

Case 1. Let $\alpha > 0$. We have

$$\zeta_\alpha = \frac{1}{\alpha \mathrm{rg}_{\mathcal{T}}^2} \geq \frac{1}{\alpha \mathrm{rg}_\alpha^2} = \frac{|a|}{(\alpha - \alpha \mathrm{rg}_\alpha - a)^2} \geq \zeta_a.$$

If $a > 0$, then multiplying the above relation by α and taking square root gives $\omega_\alpha > \omega_a$. If $a < 0$, then $\omega_a < 1 < \omega_\alpha$. Altogether,

$$\omega = \omega_\alpha = \omega_\beta = \frac{1}{\mathrm{rg}_{\mathcal{T}}}, \qquad \zeta = \zeta_\alpha = \frac{1}{\alpha \mathrm{rg}_{\mathcal{T}}^2}. \tag{2.23}$$

Using ω from (2.23), the assumption $\eta < 1/\mathrm{rg}_{\mathcal{T}}$, and (2.20), gives $\rho(R_\mu \delta H) < 1$, as desired. The theorem now follows by inserting ω and ζ from (2.23) and r from (2.18) into (2.21), and using $0 < \alpha < \beta$.

Case 2. Let $\alpha < 0$. By applying the same reasoning as in (2.22) to ω_a and ω_α, we have $\omega_a < \omega_\alpha$. Since $|\alpha| < |a|$, squaring this inequality and dividing by $|\alpha|$ gives $\zeta_\alpha > \zeta_a$. Therefore,

$$\omega = \omega_\alpha = \omega_\beta = \frac{1}{\mathrm{rg}_{\mathcal{T}}}, \qquad \zeta = \max\{\zeta_\alpha, \zeta_\beta\} = \frac{1}{\min\{|\alpha|, \beta\} \mathrm{rg}_{\mathcal{T}}^2}. \tag{2.24}$$

As in Case 1, we conclude that $\rho(R_\mu \delta H) < 1$.

From (2.23) and (2.24) we see that the latter relations hold in both cases. The theorem follows by inserting ω and ζ from (2.24) and r from (2.18) into (2.21).

□

If $\alpha = \beta$, then our bound reduces to the bound from [21, Theorem 2.48] (the term in parentheses equals one), which holds for invariant subspace of one, possibly multiple, eigenvalue. Compared to the existing relative perturbation bounds from [1, 4, 21, 11], our bound is the most general since it holds for all indefinite non-singular Hermitian matrices and applies to eigenspaces which correspond to any set of neighboring eigenvalues. For positive definite matrices one can prove Theorem 2.1 with a better type of relative gap [19]. If H is given in the factorized form $H = GAG^*$ and is perturbed through

its factor G, the perturbation bound for invariant subspace of one, possibly multiple, eigenvalue, is given in [16]. By using technique similar to the one in the proof Theorem 2.1, one can generalize this bound to subspaces which correspond to a set of neighboring eigenvalues [19].

REMARK 2.2. The bound of Theorem 2.1 differs from the bound of [21, Theorem 2.48] by the term in parentheses. This term depends on the relative size of the set $\mathcal{T}$, which is essentially the condition number $\|\widehat{H}\|\,\|\widehat{H}^{-1}\|$, where $\widehat{H}$ is the restriction of H to the observed invariant subspace. This condition number appears naturally if the interval $[\alpha,\beta]$ is filled with pathologically close eigenvalues. However, if the set $\mathcal{T}$ consists of two sets of eigenvalues, $\mathcal{T}_1 = \{\alpha,\cdots,\lambda_l\}$ and $\mathcal{T}_2 = \{\lambda_{l+1},\cdots,\beta\}$, where λ_l and λ_{l+1} are well separated, than this condition number is artificial and can be avoided as follows: let $P \equiv P_{\mathcal{T}}$, $P_{\mathcal{T}_1}$, and $P_{\mathcal{T}_2}$, be the projections onto subspaces corresponding to $\mathcal{T}$, $\mathcal{T}_1$ and $\mathcal{T}_2$, respectively. Then $P = P_{\mathcal{T}_1} + P_{\mathcal{T}_2}$, $\delta P = \delta P_{\mathcal{T}_1} + \delta P_{\mathcal{T}_2}$ and $\|\delta P\| \le \|\delta P_{\mathcal{T}_1}\| + \|\delta P_{\mathcal{T}_2}\|$, and the bound obtained by bounding $\|\delta P_{\mathcal{T}_1}\|$ and $\|\delta P_{\mathcal{T}_2}\|$ separately will be sharper than the one obtained by bounding $\|\delta P\|$ directly. Of course, this idea can be used inductively.

3. Numerical example

In this section we first describe how to compute η from Theorem 2.1 and how to estimate the accuracy of the computed invariant subspace. Then we give an example which illustrates Theorem 2.1 and compares it with the classical bounds (1.2) and (1.3). Finally, we make some concluding remarks.

Let H be a graded matrix given by (1.6). In order to compute η from (1.7), (1.11) or (1.13), we need to know $\widehat{A}$ from (1.8). $\widehat{A}$ can be computed by the highly accurate eigenreduction algorithm from [20, 14]. This algorithm first factorizes H as $H = GJG^*$ by the symmetric indefinite factorization from [15]. Here $J = \mathrm{diag}(\pm 1)$. This factorization is followed by the one-sided J-orthogonal Jacobi method on the pair G, J [20, 14]. This method forms the sequence of matrices

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

Such matrices F_k are called J-orthogonal. This sequence converges to some matrix GF which has numerically orthogonal columns. The eigenvalues of H are approximated by the diagonal elements of the matrix $\Lambda \equiv |\Lambda| J$, where $|\Lambda| = \mathrm{diag}(F^*G^*GF)$. The corresponding eigenvectors of H are approximated by the columns of the matrix by $Q \equiv GF|\Lambda|^{-1/2}$. Therefore, $\left|H\right|$ from (1.5) is given by $\left|H\right| = GFF^*G^*$. Since the matrix GF is readily available in the computer, we can compute $\widehat{A}$ from (1.8) as $\widehat{A} = D^{-*}GFF^*G^*D^{-1}$, or even simpler, we can compute just its factor $D^{-*}GF$. Therefore, if the eigenvalue problem is solved by the above highly accurate algorithm, then the computation of $\widehat{A}$ requires only little extra cost. Error bounds for this

highly accurate eigenreduction algorithm, which are given in [14], ensure that the computed $\widehat{A}$ is accurate enough. This particularly holds for well-scaled matrices, that is, for the matrices where $\widehat{A}$ is well conditioned if D is chosen as in (1.10). Once we have $\widehat{A}$, we can compute η directly from the definitions (1.7), (1.11), or (1.13), provided that we know an upper bound for $\|\delta A\|$ or ε.

REMARK 3.1. In order to estimate the accuracy of the invariant subspace which is computed by some numerical method, we assume that $\widetilde{H}$ is the original matrix, $\lambda_i, \cdots, \lambda_{i+k-1}$ are the computed eigenvalues, and the columns of $Q_{\mathcal{T}}$ are the corresponding computed eigenvectors. With this notation we can clearly use (1.2), provided that we estimate the eigenvalues $\widetilde{\lambda}_{i-1}$ and $\widetilde{\lambda}_{i+k}$ which appear in the denominator. The bound of Theorem 2.1, on the other hand, uses only original quantities. Therefore, this bound can be applied by simply inserting the computed quantities, that is, by switching the roles of H and $\widetilde{H}$, provided we know η which is generated by the algorithm. For example, if we use the above highly accurate algorithm in double precision, error analysis from [14, 15] shows that η is given by (1.13) with $\varepsilon \approx 10^{-16}$ in (1.12).

Let us give an example. Let

$$H = \begin{bmatrix} 7.7e+08 & 9.9e+01 & -5.8e+06 & -2.0e-01 & 6.1e-02 & 1.2e-01 \\ 9.9e+01 & 5.7e-04 & -7.5e+00 & -1.1e-07 & -9.9e-08 & -3.2e-08 \\ -5.8e+06 & -7.5e+00 & -2.9e+05 & -8.3e-04 & -3.9e-03 & 1.1e-03 \\ -2.0e-01 & -1.1e-07 & -8.3e-04 & 1.1e-09 & 8.5e-11 & 4.9e-11 \\ 6.1e-02 & -9.9e-08 & -3.9e-03 & 8.5e-11 & 5.7e-10 & 1.4e-10 \\ 1.2e-01 & -3.2e-08 & 1.1e-03 & 4.9e-11 & 1.4e-10 & 4.6e-10 \end{bmatrix},$$

and

$$\delta H = \begin{bmatrix} -6.8e+02 & -2.2e-05 & -2.8e+00 & 7.2e-09 & 1.3e-08 & -3.2e-08 \\ -2.2e-05 & -3.7e-11 & -1.6e-07 & 9.7e-15 & -4.3e-15 & -5.1e-15 \\ -2.8e+00 & -1.6e-07 & 7.8e-02 & 3.4e-11 & -6.4e-10 & 1.1e-09 \\ 7.2e-09 & 9.7e-15 & 3.4e-11 & 6.4e-16 & 8.0e-19 & 1.1e-17 \\ 1.3e-08 & -4.3e-15 & -6.4e-10 & 8.0e-19 & 3.5e-16 & 6.1e-18 \\ -3.2e-08 & -5.1e-15 & 1.1e-09 & 1.1e-17 & 6.1e-18 & 2.8e-16 \end{bmatrix}.$$

The eigenvalues of H are (properly rounded)

$$\lambda_1 = -3.34 \cdot 10^5, \quad \lambda_2 = 3.89 \cdot 10^{-10}, \quad \lambda_3 = 6.10 \cdot 10^{-10},$$
$$\lambda_4 = 1.10 \cdot 10^{-9}, \quad \lambda_5 = 6.94 \cdot 10^{-4}, \quad \lambda_6 = 7.70 \cdot 10^8.$$

Here δH is a component-wise relative perturbation (1.9) with $\varepsilon = 10^{-6}$. Note that $\|\delta H\| \approx 6.8 \cdot 10^2$. We have used the diagonal scaling matrix D from (1.10). Also, $\eta \approx 4.2 \cdot 10^{-6}$ is computed from (1.11) with $\| \, |A| \, \| \approx 1.7$ and $\|\widehat{A}^{-1}\| \approx 2.4$.

Perturbations of various subspaces and their bounds are shown in Table 1. The table is formed as follows: the first column describes the set of the eigenvalues which define $Q_{\mathcal{T}}$. For example, $\mathcal{T}_{23}$ means that $Q_{\mathcal{T}}$ contains eigenvectors which correspond to eigenvalues λ_2 and λ_3. The second column gives the actual value of $\|\delta P\|$, and the other columns give error bounds computed

from Theorem 2.1, (1.2) and (1.3), respectively. Since the diameter of the set $\mathcal{T}_{2345}$ is large, and this set is a union of two well separated sets $\mathcal{T}_{234}$ and $\mathcal{T}_5$, we used Remark 2.2 and computed the bound for $\|\delta P_{\mathcal{T}_{2345}}\|$ by adding the bounds for $\|\delta P_{\mathcal{T}_{234}}\|$ and $\|\delta P_{\mathcal{T}_5}\|$.

TABLE 1. Perturbation bounds.

$\mathcal{T}$	$\|\delta P\|$	Theorem 2.1	(1.2)	(1.3)
$\mathcal{T}_2$	$1.6 \cdot 10^{-7}$	$1.9 \cdot 10^{-5}$	> 1	> 1
$\mathcal{T}_{23}$	$1.2 \cdot 10^{-7}$	$3.3 \cdot 10^{-5}$	> 1	> 1
$\mathcal{T}_{234}$	$1.2 \cdot 10^{-10}$	$1.2 \cdot 10^{-5}$	$2.9 \cdot 10^{-4}$	> 1
$\mathcal{T}_{2345}$	$2.4 \cdot 10^{-12}$	$1.6 \cdot 10^{-5}$	$6.8 \cdot 10^{-10}$	$2.0 \cdot 10^{-3}$
$\mathcal{T}_5$	$1.2 \cdot 10^{-10}$	$4.2 \cdot 10^{-6}$	$3.3 \cdot 10^{-1}$	> 1
$\mathcal{T}_6$	$1.8 \cdot 10^{-8}$	$4.2 \cdot 10^{-6}$	$8.8 \cdot 10^{-7}$	$8.8 \cdot 10^{-7}$

The values of $\|\delta P\|$ were computed as

$$\|\delta P\| = \|P - \widetilde{P}\| = \|Q_{\mathcal{T}} Q_{\mathcal{T}}^T - \widetilde{Q}_{\mathcal{T}} \widetilde{Q}_{\mathcal{T}}\|,$$

where the matrices $Q_{\mathcal{T}}$ and $\widetilde{Q}_{\mathcal{T}}$ are defined in Section 1. The matrices $Q_{\mathcal{T}}$ and $\widetilde{Q}_{\mathcal{T}}$ were computed by the the above highly accurate algorithm in double precision. Since here $\| \, |A| \, \| \approx 1.7$, $\|\widehat{A}^{-1}\| \approx 2.4$, and $\varepsilon \approx 10^{-16}$, (1.13) implies that $\eta \approx 10^{-16}$. Since relative gaps are moderate in all cases, from Remark 3.1 we conclude that all of $Q_{\mathcal{T}}$ were computed to almost full accuracy. The same holds for all of $\widetilde{Q}_{\mathcal{T}}$, thus the computed values of $\|\delta P\|$ which are displayed in Table 1 are almost equal to the exact ones.

From Table 1 we can make some interesting observations which also depict the general behavior. The bound of Theorem 2.1 is usually sharper than the classical bounds (1.2) and (1.3) for subspaces which correspond to tiny (clustered) eigenvalues which have large relative gaps and small absolute gaps like $\mathcal{T}_2$, $\mathcal{T}_{23}$, $\mathcal{T}_{234}$, $\mathcal{T}_{2345}$, and $\mathcal{T}_5$. For such subspaces classical bounds can completely fail. Classical bounds are, as expected, sharper for subspaces which correspond to absolutely large eigenvalues like $\mathcal{T}_6$, but our bound is still good.

Let us conclude the paper by saying that our bound is in appropriate cases sharper than the classical norm-wise bounds which use absolute gaps. Our bound is useful for relative perturbations which occur in numerical computations, and can be used to estimate the accuracy of the computed invariant subspaces.

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