SOME NEW BOUNDS ON PERTURBATION OF SUBSPACES

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When a Hermitian linear operator A is slightly perturbed, by how much can its invariant subspaces change? Given some approximations to a cluster of neighboring eigenvalues and to the corresponding eigenvectors of a real symmetric matrix, and given a lower bound $\delta > 0$ for the gap that separates the cluster from all other eigenvalues, how much can the subspace spanned by the eigenvectors differ from that spanned by our approximations? These questions are closely related; both are investigated here. First the difference between the two subspaces is characterized in terms of certain angles through which one subspace must be rotated in order most directly to reach the other. The angles constitute the spectrum of a Hermitian operator Θ, with which is associated a commuting skew-Hermitian operator $J = -J^3$; the unitary operator that differs least from the identity and rotates one subspace into the other turns out to be $\exp(J\Theta)$. These operators unify the treatment of natural geometric, operator-theoretic and error-analytic questions concerning those subspaces. Given the gap δ, and given bounds upon either the perturbation (1st question) or a computable residual (2nd question), we obtain sharp bounds upon unitary-invariant norms of trigonometric functions of Θ. (A norm is unitary-invariant whenever $\|L\| = \|ULV\|$ for all unitary U and V. Examples are the bound-norm $\|L\|_1 \equiv \sup\|Lx\|/\|x\|$ and the square-norm $\|L\|_{sq} \equiv (\text{trace } L^*L)^{1/2}$.)

In this note we consider a finite-dimensional unitary space $\mathcal{H}$ in which the scalar product is denoted by y^*x, and $\|x\| \equiv (x^*x)^{1/2}$. Proofs of the following statements will appear elsewhere, together with extensions to infinite-dimensional Hilbert spaces and to non-compact or unbounded operators [2]. That article discusses the relation of our results to earlier work on the subject, such as [1], [3], [4].

1. **Subspaces and isometries.** There are two convenient ways to identify a subspace of $\mathcal{H}$. On the one hand, let P be the orthogonal projector ($P = P^* = P^2$) onto that subspace, which is then denoted by $P\mathcal{H}$. On the other hand, let $e_1, e_2, \cdots, e_n$ be an orthonormal basis for the subspace; then $E \equiv (e_1, e_2, \cdots, e_n)$ denotes an isometry mapping column n-vectors into the subspace, which is now interpreted as the range $\mathcal{R}(E)$. Orthonormality of the e_i's means $E^*E = ((e_i^*e_j))$ $= 1$, the identity operator on the n-space; $\mathcal{R}(E) = P\mathcal{H}$ means P $= EE^* = \sum_1^n e_ie_i^*$. Note that the subspace does not determine E

uniquely, but only to within post-multiplication by an arbitrary unitary $n\times n$ matrix. The orthogonal complement of $P\mathcal{H}$ is $\tilde{P}\mathcal{H}$ where $\tilde{P}\equiv 1-P$; then the equations $\hat{E}\hat{E}^*=\tilde{P}$ and $\hat{E}^*\hat{E}=1$ define, to within unitary post-multiplication, an isometry $\hat{E}$ complementary to E in the sense that $(E, \hat{E})$ is formally unitary:

$$(E, \hat{E})^*(E, \hat{E}) = \begin{pmatrix} E^*E & E^*\hat{E} \\ \hat{E}^*E & \hat{E}^*\hat{E} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

and $(E, \hat{E})(E, \hat{E})^* = EE^* + \hat{E}\hat{E}^* = 1.$

2. **Angles between subspaces.** Let $P\mathcal{H}=\mathcal{R}(E)$ and $Q\mathcal{H}=\mathcal{R}(F)$ be two subspaces given together with their projectors and isometries, with $n\equiv\dim P\mathcal{H}$ and $m\equiv\dim Q\mathcal{H}$. For simplicity, assume $n\leqq m$ and $n+m\leqq\dim\mathcal{H}$. The separation between these subspaces is unchanged by the following transformations:

(i) Pre-multiply E and F by the same arbitrary unitary operator.

(ii) Post-multiply E or F (or $\hat{E}$ or $\hat{F}$) by an arbitrary unitary matrix.

Transformation (i) rotates both subspaces simultaneously without altering their relative positions, while (ii) merely changes coordinates within each subspace. Consequently the separation between the subspaces is characterized by the invariants of the matrix

$$\begin{pmatrix} C \\ S \end{pmatrix} \equiv \begin{pmatrix} E^*F \\ \hat{E}^*F \end{pmatrix} = (E, \hat{E})^*F$$

when C and S are pre-multiplied by independent arbitrary unitaries or post-multiplied by the same arbitrary unitary matrix. Since $C^*C+S^*S=F^*F=1$, coordinate systems can be so chosen as to exhibit the matrices

$$C = \underbrace{\left[\begin{array}{c|c} \begin{matrix}\gamma_1 & & \\ & \ddots & \\ & & \gamma_n\end{matrix} & 0 \end{array}\right]}_{n \qquad m-n} n, \quad S = \underbrace{\left[\begin{array}{c|c} 0 & \begin{matrix}1 & & \\ & \ddots & \\ & & 1\end{matrix} \\ \hline \begin{matrix}\sigma_1 & & \\ & \ddots & \\ & & \sigma_n\end{matrix} & 0 \\ \hline 0 & 0 \end{array}\right]}_{n \qquad m-n} \begin{matrix} m-n \\ \\ n \\ \\ \end{matrix}$$

simultaneously in essentially diagonal forms, where $\gamma_i = \cos\theta_i$ and $\sigma_i = \sin\theta_i$ for angles $\theta_1 \geqq \theta_2 \geqq \cdots \geqq \theta_n$ in $0 \leqq \theta_i \leqq \pi/2$. These angles, "the angles between the subspaces," are the invariants that characterize the separation between the given subspaces. The Hermitian operator Θ can now be defined via its matrix in the foregoing coordinate system;

$$\Theta \equiv (E, \hat{E})\,\mathrm{diag}(\theta_1, \theta_2, \cdots, \theta_n, \underbrace{0, 0, \cdots, 0}_{m-n}, \theta_1, \theta_2, \cdots, \theta_n, 0, 0, \cdots)$$

$$\cdot (E, \hat{E})^*.$$

We shall also need $\Theta_0 \equiv \mathrm{diag}(\theta_1\theta_2, \cdots, \theta_n)$.

3. The direct rotation. We define a unitary operator U whose matrix, in the co-ordinate system that essentially diagonalizes C and S above, is:

$$(E,\hat{E})^* U (E,\hat{E}) = \left[\begin{array}{c|c||c|c} \begin{matrix}\gamma_1 & & \\ & \ddots & \\ & & \gamma_n\end{matrix} & 0 & \begin{matrix}-\sigma_1 & & \\ & \ddots & \\ & & -\sigma_n\end{matrix} & 0 \\ \hline 0 & \begin{matrix}1 & & \\ & \ddots & \\ & & 1\end{matrix} & 0 & 0 \\ \hline \begin{matrix}\sigma_1 & & \\ & \ddots & \\ & & \sigma_n\end{matrix} & 0 & \begin{matrix}\gamma_1 & & \\ & \ddots & \\ & & \gamma_n\end{matrix} & 0 \\ \hline 0 & 0 & 0 & \begin{matrix}1 & & \\ & \ddots & \\ & & 1\end{matrix} \end{array}\right] \begin{matrix} n \\ \\ m-n \\ \\ n \\ \\ \\ \end{matrix}$$

$$\qquad\qquad n \qquad\qquad m-n \qquad\qquad n$$

Evidently $U = \exp(J\Theta)$ for a suitable skew-Hermitian $J = -J^3$ which commutes with Θ. This unitary U is called the "direct rotation" of $P\mathcal{H}$ into $Q\mathcal{H}$ partly because $UP\mathcal{H} \subseteq Q\mathcal{H}$. But the last relation is also satisfied by many other unitaries U; what distinguishes the direct rotation from the others is the following theorem:

Of all unitary U satisfying $UP\mathcal{H}\subseteq Q\mathcal{H}$, the one which minimizes each unitary-invariant norm of $(1-U)^*(1-U)$, including in particular $\|1-U\|_1^2$ and $\|1-U\|_{sq}^2$, is the direct rotation U defined above. Furthermore, if all $\theta_i \leq \pi/3$ and $\mathcal{H}$ is a real space, every unitary-invariant norm of $(1-U)$ is minimized too.

To simplify matters, let us further assume that $P\mathcal{H}\cap\tilde{Q}\mathcal{H}=0$, so all $\theta_i<\pi/2$; then the theorem characterizes the direct rotation uniquely. And also we obtain a coordinate-free construction for the direct rotation:

Let T be the orthogonal projector onto $P\mathcal{H}\oplus(Q\mathcal{H}\cap\tilde{P}\mathcal{H})$; then the direct rotation is the principal square root of $(Q-\tilde{Q})(T-\tilde{T})$, that is, the unitary square root with spectrum in the right half-plane.

The construction is especially simple when $n=m$ because then $T=P$. (But when some $\theta_i=\pi/2$, the construction must be altered to allow for the nonuniqueness of direct rotations.)

Various other measures that have been used to describe the separation between two subspaces can be expressed in terms of Θ. For example:

$$\|\sin\Theta\|_1 = \sup\|\tilde{Q}p\| \text{ over } p\in P\mathcal{H} \text{ with } \|p\| = 1.$$

$$2\|\sin\tfrac{1}{2}\Theta\|_1 = \sup(\inf\|q-p\| \text{ over } q\in Q\mathcal{H},\ \|q\| = 1) \text{ over } p\in P\mathcal{H},\ \|p\| = 1.$$

$\|\sin\Theta_0\|=\|\tilde{Q}E\|=\|\tilde{Q}P\|$, $2\|\sin\frac{1}{2}\Theta\|=\|1-U\|$, and $\|\sin\Theta\|=\|P-Q\|$ for all unitary-invariant norms.

4. Question 1—perturbation. A Hermitian operator A is given together with some of its orthonormal eigenvectors $e_1, e_2, \cdots, e_n$; more generally, we might be given merely the invariant subspace $\mathcal{R}(E)$ which they span. This subspace and its complement $\mathcal{R}(\hat{E})$ "reduce" A in the sense that we may decompose

$$A = (E,\hat{E})\begin{pmatrix} A_0 & 0 \\ 0 & A_1\end{pmatrix}(E,\hat{E})^* = EA_0E^* + \hat{E}A_1\hat{E}^*$$

where the $n\times n$ Hermitian matrix $A_0\equiv E^*AE$ has the same spectrum as A's restriction to $\mathcal{R}(E)$ while $A_1\equiv\hat{E}^*A\hat{E}$ has the rest of A's spectrum. Adding a Hermitian perturbation H to A changes its spectrum and invariant subspaces; let $\mathcal{R}(F)$ be one of $(A+H)$'s invariant subspaces, identified perhaps by specifying an interval containing the spectrum of one of the matrices $\Lambda_0\equiv F^*(A+H)F$ or Λ_1

$\equiv \hat{F}^*(A+H)\hat{F}$ which figure in the decomposition $A+H = F\Lambda_0 F^* + \hat{F}\Lambda_1\hat{F}^*$.

How different is $\mathcal{R}(F)$ from $\mathcal{R}(E)$? This question will be answered in terms of hypotheses upon $\|H\|$ and upon a gap $\delta > 0$ between the spectra of two of the A_i and Λ_i. Another similar question will be answered at the same time.

5. **Question 2—approximation.** A Hermitian operator $A+H$ is given together with orthonormal vectors $e_1, e_2, \cdots, e_n$ intended to approximate eigenvectors $f_1, f_2, \cdots, f_n$; more generally, the subspace $\mathcal{R}(E)$ spanned by the e's might be intended to approximate an invariant subspace $\mathcal{R}(F)$ of $A+H$. Also given is a Hermitian $n\times n$ matrix A_0, usually diagonal, intended to approximate $\Lambda_0 \equiv F^*(A+H)F$; more generally, A_0's spectrum approximates that part of $(A+H)$'s spectrum associated with $\mathcal{R}(F)$. A residual $R \equiv (A+H)E - EA_0$ may be computed, and will be small when all approximations are close. Indeed, among $(A+H)$'s eigenvalues are n which may be paired with those of A_0 in such a way that no two in a pair differ by more than $\|R\|_1$; this fact may help to characterize Λ_0 and hence identify F, when $A+H$, E and A_0 are all that are given.

How different is $\mathcal{R}(F)$ from $\mathcal{R}(E)$? This question will be answered in terms of hypotheses upon $\|R\|$ and upon a gap $\delta > 0$ between the spectra of two of the A_i and Λ_i. Here A_0 and Λ_0 have already been defined, and $\Lambda_1 \equiv \hat{F}^*(A+H)\hat{F}$ as before. But A_1 is not yet defined because the partition of $A+H$ into a sum is partly arbitrary. Instead, to unify questions 1 and 2, we define as before $A \equiv EA_0E^* + \hat{E}A_1\hat{E}^*$, now a function of A_1, and thus define the Hermitian perturbation $H \equiv (A+H) - A$ as a function of A_1 satisfying $HE = R$. Some of our results are unaffected by the choice of A_1.

6. **The main results.** In each of the following theorems, those of the A_i, Λ_i, H and R which appear are to be interpreted as above, subject to additional hypotheses varying from one theorem to the next. In all cases, Θ is the angle-operator between the invariant subspaces $\mathcal{R}(E)$ of A and $\mathcal{R}(F)$ of $A+H$, and Θ_0 is as defined earlier. The norm inequalities are valid (and best-possible) for every unitary-invariant norm.

THE sin θ THEOREM. *Assume that A_0's spectrum lies in some interval while Λ_1's spectrum lies distant at least $\delta > 0$ from that interval (perhaps on both sides of it); or vice-versa. Then $\delta\|\sin\Theta_0\| \leq \|R\| \leq \|H\|$. And if the spectra of Λ_0 and A_1 are separated in the same way, $\delta\|\sin\Theta\| \leq \|H\|$.*

THE sin 2θ THEOREM. *Assume that Λ_0's spectrum lies in some interval* *while Λ_1's spectrum lies distant at least $\delta > 0$ from that interval (perhaps on both sides of it); or vice-versa. Then $\delta\|\sin 2\Theta_0\| \leqq 2\|R\|$ and $\delta\|\sin 2\Theta\| \leqq 2\|H\|$. (The last inequality is valid if, instead, the spectra of A_0 and A_1 are separated as described above for Λ_0 and Λ_1.) And if $2\|R\|_1 < \delta$ or $2\|H\|_1 < \delta$, and if A_0's spectrum lies no further than $\delta/2$ from that interval containing Λ_0's spectrum, then $\Theta_0 < \pi/4$ and $\Theta < \pi/4$ beside satisfying the inequalities above.*

The Rayleigh-Ritz method prescribes A_0 to be chosen in such a way that, given $A+H$ and E, $\|R\|$ will be minimized; namely, $A_0 = E^*(A+H)E$. For this choice, the theorems above can be sharpened.

THE tan θ THEOREM. *Assume $A_0 = E^*(A+H)E$, and assume there is a gap $\delta > 0$ between two intervals of which one contains A_0's spectrum and the other Λ_1's. Then $\delta\|\tan \Theta_0\| \leqq \|R\|$ and $\delta\|\tan \Theta\| \leqq \|H\|$.*

THE tan 2θ THEOREM. *Assume $A_0 = E^*(A+H)E$, $A_1 = \hat{E}^*(A+H)\hat{E}$, and assume there is a gap $\delta > 0$ between two intervals of which one contains A_0's spectrum and the other A_1's. Then $\delta\|\tan 2\Theta_0\| \leqq 2\|R\|$ and $\delta\|\tan 2\Theta\| \leqq 2\|H\|$. Furthermore, Λ_0 and Λ_1 may be so chosen that their spectra are on the same sides of the gap as are A_0's and A_1's respectively, and when this is done then $\Theta_0 < \pi/4$ and $\Theta < \pi/4$ beside satisfying the inequalities above.*

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