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A Sharp Version of Kahan's Theorem on Clustered Eigenvalues

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ABSTRACT

Let the $n \times n$ Hermitian matrix A have eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$, let the $k \times k$ Hermitian matrix H have eigenvalues $\mu_1 \leq \mu_2 \leq \cdots \leq \mu_k$, and let Q be an $n \times k$ matrix having full column rank, so $1 \leq k \leq n$. It is proved that there exist k eigenvalues $\lambda_{i_1} \leq \lambda_{i_2} \leq \cdots \leq \lambda_{i_k}$ of A such that

$$\max_{1 \leq j \leq k} |\mu_j - \lambda_{i_j}| \leq \frac{c}{\sigma_{\min}(Q)} \|AQ - QH\|_2$$

always holds with $c = 1$, where $\sigma_{\min}(Q)$ is the smallest singular value of Q, and $\|\cdot\|_2$ denotes the biggest singular value of a matrix. The inequality was proved for $c \leq \sqrt{2}$ in 1967 by Kahan, who also conjectured that it should be true for $c = 1$.

The Rayleigh-Ritz approximation to some k eigenvalues of an $n \times n$ Hermitian matrix A begins with k orthonormal column vectors whose span is intended to approximate an invariant subspace of A. These columns are assembled into a rectangular orthogonal matrix Q, so $Q^*Q = I_k$, the $k \times k$ identity matrix. Here "*" takes the conjugate transpose. Then the *Rayleigh quotient*

$$H = Q^*AQ = H^*$$

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is computed; its k eigenvalues approximate some eigenvalues of A to within $\pm\|AQ - QH\|_2$, where the norm $\|\cdot\|_2$ denotes the biggest singular value. But until 1967 we could not be sure that as many as k eigenvalues of A were approximated that well; for all we knew then, the k eigenvalues of H might approximate fewer than k eigenvalues of A, some more than once.

Moreover, the exigencies of approximate computation could produce columns in Q that were at best nearly orthonormal, and H at best nearly a Rayleigh quotient, and then the existing body of theory left too many questions unanswered.

In 1967, Kahan [6] answered several of those questions with the following theorem, whose proof was first published in 1980 in Parlett [9, pp. 229–233] and which was extended in 1982 to compact self-adjoint operators by Davis, Kahan, and Weinberger [4].

THEOREM 1 (Kahan). *Let the $n \times n$ Hermitian matrix A have eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_n$, let the $k \times k$ Hermitian matrix H have eigenvalues $\mu_1 \le \mu_2 \le \cdots \le \mu_k$, and let Q be an $n \times k$ matrix having full column rank, so $1 \le k \le n$. Then there exist k eigenvalues $\lambda_{i_1} \le \lambda_{i_2} \le \cdots \le \lambda_{i_k}$ of A such that*

$$\max_{1 \le j \le k} |\mu_j - \lambda_{i_j}| \le \frac{c}{\sigma_{\min}(Q)} \|AQ - QH\|_2, \tag{1}$$

where $\sigma_{\min}(Q)$ is the smallest singular value of Q, i.e.,

$$\sigma_{\min}(Q) \stackrel{\text{def}}{=} \sqrt{\textit{the smallest eigenvalue of } Q^*Q};$$

and the constant $c \le \sqrt{2}$. Here eigenvalues are counted according to multiplicity.

In some special cases, as when $k = 1$ or $k = n$, or when $Q^*Q = I_k$, or when all eigenvalues of H are sufficiently well separated, Kahan also showed that $c = 1$. He conjectured that $c = 1$ always. In this short paper, we are going to show that this is indeed true. We will prove the following theorem:

THEOREM 2. $c = 1$ *always in Theorem* 1.

By taking $k = n$ and $Q = I_n$, one can see that this theorem is actually a generalization of the Weyl-Lidskii theorem [9, p. 191].

When the theory is properly stated, it takes multiple eigenvalues and multiple approximations in its stride. When we say that there are k eigenvalues of A being approximated by the k μ_j's in Theorem 1, there is no requirement that either λ_{i_j}'s or μ_j's be distinct. In the language of computer science, these quantities are variables, not values. In the argument of this paper care has been taken not to assume that the values of any of these variables are distinct.

The proof of Theorem 2 needs the following two lemmas.

LEMMA 3. *Partition a matrix X as*

$$X = \begin{pmatrix} X_1 \\ X_2 \end{pmatrix}.$$

If the rank of X exceeds the number of rows of X_1, then $\|X_2\|_2 \geq \sigma_{\min}(X)$.

Proof. The rank of the matrix

$$\begin{pmatrix} X_1 \\ X_2 \end{pmatrix} - \begin{pmatrix} 0 \\ X_2 \end{pmatrix} = \begin{pmatrix} X_1 \\ 0 \end{pmatrix}$$

is no bigger than the number of rows of X_1, which is less than the rank of X. This means that the perturbation $\left(\begin{smallmatrix} 0 \\ X_2 \end{smallmatrix}\right)$ lowers the rank of X by at least 1; therefore [5, Theorem 2.5.2, p. 73]

$$\|X_2\|_2 = \left\| \begin{pmatrix} 0 \\ X_2 \end{pmatrix} \right\|_2 \geq \sigma_{\min}(X),$$

as required. ∎

LEMMA 4 (Davis-Kahan). *Let M and W be two Hermitian matrices. Suppose there are two disjoint intervals, each of width at least $\eta > 0$ and containing no eigenvalues of either matrix, between which intervals lie all the eigenvalues of one matrix and none of the other. Let S be a complex matrix with suitable dimensions. Then there is a unique solution X to the matrix equation $MX - XW = S$, and moreover $\eta\|X\|_2 \leq \|S\|_2$.*

The proof of this lemma can be found in [3, Theorem 5.1], and [10, Lemma 3.5, p. 251] as well.

Proof of Theorem 2. For any unitary U and V, the substitutions

$$A \leftarrow U^*AU, \qquad H \leftarrow V^*HV, \quad \text{and} \quad Q \leftarrow U^*QV \tag{2}$$

leave the theorem unchanged, so we may assume without loss of generality that

$$A = \operatorname{diag}(\lambda_1, \lambda_2, \ldots, \lambda_n) \quad \text{and} \quad H = \operatorname{diag}(\mu_1, \mu_2, \ldots, \mu_k),$$

and $\mu_1 \le \mu_2 \le \cdots \le \mu_k$. (For reasons that will be clear soon, we do not put the λ_j's in increasing order.) In what follows we will prove the theorem for diagonal A and H by induction. When $k = 1$, $\|Q\|_2 = \sigma_{\min}(Q)$ and

$$\|AQ - QH\|_2 = \|(A - \mu_1 I)Q\|_2 \ge \min_{1\le j\le n} |\lambda_j - \mu_1| \, \|Q\|_2,$$

as was to be shown.

Next assume $c = 1$ holds for $k \le m < n$. We have to show that it also holds for $k = m+1$. We use a MATLAB-like notation $X_{i:j}$ for the submatrix of X consisting of its ith to jth columns. Set $R = AQ - QH$; then it is easy to see that

$$\begin{aligned} R_{1:m} &= AQ_{1:m} - Q_{1:m}\,\mathrm{diag}(\mu_1, \dots, \mu_m), \\ R_{2:m+1} &= AQ_{2:m+1} - Q_{2:m+1}\,\mathrm{diag}(\mu_2, \dots, \mu_{m+1}). \end{aligned}$$

Notice that $\sigma_{\min}(Q) \le \sigma_{\min}(Q_{1:m})$ and $\sigma_{\min}(Q) \le \sigma_{\min}(Q_{2:m+1})$ because

$$Q^*Q = \begin{pmatrix} Q_{1:m}^* Q_{1:m} & * \\ * & * \end{pmatrix} = \begin{pmatrix} * & * \\ * & Q_{2:m+1}^* Q_{2:m+1} \end{pmatrix}.$$

So the induction hypothesis implies that there are m eigenvalues

$$\alpha_1 \le \alpha_2 \le \cdots \le \alpha_m$$

of A such that

$$\max_{1\le j\le m} |\mu_j - \alpha_j| \le \frac{\|R_{1:m}\|_2}{\sigma_{\min}(Q_{1:m})} \le \frac{\|R\|_2}{\sigma_{\min}(Q)}, \tag{3}$$

and there are also m eigenvalues

$$\beta_1 \le \beta_2 \le \cdots \le \beta_m \tag{4}$$

of A such that

$$\max_{1\le j\le m} |\mu_{j+1} - \beta_j| \le \frac{\|R_{2:m+1}\|_2}{\sigma_{\min}(Q_{2:m+1})} \le \frac{\|R\|_2}{\sigma_{\min}(Q)}. \tag{5}$$

At this point there are two possible lines of argument. One line shows that there is no loss of generality in assuming that $\alpha_i \le \beta_i$, $i = 1, 2, \dots, m$, as intuition suggests, and then considers the cardinality of $\{\alpha_i\}_{i=1}^m \cup \{\beta_i\}_{i=1}^m$. However, the following second argument seems shorter.

This argument breaks into two cases. In the first case, there exists an integer L $(1 \le L \le m)$ such that $\alpha_L < \beta_L$. In this case, we pair α_i with μ_i for $i = 1, 2, \dots, L$, and pair β_{j-1} with μ_j for $j = L+1, L+2, \dots, m+1$. By (3) and (5) the desired bound holds for all $m+1$ pairs.

On the other hand, in the second case $\alpha_j \geq \beta_j$ for all $j = 1, 2, \ldots, m$. In this case, the set $\{\beta_i\}_{i=1}^m$ can be replaced by $\{\alpha_i\}_{i=1}^m$ without violating any of the conditions (4) and (5). To confirm this, apply the Weyl-Lidskii theorem to the two 2×2 matrices

$$\begin{pmatrix} \mu_{j+1} & \\ & \mu_j \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \beta_j & \\ & \alpha_j \end{pmatrix},$$

whose difference is bounded in norm $\|\cdot\|_2$ by $\|R\|_2/\sigma_{\min}(Q)$, according to (3) and (5), so their ordered eigenvalues differ by no more than that; in particular,

$$|\mu_{j+1} - \alpha_j| \leq \frac{\|R\|_2}{\sigma_{\min}(Q)}. \tag{6}$$

Thus, in the second case we have found m ordered eigenvalues α_j of A that are all approximated within $\pm\|R\|_2/\sigma_{\min}(Q)$ by either the first m or the last m of the $m+1$ ordered μ_j's. What remains is to find one more eigenvalue γ of A approximated at least as well by at least one of the μ_j's.

Without loss of generality, we may suppose that $\alpha_1, \alpha_2, \ldots, \alpha_m$ occupy the first m positions on the diagonal of A, which may then be written

$$A = \operatorname{diag}(\alpha_1, \alpha_2, \ldots, \alpha_m) \oplus \widetilde{A}$$

to define $\widetilde{A}$. The γ we seek will be an eigenvalue of $\widetilde{A}$. Now the proof breaks into two subcases (I) and (II) according to whether γ lies between μ_1 and μ_{m+1} or not.

Subcase (I): $\widetilde{A}$ has at least one eigenvalue γ of A between μ_1 and μ_{m+1} inclusive. We shall find a place to insert γ among the α_j's. For this purpose we assign $\alpha_0 = -\infty$ and $\alpha_{m+1} = +\infty$, so that an index J must exist satisfying

$$\alpha_J \leq \gamma \leq \alpha_{J+1}. \tag{7}$$

Whether either or neither or both of the last inequalities are strict does not matter; recall what was said about multiple eigenvalues just after the statement of Theorem 2. From (7) and $(3)_{j=J+1}$ and $(6)_{j=J}$ we infer that

$$|\mu_{J+1} - \gamma| \leq \frac{\|R\|_2}{\sigma_{\min}(Q)}.$$

Consequently, the two diagonal matrices

$$\begin{aligned} &\operatorname{diag}(\alpha_1, \alpha_2, \ldots, \alpha_J) \oplus \quad \gamma \quad \oplus \operatorname{diag}(\alpha_{J+1}, \alpha_{J+2}, \ldots, \alpha_m), \\ &\operatorname{diag}(\mu_1, \mu_2, \ldots, \mu_J) \oplus \mu_{J+1} \oplus \operatorname{diag}(\mu_{J+2}, \mu_{J+3}, \ldots, \mu_{m+1}) \end{aligned}$$

have their elements in order, and corresponding elements different by at most $\|R\|_2/\sigma_{\min}(Q)$, as claimed.

Subcase (II): $\widetilde{A}$ has no eigenvalue between μ_1 and μ_{m+1} inclusive, so there must be some $\eta > 0$ such that $\widetilde{A}$ has an eigenvalue at one of $\mu_1 - \eta$ or $\mu_{m+1} + \eta$, or at both, but not between them. This η will play a role in our proof analogous to its role in Lemma 4.

Just as $\widetilde{A}$ is obtained by deleting the leading m rows and columns of A, obtain $\widetilde{Q}$ from Q and $\widetilde{R}$ from R by deleting m leading rows. Then the equation $R = AQ - QH$ implies $\widetilde{R} = \widetilde{A}\widetilde{Q} - \widetilde{Q}H$. Since the spectra of $\widetilde{A}$ and H are now separated by η, Lemma 4 implies that

$$\begin{aligned} \eta\|\widetilde{Q}\|_2 &\le \|\widetilde{R}\|_2, \\ &\le \|R\|_2 \end{aligned}$$

because $\widetilde{R}$ is a submatrix of R. Moreover, Lemma 3 implies $\|\widetilde{Q}\|_2 \ge \sigma_{\min}(Q)$ because Q has rank $m+1$, which exceeds the number m of rows deleted to produce $\widetilde{Q}$. Therefore

$$\eta \le \frac{\|\widetilde{R}\|_2}{\|\widetilde{Q}\|_2} \le \frac{\|R\|_2}{\sigma_{\min}(Q)}.$$

Now if $\gamma = \mu_1 - \eta$ is an eigenvalue of $\widetilde{A}$, and hence of A, pair γ with μ_1 and α_i with μ_{i+1} for $i = 1, 2, \ldots, m$. Otherwise $\gamma = \mu_{m+1} + \eta$ is an eigenvalues of $\widetilde{A}$, and hence of A, which we pair with μ_{m+1}, and α_i with μ_i for $i = 1, 2, \ldots, m$. Either way, we have found $m+1$ ordered eigenvalues of A that differ from their counterparts of H no more than claimed.

This completes the induction step from $k = m$ to $k = m+1$, and thus confirms Theorem 2 for every $k \le n$. ∎

Let us conclude this paper with a few remarks on possible improvements of Theorem 2 and on recent developments related to Rayleigh quotients.

REMARK 1. An improvement of Theorem 2 of immediate practical value would be a reduction in the right-hand side of (1). In the absence of information about the provenance of H, no such reduction is possible, as can be seen from simple examples with $k = 1$. On the other hand, if $Q^*Q \approx I$ and $H \approx Q^*AQ$ closely enough, and if all but k of A's eigenvalues differ from every one of H's by at least $\eta > \|AQ - QH\|_2$, then (1) can be reduced to something of the order of

$$\frac{\|AQ - QH\|_2^2}{\eta}.$$

To achieve so dramatic a reduction requires techniques like those used by N. J. Lehmann as explained in [9, pp. 198–202] or techniques used by Stewart and Sun in [10, pp. 254–257] and in [11]. In [11, Corollary 3.4] it is proved that

> if $Q^*Q = I$ and $H = Q^*AQ$, and there is a number $\eta > 0$ such that either all but k of A's eigenvalues lie outside the open interval $(\mu_1 - \eta, \mu_k + \eta)$ or all but k of A's eigenvalues lie inside the closed interval $[\mu_L + \eta, \mu_{L+1} - \eta]$ for some $1 \le L \le k-1$, and $\epsilon \stackrel{\text{def}}{=} \|AQ - QH\|_2/\eta < 1$, (8)

then

$$\max_{1\le j\le k} |\mu_j - \lambda_{i_j}| \le \frac{\|AQ - QH\|_2^2}{\eta\sqrt{1-\epsilon^2}}. \tag{9}$$

REMARK 2. Another improvement of some theoretical interest uses some other functions in place of the "max" in (1) with $c = 1$. For instance, in [6], Kahan proved that

$$\sqrt{\sum_{j=1}^{k} (\mu_k - \lambda_{i_j})^2} \le \frac{\|AQ - QH\|_F}{\sigma_{\min}(Q)}, \tag{10}$$

where $\|Z\|_F^2 \stackrel{\text{def}}{=} \operatorname{trace}(Z^*Z)$ is the sum of the squares of Z's singular values. Moreover, for the same reason as described in Remark 1, (10) is improvable provided sufficient information about H is available. In [11, Corollary 3.5] it is proved that

> if $Q^*Q = I$ and $H = Q^*AQ$, and all but k of A's eigenvalues differ from every one of H's by at least $\eta > 0$ and $\epsilon_F \stackrel{\text{def}}{=} \|AQ - QH\|_F/\eta < 1$, (11)

then

$$\sqrt{\sum_{j=1}^{k} (\mu_k - \lambda_{i_j})^2} \le \frac{\|AQ - QH\|_F^2}{\eta\sqrt{1-\epsilon_F^2}}. \tag{12}$$

We caution the reader to notice that the conditions (11) allow eigenvalues to interlace arbitrarily whereas (8) do not.

REMARK 3. As to more general unitarily invariant norms, Theorem IV.4.14 in [10] provides one kind of generalization which says if $Q^*Q = I$

and $H = Q^*AQ$, then

$$|||\mathrm{diag}(\mu_1 - \lambda_{i_1}, \mu_2 - \lambda_{i_2}, \ldots, \mu_k - \lambda_{i_k})||| \le 2\,|||AQ - QH|||\,,$$

where $|||\cdot|||$ denotes any unitarily invariant norm. Under stronger conditions (8), Sun [11, Corollary 3.4] shows

$$|||\mathrm{diag}(\mu_1 - \lambda_{i_1}, \mu_2 - \lambda_{i_2}, \ldots, \mu_k - \lambda_{i_k})||| \le \frac{|||AQ - QH|||\ \|AQ - QH\|_2}{\eta\sqrt{1-\epsilon^2}}. \tag{13}$$

In proving (13) Sun [11] relied on a $\sin\theta$ theorem from Davis and Kahan [3], which is why, the conditions (8) come in. Along similar lines, if we use a $\sin\theta$ theorem from Bhatia, Davis, and McIntosh [2], we will get a bound a little bit weaker than (13) but under weaker conditions like (11). One can prove that

> if $Q^*Q = I$ and $H = Q^*AQ$, and all but k of A's eigenvalues differ from every one of H's by at least $\eta > 0$ and $\epsilon \stackrel{\mathrm{def}}{=} \|AQ - QH\|_2/\eta < 1$, (14)

then

$$|||\mathrm{diag}(\mu_1 - \lambda_{i_1}, \mu_2 - \lambda_{i_2}, \ldots, \mu_k - \lambda_{i_k})||| \le \widehat{c}\ \frac{|||AQ - QH|||\ \|AQ - QH\|_2}{\eta\sqrt{1-\epsilon^2}},$$

where the constant

$$\widehat{c} \le \frac{\pi}{2}\int_0^{\pi} \frac{\sin\xi}{\xi}\,d\xi < 2.91 \qquad [1].$$

This inequality appears to be new, and a proof can be obtained from the third author.

REMARK 4. More generalizations of Theorem 2, which are of purely theoretical interest, are due to Liu and Xu [8], Sun [11], and Li [7], who assume that bounds upon the angles between the subspace spanned by the column vectors of Q and a k-dimensional invariant space of A are available.

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