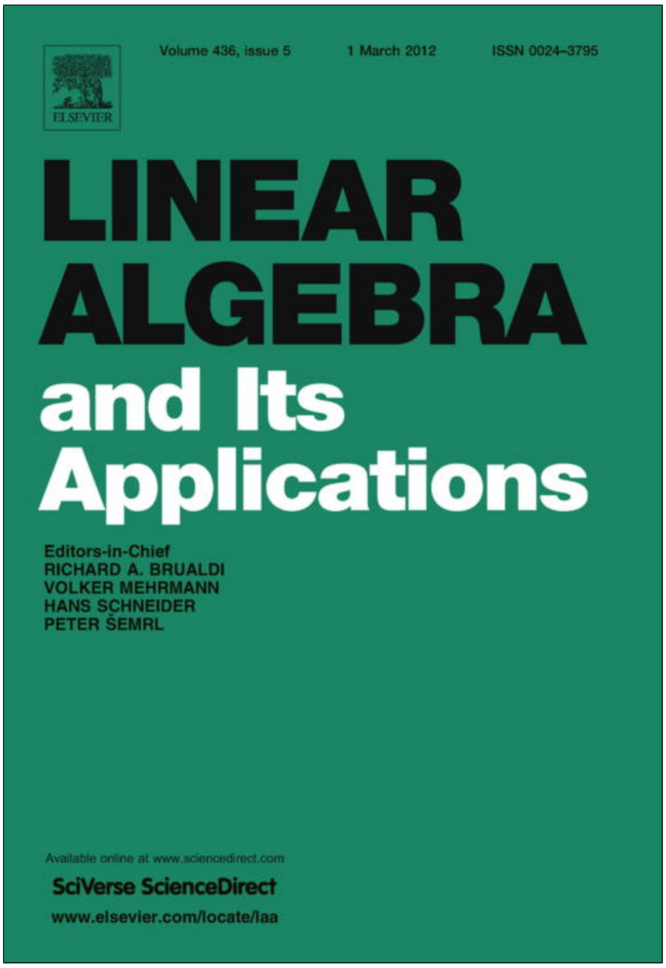
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The tan θ theorem with relaxed conditions

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ABSTRACT

The Davis–Kahan tan θ theorem bounds the tangent of the angles between an approximate and an exact invariant subspace of a Hermitian matrix. When applicable, it gives a sharper bound than the sin θ theorem. However, the tan θ theorem requires more restrictive conditions on the spectrums, demanding that the entire approximate eigenvalues (Ritz values) lie above (or below) the set of exact eigenvalues corresponding to the orthogonal complement of the invariant subspace. In this paper we show that the conditions of the tan θ theorem can be relaxed, in that the same bound holds even when the Ritz values lie both below and above the exact eigenvalues, but not vice versa.

1. Introduction

The tan θ theorem is one of the four main results in the classical and celebrated paper by Davis and Kahan [2]. Along with the other three theorems, it is a useful tool for examining the quality of a computed approximate eigenspace.

The statement of the tan θ theorem is as follows. Let A be an n-by-n Hermitian matrix, and let $X = [X_1\ X_2]$ where $X_1 \in \mathbb{C}^{n\times k}$ be an exact unitary eigenvector matrix of A so that $X^HAX = \mathrm{diag}(\Lambda_1, \Lambda_2)$ is diagonal. Also let $Q_1 \in \mathbb{C}^{n\times k}$ be an orthogonal matrix $Q_1^HQ_1 = I_k$, and define the residual matrix

$$R = AQ_1 - Q_1A_1, \quad \text{where} \quad A_1 = Q_1^HAQ_1. \tag{1}$$

The eigenvalues of A_1 are called the Ritz values with respect to Q_1. Suppose that the Ritz values $\lambda(A_1)$ lie entirely above (or below) $\lambda(\Lambda_2)$, the exact eigenvalues corresponding to X_2. Specifically, suppose that there exists $\delta > 0$ such that $\lambda(A_1)$ lies entirely in $[\beta, \alpha]$ while $\lambda(\Lambda_2)$ lies entirely in $[\alpha + \delta, \infty)$,

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or in $(-\infty, \beta - \delta]$. Then, the $\tan\theta$ theorem gives an upper bound for the tangents of the canonical angles between Q_1 and X_1,

$$\| \tan \angle(Q_1, X_1)\| \leqslant \frac{\|R\|}{\delta}, \tag{2}$$

where $\|\cdot\|$ denotes any unitarily invariant norm. $\tan \angle(Q_1, X_1)$ is the matrix whose singular values are the tangents of the k canonical angles between the n-by-k orthogonal matrices Q_1 and X_1.

The $\sin\theta$ theorem, on the other hand, asserts the same bound, but in terms of the sine instead of tangent:

$$\| \sin \angle(Q_1, X_1)\| \leqslant \frac{\|R\|}{\delta}. \tag{3}$$

An important practical use of the $\tan\theta$ and $\sin\theta$ theorems is to assess the quality of an approximation to the partial eigenpairs (Λ_1, X_1) of a large Hermitian matrix A. A typical algorithm generates a subspace Q_1 designed to approximate X_1, then performs the Rayleigh–Ritz method, see for example [1,5]. We thus have for a unitary matrix $Q = [Q_1\ Q_2]$

$$(\widetilde{A} =)\ Q^H A Q = \begin{bmatrix} A_1 & \widetilde{R}^H \\ \widetilde{R} & A_2 \end{bmatrix}, \tag{4}$$

in which A, Q_1 and A_1 are known. Note that $\|\widetilde{R}\|$ can be computed because $\|\widetilde{R}\| = \|AQ_1 - Q_1 A_1\| = \|R\|$ for any unitarily invariant norm. With some additional information on a bound for δ, we can examine the nearness of the two subspaces spanned by Q_1 and X_1 by using (2) or (3).

Let us compare the $\tan\theta$ theorem (2) and the $\sin\theta$ theorem (3). (2) is clearly sharper than (3), because $\tan\theta \geqslant \sin\theta$ for any $0 \leqslant \theta < \frac{\pi}{2}$. In particular, for the spectral norm, when $\|R\|_2 > \delta$ (3) is useless but (2) still provides nontrivial information.

However, the $\sin\theta$ theorem holds more generally than the $\tan\theta$ theorem in two respects. First, the bound (3) holds with A_1 replaced with any k-by-k Hermitian matrix M (the choice affects δ) and R replaced with $AQ_1 - Q_1 M$. The $\tan\theta$ theorem takes $M = Q_1^H A Q_1$, which is a special but important choice because it arises naturally in practice as described above, and it is optimal in the sense that it minimizes $\|R\|$ for any unitarily invariant norm [9, p. 252].

Second, and more importantly for the discussion in this paper, the hypothesis on the situation of the spectrums of A_1 and Λ_2 is less restrictive in the $\sin\theta$ theorem, allowing the Ritz values $\lambda(A_1)$ to lie on both sides of the exact eigenvalues $\lambda(\Lambda_2)$ corresponding to X_2, or vise versa. Specifically, in addition to the situation described above, the bound (3) holds also in either of the two cases:

1. $\lambda(\Lambda_2)$ lies in $[a, b]$ and $\lambda(A_1)$ lies in the *union* of $(-\infty, a-\delta]$ and $[b+\delta, \infty)$.
2. $\lambda(A_1)$ lies in $[a, b]$ and $\lambda(\Lambda_2)$ lies in the *union* of $(-\infty, a-\delta]$ and $[b+\delta, \infty)$.

We note that in the literature these two cases have not been treated separately. In particular, as discussed above, the original $\tan\theta$ theorem imposes the Ritz values $\lambda(A_1)$ to lie entirely above (or below) the eigenvalues $\lambda(\Lambda_2)$, allowing neither of the two cases.

The goal of this paper is to show that the condition in the $\tan\theta$ theorem can be relaxed by proving that the bound (2) still holds true in the first (but not in the second) case above. In other words, the conclusion of the $\tan\theta$ theorem is valid even when the Ritz values $\lambda(A_1)$ lie both below and above the exact eigenvalues $\lambda(\Lambda_2)$.

We will also revisit the counterexample described in [2] that indicates the restriction on the spectrums is necessary in the $\tan\theta$ theorem. This does not contradict our result because, as we will see, its situation corresponds to the second case above. Finally, we extend the result to the generalized $\tan\theta$ theorem, in which the dimensions of Q_1 and X_1 are allowed to be different.

Notations: $\sigma_1(X) \geqslant \cdots \geqslant \sigma_n(X)$ are the singular value of a general matrix $X \in \mathbb{C}^{m\times n}$, and $\sigma_{\max}(X) = \sigma_1(X)$ and $\sigma_{\min}(X) = \sigma_n(X)$. $\|\cdot\|$ denotes any unitarily invariant norm, $\|X\|_2 = \sigma_{\max}(X)$

the spectral norm and $\|X\|_F = \sqrt{\sum_{i,j} X_{ij}^2}$ the Frobenius norm. $\lambda(A)$ denotes the spectrum, or the set of eigenvalues of a square matrix A.

2. The $\tan\theta$ theorem under a relaxed condition on the spectrums

2.1. Preliminaries

We first prove a lemma that we use in the proof of our main result.

Lemma 2.1. *Let $X \in \mathbb{C}^{m\times n}$, $Y \in \mathbb{C}^{n\times r}$, $Z \in \mathbb{C}^{r\times s}$ have the singular value decompositions $X = U_X\Sigma_X V_X^H$, $Y = U_Y\Sigma_Y V_Y^H$ and $Z = U_Z\Sigma_Z V_Z^H$, where the singular values are arranged in descending order. Then for any unitarily invariant norm $\|\cdot\|$,*

$$\|XYZ\| \leqslant \|Y\|_2\|\widetilde{\Sigma}_X\widetilde{\Sigma}_Z\|, \tag{5}$$

where $\widetilde{\Sigma}_X = diag(\sigma_1(X), \ldots, \sigma_p(X))$, $\widetilde{\Sigma}_Z = diag(\sigma_1(Z), \ldots, \sigma_p(Z))$ are diagonal matrices of the p largest singular values where $p = \min\{m, n, r, s\}$. Moreover, analogous results hold for any combination of $\{X, Y, Z\}$, that is, $\|XYZ\| \leqslant \|X\|_2\|\widetilde{\Sigma}_Y\widetilde{\Sigma}_Z\|$ and $\|XYZ\| \leqslant \|Z\|_2\|\widetilde{\Sigma}_X\widetilde{\Sigma}_Y\|$.

Proof. In the majorization property of singular values of a matrix product $\sum_{i=1}^k \sigma_i(AB) \leqslant \sum_{i=1}^k \sigma_i(A)\sigma_i(B)$ for all $k = 1, \ldots, p$ [4, p. 177], we let $A := X$ and $B := YZ$ to get

$$\begin{aligned}\sum_{i=1}^k \sigma_i(XYZ) &\leqslant \sum_{i=1}^k \sigma_i(X)\sigma_i(YZ)\\ &\leqslant \sum_{i=1}^k \sigma_i(X)\sigma_i(Z)\|Y\|_2\\ &= \|Y\|_2\sum_{i=1}^k \sigma_i(\Sigma_X\Sigma_Z) \quad \text{for} \quad k = 1, \ldots, p.\end{aligned}$$

(5) now follows from Ky-Fan's theorem [3, p. 445]. A similar argument proves the inequality for the other two combinations. $\square$

We next recall the CS decomposition [6,8], which states that for any unitary matrix Q and its 2-by-2 partition $Q = \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22}\end{bmatrix}$ where $Q_{11} \in \mathbb{C}^{k\times\ell}$, there exist $U_1 \in \mathbb{C}^{k\times k}$, $U_2 \in \mathbb{C}^{(n-k)\times(n-k)}$, $V_1 \in \mathbb{C}^{\ell\times\ell}$ and $V_2 \in \mathbb{C}^{(n-\ell)\times(n-\ell)}$ such that

$$\begin{bmatrix} U_1 & 0 \\ 0 & U_2\end{bmatrix}^H \begin{bmatrix} Q_{11} & Q_{12} \\ Q_{21} & Q_{22}\end{bmatrix}\begin{bmatrix} V_1 & 0 \\ 0 & V_2\end{bmatrix} = \left[\begin{array}{ccc|ccc} I & & & 0 & & \\ & C & & & -S & \\ & & 0 & & & I \\ \hline 0 & & & I & & \\ & S & & & C & \\ & & I & & & 0 \end{array}\right]. \tag{6}$$

The blank submatrices are all zeros, and the zero matrices shown in (6) are not necessarily square and may be empty.

Applied to the unitary matrix $W = Q^H X = \begin{bmatrix} Q_1^H X_1 & Q_1^H X_2 \\ Q_2^H X_1 & Q_2^H X_2 \end{bmatrix}$, the CS decomposition states that there exist unitary matrices $U_1 \in \mathbb{C}^{k\times k}$, $U_2 \in \mathbb{C}^{(n-k)\times(n-k)}$, $V_1 \in \mathbb{C}^{k\times k}$ and $V_2 \in \mathbb{C}^{(n-k)\times(n-k)}$ such that $\begin{bmatrix} U_1 & 0 \\ 0 & U_2 \end{bmatrix}^H W \begin{bmatrix} V_1 & 0 \\ 0 & V_2 \end{bmatrix}$ can be expressed as $\left[\begin{array}{c|cc} C & 0 & -S \\ \hline 0 & I_{n-2k} & 0 \\ S & 0 & C \end{array}\right]$ when $k < \frac{n}{2}$, $\begin{bmatrix} C & -S \\ S & C \end{bmatrix}$ when $k = \frac{n}{2}$, and $\left[\begin{array}{cc|c} I_{2k-n} & 0 & 0 \\ 0 & C & -S \\ \hline 0 & S & C \end{array}\right]$ when $k > \frac{n}{2}$, where $C = \mathrm{diag}(\cos\theta_1, \dots, \cos\theta_p)$ and $S = \mathrm{diag}(\sin\theta_1, \dots, \sin\theta_p)$, in which $p = \min\{k, n-k\}$. The nonnegative quantities $\theta_1 \leqslant \cdots \leqslant \theta_p$ are the canonical angles between Q_1 and V_1. Note that they are also the canonical angles between Q_2 and V_2.

2.2. Main result

We now prove the $\tan\theta$ theorem under a relaxed condition.

Theorem 1. *Let $A \in \mathbb{C}^{n\times n}$ be a Hermitian matrix and let $X = [X_1\ X_2]$ be its unitary eigenvector matrix so that $X^H AX = \mathrm{diag}(\Lambda_1, \Lambda_2)$ is diagonal where X_1 and Λ_1 have k columns. Let $Q_1 \in \mathbb{C}^{n\times k}$ be orthogonal, and let $R = AQ_1 - Q_1 A_1$, where $A_1 = Q_1^H A Q_1$. Suppose that $\lambda(\Lambda_2)$ lies in $[a, b]$ and $\lambda(A_1)$ lies in the union of $(-\infty, a-\delta]$ and $[b+\delta, \infty)$. Then*

$$\|\tan\angle(Q_1, X_1)\| \leqslant \frac{\|R\|}{\delta}. \tag{7}$$

Proof. Note that $W = Q^H X$ is the unitary eigenvector matrix of $\widetilde{A} = Q^H AQ = \begin{bmatrix} A_1 & \widetilde{R}^H \\ \widetilde{R} & A_2 \end{bmatrix}$ as in (4). Partition $W = \begin{bmatrix} Q_1^H X_1 & Q_1^H X_2 \\ Q_2^H X_1 & Q_2^H X_2 \end{bmatrix} = [W_1\ W_2]$, so that the columns of W_2 are the eigenvectors of $\widetilde{A}$ corresponding to $\lambda(\Lambda_2)$. Further partition $W_2 = \begin{bmatrix} Q_1^H X_2 \\ Q_2^H X_2 \end{bmatrix} = \begin{bmatrix} W_2^{(1)} \\ W_2^{(2)} \end{bmatrix}$ so that $W_2^{(1)}$ is k-by-$(n-k)$. The first k rows of $\widetilde{A}W_2 = W_2\Lambda_2$ is

$$A_1 W_2^{(1)} + \widetilde{R}^H W_2^{(2)} = W_2^{(1)}\Lambda_2,$$

which is equivalent to

$$A_1 W_2^{(1)} - W_2^{(1)}\Lambda_2 = -\widetilde{R}^H W_2^{(2)}. \tag{8}$$

For definiteness we discuss the case $k \leqslant \frac{n}{2}$. The case $k > \frac{n}{2}$ can be treated with few modifications. By the CS decomposition we know that there exist unitary matrices $U_1 \in \mathbb{C}^{k\times k}$, $U_2 \in \mathbb{C}^{(n-k)\times(n-k)}$ and $V \in \mathbb{C}^{(n-k)\times(n-k)}$ such that $W_2^{(1)} = U_1\widetilde{S}V^H$ and $W_2^{(2)} = U_2\widetilde{C}V^H$, where $\widetilde{C} = \mathrm{diag}(I_{n-2k}, C) \in \mathbb{C}^{(n-k)\times(n-k)}$, $\widetilde{S} = [0_{k,n-2k}\ \ -S] \in \mathbb{C}^{k\times(n-k)}$ in which $C = \mathrm{diag}(\cos\theta_1, \dots, \cos\theta_k)$ and $S = \mathrm{diag}(\sin\theta_1, \dots, \sin\theta_k)$. Hence we can express (8) as

$$A_1 U_1\widetilde{S}V^H - U_1\widetilde{S}V^H\Lambda_2 = -\widetilde{R}^H U_2\widetilde{C}V^H. \tag{9}$$

We claim that $\widetilde{C}$ is nonsingular. To see this, suppose on the contrary that there exists i such that $\cos\theta_i = 0$, which makes $\widetilde{C}$ singular. Defining $j = n - 2k + i$ this means $W_2^{(2)}Ve_j = 0$ where e_j is the jth column of I_{n-k}, so the jth column of $W_2^{(2)}V$ is all zero.

Now, by $\widetilde{A}W_2 = W_2\Lambda_2$ we have $\widetilde{A}W_2V = W_2V(V^H\Lambda_2V)$. Taking the jth column yields

$$\widetilde{A}W_2Ve_j = W_2V(V^H\Lambda_2V)e_j.$$

Since W_2Ve_j is nonzero only in its first k elements, we get

$$\begin{bmatrix} A_1 \\ \widetilde{R} \end{bmatrix} W_2^{(1)}Ve_j = W_2V(V^H\Lambda_2V)e_j,$$

the first k elements of which is

$$A_1W_2^{(1)}Ve_j = W_2^{(1)}V(V^H\Lambda_2V)e_j.$$

Now define $v = W_2^{(1)}Ve_j$ and let $\gamma = (a+b)/2$. Subtracting γv we get

$$(A_1 - \gamma I)v = W_2^{(1)}V(V^H(\Lambda_2 - \gamma I)V)e_j.$$

Defining $\widehat{A}_1 = A_1 - \gamma I$ and $\widehat{\Lambda}_2 = \Lambda_2 - \gamma I$ and taking the spectral norm we get

$$\|\widehat{A}_1v\|_2 = \|W_2^{(1)}\widehat{\Lambda}_2Ve_j\|_2.$$

Note by assumption that defining $c = \frac{1}{2}(b-a)$ the eigenvalues of $\widehat{\Lambda}_2$ lie in $[-c, c]$ and those of $\widehat{A}_1$ lie in the union of $[c+\delta, \infty)$ and $(-\infty, c-\delta]$, so noting that $\|v\|_2 = \|e_j\|_2 = 1$ and $\|W_2^{(1)}\|_2 = \|\widetilde{C}\|_2 \leqslant 1$, we must have $\sigma_{\min}(\widehat{A}_1) \leqslant \|W_2^{(1)}\widehat{\Lambda}_2Ve_j\|_2 \leqslant \|\widehat{\Lambda}_2\|_2$. However, this contradicts the assumptions, which require $\delta + c < \sigma_{\min}(\widehat{A}_1)$ and $\|\widehat{\Lambda}_2\|_2 \leqslant c$. Therefore we conclude that $\widetilde{C}$ must be invertible.

Hence we can right-multiply $V\widetilde{C}^{-1}$ to (9), which yields

$$\begin{aligned} -\widetilde{R}^HU_2 &= A_1U_1\widetilde{S}V^HV\widetilde{C}^{-1} - U_1\widetilde{S}V^H\Lambda_2V\widetilde{C}^{-1} \\ &= A_1U_1\widetilde{S}\widetilde{C}^{-1} - U_1\widetilde{S}\widetilde{C}^{-1}\cdot(\widetilde{C}V^H\Lambda_2V\widetilde{C}^{-1}). \end{aligned}$$

As above we introduce a "shift" $\gamma = (a+b)/2$ such that

$$\begin{aligned} -\widetilde{R}^HU_2 &= A_1U_1\widetilde{S}\widetilde{C}^{-1} - (\gamma U_1\widetilde{S}\widetilde{C}^{-1} - \gamma U_1\widetilde{S}\widetilde{C}^{-1}) - U_1\widetilde{S}\widetilde{C}^{-1}\cdot(\widetilde{C}V^H\Lambda_2V\widetilde{C}^{-1}) \\ &= (A_1 - \gamma I)U_1\widetilde{S}\widetilde{C}^{-1} - U_1\widetilde{S}\widetilde{C}^{-1}\cdot(\widetilde{C}V^H(\Lambda_2 - \gamma I)V\widetilde{C}^{-1}) \\ &= \widehat{A}_1U_1\widetilde{S}\widetilde{C}^{-1} - U_1\widetilde{S}V^H\widehat{\Lambda}_2V\widetilde{C}^{-1}. \end{aligned}$$

Taking a unitarily invariant norm and using $\|\widetilde{R}\| = \|R\|$ and the triangular inequality yields

$$\begin{aligned} \|R\| &\geqslant \|\widehat{A}_1U_1\widetilde{S}\widetilde{C}^{-1}\| - \|(U_1\widetilde{S})(V^H\widehat{\Lambda}_2V)\widetilde{C}^{-1}\| \\ &\geqslant \sigma_{\min}(\widehat{A}_1)\|\widetilde{S}\widetilde{C}^{-1}\| - \|(U_1\widetilde{S})(V\widehat{\Lambda}_2V^H)\widetilde{C}^{-1}\|. \end{aligned}$$

We now appeal to Lemma 2.1 substituting $X \leftarrow U_1\widetilde{S}$, $Y \leftarrow V^H\widehat{\Lambda}_2V$, $Z \leftarrow \widetilde{C}^{-1}$. In doing so we note that $\widetilde{\Sigma}_X\widetilde{\Sigma}_Z = \mathrm{diag}(\tan\theta_k, \ldots, \tan\theta_1)$ so $\|\widetilde{\Sigma}_X\widetilde{\Sigma}_Z\| = \|SC^{-1}\| = \|\widetilde{S}\widetilde{C}^{-1}\| = \|\tan\angle(Q_1, X_1)\|$, so we get

$$\begin{aligned} \|R\| &\geqslant \sigma_{\min}(\widehat{A}_1)\|SC^{-1}\| - \|V^H\widehat{\Lambda}_2V\|_2\|SC^{-1}\| \\ &= \sigma_{\min}(\widehat{A}_1)\|SC^{-1}\| - \|\widehat{\Lambda}_2\|_2\|SC^{-1}\| \\ &= \|\tan\angle(Q_1, X_1)\|\left(\sigma_{\min}(\widehat{A}_1) - \|\widehat{\Lambda}_2\|_2\right). \end{aligned}$$

Using $\sigma_{\min}(A_1) - \|\Lambda_2\|_2 \geqslant (c+\delta) - c = \delta$, we conclude that

$$\|\tan\angle(Q_1, X_1)\| \leqslant \frac{\|R\|}{\sigma_{\min}(A_1) - \|\Lambda_2\|_2} \leqslant \frac{\|R\|}{\delta}. \quad \square$$

Remarks. Below are two remarks on the $\tan\theta$ theorem with relaxed conditions, Theorem 1.

- Practical situations to which the relaxed theorem is applicable but not the original include the following two cases:

  (i) When extremal (both smallest and largest) eigenpairs are sought, for example by the Lanczos algorithm (e.g., [1,7]). In this case Q_1 tends to approximately contain the eigenvectors corresponding to the largest and smallest eigenvalues of A, so we may directly have the situation in Theorem 1.

  (ii) When internal eigenpairs are sought. In this case the exact (undesired) eigenvalues $\lambda(\Lambda_2)$ lie below and above $\lambda(A_1)$, so Theorem 1 is not applicable. However, if the residual $\|R\|$ is sufficiently small then we must have $\lambda(A_1) \simeq \lambda(\Lambda_1)$ and $\lambda(A_2) \simeq \lambda(\Lambda_2)$, in which case the Ritz values $\lambda(A_2)$ lie both below and above the eigenvalues $\lambda(\Lambda_1)$. We can then invoke Theorem 1 with the subscripts 1 and 2 swapped, see below for an example.

- For the $\tan 2\theta$ theorem we cannot make a similar relaxation in the conditions on the spectrums. Note that in the $\tan 2\theta$ theorem the gap δ is defined as the separation between the two sets of Ritz values $\lambda(A_1)$ and $\lambda(A_2)$ (instead of $\lambda(\Lambda_2)$), so there is no separate situations in which one spectrum lies both below and above the other, unlike in the $\tan\theta$ theorem. To see that in such cases $\frac{\|R\|}{\widetilde{\delta}}$ (where $\widetilde{\delta}$ is the separation between $\lambda(A_1)$ and $\lambda(A_2)$) is not an upper bound of $\|\frac{1}{2}\tan 2\angle(Q_1, X_1)\|$, we consider the example (10) below, in which we have $\frac{\|R\|_2}{\widetilde{\delta}} = \frac{1/\sqrt{2}}{1/\sqrt{2}} = 1$ but $\|\frac{1}{2}\tan 2\angle(Q_1, X_1)\|_2 = \infty$.

The counterexample in [2]. Ref. [2] considers the following example in which the spectrums of A_1 and Λ_2 satisfy the conditions of the $\sin\theta$ theorem but not the original $\tan\theta$ theorem.

$$A = \begin{bmatrix} 0 & 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} & 0 \end{bmatrix}, \quad Q_1 = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}. \tag{10}$$

A has eigenvalues $0, 1, -1$, and the exact angle between Q_1 and the eigenvector $X_1 = [\frac{1}{\sqrt{2}}, \frac{1}{\sqrt{2}}, 0]^T$ corresponding to the zero eigenvalue satisfies $\tan\angle(Q_1, X_1) = 1$. We can also compute $A_1 = 0$ so $\delta = 1$, and $\|R\|_2 = 1/\sqrt{2}$. In this case $\lambda(\Lambda_2) = \{1, -1\}$ lies on both sides of $A_1 = 0$, which violates the assumption in the original $\tan\theta$ theorem. In fact, $\|R\|_2/\delta = 1/\sqrt{2}$ is not an upper bound of $\|\tan\angle(Q_1, X_1)\|_2 = 1$.

Let us now examine (10) in terms of our relaxed $\tan\theta$ theorem, Theorem 1. The above setting does not satisfy the assumption in Theorem 1 either. In particular, the situation between $\lambda(A_1)$ and $\lambda(\Lambda_2)$ corresponds to the second case in the introduction, which the relaxed $\tan\theta$ theorem does not cover. However, in light of the fact $\angle(Q_1, X_1) = \angle(Q_2, X_2)$ for all the p canonical angles, we can attempt to bound $\|\tan\angle(Q_1, X_1)\|$ via bounding $\|\tan\angle(Q_2, X_2)\|$. We have $\lambda(A_2) = \pm\frac{1}{\sqrt{2}}$ and $\lambda(\Lambda_1) = 0$, so the assumptions in Theorem 1 (in which we swap the subscripts 1 and 2) are satisfied with $\delta = 1/\sqrt{2}$. Therefore we can invoke the $\tan\theta$ theorem, and get the correct and sharp bound $\|\tan\angle(Q_2, X_2)\| \leqslant \|R\|/\delta = 1$. We note that the original $\tan\theta$ theorem still cannot be invoked because the assumptions are violated.

2.3. The generalized $\tan\theta$ theorem with relaxed conditions

Ref. [2] also proves the *generalized* $\tan\theta$ theorem, in which the dimension of Q_1 is smaller than that of X_1. Here we show that the same relaxation on the condition can be attained for the generalized $\tan\theta$ theorem. We prove the below theorem, in which X_1 now has $\ell(\geqslant k)$ columns.

Theorem 2. *Let $A \in \mathbb{C}^{n\times n}$ be a Hermitian matrix and let $X = [X_1\ X_2]$ be its unitary eigenvector matrix so that $X^HAX = \mathrm{diag}(\Lambda_1, \Lambda_2)$ is diagonal where X_1 and Λ_1 have $\ell(\geqslant k)$ columns. Let $Q_1 \in \mathbb{C}^{n\times k}$ be orthogonal, and let $R = AQ_1 - Q_1A_1$, where $A_1 = Q_1^HAQ_1$. Suppose that $\lambda(\Lambda_2)$ lies in $[a, b]$ and $\lambda(A_1)$ lies in the union of $(-\infty, a-\delta]$ and $[b+\delta, \infty)$. Then*

$$\|\tan\angle(Q_1, X_1)\| \leqslant \frac{\|R\|}{\delta}. \tag{11}$$

Proof. The proof is almost the same as that for Theorem 1, so we only highlight the differences.

We discuss the case $k \leqslant \ell \leqslant \frac{n}{2}$; other cases are analogous. We partition $W_2 = \begin{bmatrix} Q_1^HX_2 \\ Q_2^HX_2 \end{bmatrix} = \begin{bmatrix} W_2^{(1)} \\ W_2^{(2)} \end{bmatrix}$ where $W_2^{(1)}$ is k-by-$(n-\ell)$. There exist unitary matrices $U_1 \in \mathbb{C}^{k\times k}$, $U_2 \in \mathbb{C}^{(n-k)\times(n-k)}$ and $V \in \mathbb{C}^{(n-\ell)\times(n-\ell)}$ such that $W_2^{(1)} = U_1\widetilde{S}V^H$ and $W_2^{(2)} = U_2\widetilde{C}V^H$, where $\widetilde{C} = \begin{bmatrix} \mathrm{diag}\,(I_{n-k-\ell}, C) \\ 0_{\ell-k,n-\ell} \end{bmatrix} \in \mathbb{C}^{(n-k)\times(n-\ell)}$ and $\widetilde{S} = [0_{k,n-k-\ell}\quad -S] \in \mathbb{C}^{k\times(n-\ell)}$, in which $C = \mathrm{diag}(\cos\theta_1, \ldots, \cos\theta_k)$ and $S = \mathrm{diag}(\sin\theta_1, \ldots, \sin\theta_k)$. We then right-multiply (9) by $\mathrm{diag}\left(I_{n-k-\ell}, C^{-1}\right)$, which yields

$$-\widetilde{R}^HU_2 \begin{bmatrix} I_{n-\ell} \\ 0_{\ell-k,n-\ell} \end{bmatrix} = A_1U_1\widetilde{S}\mathrm{diag}\left(I_{n-k-\ell}, C^{-1}\right) - U_1\widetilde{S}V^H\Lambda_2V\mathrm{diag}\left(I_{n-k-\ell}, C^{-1}\right).$$

Noting that the k largest singular values of $\mathrm{diag}\left(I_{n-k-\ell}, C^{-1}\right)$ are $1/\cos\theta_k, \ldots, 1/\cos\theta_1$ and using Lemma 2.1 we get

$$\begin{aligned} \|R\| &\geqslant \left\| \widetilde{R}^HU_2 \begin{bmatrix} I_{n-\ell} \\ 0_{\ell-k,n-\ell} \end{bmatrix} \right\| \\ &\geqslant \sigma_{\min}(\widehat{A}_1)\|SC^{-1}\| - \|\widehat{\Lambda}_2\|_2\|SC^{-1}\| \\ &= \|\tan\angle(Q_1, X_1)\|\left(\sigma_{\min}(\widehat{A}_1) - \|\widehat{\Lambda}_2\|_2\right), \end{aligned}$$

which is (11). □

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