

Davis-Kahan Theorem

Yutong Wang
London School of Economics

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Davis-Kahan Theorem is about bounding the eigenspace or eigenvectors after the original matrix is perturbed. To understand it, basic knowledge of linear algebra is required.

Here we focus on the Symmetric matrix. Assume $A \in \mathbb{R}^{n \times n}$ is symmetric, where $A+H \in \mathbb{R}^{n \times n}$ is still symmetric (which implies the perturbation H is still symmetric). Thus we have the eigendecomposition:

$$\begin{aligned} A &= \sum_{i=1}^n \lambda_i u_i u_i^*, \\ A+H &= \sum_{i=1}^n \mu_i v_i v_i^*. \end{aligned}$$

We would like to show that if H is ‘small’ (in some sense), then u_i is close to v_i . One of the key concerns is that the order of the spectrum may change after the perturbation. See a typical example:

Example 1. Let $A = \begin{pmatrix} 1 & \varepsilon \\ \varepsilon & 1 \end{pmatrix}$, whose eigenvalues are the roots of equation $(1 - \lambda)^2 - \varepsilon^2 = 0$, i.e., $\lambda_1 = 1 + \varepsilon$, $\lambda_2 = 1 - \varepsilon$.

1 Principal Angles

1.1 Definitions

The Principal angles are defined step by step. First, we could define the principal angle between two vectors; then the principal angle between two lines (lines are 1-D subspaces) can be defined; Next, the definition can be generalised to principal angles between a line and a 2-D subspace; and eventually principal angles between any two sub-spaces (no further assumptions on the dimension of two sub-spaces).

From the process of defining, we could see that the principal angle can be defined in any inner product space. Now let’s consider Euclidean spaces only.

1. **Between vectors.** Assume $x, y \in \mathbb{R}^n$, then the principal angle between them is defined via their as:

$$\Theta_{x,y} := \arccos \frac{x^\top y}{\|x\| \|y\|}.$$

It is worth mentioning that the RHS can take any value between $[-1, 1]$. To cover the range, we allow $\theta_{x,y}$ taking value in $[0, \pi]$. It helps to construct intuition by setting $n = 2$, where all the stuff can be drawn in a 2-D paper.

2. **Between lines.** Assume still $x, y \in \mathbb{R}^n$, We are going to define the principal angle for two subspaces: $\mathbb{R}x := \{ax \mid a \in \mathbb{R}\}$ and $\mathbb{R}y := \{ay \mid a \in \mathbb{R}\}$.

$$\Theta_{\mathbb{R}x, \mathbb{R}y} := \arccos \frac{|x^\top y|}{\|x\| \|y\|} = \inf_{a \in \mathbb{R}, b \in \mathbb{R}} \arccos \frac{|(ax)^\top (by)|}{\|ax\| \|by\|}.$$

Here the infimum does not actually solve any optimisation, since the objective function does not depend on either a or b . However, this expression is convenient for generalisation.

In addition, one can see that $\cos(\theta_{\mathbb{R}x, \mathbb{R}y})$ is always non-negative, thus, allowing $\theta_{\mathbb{R}x, \mathbb{R}y} \in [0, \frac{\pi}{2}]$ is enough to cover all values.

3. **Between a line and a plane (2-D subspace).** Now assume we have a line spanned by $x \in \mathbb{R}^n$, i.e., $\mathbb{R}x = \{ax \mid a \in \mathbb{R}\}$, and a 2-D subspace spanned by vector $y, z \in \mathbb{R}^n$, i.e. $\mathbb{R}\{y, z\} := \{by + cz \mid b, c \in \mathbb{R}\}$. The (minimal) principal angle between the line and the plane is:

$$\Theta_{\mathbb{R}x, \mathbb{R}\{y, z\}}^1 := \inf_{a, b, c \in \mathbb{R}} \arccos \frac{|(ax)^\top (by + cz)|}{\|ax\| \|by + cz\|}.$$

4. **Between any two subspace of \mathbb{R}^n .** Assume the two subspaces \mathcal{E}, \mathcal{F} are spanned by $\{e_1, \dots, e_p\}$ and $\{f_1, \dots, f_q\}$, respectively. WLOG, we could assume $E = (e_1, \dots, e_p) \in \mathbb{R}^{n \times p}$ and $F = (f_1, \dots, f_q) \in \mathbb{R}^{n \times q}$ are matrices consist of two orthonormal basis.¹² By the definition of the basis, we know that any vector in space \mathcal{E} can be expressed as $E\alpha$ for $\alpha \in \mathbb{R}^p$, any vector in space \mathcal{F} can be expressed as $F\beta$ for $\beta \in \mathbb{R}^q$, the (minimal) principal angle between the two subspaces \mathcal{E}, \mathcal{F} is defined as:

$$\begin{aligned}\Theta_{\mathcal{E}, \mathcal{F}}^1 &= \inf_{\|\alpha\|=1, \|\beta\|=1} \arccos \left((E\alpha)^\top (F\beta) \right) \\ &= \inf_{\|\alpha\|=1, \|\beta\|=1} \arccos \left(\alpha^\top E^\top F \beta \right) \\ &= \arccos \sup_{\|\alpha\|=1, \|\beta\|=1} \left(\alpha^\top E^\top F \beta \right) \\ &= \arccos \left(\sigma_{\max}(E^\top F) \right).\end{aligned}$$

The second last step is because $\arccos(\cdot)$ is a decreasing function, and the last step is due to the min-max Theorem - a way to characterise singular values.

Generally, for a p -dimensional space and q -dimensional space, $r = \min\{p, q\}$ number of principal angles are needed to describe their geometric relationship.

1.2 Properties

From the most general definition of principal angles, we have seen that the principal angles between space E and F are related to singular values of the $E^\top F$. The following proposition says that it is actually fully captured by all singular values of $E^\top F$.

Proposition 1. Suppose the columns of $E \in \mathbb{R}^{n \times p}$ and $F \in \mathbb{R}^{n \times q}$ form orthogonal basis for subspaces \mathcal{E}, \mathcal{F} . Let the SVD of $E^\top F$ be $U\Sigma V^\top$, where $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_r)$ where $r = \min\{p, q\}$. Then, the column vector of all principal angles can be characterised as:

$$\Theta_{\mathcal{E}, \mathcal{F}} := \left(\Theta_{\mathcal{E}, \mathcal{F}}^1, \dots, \Theta_{\mathcal{E}, \mathcal{F}}^r \right)^\top = \left(\arccos(\sigma_1), \dots, \arccos(\sigma_r) \right)^\top. \quad (1.1)$$

Remark 1. We know that singular values of $E^\top F$ and $F^\top E$ are the same, thus those $\sigma_1, \dots, \sigma_r$ are also singular values of $F^\top E$. As a consequence, $\Theta_{\mathcal{E}, \mathcal{F}} = \Theta_{\mathcal{F}, \mathcal{E}}$, and such symmetry is the property we expect an ‘angle’ should have before we defining it.

Remark 2. This proposition also shows that the ‘principal angles between subspaces’ are well-defined. Recall that in the general definition, for subspaces \mathcal{E} and \mathcal{F} , we select orthogonal basis E and F respectively, and define the principal angle based on E and F . What if we choose a different pair of orthogonal bases E_2 and F_2 ? Will we get the same value of the principal angle? The proposition tells us: Yes! Because the singular value is unitarily invariant, which says that if we do SVD and get $E^\top F = U\Sigma V$ and $E_2^\top F_2 = U_2\Sigma_2V_2$, then $\Sigma = \Sigma_2$ (up to a permutation of diagonal elements).

An important problem is that, if we know the principal angle between \mathcal{E} and \mathcal{F} , what can we conclude about the principal angles between \mathcal{E} and \mathcal{F}_\perp ? Or the principal angles between \mathcal{E}_\perp and \mathcal{F} ? And that between \mathcal{E}_\perp and \mathcal{F}_\perp ? The next proposition gives the answer.

For better exposition purposes, we use superscripts ‘up arrow’ of a vector x^\uparrow to denote presenting the elements in a vector in ascending order, and also ‘down arrow’ x^\downarrow to denote presenting the elements in descending order.

Proposition 2. Let orthogonal complements of subspaces \mathcal{E} and \mathcal{F} be denoted as \mathcal{E}_\perp and \mathcal{F}_\perp . Then:

¹Check. It is a useful practice to get familiar with linear algebra.

²There is a bit of abuse of notations: E denotes both the basis and the subspace.

1. $[\Theta_{\mathcal{E}, \mathcal{F}}^\downarrow, 0, \dots, 0] = [\Theta_{\mathcal{E}_\perp, \mathcal{F}_\perp}^\downarrow, 0, \dots, 0],$
2. $[\Theta_{\mathcal{E}, \mathcal{F}_\perp}^\downarrow, 0, \dots, 0] = [\Theta_{\mathcal{E}_\perp, \mathcal{F}}^\downarrow, 0, \dots, 0],$
3. $[\frac{\pi}{2}, \dots, \frac{\pi}{2}, \Theta_{\mathcal{E}, \mathcal{F}}^\downarrow] = [\frac{\pi}{2} - \Theta_{\mathcal{E}, \mathcal{F}_\perp}^\uparrow, 0, \dots, 0].$

To prove the proposition, we need several results regarding projections. These contents are in section four.

2 SVD and Eigendecomposition

In this section, we review the definition of the eigenvalue and the singular value. As one way to understand it, eigenvalue is only well-defined for squared matrix, while singular value, as the generalisation, is defined for all matrices.

2.1 Eigendecomposition

Definition 1. For a squared matrix $A \in \mathbb{R}^{n \times n}$, its eigenvalue is defined as the value λ such that there exists a vector $\alpha \in \mathbb{R}^n$ satisfying:

$$A\alpha = \lambda\alpha,$$

the α is called the corresponding eigenvector.

Remark 1. With the view of ‘matrix represents linear operator’, we could think of it as: at the direction of α , the operator becomes simpler to be expressed.

Remark 2. The thought behind eigenvalue decomposition is to ‘simplify’ the matrix, and we always want to find a coordinate such that matrix A is easier. Easy in matrix context can mean ‘diagonal’. The reason

Assumption 1. A has n number of different eigenvalues, $\lambda_1 > \lambda_2 > \dots > \lambda_n$.

This is for sure the simplest but also the most seen case. Assume the corresponding eigenvectors are $\alpha_1, \dots, \alpha_n$, then:

$$A \cdot (\alpha_1, \dots, \alpha_n) = (\alpha_1, \dots, \alpha_n) \cdot \text{diag}(\lambda_1, \dots, \lambda_n).$$

There is a theorem that ensures that eigenvectors of different eigenvalues are linearly independent.

Proposition 3. If λ_1 and λ_2 are two distinct eigenvalues with corresponding eigenvectors α_1 and α_2 , then α_1 and α_2 are linear independent.

Proof. If $a, b \in \mathbb{R}$ such that $a\alpha_1 + b\alpha_2 = \mathbf{0}$, then $\mathbf{0} = A\mathbf{0} = A(a\alpha_1 + b\alpha_2) = a\lambda_1\alpha_1 + b\lambda_2\alpha_2 = \lambda_1(a\alpha_1 + b\alpha_2) + b(\lambda_2 - \lambda_1)\alpha_2 = b(\lambda_2 - \lambda_1)\alpha_2$. The only possibility is that $b = 0$. With the same reason, $a = 0$. \square

Denote $Q = (\alpha_1, \dots, \alpha_n) \in \mathbb{R}^{n \times n}$, and $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_n)$. From the proposition 3, we know that $\text{rank}(Q) = n$. Thus Q is invertible, we get an eigenvalue decomposition.

$$A = Q\Lambda Q^{-1}.$$

2.2 Matrix as Linear Operator

This section is to explain how eigenvalue decomposition helps. To see this, it is required to understand that (1) matrices are expressions of linear operators, and (2) diagonal matrices make analysis easier.

Definition 2. Matrix A and B are called *similar* if there exists an invertible matrix P such that:

$$A = P^{-1}BP.$$

Meanwhile, the mapping $B \rightarrow P^{-1}BP$ is called *similarity transformation* (if P is invertible).

Remark 2. The matrix similarity is **changing the coordinate** under which the linear operator is expressed. Suppose there is a linear operator $\mathcal{A} : V \rightarrow V$ and a basis (with order) $U = (u_1, \dots, u_n)$ of a finite dimensional V . Since $\mathcal{A}(u_i) \in V$, it can be expressed by a linear combination of $\{u_1, \dots, u_n\}$, say $\mathcal{A}(u_i) = UA_i$, where $A_i \in \mathbb{R}^{n \times 1}$. Put the result together for all $i = 1, \dots, n$:

$$\begin{aligned} \mathcal{A}\left((u_1, \dots, u_n)\right) &:= (\mathcal{A}(u_1), \dots, \mathcal{A}(u_n)) \\ &= (UA_1, \dots, UA_n) \\ &= U(A_1, \dots, A_n). \end{aligned}$$

We speak of the matrix $A = (A_1, \dots, A_n) \in \mathbb{R}^{n \times n}$ as the expression of the linear operator \mathcal{A} under the basis $U = (u_1, \dots, u_n)$. If we know the expression of the linear operator \mathcal{A} , and we know a vector $x = U\alpha = \alpha_1 u_1 + \dots + \alpha_n u_n \in V$ (say, α is the coordinate of x under basis U), then $\mathcal{A}(x) \in V$ can be expressed as

$$\begin{aligned} \mathcal{A}(x) &= \mathcal{A}(U\alpha) \\ &= \mathcal{A}(\alpha_1 u_1 + \dots + \alpha_n u_n) \\ &= \alpha_1 \mathcal{A}(u_1) + \dots + \alpha_n \mathcal{A}(u_n) \\ &= (\mathcal{A}(u_1), \dots, \mathcal{A}(u_n)) \cdot \alpha \\ &= (UA)\alpha \\ &= U(A\alpha). \end{aligned}$$

In plain English: if x has coordinate α , then the coordinate of $\mathcal{A}(x)$ is $A\alpha$.

Now suppose that we want to find the expression of \mathcal{A} under another basis $W = (w_1, \dots, w_n)$ which can be expressed as $W = UP = (Up_1, \dots, Up_n)$. According to the definition, we need the matrix B such that, $\mathcal{A}(w_1, \dots, w_n) = WB$. Since

$$\begin{aligned} \mathcal{A}(w_1, \dots, w_n) &= (\mathcal{A}(w_1), \dots, \mathcal{A}(w_n)) \\ &= (\mathcal{A}(Up_1), \dots, \mathcal{A}(Up_n)) \\ &= (UAp_1, \dots, UAp_n) \\ &= UAP, \end{aligned}$$

we have $UAP = \mathcal{A}(w_1, \dots, w_n) = WB = UPB$, which gives $B = P^{-1}AP$.

Proposition 4. If A is the matrix expression of linear operator \mathcal{A} under basis U , then the matrix expression of \mathcal{A} under basis $W = UP$ is given by:

$$B = P^{-1}AP.$$

The reason why I put this result here, is to show the idea behind the eigenvalue decomposition. From 2.2 we know that, for linear operators satisfying some regularity conditions (diagonalisable condition),

if we choose the basis properly, these linear operators can be expressed by diagonal matrices. Then another natural question arises: how does a diagonal matrix help?

On one hand, a linear operator (from a finite-dimensional space V to itself) can always be seen as a function composition of a rotation (R) and a stretch (S), although the angle of rotation and the times that it is stretched depends on the particular position (i.e. the value of x). For any $x \in V$,

$$\begin{aligned}\mathcal{A}(x) &= \|\mathcal{A}(x)\| \cdot \frac{\mathcal{A}(x)}{\|\mathcal{A}(x)\|} \\ &= S_x \circ R_x(x).\end{aligned}$$

Then if \mathcal{A} can be diagonal under a basis $U = (u_1, \dots, u_n)$, then \mathcal{A} operates on each u_i would be just a constant stretch (does not depend on how long u_i is), with an identical rotation.

On the other hand, diagonal matrices B make it easier to compute its power:

$$B^k = (\text{diag}(b_1, \dots, b_n))^k = \text{diag}(b_1^k, \dots, b_n^k).$$

Thus, when matrix A is similar to a diagonal matrix B , say $A = P^{-1}BP$, then for any $k \in \mathbb{Z}_+$,

$$A^k = (PBP^{-1})^k = P(B)^k P^{-1}.$$

2.3 Eigendecomposition of Symmetric Matrices

When A is a symmetric matrix, A is diagonalisable. Also, there is a theorem that ensures that columns in Q are orthogonal, i.e., $\langle \alpha_i, \alpha_j \rangle = \alpha_i^\top \alpha_j = 0$, for $1 \leq i \neq j \leq n$. Then, one can verify that $Q^\top Q = (\alpha_i^\top \alpha_j)_{n \times n} = (\delta_{ij})_{n \times n} = I_n$. The uniqueness of inverse also ensures that $QQ^\top = I_n$. Write it in another way, $Q^{-1} = Q^\top$, substitute it into $A = Q\Lambda Q^{-1}$, we get:

$$A = Q\Lambda Q^\top.$$

This is the reason why symmetric matrices are easier to study: generally, for a matrix Q , a typical solver for its inverse has time complexity $O(n^3)$ (although some can achieve $O(n^{2.5})$, which is still computational intensive). However, from Q to Q^\top does not involve any ‘computation’.

Proposition 5. *If $A \in \mathbb{R}^{n \times n}$ and A is symmetric, i.e., $A^\top = A$, then eigenvectors for different eigenvalues of A are orthogonal.*

Proof. Suppose x and y are eigenvectors for distinct eigenvalues λ and μ of A , then:

$$\begin{aligned}\lambda \langle x, y \rangle &= \langle \lambda x, y \rangle \\ &= \langle Ax, y \rangle \\ &= \langle x, A^\top y \rangle \\ &= \langle x, Ay \rangle \\ &= \langle x, \mu y \rangle \\ &= \mu \langle x, y \rangle\end{aligned}$$

$(\lambda - \mu) \langle x, y \rangle = 0$, the only possibility is that $\langle x, y \rangle = 0$. □

2.4 Singular Value Decomposition

Singular value decomposition can be understood as a generalisation of eigendecomposition since it can be defined for non-squared matrices. The next theorem tells us that any matrix has its SVD.

Theorem 1. (Existence of SVD.) For a matrix $A \in \mathbb{R}^{m \times n}$, denote its rank by r (implying $r \leq \min\{m, n\}$). Then A has decomposition:

$$A = U\Sigma V^\top = \sum_{i=1}^r \sigma_i u_i v_i^\top,$$

where $U = (u_1, \dots, u_r)$, $u_i \in \mathbb{R}^m$, and $V = (v_1, \dots, v_r)$, $v_i \in \mathbb{R}^n$ are two matrices consist of orthogonal columns, and $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_r)$.

Proof. For any A , $A^\top A$ is symmetric, and for any $x \in \mathbb{R}^n$, $x^\top A^\top A x = (Ax)^\top (Ax) \geq 0$, thus $A^\top A$ is positive semi-definite. If we denote the eigenvalue decomposition of $A^\top A$ as:

$$A^\top A = V\Lambda V^{-1},$$

where $\Lambda = \text{diag}(\lambda_1, \dots, \lambda_r)$. Then we know that columns in V are orthogonal due to , i.e. , $V^{-1} = V^\top$, and $\lambda_i \geq 0$.

For each v_i , $\|Av_i\|^2 = \langle Av_i, Av_i \rangle = v_i^\top A^\top A v_i = v_i^\top (\lambda_i v_i) = \lambda_i (v_i^\top v_i) = \lambda_i$. Set $\sqrt{\lambda_i} = \sigma_i$, then $\|\frac{1}{\sigma_i} Av_i\| = 1$.

Now set $u_i = \frac{1}{\sigma_i} Av_i$, then:

$$\begin{aligned} u_i^\top u_j &= \left(\frac{1}{\sigma_i} Av_i\right)^\top \frac{1}{\sigma_j} Av_j \\ &= \frac{1}{\sigma_i \sigma_j} v_i^\top A^\top A v_j \\ &= \frac{\sigma_j^2}{\sigma_i \sigma_j} v_i^\top v_j \\ &= \delta_{ij}, \end{aligned}$$

or $U^\top U = I_r$ in its matrix form. Since $AV = U\Sigma$, multiply V^\top on the right, we get: $A = U\Sigma V^\top$. \square

It can be constructed in such a thought. Note that $\text{rank}(AA^\top) = \text{rank}(A^\top A) = \text{rank}(A) = r$, if we do eigendecomposition for AA^\top and $A^\top A$, we will get:

$$\begin{aligned} AA^\top &= U\Lambda U^\top, \\ A^\top A &= V\Lambda V^\top. \end{aligned}$$

All eigenvalues of AA^\top are root of $\det(\lambda I - AA^\top) = 0$, which is equivalent to $\det(\lambda I - A^\top A) = 0$. This shows that AA^\top and $A^\top A$ have the same eigenvalues. And in fact, $\Lambda = \Sigma^2 = \text{diag}(\sigma_1^2, \dots, \sigma_r^2)$.

One characterisation of singular value is by the min-max Theorem.

Theorem 2. (Min-max Theorem) For a matrix $A \in \mathbb{R}^{m \times n}$, it has $\min\{m, n\}$ number of singular values, and they can be characterised as: for $i = 1, \dots, \min\{m, n\}$,

$$\sigma_i(A) = \min_{\dim(U)=n-i+1} \max_{x \in U, \|x\|_2=1} \|Ax\|_2$$

The importance of singular value partly lies in its unitary invariance.

Theorem 3. (Unitary invariance) For unitary matrix U and V (which makes all the matrix multiples compatible), the singular value of A and UAV are the same.

Combine the above two results, one can see that, for a symmetric (and of course, squared) matrix A , its singular value can be characterised as:

$$\sigma_i(A) = \min_{\dim(U)=n-i+1} \max_{x \in U, \|x\|_2=1, y \in U, \|y\|_2=1} \|y^\top Ax\|_2.$$

With this in mind, let's take a look at the definition of the principal angle between two subspaces. Since $\arccos(\cdot)$ is a decreasing function, to find the infimum, we want what is inside \arccos as large as possible, thus:

$$\theta_{E,F} = \arccos \sigma_{\max}(E^\top F).$$

In this way, we relate the geometry (the angle) to the algebra (the singular value). To study all angles rather than the 'principal' angle, we utilise all singular values of $E^\top F$. Note that $E^\top F \in \mathbb{R}^{l \times m}$, the singular values can be expressed as $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_k$, where $k = \min\{l, m\}$. Define the angle $\Theta_{E,F}$ between space E and F as:

$$\cos(\Theta_{E,F}) = \text{diag}(\sigma_1, \dots, \sigma_k).$$

3 Norm

Normed space is a linear space equipped with a structure called a norm. Intuitively, norm is a way of defining 'length'.

Definition 3. Given a vector space V , a real-valued function $p : V \rightarrow \mathbb{R}$ is called a norm if:

1. (Sub-additivity) $p(x + y) \leq p(x) + p(y)$ for all $x, y \in V$.
2. (Absolute homogeneity) $p(sx) = |s|p(x)$ for any scalar s .
3. (Positive definiteness) If $p(x) = 0$, then $x = \mathbf{0}$.

It is worth mentioning that, in a normed space $(V, \|\cdot\|)$, there is a naturally induced metric defined as: for any $x, y \in V$,

$$\rho(x, y) := \|x - y\|$$

3.1 Norm of Vectors

For $x \in \mathbb{R}^n$,

1. $\|x\|_2 = \left(\sum_{i=1}^n x_i^2\right)^{\frac{1}{2}}$ is a norm, called l_2 -norm.
2. $\|x\|_1 = \sum_{i=1}^n |x_i|$ is a norm, called l_1 -norm.
3. Generally, $\|x\|_p = \left(\sum_{i=1}^n |x_i|^p\right)^{\frac{1}{p}}$ is a norm (for $p \geq 1$), called l_p -norm.
4. As another extreme case, set $p \rightarrow \infty$, one has:

$$\|x\|_\infty = \lim_{p \rightarrow \infty} \left(\sum_{i=1}^n |x_i|^p\right)^{\frac{1}{p}} = \max_{i=1, \dots, n} |x_i|,$$

called the l_∞ -norm

3.2 Norm of Matrices

One way to look at a $m \times n$ matrix is to treat it as a linear operator from \mathbb{R}^n to \mathbb{R}^m under a particular basis. In this sense, the norm of matrices can be defined in the following way:

Suppose we have equipped \mathbb{R}^n with norm $\|\cdot\|_U$, and equipped \mathbb{R}^m with norm $\|\cdot\|_V$. Then, for any $A \in \mathbb{R}^{m \times n}$, there is a natural induced norm (called operator norm)³:

$$\|A\|_{U \rightarrow V} := \sup_{x \in \mathbb{R}^n} \frac{\|Ax\|_V}{\|x\|_U} = \sup_{x \in \mathbb{R}^n, \|x\|_U=1} \|Ax\|_V.$$

A lot of norms of this kind can be defined:

1. The $2 \rightarrow 2$ norm. Take the l_2 norm on \mathbb{R}^m , and also l_2 norm on \mathbb{R}^n . We have:

$$\|A\|_{2 \rightarrow 2} := \sup_{x \in \mathbb{R}^n} \frac{\|Ax\|_2}{\|x\|_2} = \sup_{x \in \mathbb{R}^n, \|x\|_2=1} \|Ax\|_2.$$

Combined with the min-max Theorem, one can see that the $2 \rightarrow 2$ norm is equal to the maximum among absolute values of all singular values.

Proposition 6. *Suppose there are three normed vector spaces, U, V, W , then for three naturally induced operator norms, the sub-multiplicative property holds, i.e., for any $A : U \rightarrow V$ and $B : V \rightarrow W$,*

$$\|BA\|_{U \rightarrow W} \leq \|B\|_{V \rightarrow W} \|A\|_{U \rightarrow V}.$$

Another important and widely-used norm is the Frobenius norm, which is quite similar to the l_2 -norm for vector if we stretch the matrix to be a vector in $\mathbb{R}^{mn \times 1}$:

Definition 4. *For $A \in \mathbb{R}^{m \times n}$, its Frobenius norm is defined by:*

$$\|A\|_F = \left(\sum_{i=1}^m \sum_{j=1}^n a_{ij}^2 \right)^{\frac{1}{2}}.$$

Several important results regarding the Frobenius norm are required.

Theorem 4. *For $A \in \mathbb{R}^{m \times n}$,*

$$\|A\|_F^2 = \text{tr}(AA^\top).$$

4 Complementary Subspace and Orthogonal Complement

These two stuff are both complementary subspaces in some sense of a subspace $U \subset V$, in some vector spaces V . Although they rely on different structures of the space V , they have similar names which may lead to misunderstanding. To put it clearly, we state their definition and distinguish them.

4.1 Complementary Subspace

To define complementary subspace, we first need the definition of ‘sum’ between two subsets of a vector space.

Definition 5. *For subsets $U, W \subset V$, their sum (denote as $U + W$) is defined as:*

$$U + W := \{u + w : u \in U \wedge w \in W\}.$$

³Verifying why it satisfies all three conditions is a practice to get familiar with the definition.

The direct sum can be defined for two sets (not necessarily to be subspaces). One can also easily verify that if U and W are subspaces of V , then $U + W$ is also a subspace of V .

Proposition 7. *If U, W are subspaces of V , then $U + W$ is also a subspace of V .*

If additionally, $U \cap W = \{0\}$ and $U + W = V$, then we say W is the complementary subspace of U . It deserves a definition.

Definition 6. *If subspaces U, W satisfying $U \cap W = \{0\}$, and $U + W = V$, then we say the ‘direct sum’ of U and W is V , and denote*

$$U \oplus W = V.$$

4.2 Orthogonal Complement

If we want to speak of ‘orthogonal’, we require the vector space to be equipped with an inner product structure.

Definition 7. *In an inner product space $(V, \langle \cdot, \cdot \rangle)$, the orthogonal complement of a subspace $U \subset V$ is defined as:*

$$U^\perp := \{v \in V : \forall u \in U, \langle u, v \rangle = 0\}.$$

4.3 Comments

For the case where $V = \mathbb{R}^2$, define $e_1 = (1, 0)^\top$, consider a subspace $U = \text{span}(e_1) = \{(\lambda, 0)^\top : \lambda \in \mathbb{R}\}$. Then simple calculation gives its orthogonal complement:

$$U^\perp = \text{span}(e_2) = \{(0, \mu)^\top : \mu \in \mathbb{R}\},$$

where $e_2 = (0, 1)^\top$. Further more, U^\perp is also a complementary subspace of U , i.e., $U \oplus U^\perp = V$. However, U^\perp is not the unique complementary subspace of U . To see this, we define $W = \text{span}((1, 1)^\top)$, then it is easy to verify that $U \oplus W = V$.

In fact, take $W = \text{span}(w)$ for any w such that $\text{rank}((e_1, w)) = 2$, we have $U \oplus W = V$.⁴

One can see that, $U \oplus W = V$ does not necessarily mean $U^\perp = W$.

5 Projection

Definition 8. *A function mapping from a vector space V to itself, $P : V \rightarrow V$, is called a projection if:*

$$P \circ P = P.$$

Basically, projections can be classified as oblique projection and orthogonal projection.

Definition 9. *P is an orthogonal projection if and only if $P^2 = P = P^\top$; projections that are not orthogonal are called oblique projections.*

For any k -dimensional subspace of \mathbb{R}^n ($k \leq n$), we could always assume it is spanned by an orthonormal basis. This is due to an algorithm to find an orthonormal basis for any subspace.

Theorem 5. *(Gram-Schmidt algorithm) Google it.*

⁴It is possible to speak of ‘space’ of complementary subspaces of U , but is not necessary here.

The logic is like this, for any k -dimensional subspace spanned by $\{u_1, \dots, u_k\}$, we could apply the Gram-Schmidt algorithm to get vectors $\{v_1, \dots, v_k\}$ such that $\text{span}\{v_1, \dots, v_k\} = \text{span}\{u_1, \dots, u_k\}$ and also $v_i \perp v_j$ for $1 \leq i \neq j \leq k$.

The following two theorems are from [Ipsen and Meyer \(1995\)](#).

Theorem 6. *If P_R and P_N are orthogonal projections to subspace R and N , then the minimum angle between space R and N can be captured by:*

$$\cos \theta = \|P_N P_R\|_2 = \|P_R P_N\|_2.$$

Proof. In fact, Suppose N is spanned by U , and R is spanned by W , then: $P_N = UU^\top$, while $P_R = WW^\top$. From the definition of the minimum angle between N and R ,

$$\begin{aligned} \cos \theta &= \sigma_{\max}(U^\top W) \\ &= \max_{\substack{u \in R, w \in N \\ \|u\|_2=1, \|w\|_2=1}} w^\top u \\ &= \max_{\substack{u \in R, w \in N \\ \|u\|_2 \leq 1, \|w\|_2 \leq 1}} w^\top u \\ &= \max_{\|x\|_2 \leq 1, \|y\|_2 \leq 1} (P_N \circ x)^\top (P_R \circ y) \\ &= \max_{\|x\|_2 \leq 1, \|y\|_2 \leq 1} x^\top P_N P_R y \\ &= \|P_N P_R\|_2 \end{aligned}$$

□

Definition 10. *Subspaces $\mathcal{E}, \mathcal{F} \subset \mathbb{R}^n$ are said to be complementary when $\mathcal{E} + \mathcal{F} = \mathbb{R}^n$ and $\mathcal{E} \cap \mathcal{F} = \emptyset$, and this is denoted by writing $\mathcal{E} \oplus \mathcal{F} = \mathbb{R}^n$. The associated oblique projector (onto \mathcal{E}) is the unique idempotent matrix⁵ P whose range is \mathcal{E} and whose nullspace is \mathcal{F} . Treat it as an operator, it acts as the identity on \mathcal{E} , and the zero operator on \mathcal{F} .*

Remark 1. ‘Complement’ and ‘Orthogonal Complement’ are different. The definition of complementary space relies on linearly independence, while it does not require the inner product structure of the space, although in Euclidean spaces there is a natural inner product $\langle x, y \rangle = x^\top y$ that makes it a Hilbert space. It is generally a hard problem. It can be simplified if we are talking about Euclidean space. The complementary subspace of $\mathcal{E} \subset \mathbb{R}^n$ can be characterised as:

$$\left\{ x \in \mathbb{R}^n : \forall y \in \mathcal{E}, x \text{ and } y \text{ are linearly independent.} \right\}$$

while the orthogonal complement of \mathcal{E} can be characterised as:

$$\mathcal{E}^\perp := \left\{ x \in \mathbb{R}^n : \forall y \in \mathcal{E}, \langle x, y \rangle = 0 \right\}.$$

The minimal angle between space \mathcal{E} and its complementary space \mathcal{F} (such that $\mathcal{E} \oplus \mathcal{F} = \mathbb{R}^n$) can be captured by the projection matrix P onto \mathcal{E} , according to the following theorem.

Theorem 7. *Let P be the oblique projector onto \mathcal{E} along \mathcal{F} , $\mathcal{E} \oplus \mathcal{F} = \mathbb{R}^n$, then:*

$$\min\{\sin(\Theta_{\mathcal{E}, \mathcal{F}})\} = \frac{1}{\|P\|_{2 \rightarrow 2}}.$$

⁵A matrix X is called idempotent iff $X^2 = X$.

Proof. By the Gram-Schmidt algorithm, we can always find orthogonal bases $U = (U_1, U_2)$ and $V = (V_1, V_2)$ such that: $\mathcal{E} = \text{span}(U_1)$, and $\mathcal{F} = \text{span}(V_2)$. From the definition of the oblique projection, we know that: $PV_2 = 0$. Thus, P can be expressed as:

$$P = (U_1, U_2) \begin{pmatrix} C & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} V_1^\top \\ V_2^\top \end{pmatrix} = U_1 C V_1^\top.$$

Use the definition of the oblique projection, $P^2 = P$, we have:

$$U_1 C V_1^\top U_1 C V_1^\top = U_1 C V_1^\top.$$

Multiply U_1^\top on the left and multiply V_1 on the right, we get:

$$C V_1^\top U_1 C = C.$$

Since C is full-rank, we get: $C = (V_1^\top U_1)^{-1}$. Thus,

$$\|P\|_2 = \|C\|_2 = \frac{1}{\min_{\|x\|_2=1} \|C^{-1}x\|_2} = \frac{1}{\min_{\|x\|_2=1} \|V_1^\top U_1 x\|_2}.$$

Applying the theorem 6, we get:

$$\begin{aligned} \cos^2 \theta &= \|P_{\mathcal{F}} P_{\mathcal{E}}\|_2^2 \\ &= \|V_2 V_2^\top U_1 U_1^\top\|_2^2 \\ &= \|V_2 V_2^\top U_1\|_2^2 \\ &= \|(I - V_1 V_1^\top) U_1\|_2^2 \\ &= \max_{\|x\|_2=1} \|(I - V_1 V_1^\top) U_1 x\|_2^2 \\ &= \max_{\|x\|_2=1} x^\top U_1^\top (I - V_1 V_1^\top) U_1 x \\ &= \max_{\|x\|_2=1} 1 - \|V_1^\top U_1 x\|_2^2 \\ &= 1 - \min_{\|x\|_2=1} \|V_1^\top U_1 x\|_2^2. \end{aligned}$$

Combining these two equations above, we get the result. \square

Theorem 8. For non-zero subspaces $\mathcal{E}, \mathcal{F} \subset \mathbb{R}^n$, let $P_{\mathcal{E}}, P_{\mathcal{F}}$ denote the orthogonal projection onto them, let θ be the minimum angle between two subspaces. Then:

- \mathcal{E} and \mathcal{F} are complementary spaces iff $P_{\mathcal{E}} - P_{\mathcal{F}}$ is non-singular.
- If \mathcal{E} and \mathcal{F} are complementary spaces, then $\sin \theta = \frac{1}{\|(P_{\mathcal{E}} - P_{\mathcal{F}})^{-1}\|_2}$

The proof is quite similar to that of theorem 7. With this theorem, It is all clear about the relationship between \mathcal{E} and \mathcal{F} , and their orthogonal complements.

Theorem 9. If a subspace of \mathbb{R}^n is spanned by an orthonormal basis $\{u_1, \dots, u_k\}$, then the matrix expression of the projection operator is given by:

$$P_u = \sum_{i=1}^k u_i u_i^\top.$$

Proof. The sketch:

1. Verifying $P_u \circ P_u = P_u$ to show it is a projection.
2. Show for any u_i , $i = 1, \dots, k$, $P_u u_i = u_i$.
3. Show for any vector v linearly independent from $\{u_1, \dots, u_k\}$, $P_u v = 0$.

□

6 Inequalities

Proposition 8. For diagonal matrix $D = \text{diag}(d_1, \dots, d_n)$ with diagonal elements lies between $[d_{\min}, d_{\max}]$, we have:

$$d_{\min} \|X\|_F \leq \|DX\|_F \leq d_{\max} \|X\|_F$$

Proof. Sketch: Treat $\|DX\|_F^2$ as a function of (d_1, \dots, d_n) , Show that it is increasing in all d_i .

$$\|DX\|_F^2 = \text{tr}(DX(DX)^\top)$$

□

7 Davis-Kahan Theorem

Now we are ready to talk about the Davis-Kahan Theorem. Recall the setting and the problem that we concern: assume we have a symmetric matrix A , and a symmetric perturbation H , with eigendecomposition:

$$\begin{aligned} A &= \sum_{i=1}^n \lambda_i u_i u_i^* = U \Lambda U^\top + U_\perp \Lambda_\perp U_\perp^\top, \\ A + H &= \sum_{i=1}^n \mu_i v_i v_i^* = V M V^\top + V_\perp M_\perp V_\perp^\top. \end{aligned}$$

With the belief that if H is small, then u_i and v_i should be very close. We are interested in quantitatively measuring how close u_i and v_i are, and relate it to some quantity of the perturbation H . Now it is clear, since $u_i, v_i \in \mathbb{R}^n$, and $\|u_i\|_2 = 1, \|v_i\|_2 = 1$, they are in a unit sphere: $u_i, v_i \in \mathcal{S}^{n-1}$. It is reasonable to measure how close they are by the principal angle between the two unit vectors. Furthermore, it is equivalent to measuring angles between the spaces generated by the first k eigenvectors $\{u_1, \dots, u_k\}$ and $\{v_1, \dots, v_k\}$.

Denote $U = (u_1, \dots, u_k)$ and $V = (v_1, \dots, v_k)$, then $P := UU^\top$ and $Q := VV^\top$ are the projection

onto space U and V .

$$\begin{aligned}
\|P - Q\|_F^2 &= \text{tr}((P - Q)(P - Q)^\top) \\
&= \text{tr}(PP^\top - QP^\top - PQ^\top - QQ^\top) \\
&= 2k - 2\text{tr}(PQ^\top) \\
&= 2k - 2\text{tr}(UU^\top(VV^\top)^\top) \\
&= 2k - 2\text{tr}(U(U^\top VV^\top)) \\
&= 2k - 2\text{tr}((U^\top VV^\top)U) \\
&= 2k - 2\text{tr}((U^\top V)(U^\top V)^\top) \\
&= 2k - 2\|U^\top V\|_F^2,
\end{aligned}$$

Since the Frobenius norm is unitary invariant, denote the eigendecomposition of $U^\top V$ as $U^\top V = W_1 \Sigma W_2^\top$, we have:

$$\begin{aligned}
\|U^\top V\|_F^2 &= \|W_1 \Sigma W_2^\top\|_F^2 \\
&= \|\Sigma\|_F^2 \\
&= \|\cos(\Theta_{U,V})\|_F^2 \\
&= \sum_{i=1}^k \cos^2(\theta_{U,V}).
\end{aligned}$$

Combine the results above, we have:

$$\begin{aligned}
\|P - Q\|_F^2 &= 2k - 2 \sum_{i=1}^k \cos^2(\theta_{U,V}) \\
&= 2 \sum_{i=1}^k \sin^2(\theta_{U,V}) \\
&= 2\|\sin(\Theta_{U,V})\|_F^2.
\end{aligned}$$

Several properties of the function $\text{tr}(\cdot)$ are used in the derivation, which is summarised in the following proposition.

Proposition 9. *For a matrix $A \in \mathbb{R}^{n \times m}$, the function $\text{tr}(\cdot) : \mathbb{R}^{n \times m} \rightarrow \mathbb{R}$ is defined as:*

$$\text{tr}(A) = \sum_{i=1}^{\min\{m,n\}} A_{ii}.$$

The function has the following properties:

1. *It is a linear function, i.e., for any A, B , $\text{tr}(A + B) = \text{tr}(A) + \text{tr}(B)$.*
2. *For compatible matrices A, B , $\text{tr}(AB) = \text{tr}(BA)$.*

We have shown how to measure the difference between u_i and v_i , and construct intuition about it. Now we are ready to upper bound the $\|U^\top V\|_F$.

Recall that we have the eigendecomposition of A and $A + H$ in matrix form,

$$\begin{aligned} A &= \sum_{i=1}^n \lambda_i u_i u_i^* = U \Lambda U^\top + U_\perp \Lambda_\perp U_\perp^\top, \\ A + H &= \sum_{i=1}^n \mu_i v_i v_i^* = V M V^\top + V_\perp M_\perp V_\perp^\top, \end{aligned}$$

where U_\perp consists of the basis of the complement subspace of $U = \text{span}\{u_1, \dots, u_k\}$, i.e., $U^\top U_\perp = \mathbf{0}$. The same applies for V .

Multiply U on the right of $H = (A + H) - A$, we get:

$$\begin{aligned} HU &= (A + H)U - AU \\ &= (V M V^\top + V_\perp M_\perp V_\perp^\top)U - (U \Lambda U^\top + U_\perp \Lambda_\perp U_\perp^\top)U \\ &= (V M V^\top)U + (V_\perp M_\perp V_\perp^\top)U - U \Lambda. \end{aligned}$$

Then, multiply V_\perp^\top on the left, we get:

$$\begin{aligned} V_\perp^\top H U &= V_\perp^\top \left((V M V^\top)U + (V_\perp M_\perp V_\perp^\top)U - U \Lambda \right) \\ &= M_\perp V_\perp^\top U - V_\perp^\top U \Lambda. \end{aligned} \tag{7.2}$$

Using the 7.2 together with some inequalities regarding the norm of matrices, and the assumption regarding the eigengap below, we could obtain the results.

7.1 Frobenius Norm Form

To prove:

$$\|\sin(\Theta_{U,V})\|_F \leq \frac{\|H\|_F}{\delta},$$

take Frobenius norm on both sides of 7.2,

$$\begin{aligned} \|V_\perp^\top H U\|_F &= \|M_\perp V_\perp^\top U - V_\perp^\top U \Lambda\|_F \\ &\geq | \|M_\perp V_\perp^\top U\|_F - \|V_\perp^\top U \Lambda\|_F | \\ &= \max \left\{ \|M_\perp V_\perp^\top U\|_F - \|V_\perp^\top U \Lambda\|_F, \|V_\perp^\top U \Lambda\|_F - \|M_\perp V_\perp^\top U\|_F \right\} \end{aligned}$$

The last step is because we are not sure which is larger, $\|V_\perp^\top U \Lambda\|_F$ or $\|M_\perp V_\perp^\top U\|_F$. Take the first situation as an example, using the inequality 8, we have:

$$\begin{aligned} \|M_\perp V_\perp^\top U\|_F - \|V_\perp^\top U \Lambda\|_F &\geq \min\{M_\perp\} \|V_\perp^\top U\|_F - \|V_\perp^\top U\|_F \max\{\Lambda\}, \\ \|V_\perp^\top U \Lambda\|_F - \|M_\perp V_\perp^\top U\|_F &\geq \min\{\Lambda\} \|V_\perp^\top U\|_F - \max\{M_\perp\} \|V_\perp^\top U\|_F. \end{aligned}$$

Here we need the assumption on the gap between eigenvalues of Λ and M_\perp ,

Assumption 2. *There exists a constant $\delta > 0$, such that $|\lambda_i - \mu_j| \geq \delta$ for all $i = 1, \dots, k, j = k+1, \dots, n$.*

With the assumption above, we have:

$$\max \left\{ \min\{M_\perp\} - \max\{\Lambda\}, \min\{\Lambda\} - \max\{M_\perp\} \right\} \geq \delta,$$

and thus,

$$\|V_\perp^\top H U\|_F \geq \delta \|V_\perp^\top U\|_F.$$

For the LHS, note that:

$$\begin{aligned}
\|V_\perp^\top HU\|_F^2 &= \text{tr}\left((V_\perp^\top HU)(V_\perp^\top HU)^\top\right) \\
&= \text{tr}\left((V_\perp^\top HU)U^\top H^\top V_\perp\right) \\
&= \text{tr}\left(V_\perp^\top HPPH^\top V_\perp\right) \\
&= \text{tr}\left(PH^\top V_\perp V_\perp^\top HP\right) \\
&= \text{tr}\left(PH^\top QQHP\right) \\
&\leq \text{tr}(H^\top H) \\
&= \|H\|_F^2.
\end{aligned}$$

For the RHS,

$$\begin{aligned}
\|V_\perp^\top U\|_F^2 &= \text{tr}\left(V_\perp^\top U(V_\perp^\top U)^\top\right) \\
&= \text{tr}\left(V_\perp^\top UU^\top V_\perp\right) \\
&= \text{tr}\left(UU^\top V_\perp V_\perp^\top\right) \\
&= \text{tr}\left(P(I_n - Q)\right) \\
&= \text{tr}(P) - \text{tr}(PQ) \\
&= k - \text{tr}(PQ) \\
&= k - \text{tr}(UU^\top VV^\top) \\
&= k - \text{tr}(U^\top VV^\top U) \\
&= k - \|\cos(\Theta_{U,V})\|_F^2 \\
&= \|\sin(\Theta_{U,V})\|_F^2.
\end{aligned}$$

Combine all the inequalities, we get:

$$\|\sin(\Theta_{U,V})\|_F \leq \frac{\|H\|_F}{\delta}.$$

7.2 $2 \rightarrow 2$ Norm Form

Similarly, we could prove that it also holds for the $2 \rightarrow 2$ norm. To be short, we use $\|\cdot\|_{op}$ to represent $2 \rightarrow 2$ -norm. To avoid the tedious discussion, we impose the eigengap assumption as follows.

Assumption 3. *The eigenvalues of Λ are contained in an interval (a, b) , and eigenvalues of M_\perp are excluded from $(a - \delta, b + \delta)$ for some $\delta > 0$.*

Denote $c := \frac{a+b}{2}$ and $r := \frac{b-a}{2}$. Take the $2 \rightarrow 2$ -norm on both sides of 7.2, we have:

$$\begin{aligned}
\|V_\perp^\top HU\|_{op} &= \|M_\perp V_\perp^\top U - V_\perp^\top U \Lambda\|_{op} \\
&= \|(M_\perp - cI)V_\perp^\top U - V_\perp^\top U(\Lambda - cI)\|_{op} \\
&\geq \|(M_\perp - cI)V_\perp^\top U\|_{op} - \|V_\perp^\top U(\Lambda - cI)\|_{op}.
\end{aligned}$$

Since the eigenvalue of $\Lambda - cI$ lies in $(-r, r)$, while the eigenvalue of $M_\perp - cI$ lies in $(-\infty, -r - \delta] \cup [r + \delta, \infty)$. Thus,

$$\begin{aligned}
\|\Lambda - cI\|_{op} &< r, \\
\|(M_\perp - cI)^{-1}\|_{op} &< \frac{1}{r + \delta}.
\end{aligned}$$

Using the sub-multiplicative property of operator norms, we get:

$$\begin{aligned}\|V_{\perp}^{\top}U\|_{op} &= \|(M_{\perp} - cI)^{-1}(M_{\perp} - cI)V_{\perp}^{\top}U\|_{op} \\ &\leq \|(M_{\perp} - cI)^{-1}\|_{op}\|(M_{\perp} - cI)V_{\perp}^{\top}U\|_{op} \\ &\leq \frac{1}{r + \delta}\|(M_{\perp} - cI)V_{\perp}^{\top}U\|_{op}.\end{aligned}$$

Also,

$$\begin{aligned}\|V_{\perp}^{\top}U(\Lambda - cI)\|_{op} &\leq \|V_{\perp}^{\top}U\|_{op}\|(\Lambda - cI)\|_{op} \\ &< r\|V_{\perp}^{\top}U\|_{op}.\end{aligned}$$

Combine two inequalities above, we have:

$$\begin{aligned}\|V_{\perp}^{\top}HU\|_{op} &\geq (r + \delta)\|V_{\perp}^{\top}U\|_{op} - r\|V_{\perp}^{\top}U\|_{op} \\ &= \delta\|V_{\perp}^{\top}U\|_{op}.\end{aligned}$$

Since the $2 \rightarrow 2$ operator norm is exactly the largest absolute eigenvalue,

$$111$$

$$\|\sin(\Theta_{U,V})\|_{2 \rightarrow 2} \leq \frac{\sqrt{k}\|H\|_{2 \rightarrow 2}}{\delta}$$

In fact, for any unitary invariant norm $\|\cdot\|$, similar results hold.

8 A Useful Variant

One of the important applications of the Davis-Kahan Theorem is in statistics, where A captures the population information (thus is an unknown parameter, from the perspective of the frequentists), and H is the error due to sampling and randomness. In this setting, our goal is typically to show that the sample version eigenvector will be quite close to the population one, thus being a good estimator. However, it is not natural to ask for eigengap between the population version and the sample version, since the sample version can actually take any value (although for some values, the probability is really small).

In light of this, there is a useful variant of Davis-Kahan Theorem (Yu et al., 2015), which has the same conclusion, but only requires the eigengap for one of the matrices, A or $A + H$ (typically we choose A), therefore allowing us to put restriction only on the population version.

8.1 Prerequisite

Some theorems (such as the Hoffman-Wielandt inequality) and lemmas are required in the proof of the variant of the Davis-Kahan theorem, and thus we put them here.

Theorem 10. (*Birkhoff-von Neumann theorem.*) *The set of all doubly stochastic matrices is the convex hull of all permutation matrices. In other words, if $X \in \mathbb{R}^{n \times n}$ is a doubly stochastic matrix, then there exists $\theta_1, \dots, \theta_k \geq 0$, $\sum_{i=1}^k \theta_i = 1$, such that:*

$$X = \theta_1 P_1 + \dots + \theta_k P_k,$$

where $P_1, \dots, P_k \in \mathbb{R}^{n \times n}$ are permutations.

Proof. of theorem 10.

Takes the minimum positive element in X , say x_{ij} . For the position (i, j) , there exists a permutation P such that $p_{ij} = 1$. Now consider $X - x_{ij}P$: the number of elements that are zero increases, and it satisfies the condition that, the summation of each column and each row are the same.

Continue this process, and we will get the decomposition. It is easy to see that the process will end after at most n^2 steps, since each step strictly makes at least one element zero.

However, it might not be unique.

(It can also be rigorously stated by induction.) □

Lemma 1. For two sequences $\{a_i\}_{i=1}^n$ and $\{b_i\}_{i=1}^n$. Reorder them such that $a_{(1)} \leq \dots \leq a_{(n)}$, and $b_{(1)} \leq \dots \leq b_{(n)}$. Then:

$$\min_{\sigma \in \mathcal{S}_n} \sum_{i=1}^n |a_i - b_{\sigma(i)}|^2 = \sum_{i=1}^n |a_{(i)} - b_{(i)}|^2.$$

Proof. of the lemma 1.

If $a_i \leq a_{i+1}$, and $b_i \geq b_{i+1}$, then:

$$\begin{aligned} (a_i - b_i)^2 + (a_{i+1} - b_{i+1})^2 &= (a_i - b_{i+1})^2 + (b_i - a_{i+1})^2 + 2(a_i - a_{i+1})(b_i - b_{i+1}) \\ &\geq (a_i - b_{i+1})^2 + (b_i - a_{i+1})^2. \end{aligned}$$

Based on this result, mathematical induction can give the result. □

Theorem 11. (Hoffman-Wielandt inequality) If $A, B \in \mathbb{C}^{n \times n}$ are normal matrices, with eigenvalues $\lambda_1(A), \dots, \lambda_n(A)$ and $\lambda_1(B), \dots, \lambda_n(B)$. Then the optimal matching of eigenvalues beats the Frobenius norm:

$$\min_{\sigma \in \mathcal{S}_n} \sum_{i=1}^n |\lambda_i(A) - \lambda_{\sigma(i)}(B)|^2 \leq \|A - B\|_F^2,$$

where \mathcal{S}_n is the set of all permutations on $\{1, \dots, n\}$.

Proof. of theorem 11.

Denote the eigenvalue decomposition of A and B , where the eigenvalues are in descending order, i.e., $\lambda_1(A) \leq \dots \leq \lambda_n(A)$, and $\lambda_1(B) \leq \dots \leq \lambda_n(B)$:

$$\begin{aligned} C &:= UAU^* = \text{diag}(\lambda_1(A), \dots, \lambda_n(A)), \\ D &:= VBV^* = \text{diag}(\lambda_1(B), \dots, \lambda_n(B)). \end{aligned}$$

By the unitary invariance of Frobenius norm, we know:

$$\begin{aligned} \|A - B\|_F^2 &= \|U^*CU - V^*DV\|_F^2 \\ &= \text{tr}\left((U^*CU - V^*DV)^2\right) \\ &= \text{tr}(C^2) + \text{tr}(D^2) - 2\text{tr}(U^*CUV^*DV) \\ &= \text{tr}(C^2) + \text{tr}(D^2) - 2\text{tr}(CUV^*DVU^*) \\ &= \text{tr}(C^2) + \text{tr}(D^2) - 2\text{tr}(CWDW^*), \end{aligned}$$

where we define $W := UV^*$. In addition, we know that:

$$\begin{aligned}
\min_{\sigma \in \mathcal{S}_n} \sum_{i=1}^n |\lambda_i(A) - \lambda_{\sigma(i)}(B)|^2 &= \sum_{i=1}^n |\lambda_{(i)}(A) - \lambda_{(i)}(B)|^2 \\
&= \sum_{i=1}^n |\lambda_i(A) - \lambda_i(B)|^2 \\
&= \|C - D\|_F^2 \\
&= \text{tr}((C - D)^2) \\
&= \text{tr}(C^2) + \text{tr}(D^2) - 2\text{tr}(CD).
\end{aligned}$$

Then it suffices to show that $\text{tr}(CWDW^*) \leq \text{tr}(CD)$. If we denote $P = (|W_{ij}|^2)_{n \times n}$, then:

$$\begin{aligned}
\text{tr}(CWDW^*) &= \sum_{i=1}^n (CWDW^*)_{ii} \\
&= \sum_{i=1}^n \sum_{k=1}^n (CW)_{ik} (DW^*)_{ki} \\
&= \sum_{i=1}^n \sum_{k=1}^n \left(\sum_{m=1}^n C_{im} W_{mk} \right) \left(\sum_{m=1}^n D_{km} (W^*)_{mi} \right) \\
&= \sum_{i=1}^n \sum_{k=1}^n C_{ii} D_{kk} |W_{ik}|^2 \\
&= \sum_{i=1}^n \sum_{k=1}^n \lambda_i(A) \lambda_i(B) P_{ik},
\end{aligned}$$

where P is a doubly stochastic matrix. If we define function $f(P) = \sum_{i=1}^n \sum_{k=1}^n C_{ii} D_{kk} P_{ik}$ on the set of (n-by-n) all doubly stochastic matrix B_n . By Birkhoff-von Neumann theorem, B_n is the convex hull of n -th order permutations, i.e. ,

$$B_n = \left\{ \sum_{i=1}^k \theta_i P_i : \forall i, \theta_i \geq 0, \sum_{i=1}^k \theta_i = 1, P_i \text{ are permutations.} \right\}$$

On one hand, it is clear that f is a linear function, thus for any $\lambda \in [0, 1]$, and any $P_1, P_2 \in B_n$,

$$f(\lambda P_1 + (1 - \lambda) P_2) = \lambda f(P_1) + (1 - \lambda) f(P_2).$$

Thus, if f can obtain its supremum, it must be at an extreme point. On the other hand, B_n is a compact set, and f is continuous, the supremum can be obtained.

In addition, to evaluate the value of f at those extreme points (permutations), Apply the lemma 1, we see that the supremum of f is obtained when $W = I$.

□

8.2 the Key Result

Theorem 12. Let $A, A + H \in \mathbb{R}^n$ be Hermitian matrices with eigenvalues $\lambda_1 \geq \dots \geq \lambda_n$ (with corresponding eigenvectors u_1, \dots, u_n) and $\mu_1 \geq \dots \geq \mu_n$ (with corresponding eigenvectors v_1, \dots, v_n), respectively. For any $0 < d \leq n$, Let Θ be the principal angle between spaces spanned by (u_1, \dots, u_d) and (v_1, \dots, v_d) , then:

$$\|\sin(\Theta)\|_F \leq \frac{2\|H\|_F}{\lambda_d - \lambda_{d+1}}.$$

Remark 1. Compared to the original version, the bound only relies on the eigengap of matrix A , while the cost is to multiply the bound by 2, which is negligible.

Remark 2. In their paper, the bound is

$$\|\sin(\Theta)\|_F \leq \frac{2 \min\{\sqrt{d}\|H\|_{\text{op}}, \|H\|_F\}}{\lambda_d - \lambda_{d+1}}.$$

To see this, one needs to change the step 8.3 in the proof:

$$\begin{aligned} \|V(M - \Lambda)\|_F &= \|M - \Lambda\|_F \\ &\leq \left\| \begin{pmatrix} M & 0 \\ 0 & M_\perp \end{pmatrix} - \begin{pmatrix} \Lambda & 0 \\ 0 & \Lambda_\perp \end{pmatrix} \right\|_F \\ &\leq \left\| I_d \begin{pmatrix} M & 0 \\ 0 & M_\perp \end{pmatrix} - I_d \begin{pmatrix} \Lambda & 0 \\ 0 & \Lambda_\perp \end{pmatrix} \right\|_F \\ &\leq \|I_d H\|_F \\ &= \sqrt{\sum_{i=1}^d (\sigma_i(H))^2} \\ &\leq \sqrt{d(\max_{j=1, \dots, n} \sigma_j(H))^2} \\ &= \sqrt{d}\|H\|_{\text{op}}. \end{aligned}$$

Proof. of the variant of Davis-Kahan.

Suppose we have eigenvalue decomposition of A and $A + H$ as follows:

$$\begin{aligned} A &= (U \ U_\perp) \begin{pmatrix} \Lambda & 0 \\ 0 & \Lambda_\perp \end{pmatrix} \begin{pmatrix} U^\top \\ U_\perp^\top \end{pmatrix} \\ A + H &= (V \ V_\perp) \begin{pmatrix} M & 0 \\ 0 & M_\perp \end{pmatrix} \begin{pmatrix} V^\top \\ V_\perp^\top \end{pmatrix} \end{aligned}$$

It is clear that $AU = U\Lambda$. After the perturbation, eigenvectors U change to V , one way to measure the change is to look at how small the residual $L = AV - V\Lambda$ is.

$$\begin{aligned} L &= AV - V\Lambda \\ &= (A + H)V - V\Lambda - HV \\ &= V(M - \Lambda) - HV. \end{aligned}$$

Taking the Frobenius norm, and applying Wielandt-Hoffman theorem, we have:

$$\begin{aligned} \|V(M - \Lambda)\|_F &= \|M - \Lambda\|_F \\ &\leq \left\| \begin{pmatrix} M & 0 \\ 0 & M_\perp \end{pmatrix} - \begin{pmatrix} \Lambda & 0 \\ 0 & \Lambda_\perp \end{pmatrix} \right\|_F \\ &\leq \|H\|_F. \end{aligned} \tag{8.3}$$

Thus, on the one hand,

$$\begin{aligned} \|L\|_F &= \|V(M - \Lambda) - HV\|_F \\ &\leq \|V(M - \Lambda)\|_F + \|HV\|_F \\ &\leq 2\|H\|_F \end{aligned}$$

On the other hand, note that $V\Lambda = IV\Lambda = (P + P_\perp)V\Lambda = (UU^* + U_\perp U_\perp^*)V\Lambda$, we could write L as:

$$\begin{aligned} L &= AV - V\Lambda \\ &= (U\Lambda U^* + U_\perp \Lambda_\perp U_\perp^*)V - (UU^* + U_\perp U_\perp^*)V\Lambda \\ &= U(\Lambda U^*V - U^*V\Lambda) + U_\perp(\Lambda_\perp U_\perp^*V - U_\perp^*V\Lambda) \end{aligned}$$

Taking the Frobenius norm for both sides, we have:

$$\begin{aligned} \|L\|_F &\geq \|U(\Lambda U^*V - U^*V\Lambda)\|_F \\ &= \|\Lambda U^*V - U^*V\Lambda\|_F. \end{aligned}$$

Now if we have the eigengap assumption:

Assumption 4. $|\lambda_i - \lambda_j| \geq \delta > 0$, for $i = 1, \dots, k$, $j = k+1, \dots, n$.

Then, $\|L\|_F \geq \delta \|\sin \Theta_{U,V}\|$. As a result,

$$\|\sin \Theta_{U,V}\|_F \leq \frac{2\|H\|_F}{\delta}.$$

□

8.3 Original version

Theorem 13. Let $\Sigma, \hat{\Sigma} \in \mathbb{R}^{p \times p}$ be symmetric, with eigenvalues $\lambda_1 \geq \dots \geq \lambda_p$, and $\hat{\lambda}_1 \geq \dots \geq \hat{\lambda}_p$ respectively. Fix $1 \leq r \leq s \leq p$ and assume that $\min(\lambda_{r-1} - \lambda_r, \lambda_s - \lambda_{s+1}) > 0$, where $\lambda_0 := \infty$ and $\lambda_{p+1} := -\infty$. Let $d := s - r + 1$, and let $V = (v_r, v_{r+1}, \dots, v_s) \in \mathbb{R}^{p \times d}$ and $\hat{V} = (\hat{v}_r, \hat{v}_{r+1}, \dots, \hat{v}_s) \in \mathbb{R}^{p \times d}$ have orthonormal columns satisfying $\Sigma v_j = \lambda_j v_j$ and $\hat{\Sigma} \hat{v}_j = \hat{\lambda}_j \hat{v}_j$ for $j = r, r+1, \dots, s$. Then

$$\|\sin \Theta(\hat{V}, V)\|_F \leq \frac{2 \min(d^{1/2} \|\hat{\Sigma} - \Sigma\|_{op}, \|\hat{\Sigma} - \Sigma\|_F)}{\min(\lambda_{r-1} - \lambda_r, \lambda_s - \lambda_{s+1})}.$$

Moreover, there exists an orthogonal matrix $\hat{O} \in \mathbb{R}^{d \times d}$ such that:

$$\|\hat{V}\hat{O} - V\|_F \leq \frac{2^{3/2} \min(d^{1/2} \|\hat{\Sigma} - \Sigma\|_{op}, \|\hat{\Sigma} - \Sigma\|_F)}{\min(\lambda_{r-1} - \lambda_r, \lambda_s - \lambda_{s+1})}$$

Remark 1. We have seen the special case when V is spanned by v_1, \dots, v_d (start from the first eigenvector). The original version allows V to be spanned by v_r, v_{r+1}, \dots, v_s . Such a difference does not add difficulties at all, since unitary transformation can exchange the order of eigenvalues as we want. The only thing required is to set $\Lambda := \text{diag}(\lambda_r, \lambda_{r+1}, \dots, \lambda_s)$.

Remark 2. Regarding the existence of the orthogonal matrix \hat{O} , if we take $\hat{O}_1, \hat{O}_2 \in \mathbb{R}^{d \times d}$ such that $\hat{O}_1^\top \hat{V}^\top V \hat{O}_2 = \text{diag}(\cos \theta_1, \dots, \cos \theta_d)$, and set $\hat{O} = \hat{O}_1 \hat{O}_2^\top$, then:

$$\begin{aligned} \|\hat{V}\hat{O} - V\|_F^2 &= \text{tr}((\hat{V}\hat{O} - V)^\top (\hat{V}\hat{O} - V)) \\ &= \text{tr}((\hat{V}\hat{O})^\top \hat{V}\hat{O} + \hat{V}^\top \hat{V} - 2\hat{O}^\top \hat{V}^\top V) \\ &= 2d - 2\text{tr}(\hat{O}_2 \hat{O}_1^\top \hat{V}^\top V) \\ &= 2d - 2\text{tr}(\hat{O}_1^\top \hat{V}^\top V \hat{O}_2) \\ &= 2d - 2\|\cos(\Theta_{V, \hat{V}})\|_F^2 \\ &= 2\|\sin(\Theta_{V, \hat{V}})\|_F^2. \end{aligned}$$

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