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Angles between subspaces and their tangents[†]

Peizhen Zhu and Andrew V. Knyazev

Abstract. Principal angles between subspaces (PABS) (also called canonical angles) serve as a classical tool in mathematics, statistics, and applications, e.g., data mining. Traditionally, PABS are introduced via their cosines. The cosines and sines of PABS are commonly defined using the singular value decomposition. We utilize the same idea for the tangents, i.e., explicitly construct matrices, such that their singular values are equal to the tangents of PABS, using several approaches: orthonormal and non-orthonormal bases for subspaces, as well as projectors. Such a construction has applications, e.g., in analysis of convergence of subspace iterations for eigenvalue problems.

Keywords. principal angles, canonical angles, singular value, projector.

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1 Introduction

The concept of principal angles between subspaces (PABS) is introduced by Jordan [12] in 1875. Hotelling [10] defines PABS in the form of canonical correlations in statistics in 1936. Traditionally, PABS are introduced and used via their sines and more commonly, because of their connection to canonical correlations, cosines; see, e.g., [4, 11, 14, 21, 23]. The properties of sines and cosines of PABS are well investigated; e.g., in [1, 13, 22].

The tangents of PABS have attracted relatively less attention, compared to the cosines, despite of the celebrated work of Davis and Kahan [3], which includes several tangent-related theorems. The tangents of PABS also appear in several other important publications on numerical matrix analysis. In [2, 5], the authors use the tangent of the largest principal angle derived from a norm of a specific matrix. In [19, Theorem 2.4, p. 252] and [21, p. 231-232] the tangents of PABS, related to singular values of a matrix—without an explicit matrix formulation—are used to analyze perturbations of invariant subspaces. The tangents of PABS are used in [6] for generalized singular value computation. Properties of an oblique

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projector (idempotent) are naturally determined by the tangents of angles between its null space and range, e.g., the spectral norm of an idempotent is the secant of the largest canonical angle between its row and column spaces; see [20] and references there.

In [2, 5, 19–21], the two subspaces have the same dimensions. In this work, for two given subspaces (not necessarily of the same dimensions) we construct a family \mathcal{F} of explicitly given matrices, such that the singular values of the matrix $T \in \mathcal{F}$ are the tangents of PABS. We find T in two different ways. First, we derive T using matrices whose columns form the (orthonormal) bases of the subspaces. Second, we present T as the product of projectors on the subspaces. We describe the action of the matrix T as a linear operator, and provide a geometric interpretation of the singular values of T . Some of our proofs are reasonably technical, although rather standard and should be accessible to a wide audience.

Our basis-based constructions include the matrices used in [2, 5, 19, 21] and extend to the case of subspaces with different dimensions. These results are motivated by and have applications in our recent and upcoming work on majorization-based analysis of convergence of the Rayleigh-Ritz method [15, Section 2.5] and subspace iterations for eigenvalue problems [24]. Let us, however, warn a non-expert reader that the tangent function is not well-suited for computations of angles close to $\pi/2$ for evident reasons. Thus, our formulas for T cannot be recommended in general for numerical evaluation of PABS in their full range of values $[0, \pi/2]$.

The basis-based approach bounds us to the matrix theory, as we represent subspaces by matrices, e.g., it makes it difficult to attempt extending our results to general infinite-dimensional Hilbert spaces by analogy with [16]. Our projector-based results are more intuitive and general, relying only on geometry of the space. However, we do not develop here an independent theory, readily applicable to principle angles between infinite-dimensional subspaces as in [16]. We still use the basis description of subspaces, but only in the proofs, using our previous matrix results. The statements are basis-free, e.g., according to Theorem 4.1 and Remark 4.1, one possible form of the operator T is a product of the orthogonal projector onto \mathcal{X}^\perp and the oblique projector that projects onto \mathcal{Y} along \mathcal{X}^\perp , where the singular values of T determine the tangents of principal angles between subspaces \mathcal{X} and \mathcal{Y} and the subspace \mathcal{X}^\perp denotes the orthogonal complement to \mathcal{X} . If the subspaces \mathcal{X} and \mathcal{Y} are in generic position, i.e., none of the PABS is zero or $\pi/2$, the statement also becomes dimensionless, i.e., does not depend on $\dim(\mathcal{X})$ or $\dim(\mathcal{Y})$.

The rest of the paper is organized as follows. We briefly review the concept and some important properties of PABS, as well as related preliminaries, in Section 2. The goal of this work is explicitly constructing a family of matrices such that their singular values are equal to the tangents of PABS. We form these matrices using bases for subspaces in Section 3 and projectors in Section 4.

2 Definition of PABS and other preliminaries

In this section, we remind the reader the concept of PABS and some fundamental properties of PABS. We first recall that an acute angle between two unit vectors x and y , i.e., with $x^H x = y^H y = 1$, is defined as

$$\cos \theta(x, y) = |x^H y|, \text{ where } 0 \leq \theta(x, y) \leq \pi/2.$$

This definition can be recursively extended to PABS; see, e.g., [1, 8, 10].

Definition 2.1. Let $\mathcal{X} \subset \mathbb{C}^n$ and $\mathcal{Y} \subset \mathbb{C}^n$ be subspaces with $\dim(\mathcal{X}) = p$ and $\dim(\mathcal{Y}) = q$. Let $m = \min(p, q)$. The principal angles $\Theta(\mathcal{X}, \mathcal{Y}) = [\theta_1, \dots, \theta_m]$, where $\theta_k \in [0, \pi/2]$, $k = 1, \dots, m$, between \mathcal{X} and \mathcal{Y} are recursively defined by

$$\cos(\theta_k) = \max_{x \in \mathcal{X}} \max_{y \in \mathcal{Y}} |x^H y| = |x_k^H y_k|,$$

subject to $\|x\| = \|y\| = 1$, $x^H x_i = 0$, $y^H y_i = 0$, $i = 1, \dots, k-1$. The vectors $\{x_1, \dots, x_m\}$ and $\{y_1, \dots, y_m\}$ are called the principal vectors.

An alternative definition of PABS, from [1, 8], is based on the singular value decomposition (SVD) and reproduced here as the following theorem.

Theorem 2.1. Let the columns of matrices $X \in \mathbb{C}^{n \times p}$ and $Y \in \mathbb{C}^{n \times q}$ form orthonormal bases for the subspaces \mathcal{X} and \mathcal{Y} , correspondingly. Let the SVD of $X^H Y$ be $U \Sigma V^H$, where U and V are unitary matrices and Σ is a $p \times q$ diagonal matrix with the real diagonal elements s_1, \dots, s_m in decreasing order with $m = \min(p, q)$. Then $\cos \Theta^\uparrow(\mathcal{X}, \mathcal{Y}) = S(X^H Y) = [s_1, \dots, s_m]$, where $\Theta^\uparrow(\mathcal{X}, \mathcal{Y})$ denotes the vector of principal angles between \mathcal{X} and \mathcal{Y} arranged in increasing order and $S(A)$ denotes the vector of singular values of A . Moreover, the principal vectors associated with this pair of subspaces are given by the first m columns of XU and YV , correspondingly.

Theorem 2.1 implies that PABS are symmetric, i.e. $\Theta(\mathcal{X}, \mathcal{Y}) = \Theta(\mathcal{Y}, \mathcal{X})$, and unitarily invariant, i.e., $\Theta(U\mathcal{X}, U\mathcal{Y}) = \Theta(\mathcal{X}, \mathcal{Y})$ for any unitary transformation U . Important properties of PABS have been established, for finite dimensional subspaces, e.g., in [11, 14, 21–23], and for infinite dimensional subspaces in [4, 16]. Relationships of principal angles between \mathcal{X} and \mathcal{Y} , and between their orthogonal complements \mathcal{X}^\perp and \mathcal{Y}^\perp , correspondingly, are investigated in [11, 14, 16] as follows.

Property 2.1. Let $\Theta^\downarrow(\mathcal{X}, \mathcal{Y})$ denote PABS arranged in decreasing order. Then:
 (1) $[\Theta^\downarrow(\mathcal{X}, \mathcal{Y}), 0, \dots, 0] = [\Theta^\downarrow(\mathcal{X}^\perp, \mathcal{Y}^\perp), 0, \dots, 0]$,

with $\max(n - \dim(\mathcal{X}) - \dim(\mathcal{Y}), 0)$ zeros on the left and $\max(\dim(\mathcal{X}) + \dim(\mathcal{Y}) - n, 0)$ zeros on the right.

$$(2) [\Theta^\downarrow(\mathcal{X}, \mathcal{Y}^\perp), 0, \dots, 0] = [\Theta^\downarrow(\mathcal{X}^\perp, \mathcal{Y}), 0, \dots, 0],$$

with $\max(\dim(\mathcal{Y}) - \dim(\mathcal{X}), 0)$ zeros on the left and $\max(\dim(\mathcal{X}) - \dim(\mathcal{Y}), 0)$ zeros on the right.

$$(3) \left[\frac{\pi}{2}, \dots, \frac{\pi}{2}, \Theta^\downarrow(\mathcal{X}, \mathcal{Y})\right] = \left[\frac{\pi}{2} - \Theta^\uparrow(\mathcal{X}, \mathcal{Y}^\perp), 0, \dots, 0\right],$$

with $\max(\dim(\mathcal{X}) - \dim(\mathcal{Y}), 0)$ $\pi/2$ s on the left and $\max(\dim(\mathcal{X}) + \dim(\mathcal{Y}) - n, 0)$ zeros on the right.

PABS are closely related to the Cosine-Sine Decomposition (CSD); e.g., [7, 17, 18]. Let $[X, X_\perp]$ and $[Y, Y_\perp]$ be unitary matrices with $X \in \mathbb{C}^{n \times p}$ and $Y \in \mathbb{C}^{n \times q}$. Applying CSD to $[X, X_\perp]^H [Y, Y_\perp]$, we obtain

$$[X \ X_\perp]^H [Y \ Y_\perp] = \begin{bmatrix} X^H Y & X^H Y_\perp \\ X_\perp^H Y & X_\perp^H Y_\perp \end{bmatrix} = \begin{bmatrix} U_1 & \\ & U_2 \end{bmatrix} D \begin{bmatrix} V_1 \\ V_2 \end{bmatrix}^H$$

with unitary matrices U_1, U_2, V_1 , and V_2 . The matrix D has the following structure:

$$D = \begin{array}{c} \begin{matrix} r & s & q-r-s & n-p-q+r & s & p-r-s \end{matrix} \\ \begin{matrix} r \\ s \\ p-r-s \\ n-p-q+r \\ s \\ q-r-s \end{matrix} \end{array} \left[\begin{array}{ccc|ccc} I & & & & O & \\ & C & & & & S \\ & & O & & & I \\ \hline O & & & -I & & \\ & S & & & -C & \\ & & I & & & O \end{array} \right], \quad (1)$$

where $C = \text{diag}(\cos(\theta_{j_1}), \dots, \cos(\theta_{j_s}))$, and $S = \text{diag}(\sin(\theta_{j_1}), \dots, \sin(\theta_{j_s}))$ such that $\theta_{j_k} \in (0, \pi/2)$ for $k = 1, \dots, s$, are all the principal angles between the subspaces $\mathcal{R}(Y)$ and $\mathcal{R}(X)$ located in the open interval $(0, \pi/2)$. Zero matrices of various sizes, not necessarily square, are denoted by O . I denotes the identity matrix. We may have different sizes of I in D . In addition, it is possible to permute the first q columns or the last $n - q$ columns of D , or the first p rows or the last $n - p$ rows and to change the sign of any column or row to obtain the variants of the CSD.

The block sizes in the matrix D are determined by the following decomposition of the space $\mathbb{C}^n = \mathfrak{M}_{00} \oplus \mathfrak{M}_{01} \oplus \mathfrak{M}_{10} \oplus \mathfrak{M}_{11} \oplus \mathfrak{M}$ into an orthogonal sum of five subspaces, as in [9, 16], defined via the column ranges $\mathcal{X} = \mathcal{R}(X)$ and $\mathcal{Y} = \mathcal{R}(Y)$, and their orthogonal complements, \mathcal{X}^\perp and \mathcal{Y}^\perp , correspondingly, in the following way:

$$\mathfrak{M}_{00} = \mathcal{X} \cap \mathcal{Y}, \quad \mathfrak{M}_{01} = \mathcal{X} \cap \mathcal{Y}^\perp, \quad \mathfrak{M}_{10} = \mathcal{X}^\perp \cap \mathcal{Y}, \quad \mathfrak{M}_{11} = \mathcal{X}^\perp \cap \mathcal{Y}^\perp.$$

Namely, $\dim(\mathfrak{M}_{00}) = r$, $\dim(\mathfrak{M}_{10}) = q - r - s$, $\dim(\mathfrak{M}_{01}) = p - r - s$, and $\dim(\mathfrak{M}_{11}) = n - p - q + r$, according to [16, Tables 1 and 2]. Decomposing $\mathfrak{M} = \mathfrak{M}_{\mathcal{X}} \oplus \mathfrak{M}_{\mathcal{X}^\perp} = \mathfrak{M}_{\mathcal{Y}} \oplus \mathfrak{M}_{\mathcal{Y}^\perp}$, where

$$\begin{aligned}\mathfrak{M}_{\mathcal{X}} &= \mathcal{X} \cap (\mathfrak{M}_{00} \oplus \mathfrak{M}_{01})^\perp, & \mathfrak{M}_{\mathcal{X}^\perp} &= \mathcal{X}^\perp \cap (\mathfrak{M}_{10} \oplus \mathfrak{M}_{11})^\perp, \\ \mathfrak{M}_{\mathcal{Y}} &= \mathcal{Y} \cap (\mathfrak{M}_{00} \oplus \mathfrak{M}_{10})^\perp, & \mathfrak{M}_{\mathcal{Y}^\perp} &= \mathcal{Y}^\perp \cap (\mathfrak{M}_{01} \oplus \mathfrak{M}_{11})^\perp,\end{aligned}$$

we get $s = \dim(\mathfrak{M}_{\mathcal{X}}) = \dim(\mathfrak{M}_{\mathcal{Y}}) = \dim(\mathfrak{M}_{\mathcal{X}^\perp}) = \dim(\mathfrak{M}_{\mathcal{Y}^\perp}) = \dim(\mathfrak{M})/2$.

Finally, we extensively use the Moore-Penrose pseudoinverse; see, e.g. [21]. The Moore-Penrose pseudoinverse $A^\dagger \in \mathbb{C}^{m \times n}$ of a matrix $A \in \mathbb{C}^{n \times m}$ satisfies the following $AA^\dagger A = A$, $A^\dagger AA^\dagger = A^\dagger$, $(AA^\dagger)^H = AA^\dagger$, $(A^\dagger A)^H = A^\dagger A$, and

- if $A = U\Sigma V^H$ is the SVD of A , then $A^\dagger = V\Sigma^\dagger U^H$;
- if A has full column rank and B has full row rank, then $(AB)^\dagger = B^\dagger A^\dagger$. However, this formula does not hold in general;
- AA^\dagger is the orthogonal projector onto the range of A , and $A^\dagger A$ is the orthogonal projector onto the range of A^H ;
- if U and V are unitary matrices then $(UAV)^\dagger = V^H A^\dagger U^H$ for any matrix A ;
- let A , B , and C be block matrices, such that

$$A = \begin{bmatrix} A_1 & O_A \end{bmatrix}, \quad B = \begin{bmatrix} B_1 \\ O_B \end{bmatrix}, \quad C = \begin{bmatrix} C_1 & O_{12} \\ O_{21} & O_2 \end{bmatrix},$$

where O_\star are various zero matrices. Then

$$A^\dagger = \begin{bmatrix} A_1^\dagger \\ O_A^H \end{bmatrix}, \quad B^\dagger = \begin{bmatrix} B_1^\dagger & O_B^H \end{bmatrix}, \quad C^\dagger = \begin{bmatrix} C_1^\dagger & O_{21}^H \\ O_{12}^H & O_2^H \end{bmatrix}.$$

3 $\tan \Theta$ in terms of the bases of subspaces

Let the orthonormal columns of matrices X , X_\perp , and Y span the subspaces \mathcal{X} , the orthogonal complement \mathcal{X}^\perp of \mathcal{X} , and \mathcal{Y} , correspondingly. Then $\cos \Theta(\mathcal{X}, \mathcal{Y}) = S(X^H Y)$ and $\cos \Theta(\mathcal{X}^\perp, \mathcal{Y}) = S(X_\perp^H Y)$ by Theorem 2.1. We begin with an example using 2D vectors. Let

$$X = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad X_\perp = \begin{bmatrix} 0 \\ 1 \end{bmatrix}, \quad \text{and} \quad Y = \begin{bmatrix} \cos \theta \\ \sin \theta \end{bmatrix},$$

where $0 \leq \theta < \pi/2$. Then, $X_{\perp}^H Y = \sin \theta$ and $X^H Y = \cos \theta$. Obviously, $\tan \theta$ is the singular value of $T = X_{\perp}^H Y (X^H Y)^{-1}$. If $\theta = \pi/2$, then the matrix $X^H Y$ is singular in this example. Moreover, if $\dim \mathcal{X} \neq \dim \mathcal{Y}$ the matrix $X^H Y$ is rectangular, so we use its Moore-Penrose pseudoinverse to form our matrix $T = X_{\perp}^H Y (X^H Y)^{\dagger}$. Now we are ready to prove our first main result.

Theorem 3.1. Let $[X, X_{\perp}]$ be a unitary matrix with $X \in \mathbb{C}^{n \times p}$. Let $Y \in \mathbb{C}^{n \times q}$

- (i) have orthonormal columns, or
- (ii) be such that $\text{rank}(Y) = \text{rank}(X^H Y)$, where $\text{rank}(X^H Y) \leq p$.

Then the positive singular values of the matrix $T = X_{\perp}^H Y (X^H Y)^{\dagger}$ satisfy

$$\tan \Theta(\mathcal{X}, \mathcal{Y}) = [\infty, \dots, \infty, S_+(T), 0, \dots, 0], \quad (2)$$

with $\min(\dim(\mathcal{X}^{\perp} \cap \mathcal{Y}), \dim(\mathcal{X} \cap \mathcal{Y}^{\perp})) \infty$'s and $\dim(\mathcal{X} \cap \mathcal{Y})$ zeros, where we denote $\mathcal{R}(X) = \mathcal{X}$ and $\mathcal{R}(Y) = \mathcal{Y}$.

In case (ii), $\min(\dim(\mathcal{X}^{\perp} \cap \mathcal{Y}), \dim(\mathcal{X} \cap \mathcal{Y}^{\perp})) = 0$.

Proof. (1) On the one hand, from equality (1), we obtain

$$T = X_{\perp}^H Y (X^H Y)^{\dagger} = U_2 \begin{bmatrix} O & & \\ & SC^{-1} & \\ & & O \end{bmatrix} U_1^H,$$

Hence, $S_+(T) = [\tan(\theta_{j_1}), \dots, \tan(\theta_{j_s})]$, where $0 < \theta_{j_1} \leq \dots \leq \theta_{j_s} < \pi/2$. On the other hand, from (1) we get $S(X^H Y) = S(\text{diag}(I, C, O))$, where the identity block is r -by- r and the zero block is $(p-r-s)$ -by- $(q-r-s)$. By Theorem 2.1, $\Theta(\mathcal{R}(X), \mathcal{R}(Y)) = [0, \dots, 0, \theta_{j_1}, \dots, \theta_{j_s}, \pi/2, \dots, \pi/2]$, where there are $r = \dim \mathcal{X} \cap \mathcal{Y}$ zeros and $\min(q-r-s, p-r-s) = \min(\dim \mathcal{X}^{\perp} \cap \mathcal{Y}, \dim \mathcal{X} \cap \mathcal{Y}^{\perp})$ values $\pi/2$.

(2) Let us denote the rank of Y be t , thus $t \leq p$. Let the SVD of Y be $U \Sigma V^H$, where U is an $n \times n$ unitary matrix and V is a $q \times q$ unitary matrix; Σ is an $n \times q$ real diagonal matrix with diagonal entries ordered by decreasing magnitude. Since $\text{rank}(Y) = t \leq q$, we can get a reduced SVD such that $Y = U_t \Sigma_t V_t^H$. Only the t column vectors of U and the t row vectors of V^H , corresponding to nonzero singular values are used, which means that Σ_t is a t -by- t invertible diagonal matrix. Based on the fact that the left singular vectors corresponding to the non-zero singular values of Y span the range of Y , $\tan \Theta(\mathcal{R}(X), \mathcal{R}(Y)) = \tan \Theta(\mathcal{R}(X), \mathcal{R}(U_t))$. Since $\text{rank}(X^H Y) = t$, we have $\text{rank}(X^H U_t \Sigma_t) = \text{rank}(X^H U_t) = t$. Let $T_1 = X_{\perp}^H U_t (X^H U_t)^{\dagger}$. We have $\tan \Theta(\mathcal{R}(X), \mathcal{R}(U_t)) = [S_+(T_1), 0, \dots, 0]$. It is worth

noting that the angles between $\mathcal{R}(X)$ and $\mathcal{R}(U_t)$ are in $[0, \pi/2)$, since $X^H U_t$ is full rank.

Our task is now to show that $T_1 = T$. By direct computation, we have

$$\begin{aligned}
 T &= X_{\perp}^H Y (X^H Y)^{\dagger} \\
 &= X_{\perp}^H U_t \Sigma_t V_t^H (X^H U_t \Sigma_t V_t^H)^{\dagger} \\
 &= X_{\perp}^H U_t \Sigma_t V_t^H (V_t^H)^{\dagger} (X^H U_t \Sigma_t)^{\dagger} \\
 &= X_{\perp}^H U_t \Sigma_t (X^H U_t \Sigma_t)^{\dagger} \\
 &= X_{\perp}^H U_t \Sigma_t \Sigma_t^{\dagger} (X^H U_t)^{\dagger} \\
 &= X_{\perp}^H U_t (X^H U_t)^{\dagger}.
 \end{aligned}$$

In two identities above we use the fact that if a matrix A is of full column rank, and a matrix B is of full row rank, then $(AB)^{\dagger} = B^{\dagger} A^{\dagger}$. Hence, $\tan \Theta(\mathcal{R}(X), \mathcal{R}(Y)) = [S_+(T), 0, \dots, 0]$ which completes the proof for the second case. \square

Remark 3.1. If $X^H Y$ has full rank, where Y may have non-orthonormal columns, we can alternatively prove Theorem 3.1 by constructing $Z = X + X_{\perp} T$ as in [19, Theorem 2.4, p.252] and [21, p.231-232]. Since $(X^H Y)^{\dagger} X^H Y = I$, the following identities $Y = P_{\mathcal{X}} Y + P_{\mathcal{X}^{\perp}} Y = X X^H Y + X_{\perp} X_{\perp}^H Y = Z X^H Y$ imply $\mathcal{R}(Y) \subseteq \mathcal{R}(Z)$. By direct calculation, we obtain that

$$X^H Z = X^H (X + X_{\perp} T) = I \text{ and } Z^H Z = (X + X_{\perp} T)^H (X + X_{\perp} T) = I + T^H T.$$

Thus, $X^H Z (Z^H Z)^{-1/2} = (I + T^H T)^{-1/2}$ is Hermitian positive definite. The matrix $Z (Z^H Z)^{-1/2}$ by construction has orthonormal columns which span the space \mathcal{Z} . Moreover, we observe that

$$S \left(X^H Z (Z^H Z)^{-1/2} \right) = (1 + S^2(T))^{-1/2}.$$

Therefore, $\tan \Theta(\mathcal{R}(X), \mathcal{R}(Z)) = [S_+(T), 0, \dots, 0]$ and $\dim(\mathcal{X}) = \dim(\mathcal{Z})$. By Theorem 3.1, $\tan \Theta_{(0, \pi/2)}(\mathcal{R}(X), \mathcal{R}(Y)) = \tan \Theta_{(0, \pi/2)}(\mathcal{R}(X), \mathcal{R}(Z))$, where all PABS in $(0, \pi/2)$ are denoted by $\Theta_{(0, \pi/2)}$. In other words, the angles in $(0, \pi/2)$ between subspaces $\mathcal{R}(X)$ and $\mathcal{R}(Y)$ are the same as those between subspaces $\mathcal{R}(X)$ and $\mathcal{R}(Z)$.

If $p = q$, we have that $\Theta(\mathcal{R}(X), \mathcal{R}(Y)) = \Theta(\mathcal{R}(X), \mathcal{R}(Z))$. We note that this approach also gives us the explicit expression $P = X_{\perp}^H Y (X^H Y)^{-1}$ for the matrix P with $S(P) = \tan \Theta(\mathcal{R}(X), \mathcal{R}(Y))$; cf. [19, Theorem 2.4, p.252] and [21, p.231-232].

Remark 3.2. For the case $Y^H Y \neq I$, the condition $\text{rank}(Y) = \text{rank}(X^H Y)$ is necessary in Theorem 3.1. For example, let

$$X = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \quad X_{\perp} = \begin{bmatrix} 0 & 0 \\ 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad \text{and} \quad Y = \begin{bmatrix} 1 & 1 \\ 0 & 1 \\ 0 & 0 \end{bmatrix}.$$

Then, we have $X^H Y = [1 \quad 1]$ and $(X^H Y)^{\dagger} = [1/2 \quad 1/2]^H$. Thus,

$$T = X_{\perp}^H Y (X^H Y)^{\dagger} = [1/2 \quad 0]^H, \quad \text{and} \quad s(T) = 1/2.$$

On the other hand, we obtain that $\tan \Theta(\mathcal{R}(X), \mathcal{R}(Y)) = 0$. From this example, we see that the result in Theorem 3.1 may fail in the case $\text{rank}(Y) > \text{rank}(X^H Y)$.

Due to the fact that PABS are symmetric, i.e., $\Theta(\mathcal{X}, \mathcal{Y}) = \Theta(\mathcal{Y}, \mathcal{X})$, the matrix T in Theorem 3.1 could be substituted with $Y_{\perp}^H X (Y^H X)^{\dagger}$, where $[Y, Y_{\perp}]$ is unitary. Moreover, the nonzero angles between the subspaces \mathcal{X} and \mathcal{Y} are the same as those between the subspaces \mathcal{X}^{\perp} and \mathcal{Y}^{\perp} . Hence, T can be presented as $X^H Y_{\perp} (X_{\perp}^H Y_{\perp})^{\dagger}$ and $Y^H X_{\perp} (Y_{\perp}^H X_{\perp})^{\dagger}$. Furthermore, for any matrix T , we have $S(T) = S(T^H)$, which implies that all conjugate transposes of T are admissible.

Let \mathcal{F} denote a family of matrices, such that the singular values of the matrix $T \in \mathcal{F}$ are the tangents of PABS. The arguments above show that any of the formulas for T in the first column of Table 1 can be used in Theorem 3.1, case (i).

Table 1. Different $T \in \mathcal{F}$ using orthonormal bases for \mathcal{X} , \mathcal{Y} , \mathcal{X}^{\perp} , and \mathcal{Y}^{\perp} , see Theorem 3.1, case (i); the top two rows also applicable to non-orthonormal basis for \mathcal{Y} if $q \leq p$, see Theorem 3.1, case (ii).

$X_{\perp}^H Y (X^H Y)^{\dagger}$	$P_{\mathcal{X}^{\perp}} Y (X^H Y)^{\dagger}$
$(Y^H X)^{\dagger} Y^H X_{\perp}$	$(Y^H X)^{\dagger} Y^H P_{\mathcal{X}^{\perp}}$
$Y_{\perp}^H X (Y^H X)^{\dagger}$	$P_{\mathcal{Y}^{\perp}} X (Y^H X)^{\dagger}$
$X^H Y_{\perp} (X_{\perp}^H Y_{\perp})^{\dagger}$	$P_{\mathcal{X}} Y_{\perp} (X_{\perp}^H Y_{\perp})^{\dagger}$
$Y^H X_{\perp} (Y_{\perp}^H X_{\perp})^{\dagger}$	$P_{\mathcal{Y}} X_{\perp} (Y_{\perp}^H X_{\perp})^{\dagger}$
$(X^H Y)^{\dagger} X^H Y_{\perp}$	$(X^H Y)^{\dagger} X^H P_{\mathcal{Y}^{\perp}}$
$(Y_{\perp}^H X_{\perp})^{\dagger} Y_{\perp}^H X$	$(Y_{\perp}^H X_{\perp})^{\dagger} Y_{\perp}^H P_{\mathcal{X}}$
$(X_{\perp}^H Y_{\perp})^{\dagger} X_{\perp}^H Y$	$(X_{\perp}^H Y_{\perp})^{\dagger} X_{\perp}^H P_{\mathcal{Y}}$

Using the fact that the singular values are invariant under unitary multiplications, we can also use $P_{\mathcal{X}^{\perp}} Y (X^H Y)^{\dagger}$ for T in Theorem 3.1, where $P_{\mathcal{X}^{\perp}}$ is an

orthogonal projector onto the subspace \mathcal{X}^\perp . Thus, every matrix $T \in \mathcal{F}$ in the first column has its analog in \mathcal{F} as in the second column in Table 1, where, again, $P_{\mathcal{X}}$, $P_{\mathcal{Y}}$, and $P_{\mathcal{Y}^\perp}$ denote the orthogonal projectors onto the subspace \mathcal{X} , \mathcal{Y} , and \mathcal{Y}^\perp , correspondingly.

Finally, if $Y^H Y \neq I$ and $\text{rank}(Y) = \text{rank}(X^H Y) \leq p$, Theorem 3.1, case (ii) holds. Using the above arguments, we see that any matrix T in the top two rows in Table 1 belongs to the family \mathcal{F} under these assumptions.

Remark 3.3. From the proof of Theorem 3.1 case (i), we immediately derive $X_\perp^H Y (X^H Y)^\dagger = -(Y_\perp^H X_\perp)^\dagger Y_\perp^H X$, and $Y_\perp^H X (Y^H X)^\dagger = -(X_\perp^H Y_\perp)^\dagger X_\perp^H Y$, which demonstrates that some entries in Table 1 differ from each other only by a sign.

Now we show that some of the matrices $T \in \mathcal{F}$ in Table 1 result in singular values $S(T)$ that also match the multiplicity of zeros in Theorem 3.1 case (ii).

Corollary 3.1. Using the notation of Theorem 3.1, let Y be full rank and $p = q$. Let $P_{\mathcal{X}^\perp}$ be an orthogonal projection onto the subspace $\mathcal{R}(X_\perp)$. Then we have $\tan \Theta(\mathcal{R}(X), \mathcal{R}(Y)) = S \left(P_{\mathcal{X}^\perp} Y (X^H Y)^{-1} \right)$.

Proof. Theorem 3.1 case (ii) involves no ∞ 's and, since Y is full rank and $p = q$, the matrix $X^H Y$ is invertible. Moreover, the number of the singular values of $P_{\mathcal{X}^\perp} Y (X^H Y)^{-1}$ is $p = q$, which is the same as the number of PABS in this case. \square

The tangents of PABS also describe properties of blocks of the triangular matrix from the QR factorization of a basis of the subspace $\mathcal{X} + \mathcal{Y}$. For brevity of presentation, we make simplifying assumptions on X and Y , avoiding the rank-revealing QR.

Corollary 3.2. Let $X \in \mathbb{C}^{n \times p}$ and $Y \in \mathbb{C}^{n \times q}$ with $q \leq p$ be matrices of full rank, and also let $X^H Y$ be full rank. Let the QR factorization of $[X \ Y]$ be

$$[X \ Y] = [Q \ Q_\perp] \begin{bmatrix} R_{11} & R_{12} \\ O & R_{22} \end{bmatrix},$$

where $Q \in \mathbb{C}^{n \times p}$ and $Q_\perp \in \mathbb{C}^{n \times (n-p+1)}$. Then

$$\tan \Theta(\mathcal{R}(X), \mathcal{R}(Y)) = [S_+(R_{22}(R_{12})^\dagger), 0, \dots, 0]$$

with $\dim(\mathcal{R}(X) \cap \mathcal{R}(Y))$ zeros.

Proof. Clearly, $X = QR_{11}$ and $Y = QR_{12} + Q_{\perp}R_{22}$. Since X has full rank, we have $\mathcal{R}(Q) = \mathcal{X}$ and R_{11} is invertible. Multiplying by Q^H on both sides of equality for Y , we get $R_{12} = Q^HY$. Moreover, $\text{rank}(Q^HY) = \text{rank}(X^HY) = \text{rank}(Y)$, since R_{11} is invertible and $X^HY = R_{11}^HQ^HY$. Multiplying the equality $Y = QR_{12} + Q_{\perp}R_{22}$ by Q_{\perp}^H gives $R_{22} = Q_{\perp}^HY$ and $R_{22}(R_{12})^{\dagger} = Q_{\perp}^HY(Q^HY)^{\dagger}$. Theorem 3.1 case (ii) holds with $[Q \ Q_{\perp}]$ substituting for $[X \ X_{\perp}]$, since we have $\text{rank}(Q^HY) = \text{rank}(Y) = p$. \square

4 $\tan \Theta$ in terms of projections onto subspaces

In the previous section, we rely on bases of subspaces to construct $T \in \mathcal{F}$. Now, we pursue a more basic geometric approach, representing subspaces by using orthogonal and oblique projectors, rather than matrices of their bases.

Theorem 4.1. Let $P_{\mathcal{X}}$, $P_{\mathcal{X}^{\perp}}$ and $P_{\mathcal{Y}}$ be orthogonal projectors onto the subspaces \mathcal{X} , \mathcal{X}^{\perp} and \mathcal{Y} , correspondingly. Then the positive singular values $S_+(T)$ of the matrix $T = P_{\mathcal{X}^{\perp}}(P_{\mathcal{X}}P_{\mathcal{Y}})^{\dagger}$ satisfy $\tan \Theta(\mathcal{X}, \mathcal{Y}) = [\infty, \dots, \infty, S_+(T), 0, \dots, 0]$, where there are $\min(\dim(\mathcal{X}^{\perp} \cap \mathcal{Y}), \dim(\mathcal{X} \cap \mathcal{Y}^{\perp}))$ ∞ 's and $\dim(\mathcal{X} \cap \mathcal{Y})$ zeros.

Proof. Let the matrices $[X \ X_{\perp}]$ and $[Y \ Y_{\perp}]$ be unitary, where $\mathcal{R}(X) = \mathcal{X}$ and $\mathcal{R}(Y) = \mathcal{Y}$. By direct calculation, we obtain

$$P_{\mathcal{X}}P_{\mathcal{Y}} = [X \ X_{\perp}] \begin{bmatrix} X^HY & O \\ O & O \end{bmatrix} \begin{bmatrix} Y^H \\ Y_{\perp}^H \end{bmatrix}. \quad (3)$$

Using properties of the Moore-Penrose pseudoinverse, reviewed in Section 2, we have

$$(P_{\mathcal{X}}P_{\mathcal{Y}})^{\dagger} = [Y \ Y_{\perp}] \begin{bmatrix} (X^HY)^{\dagger} & O \\ O & O \end{bmatrix} \begin{bmatrix} X^H \\ X_{\perp}^H \end{bmatrix}, \quad (4)$$

therefore

$$T = P_{\mathcal{X}^{\perp}}(P_{\mathcal{X}}P_{\mathcal{Y}})^{\dagger} = [P_{\mathcal{X}^{\perp}}Y(X^HY)^{\dagger} \quad O] \begin{bmatrix} X^H \\ X_{\perp}^H \end{bmatrix}.$$

Thus, $S_+(T) = S_+(P_{\mathcal{X}^{\perp}}Y(X^HY)^{\dagger})$, but the latter matrix is in Table 1. \square

Remark 4.1. We note that the null space of the product $P_{\mathcal{X}}P_{\mathcal{Y}}$ is the orthogonal sum $\mathcal{Y}^{\perp} \oplus (\mathcal{Y} \cap \mathcal{X}^{\perp})$. Thus, its orthogonal complement, $\mathcal{Y} \cap (\mathcal{Y} \cap \mathcal{X}^{\perp})^{\perp}$, is thus

the range of $(P_{\mathcal{X}}P_{\mathcal{Y}})^{\dagger}$, which implies $P_{\mathcal{Y}}(P_{\mathcal{X}}P_{\mathcal{Y}})^{\dagger} = (P_{\mathcal{X}}P_{\mathcal{Y}})^{\dagger} = (P_{\mathcal{X}}P_{\mathcal{Y}})^{\dagger}P_{\mathcal{X}}$ and so $((P_{\mathcal{X}}P_{\mathcal{Y}})^{\dagger})^2 = (P_{\mathcal{X}}P_{\mathcal{Y}})^{\dagger}P_{\mathcal{X}}P_{\mathcal{Y}}(P_{\mathcal{X}}P_{\mathcal{Y}})^{\dagger} = (P_{\mathcal{X}}P_{\mathcal{Y}})^{\dagger}$. Therefore, we conclude that $(P_{\mathcal{X}}P_{\mathcal{Y}})^{\dagger}$ is simply an idempotent that projects on \mathcal{Y} along \mathcal{X}^{\perp} .

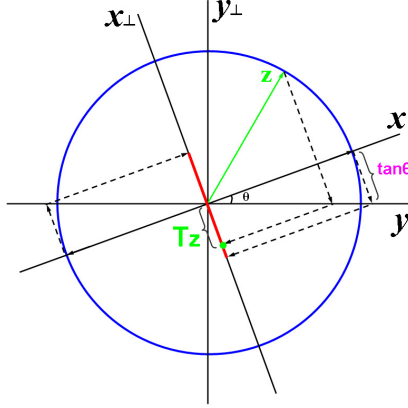


Figure 1. Geometrical meaning of $T = P_{\mathcal{X}^{\perp}}(P_{\mathcal{X}}P_{\mathcal{Y}})^{\dagger}$.

To gain geometrical insight into the action of T from Theorem 4.1 as a linear transformation, in Figure 1 we choose an arbitrary unit vector z . We project z onto \mathcal{Y} along \mathcal{X}^{\perp} , then project onto the subspace \mathcal{X}^{\perp} which is interpreted as Tz . The red segment in the graph is the image of T under all unit vectors. It is straightforward to see that $s(T) = \|T\| = \tan(\theta)$.

Using Property 2.1 and the fact that the principal angles are symmetric with respect to the subspaces \mathcal{X} and \mathcal{Y} , we observe that $P_{\mathcal{X}^{\perp}}(P_{\mathcal{X}}P_{\mathcal{Y}})^{\dagger}$ in Theorem 4.1 can alternatively be substituted with $P_{\mathcal{Y}^{\perp}}(P_{\mathcal{Y}}P_{\mathcal{X}})^{\dagger}$ or $P_{\mathcal{X}}(P_{\mathcal{X}^{\perp}}P_{\mathcal{Y}^{\perp}})^{\dagger}$. These expressions can be written in several forms, e.g., Remarks 4.1 implies

$$P_{\mathcal{X}^{\perp}}(P_{\mathcal{X}}P_{\mathcal{Y}})^{\dagger} = P_{\mathcal{X}^{\perp}}P_{\mathcal{Y}}(P_{\mathcal{X}}P_{\mathcal{Y}})^{\dagger} = (P_{\mathcal{Y}} - P_{\mathcal{X}})(P_{\mathcal{X}}P_{\mathcal{Y}})^{\dagger}.$$

From the proof of Theorem 4.1 we know that

$$P_{\mathcal{X}^{\perp}}(P_{\mathcal{X}}P_{\mathcal{Y}})^{\dagger} = [P_{\mathcal{X}^{\perp}}Y(X^HY)^{\dagger} \quad 0] \begin{bmatrix} X^H \\ X_{\perp}^H \end{bmatrix} = P_{\mathcal{X}^{\perp}}Y(X^HY)^{\dagger}X^H.$$

Similarly, we have $P_{\mathcal{X}}(P_{\mathcal{X}^{\perp}}P_{\mathcal{Y}^{\perp}})^{\dagger} = P_{\mathcal{X}}Y_{\perp}(X_{\perp}^HY_{\perp})^{\dagger}X_{\perp}^H$. Then Remark 3.3 implies $P_{\mathcal{X}^{\perp}}(P_{\mathcal{X}}P_{\mathcal{Y}})^{\dagger} = -\left(P_{\mathcal{X}}(P_{\mathcal{X}^{\perp}}P_{\mathcal{Y}^{\perp}})^{\dagger}\right)^H$. Using also Remark 4.1, we

derive

$$\begin{aligned}
 - \left(P_{\mathcal{X}^\perp} (P_{\mathcal{X}} P_{\mathcal{Y}})^\dagger \right)^H &= P_{\mathcal{X}} (P_{\mathcal{X}^\perp} P_{\mathcal{Y}^\perp})^\dagger \\
 &= P_{\mathcal{X}} P_{\mathcal{Y}^\perp} (P_{\mathcal{X}^\perp} P_{\mathcal{Y}^\perp})^\dagger \\
 &= (P_{\mathcal{Y}^\perp} - P_{\mathcal{X}^\perp}) (P_{\mathcal{X}^\perp} P_{\mathcal{Y}^\perp})^\dagger.
 \end{aligned}$$

Similar arguments justify the following chain of identities

$$\begin{aligned}
 - \left(P_{\mathcal{Y}} (P_{\mathcal{Y}^\perp} P_{\mathcal{X}^\perp})^\dagger \right)^H &= P_{\mathcal{Y}^\perp} (P_{\mathcal{Y}} P_{\mathcal{X}})^\dagger \\
 &= P_{\mathcal{Y}^\perp} P_{\mathcal{X}} (P_{\mathcal{Y}} P_{\mathcal{X}})^\dagger \\
 &= (P_{\mathcal{X}} - P_{\mathcal{Y}}) (P_{\mathcal{Y}} P_{\mathcal{X}})^\dagger.
 \end{aligned}$$

This gives a variety of different possible choices of T in Theorem 4.1.

Some of the formulas above can be simplified using the following lemma.

Lemma 4.2. *Let $\Theta(\mathcal{X}, \mathcal{Y}) < \pi/2$. Then,*

- (i) *if $\dim(\mathcal{X}) \leq \dim(\mathcal{Y})$, we have $P_{\mathcal{X}}(P_{\mathcal{X}}P_{\mathcal{Y}})^\dagger = P_{\mathcal{X}}$;*
- (ii) *if $\dim(\mathcal{X}) \geq \dim(\mathcal{Y})$, we have $(P_{\mathcal{X}}P_{\mathcal{Y}})^\dagger P_{\mathcal{Y}} = P_{\mathcal{Y}}$.*

Proof. (1). According to Remark 4.1, we get $P_{\mathcal{X}}(P_{\mathcal{X}}P_{\mathcal{Y}})^\dagger = P_{\mathcal{X}}P_{\mathcal{Y}}(P_{\mathcal{X}}P_{\mathcal{Y}})^\dagger$. By the properties of the Moore-Penrose pseudoinverse, reviewed in Section 2, $P_{\mathcal{X}}P_{\mathcal{Y}}(P_{\mathcal{X}}P_{\mathcal{Y}})^\dagger$ is the orthogonal projector onto the range $\mathcal{R}(P_{\mathcal{X}}P_{\mathcal{Y}})$ of $P_{\mathcal{X}}P_{\mathcal{Y}}$. The transformation $P_{\mathcal{X}}P_{\mathcal{Y}}$, if restricted to \mathcal{X} , is invertible, since $\Theta(\mathcal{X}, \mathcal{Y}) < \pi/2$ and $\dim(\mathcal{X}) \leq \dim(\mathcal{Y})$; thus $\mathcal{R}(P_{\mathcal{X}}P_{\mathcal{Y}}) = \mathcal{R}(P_{\mathcal{X}})$, which completes the proof of the first part.

Similarly, in part (2), $(P_{\mathcal{X}}P_{\mathcal{Y}})^\dagger P_{\mathcal{Y}} = (P_{\mathcal{X}}P_{\mathcal{Y}})^\dagger P_{\mathcal{X}}P_{\mathcal{Y}}$ is the orthogonal projector onto the range $\mathcal{R}\left((P_{\mathcal{X}}P_{\mathcal{Y}})^\dagger\right) = \mathcal{R}(P_{\mathcal{Y}}P_{\mathcal{X}}) = \mathcal{R}(P_{\mathcal{Y}})$ since $\Theta(\mathcal{X}, \mathcal{Y}) < \pi/2$ and $\dim(\mathcal{Y}) \leq \dim(\mathcal{X})$. \square

Remark 4.3. From Lemma 4.2, for the case $\dim(\mathcal{X}) \leq \dim(\mathcal{Y})$ we have

$$P_{\mathcal{X}^\perp}(P_{\mathcal{X}}P_{\mathcal{Y}})^\dagger = (P_{\mathcal{X}}P_{\mathcal{Y}})^\dagger - P_{\mathcal{X}}(P_{\mathcal{X}}P_{\mathcal{Y}})^\dagger = (P_{\mathcal{X}}P_{\mathcal{Y}})^\dagger - P_{\mathcal{X}}.$$

Since the angles are symmetric, using the second statement in Lemma 4.2 we have $(P_{\mathcal{X}^\perp}P_{\mathcal{Y}^\perp})^\dagger P_{\mathcal{Y}} = (P_{\mathcal{X}^\perp}P_{\mathcal{Y}^\perp})^\dagger - P_{\mathcal{Y}^\perp}$.

On the other hand, for the case $\dim(\mathcal{X}) \geq \dim(\mathcal{Y})$ we obtain

$$(P_{\mathcal{X}}P_{\mathcal{Y}})^\dagger P_{\mathcal{Y}^\perp} = (P_{\mathcal{X}}P_{\mathcal{Y}})^\dagger - P_{\mathcal{Y}} \text{ and } (P_{\mathcal{X}^\perp}P_{\mathcal{Y}^\perp})^\dagger P_{\mathcal{X}} = (P_{\mathcal{X}^\perp}P_{\mathcal{Y}^\perp})^\dagger - P_{\mathcal{X}^\perp}.$$

Table 2. Choices for $T \in \mathcal{F}$ with $\Theta(\mathcal{X}, \mathcal{Y}) < \pi/2$: left for $\dim(\mathcal{X}) \leq \dim(\mathcal{Y})$; right for $\dim(\mathcal{X}) \geq \dim(\mathcal{Y})$.

$(P_{\mathcal{X}}P_{\mathcal{Y}})^{\dagger} - P_{\mathcal{X}}$	$(P_{\mathcal{X}}P_{\mathcal{Y}})^{\dagger} - P_{\mathcal{Y}}$
$(P_{\mathcal{X}^{\perp}}P_{\mathcal{Y}^{\perp}})^{\dagger} - P_{\mathcal{Y}^{\perp}}$	$(P_{\mathcal{X}^{\perp}}P_{\mathcal{Y}^{\perp}})^{\dagger} - P_{\mathcal{X}^{\perp}}$

To sum up, the following formulas for T in Table 2 can also be used in Theorem 4.1. An alternative proof for $T = (P_{\mathcal{X}}P_{\mathcal{Y}})^{\dagger} - P_{\mathcal{Y}}$ is provided by Drmač in [5] for the particular case $\dim(\mathcal{X}) = \dim(\mathcal{Y})$.

Our choice of the space $\mathcal{H} = \mathbb{C}^n$ may appear natural to the reader familiar with the matrix theory, but in fact is somewhat misleading. The principal angles (and the corresponding principal vectors) between the subspaces $\mathcal{X} \subset \mathcal{H}$ and $\mathcal{Y} \subset \mathcal{H}$ are exactly the same as those between the subspaces $\mathcal{X} \subset \mathcal{X} + \mathcal{Y}$ and $\mathcal{Y} \subset \mathcal{X} + \mathcal{Y}$, i.e., we can reduce the space \mathcal{H} to the space $\mathcal{X} + \mathcal{Y} \subset \mathcal{H}$ without changing PABS. This reduction changes the definition of the subspaces \mathcal{X}^{\perp} and \mathcal{Y}^{\perp} and, thus, of the matrices X_{\perp} and Y_{\perp} that column-span the subspaces \mathcal{X}^{\perp} and \mathcal{Y}^{\perp} . All our statements that use the subspaces \mathcal{X}^{\perp} and \mathcal{Y}^{\perp} or the matrices X_{\perp} and Y_{\perp} therefore have their new analogs, if the space $\mathcal{X} + \mathcal{Y}$ substitutes for \mathcal{H} . The formulas $P_{\mathcal{X}^{\perp}} = I - P_{\mathcal{X}}$ and $P_{\mathcal{Y}^{\perp}} = I - P_{\mathcal{Y}}$, look the same, but the identity operators are different in the spaces $\mathcal{X} + \mathcal{Y}$ and \mathcal{H} .

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