On the Cone of Positive Semidefinite Matrices

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ABSTRACT

A survey of some general properties of the cone of positive semidefinite matrices, its faces, two isometric isomorphisms, and linear transformations on it is given.

I. INTRODUCTION

In recent years an impressive body of literature in linear algebra has been developed in the area of cones. In his "Theory of Cones" [1] Barker gives a survey of interrelationships among the geometric properties of, face lattices of, and order preserving linear maps on general cones. He closes with a short section on the cone PSD of positive semidefinite matrices.

This paper is an extension of that paper; it is a survey of the general properties of PSD, the faces of PSD, (two) isometric isomorphisms for PSD, and linear transformations on PSD.

Let V be a finite dimensional real or complex vector space with $L(V)$ the space of all linear transformations on V. A subset $K \subseteq V$ is said to be a cone iff $x, y \in K$, $\alpha, \beta \geqslant 0$ implies that $\alpha x + \beta y \in K$. A cone K is said to be pointed iff $K \cap (-K) = \{0\}$; full iff the (topological) interior of K is nonempty; and reproducing iff $\operatorname{span} K = V$.

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A pointed cone in K induces a partial order if we define $x \leqslant y$ by $y - x \in K$. A subset $F \subseteq K$ is said to be a face iff F is a subcone of K such that $0 \leqslant x \leqslant y$ and $y \in F$ imply $x \in F$. An extremal of K is a face E of dimension one (i.e., span E is of dimension one as a subspace of V). In an inner product space, the dual cone of K is defined as $K^* = \{x \in V \mid \mathrm{re}(x, y) \geqslant 0 \text{ for all } y \in K\}$. Also, $\pi(K) = \{T \in L(V) \mid T(K) \subseteq K\}$ and $\pi(K_1, K_2) = \{T \in L(V, W) \mid T(K_1) \subseteq K_2\}$, where K_1 and K_2 are cones in the vector spaces V and W respectively.

A matrix A is said to be positive semidefinite (definite) iff A is hermitian with all eigenvalues nonnegative (positive). For equivalent formulations see [9] or [10]. The set of all n by n positive semidefinite (definite) matrices will be represented by PSD (PD) in both of its usual ambient spaces, viz., $M_n = M_n(\mathbb{C})$, the complex space of n by n matrices over $\mathbb{C}$, and $\mathscr{H}_n$, the real space of all hermitian matrices in M_n. Finally $\mathscr{H}\mathscr{P}_{n,q}$ and $\mathscr{C}\mathscr{P}_{n,q}$ will denote the cones of hermitian preserving and completely positive maps in $L(M_n, M_q)$, with the second subscript suppressed whenever $n = q$.

II. GENERAL PROPERTIES OF PSD

In Table 1 we list some of the basic cone properties of PSD with respect to its two standard ambient spaces. A few remarks on these properties:

(1) Berman and Ben Israel [6, p. 142] and Berman [5, p. 55] show that PSD is self-dual in $\mathscr{H}_n$.

(2) Since $iI \notin$ PSD but $iI \in$ PSD*, PSD is *not* self-dual in M_n. Further, there is no $A \in$ PSD such that $\mathrm{re}(A, iI) > 0$. Hence, int $PSD = \phi$ in M_n.

(3) The set $\{E_{ii} \mid i = 1, \ldots, n\} \cup \{E_{ii} + E_{jj} + E_{ij} + E_{ji} \mid i < j;\ i, j = 1, \ldots, n\} \cup \{E_{ii} + E_{jj} + \iota E_{ij} - \iota E_{ji} \mid i < j;\ i, j = 1, \ldots, n\}$ is a subset of PSD

TABLE 1

Property	Ambient space: $\mathscr{H}_n$ over $\mathbb{R}$	$M_n(\mathbb{C})$ over $\mathbb{C}$
Cone	Yes	Yes
Pointed	Yes	Yes
Closed	Yes	Yes
Self-dual	Yes	No
Full	Yes	No
Reproducing	Yes	Yes
Polyhedral	No	No
Simplicial	No	No
Interior PSD	PD	Empty set

which is a basis for both the real space $\mathscr{H}_n$ and the complex space M_n. Thus, PSD is reproducing in both $\mathscr{H}_n$ and M_n.

(4) A discussion of some interesting results concerning PD is given by Taussky in [15] and [16].

III. FACES OF PSD

If S is a subset of a cone K, then $\Phi(S)$ will denote the smallest face of K containing S; $\Phi(S) = \bigcap\{F \lhd K \mid S \subseteq F\}$.

Let $\mathscr{O}_n$ be the set of orthogonal projections, i.e., $A \in \mathscr{O}_n$ iff $A \in \mathscr{H}_n$ and $A^2 = A$. With the usual order on projections, viz., $A \leqslant B$ iff $\operatorname{Rng} A \subseteq \operatorname{Rng} B$, and $A \wedge B$ and $A \vee B$ defined to be the orthogonal projections onto $\operatorname{Rng} A \cap \operatorname{Rng} B$ and $\operatorname{Rng} A + \operatorname{Rng} B$ respectively, $\mathscr{O}_n$ is a lattice isomorphic to both the lattice of all subspaces of $\mathbb{C}^n$ and the face lattice $F(\mathrm{PSD})$. Barker and Carlson [2, p. 29] give us

THEOREM 3.1. *The map from $\mathscr{O}_n$ to $F(\mathrm{PSD})$ given by $A \mapsto \Phi(A)$ is an order preserving lattice isomorphism.*

Barker and Carlson [2] have characterized the minimal face containing a positive semidefinite matrix as follows:

THEOREM 3.2. *Let $A, B \in \mathrm{PSD}$. Then*

$$B \in \Phi(A) \quad \textit{iff} \quad \mathscr{N}(B) \supseteq \mathscr{N}(A) \quad \textit{iff} \quad \operatorname{Rng} A \subseteq \operatorname{Rng} B$$

and

$$\Phi(A) = \Phi(B) \quad \textit{iff} \quad \mathscr{N}(A) = \mathscr{N}(B) \quad \textit{iff} \quad \operatorname{Rng} A = \operatorname{Rng} B.$$

Further, Barker and Schneider [4, *p.* 224] *give the following characterization for a face of any cone, which we specialize to PSD:*

THEOREM 3.3. *Let $F \in \mathscr{F}(\mathrm{PSD})$. Then $F = \Phi(A)$ iff $A \in F^{\Delta}$, the relative interior of F.*

We are led to a new characterization. (Note that $A^{(i)}$ denotes the ith column of A.)

THEOREM 3.4. *Every face of* PSD *is of the form*

$$F_X = \{A \in \mathrm{PSD} \mid A^{(i)} \in X^{\perp},\ i = 1, \ldots, n\}$$

where X is a subspace of $\mathbb{C}^n$. Conversely, given a subspace $X \subseteq \mathbb{C}^n$, F_X is a face of PSD.

Proof. Let $F \in \mathscr{F}(\mathrm{PSD})$. By Theorem 3.3, $F = \Phi(B)$ for some (any) $B \in F^{\Delta}$. Let $X = \mathscr{N}(B)$. By Theorem 3.2, $A \in F$ iff $\mathscr{N}(A) \supseteq X$ iff $Ax = 0$ for all $x \in X$ iff $A^{(i)} \in X^{\perp}$, $i = 1, \ldots, n$. Thus, $F = F_X$.

Given a subspace $X \subseteq \mathbb{C}^n$, $X = \mathscr{N}(B)$ for some projection B, which is *a priori* in PSD. We have that $F_X = \Phi(B)$ is a face of PSD. ∎

Since $\mathscr{N}(\Sigma_{i \in M} E_{ii}) = \mathrm{span}\{e_j \mid j \notin M\}$, where $\{e_j\}$ is the standard ordered basis for $\mathbb{C}^n$, we have

COROLLARY 3.5. *If $M \subseteq \{1, \ldots, n\}$, then*

$$\Phi\Big(\sum_{i \in M} E_{ii}\Big) = \{A \in \mathrm{PSD} \mid a_{jk} = 0 \text{ if } (j,k) \notin M \times M\}.$$

This result immediately specializes to $\Phi(I) = \mathrm{PSD}$ and $\Phi(\Sigma_{i \in \{1, \ldots, r\}} E_{ii}) = \mathrm{PSD}_r \oplus 0_{n-r}$.

Our next result includes the fact that all faces of PSD are isomorphic to PSD_r for some $0 \leqslant r \leqslant n$. Also see Schneider [12, p. 13].

THEOREM 3.6. *If $B \in \mathrm{PSD}$ is of rank r, then there exists a unitary U such that $\Phi(B) = U(PSD_r \oplus 0_{n-r})U^*$ (yielding a natural isomorphism between $\Phi(B)$ and PSD_r). Conversely, if U is unitary, then $U(PSD_r \oplus 0_{n-r})U^*$ is a face of* PSD_n, $r = 0, \ldots, n$.

Proof. Let $B \in \mathrm{PSD}$ be of rank r. By Theorem 3.3 $\Phi(B) = \{A \in \mathrm{PSD} \mid \mathrm{Rng}\, A \subseteq \mathrm{Rng}\, B\}$. Letting $\hat{\mathscr{B}} = \{b_1, \ldots, b_r\}$ be an orthonormal basis for $\mathrm{Rng}\, B$, we extend it to an orthonormal basis for $\mathbb{C}^n$, say $\mathscr{B} = \{b_1, \ldots, b_r, \ldots, b_n\}$. Letting $U = (b_1 \ \cdots \ b_n) \in M_n(\mathbb{C})$, U is unitary, and the representation of A with respect to $\mathscr{B}$ is $U^*AU = \hat{A}$. Since $\mathrm{Rng}\, A \subseteq \mathrm{Rng}\, B$, $Ax \in \mathrm{span}\, \hat{\mathscr{B}}$ for all $x \in \mathbb{C}^n$; hence for the last $n - r$ rows of $\hat{A}$ we have $\hat{A}_{(r+1)} = \cdots = \hat{A}_{(n)} = 0$. Since $\hat{A} \in \mathscr{H}_n$, we also have the columns $\hat{A}^{(r+1)} = \cdots = \hat{A}^{(n)} = 0$; thus $A \in \mathrm{PSD}_r \oplus 0_{n-r}$.

Now if $U^*AU \in \mathrm{PSD}_r \oplus 0_{n-r}$, then $\mathrm{Rng}\, A \subseteq \mathrm{Rng}\, B$, which implies that $A \in \Phi(B)$. Thus, $U^*\Phi(B)U = PSD_r \oplus O_{n-r}$.

Conversely, let unitary U be given and let P_r be the orthogonal projection onto $\operatorname{span}\{U^{(1)},\dots,U^{(r)}\}$, $r=0,\dots,n$. As above, we have that $U(\mathrm{PSD}_r\oplus 0_{n-r})U^* = \Phi(P_r)$, a face of PSD. ■

This immediately resolves the question of which nonnegative integers are the dimensions of (all) faces of PSD.

COROLLARY 3.7. *All faces of* PSD_n *have dimension* k^2 *for some* $0\leqslant k\leqslant n$.

The extremals (dimension one faces) of PSD have been described by Barker and Carlson [2]. We further characterize them as follows:

THEOREM 3.8. *The following are equivalent*:

(i) $\Phi(A)$ *is an extremal in* PSD.
(ii) *For some* $\alpha>0$, αA *is a rank* 1 *hermitian projection.*
(iii) $A\in\mathscr{H}_n$ *has one positive eigenvalue and* $n-1$ *zero eigenvalues.*
(iv) *For some* $\alpha>0$, $\alpha A = xx^*$ *where* x *is an eigenvector of* A.

Proof. Corollary 4 of Barker and Carlson [2] gives us (i) $\leftrightarrow$ (ii). Clearly (ii) $\Rightarrow$ (iii). Conversely, let A satisfy (iii). Then there exists a basis of $\mathbb{C}^n$, say $\{x_1,\dots,x_n\}$, such that $Ax_1=\alpha x_1$, where $\|x_1\|^2=\alpha>0$ and $Ax_i=0x_i=0$, $i=2,\dots,n$. Then $A=x_1x_1^*$ is easily shown to be a rank 1 projection. Finally, (iv) is contained in (iii) $\Rightarrow$ (ii); (iv) $\Rightarrow$ (ii) is immediate. ■

In a pointed semiring C of linear transformations a (left, right) ideal which is also a face is said to be a (left, right) facial ideal. Tam [14] gives a discussion of the facial ideals of $\pi(K)$ for any cone K. The faces of PSD are intimately related to the facial ideals of $\mathscr{C}\mathscr{P}_n$ (see Section IV of this paper) as follows (cf. [3, p. 226]):

THEOREM 3.9. *If* F,G *are faces in* PSD, *then* $\{\mathscr{T}\in\mathscr{C}\mathscr{P}_n\,|\operatorname{Rng}\mathscr{T}\subseteq\operatorname{span}F\}$ *is a right facial ideal in* $\mathscr{C}\mathscr{P}_n$, *and* $\{\mathscr{T}\in\mathscr{C}\mathscr{P}_n\,|\operatorname{Ker}\mathscr{T}\supseteq G\}$ *is a left facial ideal in* $\mathscr{C}\mathscr{P}_n$.

IV. LINEAR TRANSFORMATIONS ON PSD

A linear transformation $\mathscr{T}: M_n\to M_q$ is said to be completely positive iff $1_s\otimes\mathscr{T}$ is positive semidefinite preserving for all positive integers s, where $1_s\otimes\mathscr{T}: M_s(M_n)\to M_s(M_q)$ is defined by $1_s\otimes\mathscr{T}((A_{ij})_{1\leqslant i,j\leqslant s}) = (\mathscr{T}(A_{ij}))_{1\leqslant i,j\leqslant s}$. See [11] for a listing of characterizations.

Letting $\mathscr{CP}_{n,q}$ be the cone of all such completely positive maps, Barker, Hill, and Haertel [3, p. 223] give the following:

THEOREM 4.1. *The cones* $\mathscr{CP}_{n,q}$ *and* PSD_{nq} *are isometrically isomorphic.*

For further results on $\mathscr{CP}_{n,q}$ see Choi [7] or Poluikis and Hill [11]. We shall now give a different isometric isomorphism for PSD, which we shall use to characterize π(PSD). Toward this end we observe

LEMMA 4.2. *The map of* $\mathscr{H}_n$ *onto* $\mathbb{R}^{n^2}$ *given by* $H \to h$ *where* $H = (a_{ij})$ *and* $h = (a_{11}, \sqrt{2}\,\mathrm{Re}\,a_{12}, \sqrt{2}\,\mathrm{Im}\,a_{12}, \ldots, a_{22}, \sqrt{2}\,\mathrm{Re}\,a_{23}, \sqrt{2}\,\mathrm{Im}\,a_{23}, \ldots, a_{nn})^T$ *is an isometric isomorphism.*

Throughout this discussion we shall use the same Latin letter in upper and lower case to indicate this correspondence.

Note that for $n = 2$ our map is

$$\begin{pmatrix} a & b+ic \\ b-ic & d \end{pmatrix} \mapsto \begin{pmatrix} a \\ \sqrt{2}\,b \\ \sqrt{2}\,c \\ d \end{pmatrix}.$$

Now define $\mathscr{K} = \{h \in \mathbb{R}^{n^2} \mid H \in \mathrm{PSD}\} \subseteq \mathbb{R}^{n^2}$. Then we have

THEOREM 4.3. *The cones PSD and* $\mathscr{K}$ *are isometrically isomorphic.*

It is immediate that $\mathscr{K}$ is a closed, pointed, full, self-dual cone; F is a face of PSD iff $f = \{x \in \mathbb{R}^{n^2} \mid X \in F\}$ is a face of $\mathscr{K}$. Further, considering the standard ordered bases of $\mathscr{H}_n$ and $\mathbb{R}^{n^2}$, dyad products match up; i.e., $(Y \otimes_D Z)X \mapsto (yz^T)x$.

A classical problem in matrix theory has been to characterize those linear transformations which map PSD into PSD: the set π(PSD). Addressing this problem, we identify $\pi(\mathrm{PSD}) \subseteq L(\mathscr{H}_n)$ with $\pi(\mathscr{K}) \subseteq M_{n^2}(\mathbb{R})$.

A theorem of Tam [13, p. 281] immediately gives us the following characterization of the dual of π(PSD):

THEOREM 4.4. $\pi(PSD)^* = \{\Sigma Y_i \otimes_D Z_i \mid Y_i, Z_i \in \mathrm{PSD}\}$.

The $\pi(\mathscr{K})^* = \{\Sigma y_i z_i^T \mid y_i, z_i \in \mathscr{K}\}$ formulation for our $\mathscr{K}$ (it holds for a general $K \subseteq \mathbb{R}^n$) led us to the following theorem. Having it, a much quicker proof uses $K^* = K$ to show inclusion both ways.

THEOREM 4.5. $\pi(\mathscr{K}) = \{A \in M_{n^2}(\mathbb{R}) \mid y^T Ax \geqslant 0$ *for all* $y, z \in \operatorname{Ext} \mathscr{K}\}$.

This is really no stronger version of the result than $\pi(\mathscr{K}) = \{A \in M_{n^2}(\mathbb{R}) \mid y^T Az \geqslant 0$ for all $y, z \in \mathscr{K}\}$. [Note that we have characterized Ext(PSD) in Theorem 3.8.] Also, Theorem 4.5 reformulates as $\pi(\mathrm{PSD}) = \{\mathscr{T} \in \mathrm{HP} \mid (Y, \mathscr{T}(Z)) \geqslant 0$ for all $Y, Z \in \mathrm{PSD}\}$.

Since every bilinear functional on $\mathscr{H}_n$ can be represented by a matrix $A \in M_{n^2}(\mathbb{R})$ via $\mathscr{A}(X, Y) = x^T Ay$, Theorem 4.5 immediately translates to $\pi(\mathrm{PSD}) = \{\mathscr{A} \in \mathscr{H}_n \otimes \mathscr{H}_n \mid \mathscr{A}(X, Y) \geqslant 0$ for all $X, Y \in \mathrm{PSD}\}$, a formulation observed by Barker.

Given a sequence $\mathsf{H} = (H_1, \dots, H_n)$ of elements of $\mathscr{H}_n$, the smallest cone containing $\{(\operatorname{tr} H_1 P, \dots, \operatorname{tr} H_m P) \mid P \in \mathscr{B} \cap \mathrm{PSD}\}$, where $\mathscr{B}$ is the set of elements of norm 1, is said to be the joint angular field of values of $H_1, \dots, H_n$, denoted by $\mathscr{J}(\mathsf{H})$. Barker, Hill, and Haertel [3, p. 228] use this concept for the following characterization of positive semidefinite preserving:

THEOREM 4.6. *Let* $\mathsf{H} = \{H_i\}_{i=1}^m$ *and* $\mathsf{K} = \{K_i\}_{i=1}^m$ *be sequences in* $\mathscr{H}_n$ *and* $\mathscr{H}_m$ *respectively. Then* $\mathscr{B} = \sum H_i \otimes K_i \in \pi(\mathrm{PSD}_q, \mathrm{PSD}_n)$ *iff* $\mathscr{J}(\mathsf{H}) \subseteq \mathscr{J}(\mathsf{K})^*$ *or* $\mathscr{J}(\mathsf{K}) \subseteq \mathscr{J}(\mathsf{H})^*$.

The above two theorems characterize linear transformations which map PSD into itself. Schneider [12, p. 15] gives an analogous characterization for surjective maps:

THEOREM 4.7. *If* $\mathscr{T} \in \pi(\mathrm{PSD})$ *is onto, then there exists a nonsingular matrix A such that either* $\mathscr{T}(A) = AHA^*$ *or* $\mathscr{T}(A) = AH^TA^*$ *for all* $H \in \mathscr{H}_n$.

The relations among the cone of positive semidefinite preservers, its dual, and the completely positives are also given in [3], viz.,

THEOREM 4.8. $\pi(\mathrm{PSD}_n) \supseteq \mathscr{C}\mathscr{P}_n \supseteq \pi(\mathrm{PSD}_n)^*$, *and for* $n > 1$ *the inclusions are strict.*

DePillis [8, p. 136] gives the result that if $\mathscr{T} \in L(M_n)$, then there exist $\mathscr{A}_1, \mathscr{A}_2, \mathscr{A}_3, \mathscr{A}_4 \in \pi(\mathrm{PSD})$ such that $\mathscr{T} = (\mathscr{A}_1 - \mathscr{A}_2) + i(\mathscr{A}_3 - \mathscr{A}_4)$, i.e., $\pi(\mathrm{PSD})$ generates $L(M_n)$ in the same way that PSD generates M_n. Barker, Hill, and Haertel's Table 1 [3, p. 225] shows that this result holds for completely positive $\mathscr{A}_1, \dots, \mathscr{A}_4$. This table lists well-known generalizations of $\mathbb{R} \subset \mathbb{C}$ properties to $\mathscr{H}_n \subset M_n$ to third-stage generalizations of the hermitian preservers $\mathscr{H}\mathscr{P}_{n,q} \subset L(M_n, M_q)$.

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