The extreme rays of the 6×6 copositive cone

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Outline

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Copositive cone

Definition

A real symmetric $n \times n$ matrix A such that $x^T A x \geq 0$ for all $x \in \mathbb{R}^n_+$ is called copositive.

the set of all such matrices is a regular convex cone, the copositive cone $\mathcal{C}^n$

$(\mathcal{C}^n)^* = conv\{xx^T : x \in R^n_+\}$ - completely positive cone

the cone $\mathcal{C}^n$ is difficult to describe and has many applications in optimization

- graph stability number
- graph clique number
- graph chromatic number
- standard quadratic optimization problem
- quadratic programming
- convex quadratic underestimator over polytope
- mixed-integer programs

Standard Quadratic Optimization Problem

- min $x^T A x$
  s.t. $x \in \mathbb{R}^n_+, e^T x = 1$

  It's reformulation [Bomze et al.'00]:

- min $\langle A, X \rangle$
  s.t. $x \in \mathbb{R}^n_+, \langle E, X \rangle = 1, X \in (\mathcal{C}^n)^*$

Convex underestimation

- Find best convex quadratic underestimator:
  $g_P(x) = x^T A x + 2b^T x + c, A \in \mathcal{S}^n_+$ of non-convex functions
  $f(x) = x^T Q x$ over polytope $P = conv\{v_1, ..., v_n\}$
  s.t. $f(x) \geq g_P(x), \forall x \in P$.

  [Locatelli/Schoen '10]
- Can be reformulated as:
  $\min \langle E + I, X \rangle$
  s.t. $X = Q_P - U_P, X \in \mathcal{C}^n$,
  where $Q_P = V^T Q V$,
  $U_P = V^T A V + (V^T b)e^T + e(V^T b) + cE, A \in \mathcal{S}^n_+$

Graph clique number

Given an undirected graph $G = (V, E)$
Clique $S \subset V$ is maximal if S is not contained in a larger clique
Finding the clique number $w(G) = S_{max}$ is an NP-complete combinatorial optimization problem

- $w(G) = max\{S : S \text{ clique in } G\}$

  [Motzkin/Straus '65, Bomze et al.'00]
- $\frac{1}{w(G)} = min\{\langle Q_G, X\rangle : \langle E, X\rangle = 1, X \in (\mathcal{C}^n)^*\} =$
  $= max\{y \in \mathbb{R} : Q_G - yE \in \mathcal{C}^n\}, Q_G = E - A_G$

Reduce problem to line search.

Classical results

Exceptional copositive matrices

Related cones:

- completely positive cone $(\mathcal{C}^n)^*$
- sum $\mathcal{N}^n + \mathcal{S}_+^n$ of nonnegative and positive semi-definite cone
- doubly nonnegative cone $\mathcal{N}^n \cap \mathcal{S}_+^n$

$$(\mathcal{C}^n)^* \subset \mathcal{N}^n \cap \mathcal{S}_+^n \subset \mathcal{N}^n + \mathcal{S}_+^n \subset \mathcal{C}^n$$

the cones $\mathcal{N}^n$, $\mathcal{S}_+^n$ and their sum are semi-definite representable and hence easy to describe

Theorem (Diananda 1962)

For $n \leq 4$ the cones $\mathcal{C}^n$ and $\mathcal{N}^n + \mathcal{S}_+^n$ coincide.

Definition

A copositive matrix $A \in \mathcal{C}^n \setminus (\mathcal{N}^n + \mathcal{S}_+^n)$ is called exceptional.

exceptional copositive matrices exist for $n \geq 5$

Extreme rays

Definition

Let $K \subset \mathbb{R}^n$ be a regular convex cone. An non-zero element $u \in K$ is called extreme if it cannot be decomposed into a sum of other elements of K in a non-trivial manner. In other words, $u = v + w$ with $v, w \in K$ imply $v = \alpha u$, $w = \beta u$ for some $\alpha, \beta \geq 0$.
The conic hull of an extreme element is called extreme ray.

applications:

suppose $K \subset \mathcal{S}^n$ is an inner approximation of $\mathcal{C}^n$, i.e., $K \subset \mathcal{C}^n$
if all extreme rays of $\mathcal{C}^n$ are contained in K, then $K = \mathcal{C}^n$
knowledge of the extreme rays of $\mathcal{C}^n$ allows to test the exactness of inner approximations

Classical results

in [Hall, Newman 63] the extreme rays of $\mathcal{C}^n$ belonging to $\mathcal{N}^n + \mathcal{S}^n_+$ have been described:

- the extreme rays of $\mathcal{N}^n$: E_{ii} and $E_{ij} + E_{ji}$
- rank 1 matrices $A = xx^T$ with x having both positive and negative elements

- Baumert 1966: duplicating rows and columns allows to construct new extreme rays from known ones
- Hoffman, Pereira 1973: extreme rays of $\mathcal{C}^n$ with elements in $\{-1, 0, +1\}$

Reduced copositive matrices

Definition (Dickinson, Dür, Gijben, Hildebrand 2013)

A copositive matrix $A \in \mathcal{C}^n$ is called reduced with respect to a subset $\mathcal{M} \subset \mathcal{S}^n$ if it cannot be in a non-trivial manner represented as a sum $A = B + C$ with B copositive and $C \in \mathcal{M}$.

reducedness with respect to $\mathcal{N}^n$ and $\mathcal{S}_+^n$ is necessary for being exceptional extremal

reducedness with respect to $\mathcal{N}^n$

- Diananda 62: first studied
- Hall, Newman 63: reduced matrices satisfy $A_{ij} \leq \sqrt{A_{ii}A_{jj}}$
- Baumert 65: sufficient conditions

(Minimal) zero support sets

Definition (Baumert 65)

A non-zero nonnegative vector $u \in \mathbb{R}^n_+$ is called zero of $A \in \mathcal{C}^n$ if $u^T A u = 0$. The index set $\operatorname{supp} u = \{i \mid u_i > 0\}$ is called the support of u.
The set of supports of all zeros of A is called the zero support set (initially zero pattern) of A.

Definition

A zero u of a copositive matrix A is called minimal if there exists no zero v of A such that the inclusion $\operatorname{supp} v \subset \operatorname{supp} u$ holds strictly.
The set of supports of all minimal zeros of A is called the minimal zero support set of A.

the (minimal) zero support set is a subset of $2^{\{1,\dots,n\}}$

Scaling and Permutations

- the transformation $A \mapsto DAD$ preserves the copositive cone and the minimal zero support set of A, where D is diagonal matrix with strictly positive diagonal
- $A \in S^n$, permutation matrix $P \in \mathbb{R}^{n \times n}$. Then $A \mapsto PAP^T$ preserves the copositive cone and $\mathcal{V}^{PAP^T} = P\mathcal{V}^A$, where P permute elements of zeros.

Reducedness

Theorem (Dickinson, Dür, Gijben, Hildebrand 2013)

Let $A \in \mathcal{C}^n$, $n \geq 2$, and let $1 \leq i, j \leq n$. Then the following conditions are equivalent.

(i) *A is reduced with respect to E_{ij},*

(ii) *there exists a zero u of A such that $(Au)_i = (Au)_j = 0$ and $u_i + u_j > 0$.*

"zero" can be replaced with "minimal zero"

Theorem

A copositive matrix $A \in \mathcal{C}^n$ is reduced with respect to the cone $\mathcal{S}_+^n$ if and only if the linear span of the minimal zeros of A equals $\mathbb{R}^n$. Equivalently, the number of linearly independent minimal zeros equals n.

in particular, the number of minimal zero supports is at least n

Low dimensions

the number of equivalence classes (with respect to the action of S_n) of minimal zero support sets of matrices $A \in \mathcal{C}^n$ which satisfy all restrictions derived for reduced matrices is

- 0 for $n \leq 4$
- 2 for $n = 5$
- 44 for $n = 6$
- 12378 for $n = 7$

Extremal rays of $\mathcal{C}^5$

the two equivalence classes of minimal zero support sets have representatives

$$\{\{1,2\},\{2,3\},\{3,4\},\{4,5\},\{1,5\}\},$$

$$\{\{1,2,3\},\{2,3,4\},\{3,4,5\},\{1,4,5\},\{1,2,5\}\}$$

realized by the Horn matrix and the matrices

$$T(\psi) = \begin{pmatrix} 1 & -\cos\psi_4 & \cos(\psi_4+\psi_5) & \cos(\psi_2+\psi_3) & -\cos\psi_3 \\ -\cos\psi_4 & 1 & -\cos\psi_5 & \cos(\psi_5+\psi_1) & \cos(\psi_3+\psi_4) \\ \cos(\psi_4+\psi_5) & -\cos\psi_5 & 1 & -\cos\psi_1 & \cos(\psi_1+\psi_2) \\ \cos(\psi_2+\psi_3) & \cos(\psi_5+\psi_1) & -\cos\psi_1 & 1 & -\cos\psi_2 \\ -\cos\psi_3 & \cos(\psi_3+\psi_4) & \cos(\psi_1+\psi_2) & -\cos\psi_2 & 1 \end{pmatrix}$$

with $\psi_1,\dots,\psi_5 > 0$ and $\sum_{k=1}^5 \psi < \pi$

the Horn matrix is of the form $T(\psi)$ with $\psi = 0$

these correspond to the exceptional extreme rays of $\mathcal{C}_5$

The extreme rays of the 6×6 copositive cone

All cases

No.	No. in [17]	supp $\mathcal{V}^A_{\min}$
1	2	{1,2},{1,3},{1,4},{2,5},{3,6},{4,5,6}
2	3	{1,2},{1,3},{1,4},{2,5},{3,5,6},{4,5,6}
3	4	{1,2},{1,3},{1,4},{2,5,6},{3,5,6},{4,5,6}
4	5	{1,2},{1,3},{2,4},{3,4,5},{1,5,6},{4,5,6}
5	6	{1,2},{1,3},{1,4,5},{2,4,6},{3,4,6},{4,5,6}
6	8	{1,2},{1,3},{2,4,5},{3,4,5},{2,4,6},{3,5,6}
7	9	{1,5},{2,6},{1,2,3},{2,3,4},{3,4,5},{4,5,6}
8	13	{1,2},{1,3,4},{1,3,5},{2,4,6},{3,4,6},{2,5,6}
9	15	{1,2},{1,3,4},{1,3,5},{2,4,6},{3,4,6},{4,5,6}
10	16	{1,2},{1,3,4},{1,3,5},{2,4,6},{3,5,6},{4,5,6}
11	21	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{2,4,6},{3,4,6}
12	22	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{2,4,6},{3,5,6}
13	34	{1,2,3},{2,3,4},{3,4,5},{4,5,6},{1,5,6},{1,2,6}
14	36	{1,2},{1,3},{1,4},{2,5},{4,5},{3,6},{5,6}
15	37	{1,2},{1,3,4},{1,3,5},{1,4,6},{2,5,6},{3,5,6},{4,5,6}
16	41	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{2,4,6},{3,4,6},{3,5,6}
17	42	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{2,4,6},{3,5,6},{4,5,6}
18	43	{1,2,3},{2,3,4},{3,4,5},{1,4,5},{1,2,5},{3,4,6},{1,4,6},{1,2,6}
19	23	{3,4,5},{1,4,5},{1,2,5},{1,2,3},{1,5,6},{2,3,4,6}
20	1	{1,2},{1,3},{1,4},{2,5},{3,6},{5,6}
21	11	{1,2},{1,3,4},{1,3,5},{1,4,6},{2,5,6},{3,5,6}
22	12	{1,2},{2,3,4},{3,4,5},{4,5,6},{2,5,6},{2,3,6}
23	17	{1,2},{1,3,4},{2,3,5},{3,4,5},{2,4,6},{3,4,6}
24	24	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{3,4,6},{3,5,6}
25	25	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{3,4,6},{4,5,6}
26	28	{1,2,3},{1,2,4},{1,3,5},{2,4,5},{3,4,5},{2,3,6}
27	30	{1,2,3},{1,2,4},{1,3,5},{2,4,5},{3,4,6},{3,5,6}
28	32	{1,2,3},{1,2,4},{1,3,5},{2,4,5},{1,5,6},{4,5,6}
29	39	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{1,4,6},{2,5,6},{3,5,6}
30	7	{1,2},{1,3},{2,4,5},{3,4,5},{2,4,6},{3,4,6}
31	10	{1,2},{1,3,4},{1,3,5},{2,3,6},{3,4,6},{3,5,6}
32	14	{1,2},{1,3,4},{1,3,5},{2,4,6},{3,4,6},{3,5,6}
33	18	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{1,4,6},{1,5,6}
34	19	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{1,4,6},{2,5,6}
35	20	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{1,4,6},{3,5,6}
36	26	{1,2,3},{1,2,4},{1,3,5},{1,4,5},{2,3,6},{2,4,6}
37	27	{1,2,3},{1,2,4},{1,3,5},{1,4,5},{2,3,6},{3,4,6}
38	38	{1,2},{1,3,4},{1,3,5},{2,4,6},{3,4,6},{2,5,6},{3,5,6}
39	40	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{1,4,6},{3,5,6},{4,5,6}
40	44	{1,2,3},{1,2,4},{1,3,5},{1,4,5},{2,3,6},{2,4,6},{3,5,6},{4,5,6}
41	35	{1,2,3,4},{2,3,4,5},{3,4,5,6},{1,4,5,6},{1,2,5,6},{1,2,3,6}
42	33	{1,2,5},{1,4,5},{1,2,3},{3,4,5},{2,3,6},{3,4,6}
43	31	{1,2,5},{1,4,5},{1,2,3},{3,4,5},{1,3,6},{3,5,6}
44	29	{1,2,3},{1,2,4},{1,3,5},{2,4,5},{2,3,6},{2,5,6}

General algorithm

- Parametrization
- First order conditions
- Copositivity and absence of additional minimal zeros
- Extremality

Parametrization

- Diagonal elements of A are positive and normalized to 1 by $A \mapsto DAD$
- Hall and Newman: $A_{ij} = -\cos\phi_{ij}, \phi_{ij} \in [0, \pi], \forall i, j$.
- Zeros imposes conditions on the elements A_{ij}
- A_{ij} not covered by zeros are parameterized by $b_i \in [-1, 1]$.

Lemma

Let $A \in \mathcal{C}_n$ with $A_{ii} = 1$ for all i, and let $u \in \mathcal{V}^A_{\text{min}}$ with $\operatorname{supp} u = \{i, j\}$ for some indices $i, j \in \{1, \ldots, n\}$. Then $A_{ij} = -1$ and the two positive elements of u are equal.

Parametrization

Lemma

Let $A \in \mathcal{C}_n$ be extremal and $A_{ii} = 1$ for all i. Suppose $\{i,j\},\{j,k\} \in \operatorname{supp} \mathcal{V}^A_{\min}$, where i,j,k are mutually different indices. Then $A_{\{i,j,k\}}$ is a rank 1 positive semi-definite matrix with $A_{ik} = -A_{ij} = -A_{jk} = 1$.

Lemma

Let $A \in \mathcal{C}_n$ have unit diagonal and suppose there exists a minimal zero u of A with support $\{i,j,k\}$, where $i,j,k \in \{1,\dots,n\}$ are mutually different indices. Then the submatrix $A_{\{i,j,k\}}$ is given by

$$\begin{pmatrix} 1 & -\cos\phi_k & -\cos\phi_j \\ -\cos\phi_k & 1 & -\cos\phi_i \\ -\cos\phi_j & -\cos\phi_i & 1 \end{pmatrix},$$

where $\phi_i,\phi_j,\phi_k \in (0,\pi)$ and $\phi_i + \phi_j + \phi_k = \pi$. Moreover, there exists $\lambda > 0$ such that $\lambda u_{\{i,j,k\}} = (\sin\phi_i, \sin\phi_j, \sin\phi_k)^T$.

Linear dependency of minimal zeros

Reducedness of $A \in \mathcal{C}_n$ with respect to $\mathcal{S}^n_+$:

In cases 30-42 there is linear dependency of the minimal zeros, so this excludes the extremality

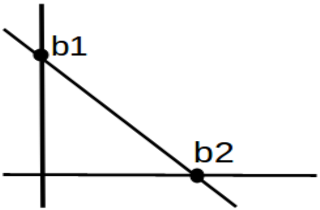
First order conditions

- If $u \in \mathcal{V}^A$, then $Au \geq 0$ and $(Au)_i$ is zero whenever $u_i > 0$
- Zeros imposes conditions on the elements A_{ij}
- b_i are expressed explicitly as a function of the angles ϕ_{ij}

First order conditions

Lemma

Let $\mathcal{I} \subset 2^{\{1,\dots,n\}}$ be an index set and let $A \in \mathcal{C}_n$ be an exceptional extremal copositive matrix such that $A_{ii} = 1$ for all i and such that $\operatorname{supp} \mathcal{V}^A_{\min} = \mathcal{I}$. Let $\mathcal{B}$ be the set of all matrices $B \in S^n$ such that $B_{ij} = A_{ij}$ for all elements A_{ij} covered by $\mathcal{I}$, and $Bu \geq 0$ for all minimal zeros $u \in \mathcal{V}^A_{\min}$.
Then A is an extremal element of the polyhedron $\mathcal{B}$. In particular, there exists a subset of equalities $(Au^j)_k = 0$ which determine the values of the uncovered elements of A uniquely.



Incompatibile F.O.C

In cases 43, 44 happens that first order conditions are incompatible constraints on the angles. There are no copositive matrices with the corresponding minimal zero support set.

Copositivity

Theorem

A matrix $A \in S^n$ is copositive if and only if for every non-empty index set $I \subset \{1, \ldots, n\}$, the submatrix A_I is copositive or there exists $v \in \mathbb{R}^n \setminus (-\mathbb{R}^n_+)$ with $\operatorname{supp} v \subseteq I \subseteq \operatorname{supp}_{\geq 0}(Av)$.

Copositivity

- For $|I| = \{1, 2\}, v = \sum_{i \in I} e_i$
- For I containing the support of a minimal zero u we may take $v = u$ and $|I| = \{5, 6\}$ turn always out to be supersets of a minimal zero support
- $|I| = 4$ we provide a vector v for each case individually

List of vectors

Case No.	Index subset	Certifying vectors v
1	$\{2,3,4,5\}$	$e_3 - e_2$
2	$\{2,3,4,5\}, \{2,3,4,6\}$	$e_3 - e_2, e_2 + e_6$
3	$\{2,3,4,5\}, \{2,3,4,6\}$	$e_2 + e_5, e_2 + e_6$
4	$\{2,3,5,6\}$	$e_5 + e_6$
5	$\{2,3,4,5\}, \{2,3,5,6\}$	$e_3 - e_2, e_2 - e_3$
6	$\{1,4,5,6\}$	$e_4 + e_5$
7	$\{1,3,4,6\}$	$e_3 + e_4$
8	$\{1,4,5,6\}, \{2,3,4,5\}$	$e_4 + e_6$, $e_3 + e_4$ $(\phi_1 \leq 2\phi_3)$ or $e_3 + e_5$ $(\phi_3 \leq 2\phi_1)$
9	$\{2,3,4,5\}, \{2,3,5,6\}$	$e_3 + e_4$, $e_5 + e_6$ (9.1) or $e_2 + e_6$ (9.2)
10	$\{2,3,4,5\}$	$e_3 + e_5$
11	$\{1,3,4,5\}, \{2,3,4,5\}$	$e_1 + e_3, e_2 + e_4$
	$\{1,4,5,6\}$	$\sin(\phi_6 - \phi_3)e_1 - \sin(\phi_2 + \phi_6)e_4 + \sin(\phi_2 + \phi_3)e_5$
	$\{2,3,5,6\}$	$\sin(\phi_1 + \phi_2 + \phi_6)e_2 - \sin\phi_6 e_3 + \sin(\phi_1 + \phi_2)e_5$
12	$\{1,3,4,5\}, \{2,3,4,5\}$	$e_1 + e_3, e_2 + e_4$
	$\{1,4,5,6\}$	$\sin(\phi_4 - \phi_3)e_1 - \sin(\phi_2 + \phi_4)e_4 + \sin(\phi_2 + \phi_3)e_5$
13	$\{1,2,4,5\}, \{1,3,4,6\}, \{2,3,5,6\}$	$e_4 \cos\phi_4 + e_5$, $e_1 + e_6$, $e_2 + \cos\phi_2 e_3$
15	$\{2,3,4,5\}, \{2,3,4,6\}$	$e_3 + e_5, e_4 + e_6$
16	$\{1,4,5,6\}$	$e_5 + e_6$ $(2\phi_6 \geq \phi_7)$ or $e_4 \cos\phi_6 + e_6$ $(\phi_6 \leq \phi_7)$
	$\{1,3,4,5\}, \{2,3,4,5\}$	$e_1 + e_3, e_2 + e_4$
17	$\{1,3,4,5\}, \{2,3,4,5\}$	$e_1 + e_3$, $e_2 + e_4$
18	$\{1,3,5,6\}, \{2,3,5,6\}$	$e_1 + e_5$ $(-\phi_3 \leq 2\phi_6)$ or $e_1 + e_6$ $(\phi_6 \leq \phi_3)$, $e_2 + e_3$,
	$\{2,4,5,6\}$	$e_4 + e_5$ $(2\phi_6 \leq \phi_2)$ or $e_4 + e_6$ $(-\phi_2 \leq \phi_6)$

Copositivity

- $|I| = 3$ we check copositivity of A_I by the following criterion:

Lemma

Let

$$A = \begin{pmatrix} 1 & -\cos\phi_1 & -\cos\phi_2 \\ -\cos\phi_1 & 1 & -\cos\phi_3 \\ -\cos\phi_2 & -\cos\phi_3 & 1 \end{pmatrix} \in S^3$$

with $\phi_1, \phi_2, \phi_3 \in [0, \pi]$. *Then* A *is copositive if and only if* $\phi_1 + \phi_2 + \phi_3 \geq \pi$.

Absence of additional minimal zeros

Lemma

Let $A \in \mathcal{C}_n$ and let w be a minimal zero of A with support set I. Let $u \in \mathbb{R}^n \setminus (-\mathbb{R}^n_+)$ be such that $\operatorname{supp} u \subset I \subset \operatorname{supp}_{\geq 0}(Au)$. Set $B = A_I$ and $v = u_I$. Then v is proportional to w_I with a positive proportionality constant and $Bv = 0$.

- For $I = \{i, j, k\}$ the absence can in many cases be certified by verifying the strict inequality $\phi_i + \phi_j + \phi_k > \pi$
- For $|I| \geq 4$ the absence is certified for all occurring cases
- In other cases this inequality has to be added as a constraint

Existence of additional min. zeros

In cases 20-29 one of non-strict inequalities happens to be possible only as the equality $\phi_i + \phi_j + \phi_k = \pi$, which leads to the conclusion that a minimal zero with corresponding support I does indeed exist and this excludes these cases.

Extremality

Theorem

Let $A \in \mathcal{C}^n$. Then A is not extremal if and only if there exists a matrix $B \in S^n$, not proportional to A, such that $(Bu)_i = 0$ $\forall u \in \mathcal{V}^A_{\min}, i \notin \operatorname{supp} Au$.

- It is linear system and we need to determine its rank

Our approach to check extremality

Reduction of system by linear change of variables:
$F^T u_i = 0, B_I = (FPF^T)_I$
$F^T u_j = 0, B_J = (GQG^T)_J, j \neq i$

$$FPF^T = \begin{pmatrix} b_{11} & b_{12} & b_{13} & \star & \star & \star \\ b_{12} & b_{22} & b_{23} & b_{24} & \star & b_{26} \\ b_{13} & b_{23} & b_{33} & b_{34} & b_{35} & b_{36} \\ \star & b_{24} & b_{34} & b_{44} & b_{45} & b_{46} \\ \star & \star & b_{35} & b_{45} & b_{55} & \star \\ \star & b_{26} & b_{36} & b_{46} & \star & b_{66} \end{pmatrix}, \quad GQG^T = \begin{pmatrix} b_{11} & b_{12} & \star & b_{14} & b_{15} & b_{16} \\ b_{12} & b_{22} & \star & \star & b_{25} & b_{26} \\ \star & \star & \star & \star & \star & \star \\ b_{14} & \star & \star & b_{44} & b_{45} & \star \\ b_{15} & b_{25} & \star & b_{45} & b_{55} & b_{56} \\ b_{16} & b_{26} & \star & \star & b_{56} & b_{66} \end{pmatrix}.$$

Got equations to express more entries of B as a function of P

Extremality results

Cases 1-5, 11, 12, 17, 18: the extremal matrices correspond to the interior of the polytope of possible angles.
Cases 7, 8, 13, 15, 16: parts of the boundary of the polytope also correspond to extremal matrices
Cases 7-10, 13: there exist submanifolds in the interior of the polytope corresponding to non-extremal matrices.

Extreme rays of the cone $\mathcal{C}^6$

Case NE

The non-exceptional extreme rays are generated by products $DPAP^TD$ with central factor $A = E_{11}, E_{12}, aa^T$, where a is one of the columns of the matrix

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & -1 & -1 & 1 & 1 & 1 & 1 & 1 & 1 \\ 0 & 0 & -1 & -1 & -1 & -1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 0 & -1 & -1 & -1 & -1 & 1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & -1 \end{pmatrix}.$$

Case O5

$$\begin{pmatrix} 1 & -\cos\phi_1 & \cos(\phi_1+\phi_2) & \cos(\phi_4+\phi_5) & -\cos\phi_5 & 0 \\ -\cos\phi_1 & 1 & -\cos\phi_2 & \cos(\phi_2+\phi_3) & \cos(\phi_1+\phi_5) & 0 \\ \cos(\phi_1+\phi_2) & -\cos\phi_2 & 1 & -\cos\phi_3 & \cos(\phi_3+\phi_4) & 0 \\ \cos(\phi_4+\phi_5) & \cos(\phi_2+\phi_3) & -\cos\phi_3 & 1 & -\cos\phi_4 & 0 \\ -\cos\phi_5 & \cos(\phi_1+\phi_5) & \cos(\phi_3+\phi_4) & -\cos\phi_4 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix},$$

where either $\phi_1 = \cdots = \phi_5 = 0$, or $\phi_i > 0$ for $i = 1, \dots, 5$ and $\sum_{i=1}^5 \phi_i < \pi$.

Case 1

$$\begin{pmatrix} 1 & -1 & -1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 & -1 & \cos\phi_2 \\ -1 & 1 & 1 & 1 & \cos\phi_2 & -1 \\ -1 & 1 & 1 & 1 & -\cos\phi_1 & \cos(\phi_1+\phi_2) \\ 1 & -1 & \cos\phi_2 & -\cos\phi_1 & 1 & -\cos\phi_2 \\ 1 & \cos\phi_2 & -1 & \cos(\phi_1+\phi_2) & -\cos\phi_2 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_1 + \phi_2 < \pi$.

Case 2

$$\begin{pmatrix} 1 & -1 & -1 & -1 & 1 & \cos\phi_2 \\ -1 & 1 & 1 & 1 & -1 & \cos\phi_1 \\ -1 & 1 & 1 & 1 & \cos(\phi_1+\phi_2) & -\cos\phi_2 \\ -1 & 1 & 1 & 1 & \cos(\phi_1+\phi_3) & -\cos\phi_3 \\ 1 & -1 & \cos(\phi_1+\phi_2) & \cos(\phi_1+\phi_3) & 1 & -\cos\phi_1 \\ \cos\phi_2 & \cos\phi_1 & -\cos\phi_2 & -\cos\phi_3 & -\cos\phi_1 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_2 < \phi_3 < \pi - \phi_1$.

Case 3

$$\begin{pmatrix} 1 & -1 & -1 & -1 & -\cos(\phi_1+\phi_2) & \cos\phi_4 \\ -1 & 1 & 1 & 1 & \cos(\phi_1+\phi_2) & -\cos\phi_2 \\ -1 & 1 & 1 & 1 & \cos(\phi_1+\phi_3) & -\cos\phi_3 \\ -1 & 1 & 1 & 1 & \cos(\phi_1+\phi_4) & -\cos\phi_4 \\ -\cos(\phi_1+\phi_2) & \cos(\phi_1+\phi_2) & \cos(\phi_1+\phi_3) & \cos(\phi_1+\phi_4) & 1 & -\cos\phi_1 \\ \cos\phi_4 & -\cos\phi_2 & -\cos\phi_3 & -\cos\phi_4 & -\cos\phi_1 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_4 < \phi_3 < \phi_2 < \pi - \phi_1$.

Case 4

$$\begin{pmatrix} 1 & -1 & -1 & 1 & \cos(\phi_3+\phi_4) & -\cos\phi_4 \\ -1 & 1 & 1 & -1 & \cos\phi_2 & \cos\phi_4 \\ -1 & 1 & 1 & -\cos\phi_1 & \cos(\phi_1+\phi_2) & \cos\phi_4 \\ 1 & -1 & -\cos\phi_1 & 1 & -\cos\phi_2 & \cos(\phi_2+\phi_3) \\ \cos(\phi_3+\phi_4) & \cos\phi_2 & \cos(\phi_1+\phi_2) & -\cos\phi_2 & 1 & -\cos\phi_3 \\ -\cos\phi_4 & \cos\phi_4 & \cos\phi_4 & \cos(\phi_2+\phi_3) & -\cos\phi_3 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_1 + \phi_2 + \phi_3 + \phi_4 < \pi$.

Case 5

$$\begin{pmatrix} 1 & -1 & -1 & \cos(\phi_2+\phi_5) & -\cos\phi_5 & \cos\phi_3 \\ -1 & 1 & 1 & \cos(\phi_1+\phi_4) & \cos\phi_5 & -\cos\phi_4 \\ -1 & 1 & 1 & \cos(\phi_1+\phi_3) & \cos\phi_5 & -\cos\phi_3 \\ \cos(\phi_2+\phi_5) & \cos(\phi_1+\phi_4) & \cos(\phi_1+\phi_3) & 1 & -\cos\phi_2 & -\cos\phi_1 \\ -\cos\phi_5 & \cos\phi_5 & \cos\phi_5 & -\cos\phi_2 & 1 & \cos(\phi_1+\phi_2) \\ \cos\phi_3 & -\cos\phi_4 & -\cos\phi_3 & -\cos\phi_1 & \cos(\phi_1+\phi_2) & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_1 + \phi_2 + \phi_4 + \phi_5 < \pi, \phi_3 < \phi_4$.

Case 6

$$\begin{pmatrix} 1 & -1 & -1 & \cos\phi_2 & \cos\phi_1 & \cos\phi_5 \\ -1 & 1 & 1 & -\cos\phi_2 & \cos(\phi_2+\phi_3) & \cos(\phi_2+\phi_4) \\ -1 & 1 & 1 & \cos(\phi_1+\phi_3) & -\cos\phi_1 & -\cos\phi_5 \\ \cos\phi_2 & -\cos\phi_2 & \cos(\phi_1+\phi_3) & 1 & -\cos\phi_3 & -\cos\phi_4 \\ \cos\phi_1 & \cos(\phi_2+\phi_3) & -\cos\phi_1 & -\cos\phi_3 & 1 & \cos(\phi_1+\phi_5) \\ \cos\phi_5 & \cos(\phi_2+\phi_4) & -\cos\phi_5 & -\cos\phi_4 & \cos(\phi_1+\phi_5) & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_1 + \phi_3 + \phi_5 < \phi_4, \phi_2 + \phi_4 + \phi_5 < \pi$.

Case 7

$$\begin{pmatrix} 1 & -\cos\phi_1 & \cos(\phi_1+\phi_2) & \cos\phi_4 & -1 & \cos\phi_1 \\ -\cos\phi_1 & 1 & -\cos\phi_2 & \cos(\phi_2+\phi_3) & \cos\phi_1 & -1 \\ \cos(\phi_1+\phi_2) & -\cos\phi_2 & 1 & -\cos\phi_3 & \cos(\phi_3+\phi_4) & \cos\phi_2 \\ \cos\phi_4 & \cos(\phi_2+\phi_3) & -\cos\phi_3 & 1 & -\cos\phi_4 & \cos(\phi_4+\phi_5) \\ -1 & \cos\phi_1 & \cos(\phi_3+\phi_4) & -\cos\phi_4 & 1 & -\cos\phi_5 \\ \cos\phi_1 & -1 & \cos\phi_2 & \cos(\phi_4+\phi_5) & -\cos\phi_5 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_1 \le \phi_5, \phi_1 + \phi_2 + \phi_3 + \phi_4 < \pi, \phi_2 + \phi_3 + \phi_4 + \phi_5 < \pi, \phi_1 + \phi_5 \ne \pi$.

Case 8

$$\begin{pmatrix} 1 & -1 & -\cos\phi_2 & \cos(\phi_1+\phi_2) & \cos(\phi_2+\phi_3) & \cos\phi_5 \\ -1 & 1 & \cos\phi_2 & \cos(\phi_4+\phi_5) & \cos(\phi_5+\phi_6) & -\cos\phi_5 \\ -\cos\phi_2 & \cos\phi_2 & 1 & -\cos\phi_1 & -\cos\phi_3 & \cos(\phi_1+\phi_4) \\ \cos(\phi_1+\phi_2) & \cos(\phi_4+\phi_5) & -\cos\phi_1 & 1 & \cos(\phi_1-\phi_3) & -\cos\phi_4 \\ \cos(\phi_2+\phi_3) & \cos(\phi_5+\phi_6) & -\cos\phi_3 & \cos(\phi_1-\phi_3) & 1 & -\cos\phi_6 \\ \cos\phi_5 & -\cos\phi_5 & \cos(\phi_1+\phi_4) & -\cos\phi_4 & -\cos\phi_6 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_3 + \phi_4 \le \phi_1 + \phi_6, \phi_2 + \phi_3 + \phi_5 + \phi_6 \le \pi, \phi_1 + \phi_4 < \phi_3 + \phi_6$ with either $\phi_2 + \phi_3 \ne \phi_5 + \phi_6$ or with $\phi_2 + \phi_3 = \phi_5 + \phi_6 = \frac{\pi}{2}$ or with $\phi_2 + \phi_3 = \phi_5 + \phi_6, \phi_1 + \phi_6 = \phi_3 + \phi_4$.

Case 9.1

$$\begin{pmatrix} 1 & -1 & -\cos\phi_2 & \cos(\phi_1+\phi_2) & \cos(\phi_2+\phi_3) & \cos\phi_5 \\ -1 & 1 & \cos\phi_2 & \cos(\phi_4+\phi_5) & \cos(\phi_5-\phi_6) & -\cos\phi_5 \\ -\cos\phi_2 & \cos\phi_2 & 1 & -\cos\phi_1 & -\cos\phi_3 & \cos(\phi_1+\phi_4) \\ \cos(\phi_1+\phi_2) & \cos(\phi_4+\phi_5) & -\cos\phi_1 & 1 & \cos(\phi_4+\phi_6) & -\cos\phi_4 \\ \cos(\phi_2+\phi_3) & \cos(\phi_5-\phi_6) & -\cos\phi_3 & \cos(\phi_4+\phi_6) & 1 & -\cos\phi_6 \\ \cos\phi_5 & -\cos\phi_5 & \cos(\phi_1+\phi_4) & -\cos\phi_4 & -\cos\phi_6 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_2 + \phi_3 < \pi, \phi_2 + \phi_3 + \phi_5 < \pi + \phi_6, \phi_1 + \phi_4 + \phi_6 < \phi_3, \phi_2 + \phi_3 + \phi_6 < \pi + \phi_5$, excluding $\phi_2 + \phi_3 + \phi_6 = \phi_5$.

Case 9.2

$$\begin{pmatrix} 1 & -1 & -\cos\phi_2 & \cos(\phi_1+\phi_2) & \cos(\phi_2+\phi_3) & \cos\phi_5 \\ -1 & 1 & \cos\phi_2 & \cos(\phi_4+\phi_5) & -\cos(\phi_2+\phi_3) & -\cos\phi_5 \\ -\cos\phi_2 & \cos\phi_2 & 1 & -\cos\phi_1 & -\cos\phi_3 & \cos(\phi_1+\phi_4) \\ \cos(\phi_1+\phi_2) & \cos(\phi_4+\phi_5) & -\cos\phi_1 & 1 & \cos(\phi_4+\phi_6) & -\cos\phi_4 \\ \cos(\phi_2+\phi_3) & -\cos(\phi_2+\phi_3) & -\cos\phi_3 & \cos(\phi_4+\phi_6) & 1 & -\cos\phi_6 \\ \cos\phi_5 & -\cos\phi_5 & \cos(\phi_1+\phi_4) & -\cos\phi_4 & -\cos\phi_6 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_2 + \phi_3 < \pi, \phi_2 + \phi_3 + \phi_5 < \pi + \phi_6, \phi_1 + \phi_4 + \phi_6 < \phi_3, \phi_2 + \phi_3 + \phi_6 > \pi + \phi_5$.

Extreme rays of the cone $\mathcal{C}^6$

Case 10

$$\begin{pmatrix} 1 & -1 & -\cos\phi_2 & \cos(\phi_1+\phi_2) & \cos(\phi_2+\phi_3) & \cos\phi_5 \\ -1 & 1 & \cos\phi_2 & \cos(\phi_4+\phi_5) & \cos(\phi_5-\phi_6) & -\cos\phi_5 \\ -\cos\phi_2 & \cos\phi_2 & 1 & -\cos\phi_1 & -\cos\phi_3 & \cos(\phi_3+\phi_6) \\ \cos(\phi_1+\phi_2) & \cos(\phi_4+\phi_5) & -\cos\phi_1 & 1 & \cos(\phi_4+\phi_6) & -\cos\phi_4 \\ \cos(\phi_2+\phi_3) & \cos(\phi_5-\phi_6) & -\cos\phi_3 & \cos(\phi_4+\phi_6) & 1 & -\cos\phi_6 \\ \cos\phi_5 & -\cos\phi_5 & \cos(\phi_3+\phi_6) & -\cos\phi_4 & -\cos\phi_6 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_1+\phi_2+\phi_4+\phi_5 < \pi, \phi_3+\phi_4+\phi_6 < \phi_1, \phi_2+\phi_3+\phi_6 \neq \phi_5$.

Case 11

$$\begin{pmatrix} 1 & -\cos\phi_2 & -\cos\phi_1 & \cos(\phi_2+\phi_3) & \cos(\phi_2+\phi_6) & \cos(\phi_1+\phi_4) \\ -\cos\phi_2 & 1 & \cos(\phi_1+\phi_2) & -\cos\phi_3 & -\cos\phi_6 & \cos(\phi_3+\phi_5) \\ -\cos\phi_1 & \cos(\phi_1+\phi_2) & 1 & \cos(\phi_4+\phi_5) & -\cos(\phi_1+\phi_2+\phi_6) & -\cos\phi_4 \\ \cos(\phi_2+\phi_3) & -\cos\phi_3 & \cos(\phi_4+\phi_5) & 1 & \cos(\phi_3-\phi_6) & -\cos\phi_5 \\ \cos(\phi_2+\phi_6) & -\cos\phi_6 & -\cos(\phi_1+\phi_2+\phi_6) & \cos(\phi_3-\phi_6) & 1 & b_3 \\ \cos(\phi_1+\phi_4) & \cos(\phi_3+\phi_5) & -\cos\phi_4 & -\cos\phi_5 & b_3 & 1 \end{pmatrix},$$

$b_3 = \frac{-\cos(\phi_3-\phi_6)\sin(\phi_4)+\cos(\phi_1+\phi_2+\phi_6)\sin(\phi_5)}{\sin(\phi_4+\phi_5)}$, $\phi_i > 0, \phi_1+\phi_2+\phi_3+\phi_4+\phi_5 < \pi, \pi-\phi_1-\phi_4-\phi_5+\phi_3-\phi_2 < 2\phi_6 < \pi-\phi_1+\phi_5+\phi_3+\phi_4-\phi_2$.

Case 12

$$\begin{pmatrix} 1 & -\cos\phi_2 & -\cos\phi_1 & \cos(\phi_2+\phi_3) & \cos(\phi_2+\phi_4) & \cos(\phi_1+\phi_5) \\ -\cos\phi_2 & 1 & \cos(\phi_1+\phi_2) & -\cos\phi_3 & -\cos\phi_4 & \cos(\phi_3+\phi_6) \\ -\cos\phi_1 & \cos(\phi_1+\phi_2) & 1 & b_1 & \cos(\phi_5+\phi_7) & -\cos\phi_5 \\ \cos(\phi_2+\phi_3) & -\cos\phi_3 & b_1 & 1 & \cos(\phi_3-\phi_4) & -\cos\phi_6 \\ \cos(\phi_2+\phi_4) & -\cos\phi_4 & \cos(\phi_5+\phi_7) & \cos(\phi_3-\phi_4) & 1 & -\cos\phi_7 \\ \cos(\phi_1+\phi_5) & \cos(\phi_3+\phi_6) & -\cos\phi_5 & -\cos\phi_6 & -\cos\phi_7 & 1 \end{pmatrix},$$

$b_1 = \frac{\sin(\phi_5+\phi_7)\cos\phi_6 - \cos(\phi_3-\phi_4)\sin\phi_5}{\sin\phi_7}$, $\phi_i > 0, \phi_1+\phi_2+\phi_4+\phi_5+\phi_7 < \pi, \phi_4+\phi_7 > \phi_3+\phi_6, \phi_4+\phi_6 > \phi_3+\phi_7, \phi_7+\phi_3+\phi_6 > \phi_4$.

Case 13.1

$$\begin{pmatrix} 1 & -\cos\phi_1 & \cos(\phi_1+\phi_2) & -\cos(\phi_1+\phi_2+\phi_3) & \cos(\phi_5+\phi_6) & -\cos\phi_6 \\ -\cos\phi_1 & 1 & -\cos\phi_2 & \cos(\phi_2+\phi_3) & -\cos(\phi_2+\phi_3+\phi_4) & \cos(\phi_1+\phi_6) \\ \cos(\phi_1+\phi_2) & -\cos\phi_2 & 1 & -\cos\phi_3 & \cos(\phi_3+\phi_4) & -\cos(\phi_3+\phi_4+\phi_5) \\ -\cos(\phi_1+\phi_2+\phi_3) & \cos(\phi_2+\phi_3) & -\cos\phi_3 & 1 & -\cos\phi_4 & \cos(\phi_4+\phi_5) \\ \cos(\phi_5+\phi_6) & -\cos(\phi_2+\phi_3+\phi_4) & \cos(\phi_3+\phi_4) & -\cos\phi_4 & 1 & -\cos\phi_5 \\ -\cos\phi_6 & \cos(\phi_1+\phi_6) & -\cos(\phi_3+\phi_4+\phi_5) & \cos(\phi_4+\phi_5) & -\cos\phi_5 & 1 \end{pmatrix},$$

$\phi_i > 0, \sum_{j=1}^6 \phi_j < 2\pi, \phi_i+\phi_{i+1} < \pi, i = 1,\dots,5, \phi_1+\phi_6 < \pi, \phi_1+\phi_2+\phi_3 \geq \phi_4+\phi_5+\phi_6, \phi_2+\phi_3+\phi_4 \geq \phi_1+\phi_5+\phi_6, \phi_3+\phi_4+\phi_5 \geq \phi_1+\phi_2+\phi_6$, such that $\sum_{j=1}^6 \phi_j \neq \pi$, or at least two of the non-strict inequalities are equalities.

Case 13.2

$$\begin{pmatrix} 1 & -\cos\phi_1 & \cos(\phi_1+\phi_2) & -\cos(\phi_1+\phi_2+\phi_3) & \cos(\phi_5+\phi_6) & -\cos\phi_6 \\ -\cos\phi_1 & 1 & -\cos\phi_2 & \cos(\phi_2+\phi_3) & -\cos(\phi_1+\phi_5+\phi_6) & \cos(\phi_1+\phi_6) \\ \cos(\phi_1+\phi_2) & -\cos\phi_2 & 1 & -\cos\phi_3 & \cos(\phi_3+\phi_4) & -\cos(\phi_3+\phi_4+\phi_5) \\ -\cos(\phi_1+\phi_2+\phi_3) & \cos(\phi_2+\phi_3) & -\cos\phi_3 & 1 & -\cos\phi_4 & \cos(\phi_4+\phi_5) \\ \cos(\phi_5+\phi_6) & -\cos(\phi_1+\phi_5+\phi_6) & \cos(\phi_3+\phi_4) & -\cos\phi_4 & 1 & -\cos\phi_5 \\ -\cos\phi_6 & \cos(\phi_1+\phi_6) & -\cos(\phi_3+\phi_4+\phi_5) & \cos(\phi_4+\phi_5) & -\cos\phi_5 & 1 \end{pmatrix},$$

$\phi_i > 0, \sum_{j=1}^6 \phi_j < 2\pi, \phi_i+\phi_{i+1} < \pi, i = 1,\dots,5, \phi_1+\phi_6 < \pi, \phi_1+\phi_2+\phi_3 \geq \phi_4+\phi_5+\phi_6, \phi_2+\phi_3+\phi_4 \leq \phi_1+\phi_5+\phi_6, \phi_3+\phi_4+\phi_5 \geq \phi_1+\phi_2+\phi_6$, such that $\sum_{j=1}^6 \phi_j \neq \pi$, or at least two of the non-strict inequalities are equalities.

Case 14

$$\begin{pmatrix} 1 & -1 & -1 & -1 & 1 & 1 \\ -1 & 1 & 1 & 1 & -1 & 1 \\ -1 & 1 & 1 & 1 & 1 & -1 \\ -1 & 1 & 1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & 1 & -1 & 1 \end{pmatrix}.$$

Case 15

$$\begin{pmatrix} 1 & -1 & -\cos\phi_2 & -\cos\phi_1 & \cos(\phi_2+\phi_3) & \cos(\phi_1+\phi_4) \\ -1 & 1 & \cos\phi_2 & \cos\phi_1 & \cos(\phi_5+\phi_6) & -\cos\phi_6 \\ -\cos\phi_2 & \cos\phi_2 & 1 & \cos(\phi_1+\phi_2) & -\cos\phi_3 & \cos(\phi_3+\phi_5) \\ -\cos\phi_1 & \cos\phi_1 & \cos(\phi_1+\phi_2) & 1 & \cos(\phi_4+\phi_5) & -\cos\phi_4 \\ \cos(\phi_2+\phi_3) & \cos(\phi_5+\phi_6) & -\cos\phi_3 & \cos(\phi_4+\phi_5) & 1 & -\cos\phi_5 \\ \cos(\phi_1+\phi_4) & -\cos\phi_6 & \cos(\phi_3+\phi_5) & -\cos\phi_4 & -\cos\phi_5 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_1+\phi_2+\phi_3+\phi_4+\phi_5 < \pi, \phi_2+\phi_3+\phi_5+\phi_6 \leq \pi, \phi_6 \geq \phi_1+\phi_4$.

Case 16

$$\begin{pmatrix} 1 & -\cos\phi_2 & -\cos\phi_1 & \cos(\phi_2+\phi_3) & \cos(\phi_2+\phi_4) & \cos(\phi_1+\phi_5) \\ -\cos\phi_2 & 1 & \cos(\phi_1+\phi_2) & -\cos\phi_3 & -\cos\phi_4 & \cos(\phi_3+\phi_6) \\ -\cos\phi_1 & \cos(\phi_1+\phi_2) & 1 & \cos(\phi_5+\phi_6) & \cos(\phi_5+\phi_7) & -\cos\phi_5 \\ \cos(\phi_2+\phi_3) & -\cos\phi_3 & \cos(\phi_5+\phi_6) & 1 & \cos(\phi_6-\phi_7) & -\cos\phi_6 \\ \cos(\phi_2+\phi_4) & -\cos\phi_4 & \cos(\phi_5+\phi_7) & \cos(\phi_6-\phi_7) & 1 & -\cos\phi_7 \\ \cos(\phi_1+\phi_5) & \cos(\phi_3+\phi_6) & -\cos\phi_5 & -\cos\phi_6 & -\cos\phi_7 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_1+\phi_2+\phi_4+\phi_5+\phi_7 \leq \pi, \phi_4+\phi_7 > \phi_3+\phi_6, \phi_4+\phi_6 \geq \phi_3+\phi_7$.

Case 17

$$\begin{pmatrix} 1 & -\cos\phi_2 & -\cos\phi_1 & \cos(\phi_2+\phi_3) & \cos(\phi_2+\phi_4) & \cos(\phi_1+\phi_5) \\ -\cos\phi_2 & 1 & \cos(\phi_1+\phi_2) & -\cos\phi_3 & -\cos\phi_4 & \cos(\phi_3+\phi_6) \\ -\cos\phi_1 & \cos(\phi_1+\phi_2) & 1 & \cos(\phi_5-\phi_6) & \cos(\phi_5+\phi_7) & -\cos\phi_5 \\ \cos(\phi_2+\phi_3) & -\cos\phi_3 & \cos(\phi_5-\phi_6) & 1 & \cos(\phi_6+\phi_7) & -\cos\phi_6 \\ \cos(\phi_2+\phi_4) & -\cos\phi_4 & \cos(\phi_5+\phi_7) & \cos(\phi_6+\phi_7) & 1 & -\cos\phi_7 \\ \cos(\phi_1+\phi_5) & \cos(\phi_3+\phi_6) & -\cos\phi_5 & -\cos\phi_6 & -\cos\phi_7 & 1 \end{pmatrix},$$

$\phi_i > 0, \phi_3+\phi_6+\phi_7 < \phi_4, \phi_1+\phi_5+\phi_7+\phi_2+\phi_4 < \pi$.

Case 18

$$\begin{pmatrix} 1 & -\cos\phi_4 & \cos(\phi_4+\phi_5) & \cos(\phi_2+\phi_3) & -\cos\phi_3 & -\cos(\phi_3+\phi_6) \\ -\cos\phi_4 & 1 & -\cos\phi_5 & \cos(\phi_1+\phi_5) & \cos(\phi_3+\phi_4) & \cos(\phi_3+\phi_4+\phi_6) \\ \cos(\phi_4+\phi_5) & -\cos\phi_5 & 1 & -\cos\phi_1 & \cos(\phi_1+\phi_2) & \cos(\phi_1+\phi_2-\phi_6) \\ \cos(\phi_2+\phi_3) & \cos(\phi_1+\phi_5) & -\cos\phi_1 & 1 & -\cos\phi_2 & -\cos(\phi_2-\phi_6) \\ -\cos\phi_3 & \cos(\phi_3+\phi_4) & \cos(\phi_1+\phi_2) & -\cos\phi_2 & 1 & \cos\phi_6 \\ -\cos(\phi_3+\phi_6) & \cos(\phi_3+\phi_4+\phi_6) & \cos(\phi_1+\phi_2-\phi_6) & -\cos(\phi_2-\phi_6) & \cos\phi_6 & 1 \end{pmatrix},$$

$\phi_1,\dots,\phi_5 > 0, \phi_1+\phi_2+\phi_3+\phi_4+\phi_5 < \pi, -\phi_3 < \phi_6 < \phi_2$.

Case 19

$$\begin{pmatrix} 1 & -\cos\phi_4 & \cos(\phi_4+\phi_5) & \cos(\phi_2+\phi_3) & -\cos\phi_3 & \cos(\phi_3+\phi_6) \\ -\cos\phi_4 & 1 & -\cos\phi_5 & a_{24} & \cos(\phi_3+\phi_4) & -\cos\phi_7 \\ \cos(\phi_4+\phi_5) & -\cos\phi_5 & 1 & -\cos\phi_1 & \cos(\phi_1+\phi_2) & a_{36} \\ \cos(\phi_2+\phi_3) & a_{24} & -\cos\phi_1 & 1 & -\cos\phi_2 & \cos(\phi_6-\phi_2) \\ -\cos\phi_3 & \cos(\phi_3+\phi_4) & \cos(\phi_1+\phi_2) & -\cos\phi_2 & 1 & -\cos\phi_6 \\ \cos(\phi_3+\phi_6) & -\cos\phi_7 & a_{36} & \cos(\phi_6-\phi_2) & -\cos\phi_6 & 1 \end{pmatrix},$$

Extreme rays of the cone $\mathcal{C}^6$

Dimensions of exceptional extremal matrices with unit diagonal:

Case No.	Dim.	Case No.	Dim.	Case No.	Dim.	Case No.	Dim.
1	2	6	5	11	6	16	7,6,6,5
2	3	7	5,4	12	7	17	7
3	4	8	6,5,5,4	13	6,6,5,5,4,3	18	6
4	4	9	6,6	14	0	19	8,7
5	5	10	6	15	6,5,5		

Respective maximal dimension equals the number of free parameters in the expressions for the factor A

Extreme rays of the cone $\mathcal{C}^6$

Generators and types of the non-trivial symmetry groups of minimal zero support sets with the additional inequalities on ϕ_i

Case No.	Generator(s)	Group	Inequalities
1	$(1,3,2,4,6,5)$	S_2	
2	$(1,2,4,3,5,6)$	S_2	$\phi_2 \leq \phi_3$
3	$(1,3,2,4,5,6)$; $(1,2,4,3,5,6)$; $(1,2,3,4,6,5)$	$S_3 \times S_2$	$\phi_4 \leq \phi_3 \leq \phi_2$
5	$(1,3,2,4,5,6)$	S_2	$\phi_3 \leq \phi_4$
6	$(1,3,2,5,4,6)$	S_2	$\phi_2 + \phi_4 + \phi_5 \leq \pi$
7	$(6,5,4,3,2,1)$	S_2	$\phi_1 \leq \phi_5$
8	$(2,1,6,4,5,3)$	S_2	$\phi_3 + \phi_4 \leq \phi_1 + \phi_6$
11	$(2,1,4,3,5,6)$	S_2	
13	$(6,5,4,3,2,1)$; $(6,1,2,3,4,5)$	D_6	$\phi_1 + \phi_2 + \phi_3 \geq \phi_4 + \phi_5 + \phi_6$, $\phi_3 + \phi_4 + \phi_5 \geq \phi_1 + \phi_2 + \phi_6$
14	$(1,4,3,2,5,6)$; $(5,2,6,4,1,3)$	S_2^2	
15	$(1,2,4,3,6,5)$	S_2	
16	$(3,6,1,4,5,2)$	S_2	$\phi_4 + \phi_6 \geq \phi_3 + \phi_7$
17	$(2,1,4,3,5,6)$	S_2	
18	$(1,2,3,4,6,5)$; $(4,3,2,1,5,6)$	S_2^2	
19	$(5,4,3,2,1,6)$	S_2	$\phi_7 - \phi_3 - \phi_4 - \phi_6 \geq \phi_6 + \phi_9 - \pi - \phi_2$

All cases

No.	No. in [17]	supp $\mathcal{V}^A_{\min}$	result
1	2	{1,2},{1,3},{1,4},{2,5},{3,6},{4,5,6}	exceptional extremal
2	3	{1,2},{1,3},{1,4},{2,5},{3,5,6},{4,5,6}	matrices with this
3	4	{1,2},{1,3},{1,4},{2,5,6},{3,5,6},{4,5,6}	minimal zero support
4	5	{1,2},{1,3},{2,4},{3,4,5},{1,5,6},{4,5,6}	set exist
5	6	{1,2},{1,3},{1,4,5},{2,4,6},{3,4,6},{4,5,6}	
6	8	{1,2},{1,3},{2,4,5},{3,4,5},{2,4,6},{3,5,6}	
7	9	{1,5},{2,6},{1,2,3},{2,3,4},{3,4,5},{4,5,6}	
8	13	{1,2},{1,3,4},{1,3,5},{2,4,6},{3,4,6},{2,5,6}	
9	15	{1,2},{1,3,4},{1,3,5},{2,4,6},{3,4,6},{4,5,6}	
10	16	{1,2},{1,3,4},{1,3,5},{2,4,6},{3,5,6},{4,5,6}	
11	21	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{2,4,6},{3,4,6}	
12	22	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{2,4,6},{3,5,6}	
13	34	{1,2,3},{2,3,4},{3,4,5},{4,5,6},{1,5,6},{1,2,6}	
14	36	{1,2},{1,3},{1,4},{2,5},{4,5},{3,6},{5,6}	
15	37	{1,2},{1,3,4},{1,3,5},{1,4,6},{2,5,6},{3,5,6},{4,5,6}	
16	41	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{2,4,6},{3,4,6},{3,5,6}	
17	42	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{2,4,6},{3,5,6},{4,5,6}	
18	43	{1,2,3},{2,3,4},{3,4,5},{1,4,5},{1,2,5},{3,4,6},{1,4,6},{1,2,6}	
19	23	{3,4,5},{1,4,5},{1,2,5},{1,2,3},{1,5,6},{2,3,4,6}	
20	1	{1,2},{1,3},{1,4},{2,5},{3,6},{5,6}	copositivity and
21	11	{1,2},{1,3,4},{1,3,5},{1,4,6},{2,5,6},{3,5,6}	extremality enforce
22	12	{1,2},{2,3,4},{3,4,5},{4,5,6},{2,5,6},{2,3,6}	additional minimal
23	17	{1,2},{1,3,4},{2,3,5},{3,4,5},{2,4,6},{3,4,6}	zero supports
24	24	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{3,4,6},{3,5,6}	
25	25	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{3,4,6},{4,5,6}	
26	28	{1,2,3},{1,2,4},{1,3,5},{2,4,5},{3,4,5},{2,3,6}	
27	30	{1,2,3},{1,2,4},{1,3,5},{2,4,5},{3,4,6},{3,5,6}	
28	32	{1,2,3},{1,2,4},{1,3,5},{2,4,5},{1,5,6},{4,5,6}	
29	39	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{1,4,6},{2,5,6},{3,5,6}	
30	7	{1,2},{1,3},{2,4,5},{3,4,5},{2,4,6},{3,4,6}	linear span of
31	10	{1,2},{1,3,4},{1,3,5},{2,3,6},{3,4,6},{3,5,6}	minimal zeros is
32	14	{1,2},{1,3,4},{1,3,5},{2,4,6},{3,4,6},{3,5,6}	a proper subspace
33	18	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{1,4,6},{1,5,6}	
34	19	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{1,4,6},{2,5,6}	
35	20	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{1,4,6},{3,5,6}	
36	26	{1,2,3},{1,2,4},{1,3,5},{1,4,5},{2,3,6},{2,4,6}	
37	27	{1,2,3},{1,2,4},{1,3,5},{1,4,5},{2,3,6},{3,4,6}	
38	38	{1,2},{1,3,4},{1,3,5},{2,4,6},{3,4,6},{2,5,6},{3,5,6}	
39	40	{1,2,3},{1,2,4},{1,2,5},{1,3,6},{1,4,6},{3,5,6},{4,5,6}	
40	44	{1,2,3},{1,2,4},{1,3,5},{1,4,5},{2,3,6},{2,4,6},{3,5,6},{4,5,6}	
41	35	{1,2,3,4},{2,3,4,5},{3,4,5,6},{1,4,5,6},{1,2,5,6},{1,2,3,6}	
42	33	{1,2,5},{1,4,5},{1,2,3},{3,4,5},{2,3,6},{3,4,6}	
43	31	{1,2,5},{1,4,5},{1,2,3},{3,4,5},{1,3,6},{3,5,6}	first order conditions
44	29	{1,2,3},{1,2,4},{1,3,5},{2,4,5},{2,3,6},{2,5,6}	are incompatible

Essential cases

Definition

Let $\mathcal{M}_n$ be the stratified real algebraic manifold of extreme rays of the copositive cone $\mathcal{C}_n$. A stratum $\mathcal{S}$ of $\mathcal{M}_n$ is called essential if there does not exist a stratum $\mathcal{S}' \neq \mathcal{S}$ such that $\mathcal{S} \subset \partial \mathcal{S}'$.

Case 19 of dimension 14 is essential, because no other stratum has larger dimension.

Future outlook

- Suppose $K \subset \mathcal{S}^n$ is an inner approximation of $\mathcal{C}^n$, i.e., $K \subset \mathcal{C}^n$ if all extreme rays of $\mathcal{C}^n$ are contained in K, then $K = \mathcal{C}^n$ knowledge of the extreme rays of $\mathcal{C}^n$ allows to test the exactness of inner approximations
- What are the essential cases?
- Check $X \in \mathcal{C}^6 => DXD \in ? K_n^1$

Thank you for your attention!

Preprint is available on:
http://www.optimization-online.org/DB_HTML/2019/11/7489.html