On the structure of the 5 x 5 copositive cone

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Outline

Context and problem description

- Extreme and reduced rays
- Existing results
- Zero patterns
- Covering conditions

Results

- Reducedness and weak covering condition
- 3×3 copositive matrices
- Extreme and reduced matrices
- Semi-definite representation

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 $\mathcal{C}_n$

- many applications in optimization
- difficult to describe

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 $\mathcal{N}_n \cap \mathcal{S}_n^+$

$$\mathcal{C}_n^* \subset \mathcal{N}_n \cap \mathcal{S}_n^+ \subset \mathcal{N}_n + \mathcal{S}_n^+ \subset \mathcal{C}_n$$

Extreme rays

Definition

Let $K \subset \mathbb{R}^n$ be a regular convex cone. An nonzero 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 $\alpha, \beta \geq 0$.

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

in [Hoffman, Pereira 1973] the extreme rays of $\mathcal{C}_n$ with elements in $\{-1, 0, +1\}$ have been described

Reduced rays

Definition (Diananda 62, Baumert 65)

A copositive matrix $A \in \mathcal{C}_n$ is called reduced if it cannot be represented as a sum of a copositive and a nonnegative matrix in a non-trivial manner. In other words, $A = B + C$ with $B \in \mathcal{C}_n$ and $C \in \mathcal{N}_n$ imply $B = A$ and $C = 0$.

Lemma

Let $A \in \mathcal{C}_n$ be an extreme matrix. Then A is either reduced or nonnegative.

Problem formulation

Describe all extreme and reduced rays of $\mathcal{C}_5$.

Why 5×5

Theorem (Diananda 62)

Let $n \leq 4$. Then the copositive cone $\mathcal{C}_n$ is the sum of the nonnegative cone $\mathcal{N}_n$ and the positive semi-definite cone $\mathcal{S}_n^+$.

the Horn form

$$H = \begin{pmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{pmatrix}$$

is an example of a matrix in $\mathcal{C}_5 \setminus (\mathcal{N}_5 + \mathcal{S}_5^+)$

Literature

work on $\mathcal{C}_5$ and related 5×5 matrix cones

- L.D. Baumert, 1965–1967: PhD thesis and two papers on the extreme rays of $\mathcal{C}_5$
- B. Ycart, 1982: extreme rays of the doubly nonnegative cone
- C. Xu, 2001: completely positive cone
- A. Berman, C. Xu, 2004: completely positive cone
- S. Burer, K. Anstreicher, M. Dür, 2009: separation of doubly nonnegative matrices from $\mathcal{C}_5^*$
- H. Dong, K. Anstreicher, 2010: separation of DNN matrices from $\mathcal{C}_5^*$
- S. Burer, H. Dong, 2010: separation of DNN matrices from $\mathcal{C}_5^*$
- N. Shaked-Monderer, I. Bomze, F. Jarre, W. Schachinger, 2012: CP-rank

Scaling group

the group $\mathbb{R}^n_{++}$ acts on $\mathcal{C}_n$ by $d : A \mapsto \operatorname{diag}(d) A \operatorname{diag}(d)$

for every $A \in \mathcal{C}_n$, there exists a normalized A' in the orbit of A such that

$$\operatorname{diag} A' \in \{0, 1\}^n$$

if $\operatorname{diag} A' \not> 0$, then $\operatorname{diag} A \not> 0$ and $A \in \mathcal{C}_{n-1} + \mathcal{N}_n$
we may assume $\operatorname{diag} A = \mathbf{1}$ w.l.o.g.

the permutation group S_n acts on $\mathcal{C}_n$ by $P : A \mapsto PAP^T$
this action respects the property of being normalized with respect to the action of $\mathbb{R}^n_{++}$

these groups leave also $\mathcal{N}_n$ and $\mathcal{S}^+_n$ invariant $\Rightarrow$ they respect the property of being reduced

Zero patterns

Theorem (Diananda 62)

Let $A \in \mathcal{C}_n$ be a copositive matrix and $x \in \mathbb{R}^n_+$ a vector such that $x^T Ax = 0$. Let I be the set of indices i such that $x_i > 0$.
Then the principal submatrix $A_{I,I}$ is positive semi-definite.

Definition (Baumert 65)

A copositive matrix $A \in \mathcal{C}_n$ is said to have a zero with pattern $I \subset \{1, \dots, n\}$ if there exists $x \in \mathbb{R}^n_+$ such that $x^T Ax = 0$ and $I = \{i \mid x_i > 0\}$.
The zero pattern $\mathcal{P}(A)$ of A is the set of the patterns of all its zeros.

Covering conditions

Lemma (Baumert 66)

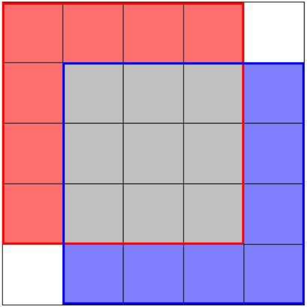
Let $A \in \mathcal{C}_n$ and i be such that for all $I \in \mathcal{P}(A)$ we have $i \notin I$. Then there exists $\varepsilon > 0$ such that $A - \varepsilon E_{ii} \in \mathcal{C}_n$. The converse also holds.

hence $\bigcup_{I \in \mathcal{P}(A)} I = \{1, \ldots, n\}$ is necessary for A being reduced

Definition

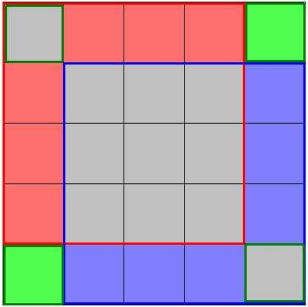
Let $A \in \mathcal{C}_n$. Call the zero pattern $\mathcal{P}(A)$ of A covering if

$$\bigcup_{I \in \mathcal{P}(A)} I^2 = \{1, \ldots, n\}^2.$$



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

not covered



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

covered

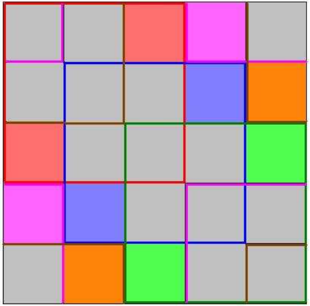
Zero patterns of extreme and reduced forms

Theorem (Baumert 67)

Let $A \in \mathcal{C}_5$ be an extreme copositive matrix whose zero pattern $\mathcal{P}(A)$ is covering. Then one of the following possibilities holds:

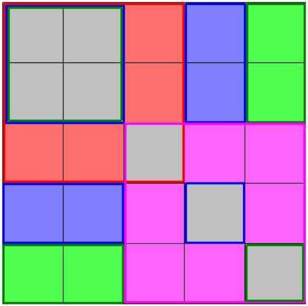
- *A is positive semi-definite*
- *A is in the orbit of the Horn form*
- *$\mathcal{P}(A)$ consists of exactly 5 elements with cardinality 3 and which are related by a permutation of order 5*

In the last case, there exists exactly 1 zero with each given pattern, and this case occurs.
If "extreme" is replaced by "reduced", then the pattern $\{\{123\}, \{124\}, \{125\}, \{345\}\}$ and its permutations may occur additionally.



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

extreme



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

reduced but not extreme

Sketch of proof

- assume $\operatorname{diag} A = \mathbf{1}$, no zeros with 1 positive element
- $|A_{ij}| \leq 1$ for all i, j [Baumert 65]
- if A has a zero with 4 or 5 positive elements, then A is PSD [Diananda 62]
- if a zero has pattern $\{i, j\}$, then $A_{ij} = -1$
- no more than 6 zeros with 2 positive elements
- if there are zeros with patterns $\{i, j\}, \{j, k\}$, then $A_{ik} = 1$
- zero patterns with zeros with 2 and 3 positive elements considered case by case

Baumerts mistake

in his thesis Baumert falsely assumed that the covering condition is equivalent to reducedness [Baumert 65, Theorem 3.3]

that is why he considered only copositive matrices with covering zero patterns

in fact, the covering condition is sufficient, but not necessary for reducedness

What is the correct condition describing reducedness?

Associated pattern

Definition

Let $A \in \mathcal{C}_n$ be a copositive matrix and $x \in \mathbb{R}_+^n$ a zero of A with pattern I. The index set $J = \{j \notin I \mid (Ax)_j = 0\}$ is called associated pattern of the zero x.

The associated zero pattern $\mathcal{AP}(A)$ of A is the set of the pairs (I, J) of (associated) patterns of all its zeros.

Lemma (Baumert 65,66)

Let $A \in \mathcal{C}_n$ be a copositive matrix and $x \in \mathbb{R}_+^n$ a zero of A with pattern I and associated pattern J. Then the principal submatrix $A_{I\cup J, I\cup J}$ can be decomposed as $B + C$, where B is positive semi-definite and C is copositive with support in J.

Consequences

Corollary

Let $A \in \mathcal{C}_n$ be a copositive matrix and $x \in \mathbb{R}^n_+$ a zero of A with pattern I and associated pattern J. Then for every $j \in J$, the principal submatrix $A_{I\cup\{j\},I\cup\{j\}}$ is positive semi-definite.

Corollary

Let $A \in \mathcal{C}_n$ be a copositive matrix and $x \in \mathbb{R}^n_+$ a zero of A with pattern I and associated pattern J. Suppose $|J| \leq 4$ and set $m\ |I| + |J|$. Then the principal submatrix $A_{I\cup J,I\cup J}$ is in $\mathcal{S}^+_m + \mathcal{N}_m$. In particular, if $I \cup J = \{1, \ldots, n\}$, then $A \in \mathcal{S}^+_n + \mathcal{N}_n$.

Characterization of reducedness

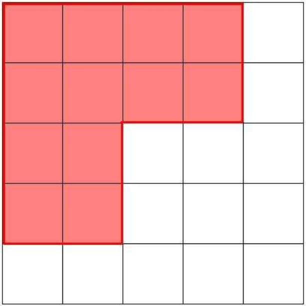
Definition

Let $A \in \mathcal{C}_n$. Call the associated zero pattern $\mathcal{AP}(A)$ of A weakly covering if

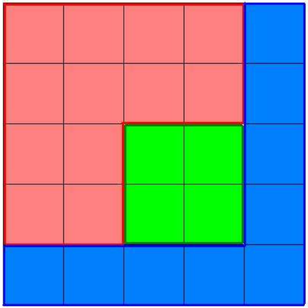
$$\bigcup_{(I,J)\in\mathcal{AP}(A)} (I^2 \cup I \times J \cup J \times I) = \{1, \ldots, n\}^2.$$

Theorem (DDGH, 12)

Let $A \in \mathcal{C}_n$. Then A is reduced if and only if its associated zero pattern $\mathcal{AP}(A)$ is weakly covering.



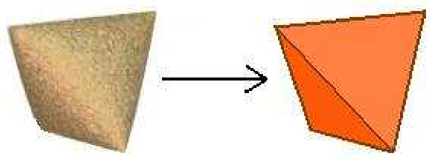
I = {1,2}, J = {3,4}



({1,2},{3,4}), ({5},{1,2,3,4}), ({3,4},{})

3×3 copositive matrices

the set $\{A \in \mathcal{S}_3^+ \mid \operatorname{diag} A = \mathbf{1}\}$ is bounded by the Cayley surface
the element-wise map $x \mapsto \frac{2}{\pi} \arcsin x$ transforms it into a tetrahedron with the same vertices



we have $\mathcal{C}_3 = \mathcal{S}_3^+ + \mathcal{N}_3$
hence the reduced matrices in $\mathcal{C}_3$ with $\operatorname{diag} A = \mathbf{1}$ have the form

$$A = \begin{pmatrix} 1 & -\cos\varphi_3 & -\cos\varphi_2 \\ -\cos\varphi_3 & 1 & -\cos\varphi_1 \\ -\cos\varphi_2 & -\cos\varphi_1 & 1 \end{pmatrix}$$

with $\varphi_k \geq 0$, $\varphi_1 + \varphi_2 + \varphi_3 = \pi$

T-matrices

let $A \in \mathcal{C}_5$ be a copositive matrix with zero pattern $\{\{1,2,3\},\{2,3,4\},\{3,4,5\},\{4,5,1\},\{5,1,2\}\}$

then A must be of the form

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

with $\psi_1,\dots,\psi_5 > 0$

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

Extreme rays

Theorem (H., 11)

Let $\psi \in [0,\pi)^5$*. Then* $T(\psi)$ *is copositive with zero pattern* $\{\{1,2,3\},\{2,3,4\},\{3,4,5\},\{4,5,1\},\{5,1,2\}\}$ *if and only if* $\psi_k > 0$ *for all* k *and* $\psi_1 + \cdots + \psi_5 < \pi$*. In this case* $T(\psi)$ *is an extreme ray of* $\mathcal{C}_5$*. Every extreme ray which is not in* $\mathcal{S}_5^+$ *or* $\mathcal{N}_5$ *or in the orbit of the Horn form can be brought to such a* $T(\psi)$ *by the action of* $\operatorname{Aut}\mathcal{C}_5$*.*

sketch of proof

- no other zero patterns can occur
- every 4×4 submatrix in $\mathcal{S}_4^+ + \mathcal{N}_4 \Rightarrow \sum_k \psi_k < \pi$
- $\det T(\psi) > 0 \Rightarrow T(\psi) \in \mathcal{C}_5$
- zeros determine the parameters $\psi \Rightarrow T(\psi)$ extremal

Reduced rays

Theorem (DDGH, 12)

Let $\psi \in [0, \pi)^5$. *Then* $T(\psi)$ *is*

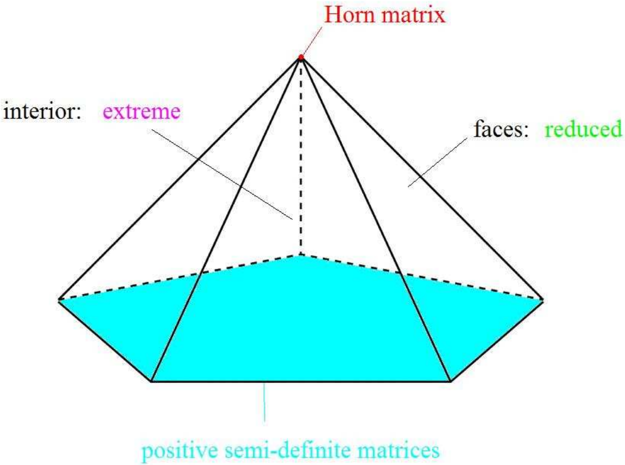
- *copositive if and only if* $\psi_1 + \cdots + \psi_5 \leq \pi$
- *positive semi-definite if and only if* $\psi_1 + \cdots + \psi_5 = \pi$
- *if* $\psi_1 + \cdots + \psi_5 < \pi$, *then* $T(\psi)$ *is reduced*

Every reduced matrix in $\mathcal{C}_5$ *which is not in* $\mathcal{S}_5^+$ *can be brought into the form* $T(\psi)$ *by the action of* $\mathrm{Aut}\,\mathcal{C}_5$.

sketch of proof

- zero pattern $\{\{123\}, \{124\}, \{125\}, \{345\}\}$ cannot occur
- weakly covering patterns which are not covering checked one by one
- PSD factorization of $T(\psi)$ for $\sum_k \psi_k = \pi$ found explicitly
- decomposition into sum of extreme matrices for $\min_k \psi_k = 0$ found explicitly

T-matrices in ψ-space



the base is a 4-dimensional simplex

Dimensions of faces

the reduced matrices which are not PSD and not extreme can be brought to the form $T(\psi)$ with

$$\sum_k \psi_k < \pi, \quad 0 = \min_k \psi_k < \max_k \psi_k$$

the dimensions of the faces of these matrices are

- 4 if the zero pattern is one of $\{\{15\},\{23\},\{234\},\{34\}\}$, $\{\{234\},\{12\},\{45\}\}$ or equivalent
- 2 otherwise

the first two patterns correspond to

$$\psi_1 = \psi_3 = \psi_5 = 0, \qquad \psi_2, \psi_4 > 0,$$

$$\psi_2 = \psi_4 = 0, \qquad \psi_1, \psi_3, \psi_5 > 0$$

respectively

Semi-definite representation of diag $A = \mathbf{1}$ section

Theorem (DDGH, 12)

Let A be a real symmetric 5×5 matrix with $\operatorname{diag} A = \mathbf{1}$. Then A is copositive if and only if the 6-th order polynomial

$$p(x) = \left(\sum_{i,j=1}^{5} A_{ij} x_i^2 x_j^2 \right) \cdot \left(\sum_{i=1}^{5} x_i^2 \right)$$

is a sum of squares.

this condition corresponds to the first level in the Parrilo hierarchy of semi-definite inner approximations of the copositive cone

the condition $\operatorname{diag} A = \mathbf{1}$ is essential: the k-th level Parrilo condition

$$\left(\sum_{i,j=1}^{5} A_{ij} x_i^2 x_j^2 \right) \cdot \left(\sum_{i=1}^{5} x_i^2 \right)^k \qquad \text{is a SOS}$$

is not necessary for $A \in \mathcal{C}_5$ for every $k \in \mathbb{N}$

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Thank you!