Copositive Matrices, their Dual, and the Recognition Problem

Cordelia(Yuqiao) Li

Advisor: Dr. Charles Johnson

Department of Mathematics, William & Mary

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Overview

1. Introduction
2. Known Theorems
3. Conjectures & Evidence

What are copositive matrices?

Definition

Let $\mathbb{S}_n$ be the set of all real n-by-n symmetric matrices. Then, $A \in \mathbb{S}_n$ is *copositive* (CoP) if its quadratic form $x^T A x \geq 0$ for all **nonnegative** vectors $x \in \mathbb{R}_n$.

- A generalization of positive semidefinite (PSD) matrices: for a PSD matrix B, $x^T B x \geq 0$ for all vectors $x \in \mathbb{R}_n$.
- All copositive matrices form a convex cone.
  - Convex cone: closed under linear combinations with positive coefficients.
- Copositive matrices were first defined by T. S. Motzkin in 1952.

Why do we care?

Copositive (CoP) matrices have many applications:

- In **optimization theory:** copositivity offers a unified convex way to reformulate nonconvex mixed quadratic programs into convex programs [10].
- In **differential equations**: CoP matrices have applications in quadratic differential equations [7].
- In **theoretical economics**: can be used to model discrete markets and games [9].
- Strong modeling power, but hard: new theory & checking copositivity is NP-hard.

Thus, CoP matrices are really useful, but more studies are needed.

Checking copositivity

In 1960, Kaplan provides the following way to check copositivity:

Theorem (Kaplan, 1960 [3])

Let $A \in \mathbb{S}_n$. Then A is copositive if and only if every principal submatrix B of A has no eigenvector $v > 0$ with associated eigenvalue $\lambda < 0$.

- This theorem provides us with a systematic way to check copositivity.
- However: NP-hard & exponential efforts.

Some entrywise properties

In [6], Bundfuss presents the following four entrywise properties for CoP matrices:

Proposition [6]

Let $A = [a_{ii}]$ be a CoP matrix. Then:

(i) $a_{ij} \geq 0$ for all i.

(ii) If $a_{ii} = 0$, then $a_{ij} \geq 0$ for all j.

(iii) $a_{ij} \geq -\sqrt{a_{ii} a_{jj}}$ for all i and all j.

Spectral of CoP matrices

Definition

The *spectral radius* of a matrix A is the largest absolute value of A's eigenvalues.

Theorem [11]

Let A be CoP. Then, the spectral radius $\rho(A)$ is an eigenvalue of A.

i.e., CoP matrices have the Perron property.

Ordinary vs. Exceptional

Let $\mathbb{S}_n$ be the set of n-by-n real symmetric matrices.
Let $\mathcal{C}_n = \{A \in \mathbb{S}_n : A \text{ is copositive (CoP)}\}$
$\mathcal{P}_n = \{A \in \mathbb{S}_n : A \text{ is positive semidefinite (PSD)}\}$;
$\mathcal{N}_n = \{A \in \mathbb{S}_n : A \text{ is nonnegative (sN)}\}$ (entry-wise nonnegative).

Theorem (Diananda, 1961 [4])

In general, $\mathcal{P}_n + \mathcal{N}_n \subset \mathcal{C}_n$. For $n \leq 4, \mathcal{P}_n + \mathcal{N}_n = \mathcal{C}_n$.

Definition

A CoP matrix is *exceptional* if it is not the sum of a PSD matrix and an sN matrix. Otherwise, we say the matrix is *ordinary*.

Thus, if the size of a CoP matrix is less than or equal to 4, then this CoP matrix is ordinary.

Example: 5-by-5 exceptional CoP

Examples

The Horn Matrix:

$$A = \begin{bmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{bmatrix}$$

The Horn matrix is exceptional CoP and cannot be decomposed into PSD + sN.

Example: ordinary CoP

Examples

$$A = \begin{bmatrix} 1 & 3 & -1 \\ 3 & 1 & 1 \\ -1 & 3 & 2 \end{bmatrix} = \begin{bmatrix} 1 & 0 & -1 \\ 0 & 1 & 1 \\ -1 & 1 & 1 \end{bmatrix} + \begin{bmatrix} 0 & 3 & 0 \\ 3 & 0 & 2 \\ 0 & 2 & 1 \end{bmatrix}.$$

CoP PSD sN

Here, A is ordinary CoP, and A can be decomposed into PSD + sN.

CoP-preserved operations

Start from something easy: CoP matrices with entries from $\{1, -1\}$ or $\{1, -1, 0\}$.

Then, $A \in \mathbb{S}_n$ is CoP if and only if all of its principal submatrices do not contain the following "forbidden" patterns (up to permutation similarity) [1]:

"Forbidden" patterns

$$\begin{bmatrix} 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{bmatrix} \quad \& \quad \begin{bmatrix} 1 & -1 & -1 \\ -1 & 1 & 0 \\ -1 & 0 & 1 \end{bmatrix}$$

Example: $\{1, 0, -1\}$

In this case, it is easier to check copositivity. (In an n-by-n matrix, there are a total of $\binom{n}{3}$ 3-by-3 principal submatrix.)

Examples

$$A = \begin{bmatrix} 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 \\ -1 & 1 & 1 & 0 \\ -1 & 1 & 0 & 1 \end{bmatrix}$$

Then, A is not CoP.

Hadamard Product & Kronecker Product

- Positive semidefiniteness is preserved under Hadamard and Kronecker products.
- Since CoP matrices are generalizations of PSD matrices, we wonder if copositivity would also be preserved.

Definition

Let $A = (a_{ij}), B = (b_{ij}), A, B \in M_n$. The *Hadamard product* of A and B, denoted by $A \circ B$, is an entrywise multiplication: $A \circ B = (a_{ij} b_{ij})$.

Definition

Let $A = (a_{ij}) \in M_{m,n}, B \in M_{p,q}$. Then, the *Kronecker product* of A and B, denoted by $A \otimes B$, is a pm-by-qn matrix:

$$\mathrm{A} \otimes \mathrm{B} = \begin{bmatrix} a_{11}\mathrm{B} & \cdots & a_{1n}\mathrm{B} \\ \vdots & \ddots & \vdots \\ a_{m1}\mathrm{B} & \cdots & a_{mn}\mathrm{B} \end{bmatrix}$$

Hadamard Product & Kronecker Product

Examples

Let $A = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & -1 \\ 1 & -1 & 1 \end{bmatrix}$, $B = \begin{bmatrix} 1 & -1 & -1 \\ -1 & 1 & 1 \\ -1 & 1 & 1 \end{bmatrix}$. Then, $A \circ B = \begin{bmatrix} 1 & -1 & -1 \\ -1 & 1 & -1 \\ -1 & -1 & 1 \end{bmatrix}$.

Remark

Let $A = (a_{ij}), B = (b_{ij}), A, B \in M_n$. Then, $A \circ B$ is a principal submatrix of $A \otimes B$.

Thus, the Hadamard (and also Kronecker) product of two general CoP matrices is not CoP.

What about some special CoP matrices Hadamard/Kronecker product with CoP matrices?

Dual cone: completely positive matrices

Definition

Let $A \in \mathbb{S}_n$. A is *completely positive(CP)* if A can be factorized as $A = BB^T$ for nonnegative matrix $B \in M_{n,m}$. CP matrices are special PSD matrices and also CoP matrices.

The set of all CP matrices also form a convex cone, and it is the dual cone of CoP matrices[8].

Definition

For a cone $K \subset \mathbb{S}_n$, the dual cone is: $K^* = \left\{ Y \in \mathbb{S}_n : \mathrm{Tr}\left(Y^T X\right) \geq 0 \quad \forall X \in K \right\}$.

Since $x^T A x = \mathrm{Tr}\left(A^T x x^T\right)$, all matrices of the form xx^T with $x \geq 0$ are in the dual cone of $\mathcal{C}_n$.

Thus, all CP matrices form a dual cone of CoP matrices.

Hadamard Product & Kronecker Product

Let A be a CoP matrix. Then:

Theorem [1]

$B \circ A$ is copositive if and only if B is CP.

Theorem

$B \otimes A$ is copositive if and only if B is CP.

Other matrix operations: polynomial?

For PSD matrices: if A is PSD, then $p(A)$ is PSD if $p(t) \geq 0$ for all $t \geq 0$.
(If λ is an eigenvalue for A, then $p(\lambda)$ is an eigenvalue for $p(A)$.)

Question

Which polynomial preserves copositivity?

This leads us to consideration of powers.

- Even power: Yes, definitely.
- Odd power: Not always.
  - Example of CoP being preserved: all PSD matrices.
  - Example of CoP not being preserved: Horn matrix.

Odd powers?

Examples

The Horn Matrix:

$$A = \begin{bmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{bmatrix}, A^3 = \begin{bmatrix} 13 & -11 & 5 & 5 & -11 \\ -11 & 13 & -11 & 5 & 5 \\ 5 & -11 & 13 & -11 & 5 \\ 5 & 5 & -11 & 13 & -11 \\ -11 & 5 & 5 & -11 & 13 \end{bmatrix}$$

Let B be the principal submatrix of A^3 with the first three rows & columns. Then, B has eigenvalue $\lambda = -0.2560$ with eigenvector $v = \begin{bmatrix} 0.4586 \\ 0.7611 \\ 0.4586 \end{bmatrix}$.

Thus, A^3 is not CoP by Kaplan's Theorem.

Note: the Horn matrix is exceptional (cannot be decomposed into PSD + sN).

Odd powers: ordinary vs. exceptional

Why is Horn matrix no longer CoP after cubing?

- We decided to run some simulations with ordinary & exceptional matrices.
- Recall: a matrix is ordinary if it can be decomposed into PSD + sN.
- It is easy to generate random ordinary CoP matrices, but hard to generate exceptional CoP matrices.
    - There are some studies on exceptional CoP matrices with certain structures[2], but only some limited cases.

Odd powers: ordinary vs. exceptional

We did simulations with size $n = 5, 6, 7, 8$, each with more than 100,000 random ordinary matrices. We reaches the following conjecture:

Conjecture

Let $A \in \mathcal{C}_n$. Then A^3 is CoP if and only if A is ordinary (that is, $A \in \mathcal{P}_n + \mathcal{N}_n$).

What is the difference between ordinary CoP & exceptional CoP?

Ordinary Recognition & Decomposition Problem

Here, we introduce the ordinary recognition & decomposition problem:

Question

- Given a CoP matrix, how to tell whether it is ordinary or not?
- If we have an ordinary CoP matrix, how to decompose it into PSD + sN?

Ordinary Recognition & Decomposition Problem

To discuss this problem, we note the following matrix properties:

1. Let A be an ordinary CoP with one possible decomposition $A = P + N$ (P is PSD, N is nonnegative). Then, P contains all negative entries of A.
2. For a PSD matrix, if we make the diagonals even more positive, it does not destroy the positive semi-definiteness.

$$P_1 = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix} \Rightarrow P_2 = \begin{bmatrix} 3 & -1 \\ -1 & 3 \end{bmatrix}$$

3. Thus, if N has some positive values on the diagonal, then we can move the positive diagonal weight all to P; the new decomposition will still be a valid ordinary decomposition.

Ordinary Recognition $\Rightarrow$ PSD Completion Problem

The ordinary recognition problem is equivalent to a restricted type of PSD completion problem. Let $A \in \mathcal{C}_n$.

Let $D \in \mathbb{S}_n$ contain only the diagonal entries of A;
let $N \in \mathbb{S}_n$ contain only the negative off-diagonal entries of A;
let $P \in \mathbb{S}_n$ contain only the positive off-diagonal entries of A.
Let $B = N + D$, and let the zero entries be unspecified. Then, we make this conjecture:

Conjecture

A is ordinary if and only if B has a PSD completion with entries no more than P.

$$A = \begin{bmatrix} a & -d & f \\ -d & b & -e \\ f & -e & c \end{bmatrix}; \Rightarrow B = \begin{bmatrix} a & -d & * \\ -d & b & -e \\ * & -e & c \end{bmatrix}$$

Ordinary Recognition ⇒ PSD Completion

If this conjecture is true, then we will have a great way to recognize ordinary CoP matrices and decompose them systematically.

Specifically, we start with a "skeleton" and gradually transfer positive weight from P to B. If we use up everything but still not yet gotten a PSD matrix, then it is exceptional.

$$A = \begin{bmatrix} a & -d & f \\ -d & b & -e \\ f & -e & c \end{bmatrix}; \Rightarrow \text{"Skeleton"}\, B = \begin{bmatrix} a & -d & 0 \\ -d & b & -e \\ 0 & -e & c \end{bmatrix}$$

Example: 3-by-3

Examples

A 3-by-3 example (size ≤ 4 : all ordinary):

$$A = \begin{bmatrix} 13 & -9 & 28 \\ -9 & 12 & -11 \\ 28 & -11 & 20 \end{bmatrix}; B = \begin{bmatrix} 13 & -9 & 0 \\ -9 & 12 & -11 \\ 0 & -11 & 20 \end{bmatrix}$$

B is not PSD with a negative eigenvalue $\lambda = -0.16$.
If we transfer some weight from the positive off-diagonal entry in A to B :
$B' = \begin{bmatrix} 13 & -9 & 1 \\ -9 & 12 & -11 \\ 1 & -11 & 20 \end{bmatrix}$ is PSD; $B' + (A - B')$ is a ordinary decomposition of A.

There can be many ways to decompose an ordinary CoP matrix.

Example: Horn matrix

Examples

Horn matrix (exceptional): $A = \begin{bmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{bmatrix}$;

$$D = I_5, P = \begin{bmatrix} 0 & 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 & 1 \\ 1 & 0 & 0 & 0 & 1 \\ 1 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \end{bmatrix}; B = \begin{bmatrix} 1 & -1 & 0 & 0 & -1 \\ -1 & 1 & -1 & 0 & 0 \\ 0 & -1 & 1 & -1 & 0 \\ 0 & 0 & -1 & 1 & -1 \\ -1 & 0 & 0 & 1 & -1 \end{bmatrix}.$$

B has no PSD completion here; if we transfer the positive off-diagonal weight on P to B, we can never get a PSD matrix.

3-by-3 Ordinary Decomposition

We start from 3-by-3 ordinary CoP matrices and want to come up with a general scheme of ordinary decomposition.

- Wlog, we can take diagonals to be 1's using diagonal equivalence.
- Let $d, e, f \geq 0$, then we have 4 cases (up to permutation similarity):

$$A_1 = \begin{bmatrix} 1 & d & f \\ d & 1 & e \\ f & e & 1 \end{bmatrix}; A_2 = \begin{bmatrix} 1 & -d & f \\ -d & 1 & e \\ f & e & 1 \end{bmatrix}; A_3 = \begin{bmatrix} 1 & -d & f \\ -d & 1 & -e \\ f & -e & 1 \end{bmatrix}; A_4 = \begin{bmatrix} 1 & -d & -f \\ -d & 1 & -e \\ -f & -e & 1; \end{bmatrix}$$

3-by-3 Ordinary Decomposition

- Claim: we only need to consider A_3.

$$A_1 = \begin{bmatrix} 1 & d & f \\ d & 1 & e \\ f & e & 1 \end{bmatrix} = I_3 + \begin{bmatrix} 0 & d & f \\ d & 0 & e \\ f & e & 0 \end{bmatrix};$$

$$A_2 = \begin{bmatrix} 1 & -d & f \\ -d & 1 & e \\ f & e & 1 \end{bmatrix} = \begin{bmatrix} 1 & -d & 0 \\ -d & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} + \begin{bmatrix} 0 & 0 & f \\ 0 & 0 & e \\ f & e & 0 \end{bmatrix}.$$

- Recall: since A_2 is CoP, $a_{ij} \geq -\sqrt{a_{ii}a_{jj}}$. Thus, $d^2 \leq 1$.

3-by-3 Ordinary Decomposition

$$A_3 = \begin{bmatrix} 1 & -d & f \\ -d & 1 & -e \\ f & -e & 1 \end{bmatrix} = \begin{bmatrix} 1 & -d & 0 \\ -d & 1 & -e \\ 0 & -e & 1 \end{bmatrix} + \begin{bmatrix} 0 & 0 & f \\ 0 & 0 & 0 \\ f & 0 & 0 \end{bmatrix};$$

$$A_4 = \begin{bmatrix} 1 & -d & -f \\ -d & 1 & -e \\ -f & -e & 1. \end{bmatrix};$$

A_4 is automatically PSD, so we only need to consider A_3.

3-by-3 Ordinary Decomposition

Now, let $A = A_3 = \begin{bmatrix} 1 & -d & f \\ -d & 1 & -e \\ f & -e & 1 \end{bmatrix}$; $B = \begin{bmatrix} 1 & -d & 0 \\ -d & 1 & -e \\ 0 & -e & 1 \end{bmatrix}$.

Let $B' = \begin{bmatrix} 1 & -d & f' \\ -d & 1 & -e \\ f' & -e & 1 \end{bmatrix} (0 \leq f' \leq f)$.

Suppose B is not PSD, and we want to make B' become PSD by picking a suitable value f'.

3-by-3 Ordinary Decomposition

$$B = \begin{bmatrix} 1 & -d & 0 \\ -d & 1 & -e \\ 0 & -e & 1 \end{bmatrix}; B' = \begin{bmatrix} 1 & -d & f' \\ -d & 1 & -e \\ f' & -e & 1 \end{bmatrix} (0 \le f' \le f).$$

Question

Do we ever have to make a negative entry more negative to get an ordinary decomposition?

Ans: No. Since $d^2 \le 1$, $\det(\begin{bmatrix} 1 & -d \\ -d & 1 \end{bmatrix}) \ge 0$. we need $\det(B') \ge 0$.

But $\det(B) = 1 - d^2 - e^2$. If d and e increase, then $\det(B)$ will be more negative.
Thus, we only need to adjust the nonnegative entries.

3-by-3 Ordinary Decomposition

$$B = \begin{bmatrix} 1 & -d & 0 \\ -d & 1 & -e \\ 0 & -e & 1 \end{bmatrix}; B' = \begin{bmatrix} 1 & -d & f' \\ -d & 1 & -e \\ f' & -e & 1 \end{bmatrix}, (0 \leq f' \leq f).$$

Then, $\det(B') = -f'^2 + 2def' - d^2 - e^2 + 1$.

At $\det(B') = 0$, we solve the quadratic equation: $f' = de \pm \sqrt{(d-1)(d+1)(e-1)(e+1)}$.

For easier notation, let
$f_1 = de - \sqrt{(d-1)(d+1)(e-1)(e+1)}, \quad f_2 = de + \sqrt{(d-1)(d+1)(e-1)(e+1)}$.
Note that $f_1, f_2 > 0$.

Then, the determinant changes as the following:

1. When $0 < f' < f_2$, $\det(B') < 0$;
2. When $f_1 < f' < f_2$, $\det(B') > 0$;
3. When $f' > f_2$, $\det(B') < 0$.

3-by-3 Ordinary Decomposition

$$B = \begin{bmatrix} 1 & -d & 0 \\ -d & 1 & -e \\ 0 & -e & 1 \end{bmatrix}; B' = \begin{bmatrix} 1 & -d & f' \\ -d & 1 & -e \\ f' & -e & 1 \end{bmatrix}, (0 \leq f' \leq f).$$

Let us denote the smallest eigenvalue & eigenvector of B' by λ_s and v_s.
When $f = 0$: $\lambda_s < 0$, and λ_s is the only negative eigenvalue of B' due to interlacing inequality.
Also, $v_s > 0$.

Recall: Kaplan's Theorem: B' is CoP if & only if it has no $\lambda < 0$ with $v > 0$.

Let us trace λ_s and v_s as f' increases.

Experiment Observations

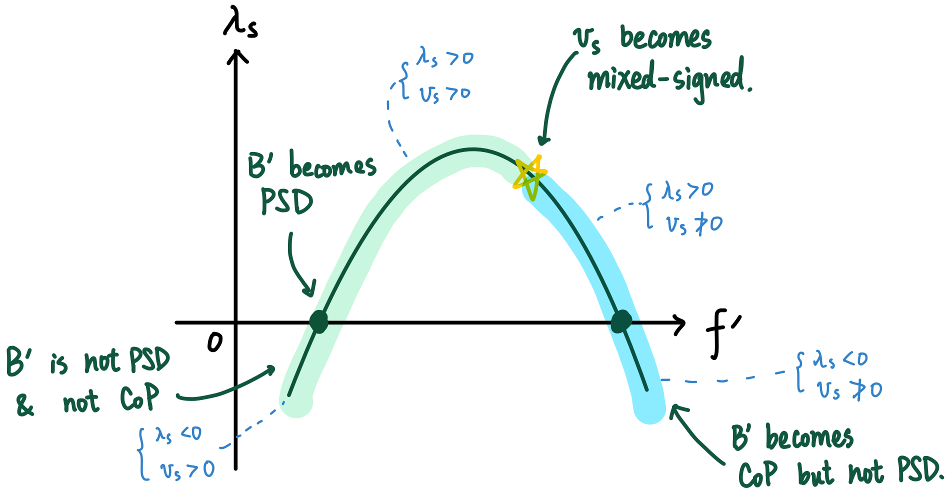
$$B = \begin{bmatrix} 1 & -d & 0 \\ -d & 1 & -e \\ 0 & -e & 1 \end{bmatrix}; B' = \begin{bmatrix} 1 & -d & f' \\ -d & 1 & -e \\ f' & -e & 1 \end{bmatrix}, (0 \leq f' \leq f).$$

We remark the following observations from computational experiments:

Observations

- When $0 \leq f' < f_1 : \lambda_s < 0$, and $v_s > 0 \Rightarrow$ **not CoP**.
- At $f' = f_1 : \lambda_s = 0, v_s > 0 \Rightarrow$ **PSD**.
- At $f_1 < f' < f_2$, there is a point where v_s start to have mixed signs $\Rightarrow$ **PSD**.
- At $f' > f_2 : \lambda_s < 0, v_s$ has mixed signs $\Rightarrow$ **CoP**.

Experiment Observations



Experiment Observations

- Thus, as we increase f', B' becomes an element in $\mathcal{P}_n$ before it becomes an element in $\mathcal{C}_n/\mathcal{P}_n$.
- If this is true, then we will have a valid way to decompose 3-by-3 ordinary CoP matrices.

Spectrum of ordinary CoP matrices

In these experiments, we had some interesting observation related to spectrum of ordinary CoP matrices.

Finally, we want to draw some connections of spectrum of ordinary CoP matrices to the spectrum of sN matrices.

- The sN inverse eigenvalue problem is unsolved.
- If we take PSD $+$ sN, the eigenvalues never decrease.

References

[1] Charles R. Johnson, Ronald L. Smith, Michael J. Tsatsomeros. *Matrix Positivity*, Cambridge University Press.

[2] Charles R. Johnson, Robert B. Reams, Sufflcient conditions to be exceptional , *Spec. Matrices*, 4 (2016),67–72.

[3] Wilfred Kaplan, A test for copositive matrices , *Lin. Alg. Appl*, 313 (2000), 203–206.

[4] P. H. Diananda, On non-negative forms in real variables some or all of which are non-negative, *Camb. Philos* I (1961), 17–25.

[5] Peter J.C. Dickinson *The Copositive Cone, the Completely Positive Cone and their Generalisations* PhD Thesis, University of Groningen, 2012.

[6] S. Bundfuss, *Copositive Matrices, Copositive Programming, and Applications*, TU Darmstadt, 2009.

[7] K.P. Hadeler, On Copositive Matrices *Lin. Alg. Appl.* , 49 (1983), 79-89.

[8] M. Hall, Jr. and M. Newman, Copositive and completely positive quadratic forms, *Proc. Cambridge Philos. Soc.*, 59 (1963), 329-339.

[9] Cheng Guo, Merve Bodur, Joshua A. Taylor, *Copositive Duality for Discrete Markets and Games*, available at `https://arxiv.org/abs/2101.05379`

[10] Samuel Burer, Copositive Programming, *Handbook on Semidefinite, Conic and Polynomial Optimization*, Springer, 2011.

[11] E. Haynsworth and A. J. Hoffman, Two remarks on copositive matrices, *Lin. Alg. Appl.*, 2(1969), 387-392.

Thank you!