Completely positive and copositive matrices and optimization

Bob's birthday conference

The Chinese University of Hong Kong November 17, 2013

Why CP matrices?

CP, COP matrices & Optimization

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Completely positive matrices (and the related copositive matrices) are of interest in mathematical optimization:

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Completely positive matrices (and the related copositive matrices) are of interest in mathematical optimization:

Every nonconvex quadratic optimization problem over the simplex,

$$\max\{x^T Q x \mid e^T x = 1, x_i \ge 0 \ \forall i\},\$$

has an equivalent completely positive formulation (with $J = ee^{T}$):

$$\max\{\langle Q, X \rangle \,|\, \langle J, X \rangle = 1, X \text{ is } CP\}.$$

Thus a nonconvex NP-hard optimization problem is transformed into a linear problem in matrix variables over a convex cone of matrices, shifting the difficulty of the problem entirely into the cone constraint. This makes understanding the cone crucial for tackling the problem.

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Definitions

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The converse holds only for $n \leq 4$.

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Basic Problems

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Basic Problems

• Identify / characterize CP matrices.

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• Identify / characterize CP matrices.

• Compute / estimate cp-ranks.

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Basic Problems

• Identify / characterize CP matrices.

• Compute / estimate cp-ranks.

Both are open and hard.

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$$A \text{ is PSD } \Leftrightarrow A = \begin{bmatrix} v_1^T \\ v_2^T \\ \vdots \\ v_n^T \end{bmatrix} \begin{bmatrix} v_1 & v_2 & \cdots & v_n \end{bmatrix} = \begin{bmatrix} \langle v_i, v_j \rangle \end{bmatrix},$$

where v_1, \dots, v_n are vectors in an *m*-dimensional Euclidean space

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A is CP $\Leftrightarrow v_1, \ldots, v_n$ can be isometrically embedded in the nonnegative orthant of some *k*-dimensional Euclidean space. cp-rank A = minimal such *k*.

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Proves:

Theorem

A is DNN and rank $A = 2 \Rightarrow A$ is CP and cp-rank A = 2.

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4 unit vectors in \mathbb{R}^3 :

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Definition

 $\forall A \in \mathbb{R}^{n \times n}$ symmetric, the **graph** of *A*, *G*(*A*), is the simple undirected graph with vertices $\{1, \ldots, n\}$, where *ij* is an edge if and only if $a_{ji} = a_{ij} \neq 0$.

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 $B \ge 0 \Rightarrow$ no cancellations in the sum $\Rightarrow \forall i$, supp b_i is a clique in G(A).
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Theorem

A graph *G* is CP \Leftrightarrow *G* contains no long (length \geq 5) odd cycle.

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The key: A No Long Odd Cycle graph looks like that:



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Each block is bipartite

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Each block is bipartite / has at most 4 vertices

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Each block is bipartite / has at most 4 vertices / consists of triangles with a common base.

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Theorem

Every CP matrix A with G(A) = G satisfies cp-rank $A = \operatorname{rank} A$ if and only if G contains no even cycle, and no triangle-free graph with more edges than vertices.

Shaked-Monderer (2001)

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The key: Such a graph looks like that:



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Each block is an edge

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Each block is an edge / an odd cycle;

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Each block is an edge / an odd cycle; at most one odd cycle is long.

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Problem

Find a (sharp) upper bound on the cp-ranks of matrices in \mathcal{CP}_n .

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• For $n \leq 4$: $A \in CP_n \Rightarrow cp$ -rank $A \leq n$.

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Bound definitely > *n*: $\forall n \ge 5$, $\exists A \in CP_n$ with cp-rank $A = \lfloor n^2/4 \rfloor$.

The DJL conjecture

$\forall n \ge 4: A \in \mathcal{CP}_n \implies \text{cp-rank } A \le \lfloor n^2/4 \rfloor.$ Drew, Johnson & Loewy (1994)

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Common thread in most results: deal with matrices on ∂CP_n .

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Long known result

The maximum cp-rank on CP_n is attained on int CP_n .

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Long asked question

Is the maximum also attained on the boundary?

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CP, COP matrices & Optimization

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Theorem 1

 $\forall n \geq 2$, the maximum of the cp-rank on CP_n is attained at a nonsingular matrix on ∂CP_n .

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• $A \in \operatorname{int} CP_n \iff A = BB^T$, $B \ge 0$ has rank *n* & a positive column. Dür & Still (2008), Dickinson (2010)

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Definitions

CP, COP matrices & Optimization

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For $n \ge 5$ there are also others. Example: the Horn matrix

$$H = \begin{bmatrix} 1 & -1 & 1 & 1 & -1 \\ -1 & 1 & -1 & 1 & 1 \\ 1 & -1 & 1 & -1 & 1 \\ 1 & 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & -1 & 1 \end{bmatrix} \text{ and more.}$$

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 COP_n is a closed convex cone.

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CP_n, COP_n

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Basic Problems

CP, COP matrices & Optimization

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• Charachterize extreme rays of COP_n .

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Hall & Newman (1963)

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- n = 5: Hildebrand matrices

Hildebrand (2012)

CP, COP matrices & Optimization

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The Barioli-Berman bound is not sharp for $n \ge 5$:

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 $\forall A \in \mathcal{CP}_n, n \geq 5$, cp-rank $A \leq \binom{n+1}{2} - 4$.

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Comments

CP, COP matrices & Optimization

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Comments

Theorem 3 bound definitely not sharp for n = 5, 6, most probably not sharp for n > 6.

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Theorem 3 bound definitely not sharp for n = 5, 6, most probably not sharp for n > 6.

Theorem 5 bound may not be sharp.

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Copositive optimization

Burer has shown that every optimization problem with quadratic objective function, linear constraints, and binary variables can be equivalently written as a linear problem over the completely positive cone. This includes many NP-hard combinatorial problems. The complexity of these problems is then shifted entirely into the cone constraint. In fact, even checking whether a given matrix is completely positive is an NP-hard problem.

Replacing the completely positive cone by a tractable cone like the cone of doubly nonnegative matrices results in a relaxation of the problem providing a bound on its optimal value. For matrices of order $n \le 4$, the doubly nonnegative cone equals the completely positive which means that the relaxation is exact. For order $n \ge 5$, however, there are doubly nonnegative matrices that are not completely positive.

Copositive cuts

Thus, in general, an optimal solution of the doubly nonnegative relaxation is not completely positive. Therefore, it is desirable to add a cut, i.e., a linear constraint that separates the obtained solution from the completely positive cone, in order to get a tighter relaxation yielding a better bound.

In [B, Duer, Shaked-Monderer and Witzel] we construct cutting planes to separate doubly nonnegative matrices which are not completely positive from the completely positive cone. In other words, given $X \in \mathcal{DNN}_n \setminus \mathcal{CP}_n$, we aim to find a $K \in \mathcal{COP}_n$ such that $\langle K, X \rangle < 0$.

Copositive cuts contd.



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Copositive cuts contd.



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Generating copositive cuts

The basic idea of our approach is stated in the following theorems:

Theorem

 $X \in \mathcal{CP}_n \Leftrightarrow \exists K \in \mathcal{COP}_n$ such that $K \circ X \notin \mathcal{COP}_n$.

Theorem

Let $X \in \mathcal{DNN}_n \setminus \mathcal{CP}_n$, and let $K \in \mathcal{COP}_n$ be such that $K \circ X \notin \mathcal{COP}_n$. Then for every nonnegative $u \in \mathbb{R}^n$ such that $u^T(K \circ X)u < 0$, the copositive matrix $K \circ uu^T$ is a cut separating X from \mathcal{CP}_n .

Proof.

$$\langle K \circ u u^T, X \rangle = u^T (K \circ X) u < 0.$$

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Generating copositive cuts contd.

If $K \circ X \notin COP_n$, as assumed in the theorem, then by Kaplan's copositivity characterization, $K \circ X$ has a principal submatrix having a positive eigenvector corresponding to a negative eigenvalue. This shows that such *u* can be chosen as this eigenvector with zeros added to get a vector in \mathbb{R}^n .

The following property is obvious but useful, since it allows to construct cutting planes based on submatrices instead of the entire matrix.

Lemma

Assume that $K \in COP_n$ is a copositive matrix that separates a matrix X from CP_n . If $A \in \mathbb{R}^{n \times p}$ and $B \in \mathbb{R}^{n \times p}$ are arbitrary matrices with B symmetric, then the copositive matrix

$$\begin{bmatrix} K & 0 \\ 0 & 0 \end{bmatrix} \text{ is a cut that separates } \begin{bmatrix} X & A \\ A^T & B \end{bmatrix} \text{ from } \mathcal{CP}_{n+p}.$$

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Generating copositive cuts contd.

We assume that the matrices that we want to separate from the completely positive cone are irreducible, since any reducible symmetric matrix can be written as a block diagonal matrix and then the problem can be split into subproblems of smaller dimension where each of the diagonal blocks is considered separately.

Note that for a cut it is desirable to have an extreme copositive matrix K rather than just a copositive K, since an extremal matrix will provide a supporting hyperplane and therefore a better (deeper) cut.

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Separating a triangle-free doubly nonnegative matrix

We assume that our matrix $X \in DNN_n$ has $X_{ii} \neq 0$, otherwise the corresponding row and column would be zero, and we can base our cut on a submatrix with no zero diagonal elements. Furthermore, by applying a suitable scaling if necessary we can assume that diag (X) = e.

Now suppose that an irreducible $X \in DNN_n$ has a triangle-free graph G(X). Then we have

X = I + C, diag (X) = e, G(X) is connected and triangle-free. (1)

The matrix *C* has zero diagonal and G(C) = G(X).

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Separating a triangle-free doubly nonnegative matrix

We now characterize complete positivity of X in terms of the spectral radius of C.

Lemma

A matrix $X \in DNN_n$ of the form (1) is completely positive if and only if the spectral radius ρ of C fulfills $\rho \leq 1$.

Proof.

Since G(X) is triangle-free, $X \in COP_n$ if and only if its comparison matrix M(X) is an *M*-matrix, which means that M(X) can be written as $M(X) = \alpha I - P$ with $P \ge 0$ and $\alpha \ge \rho(P)$. In our case, we have

$$M(X)=I-C,$$

which immediately gives the result.

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Separating a triangle-free doubly nonnegative matrix

For the separation of a doubly nonnegative matrix in the form (1) which is not completely positive from CP_n , we will use a $\{-1, 0, 1\}$ -matrix: Given a triangle-free graph *G*, let *A* be defined by:

$$A_{ij} = \begin{cases} -1 & \text{if } \{i, j\} \text{ is an edge of } G, \\ +1 & \text{if the distance between } i \text{ and } j \text{ in } G \text{ is } 2, \end{cases}$$
(2)
0 & otherwise.

We call this matrix the *Hoffman-Pereira matrix* corresponding to *G*. By [Hoffman and Pereira (1973)] the matrix *A* is copositive whenever *G* is triangle-free. If the diameter of *G* is 2, then the Hoffman-Pereira matrix does not have zero entries, and is extreme. This is the case for n = 5, and *A* is then the Horn matrix.

Separating a triangle-free doubly nonnegative matrix

Theorem

Let $X \in DNN_n \setminus CP_n$ be of the form (1), let u be the Perron vector of C, and let A be the Hoffman-Pereira matrix corresponding to G(X). Then

- (a) u > 0 and $u^T M(X) u < 0$,
- (b) $M(X) = X \circ A$ and

$$K := A \circ u u^T$$

is a copositive matrix separating X from CP_n .

Separating a triangle-free doubly nonnegative matrix

- Proof.
- (a) The assumption that G(X) is connected means that X, and therefore C, is irreducible, which implies that u > 0 by the Perron-Frobenius Theorem. Also,

$$u^{\mathsf{T}} M(X) u = u^{\mathsf{T}} u - u^{\mathsf{T}} C u = u^{\mathsf{T}} u (1 - \rho) < 0.$$

(b) It is easy to see that $M(X) = X \circ A$, and we have

$$\langle X, A \circ u u^T \rangle = \langle X \circ A, u u^T \rangle = u^T (X \circ A) u = u^T M(X) u < 0.$$

Since u > 0 and A is copositive, the matrix $K := A \circ uu^T$ is copositive, which by the above is a cut that separates X from CP_n .

Note that since u > 0, the cut matrix *K* is extreme if and only if the Hoffman-Pereira matrix *A* is extreme. This happens, e.g., when the graph G(X) is an odd cycle.

Application to the stable set problem

We illustrate the separation procedure by applying it to some instances of the stable set problem.

As shown in [de Klerk and Pasechnik (2002)], the problem of computing the stability number α of a graph *G* can be stated as a completely positive optimization problem:

$$\alpha = \max\{\langle \boldsymbol{E}, \boldsymbol{X} \rangle : \langle \boldsymbol{I}, \boldsymbol{X} \rangle = 1, \ \langle \boldsymbol{A}_{\boldsymbol{G}}, \boldsymbol{X} \rangle = 0, \ \boldsymbol{X} \in \mathcal{CP}_n\}$$
(3)

where A_G denotes the adjacency matrix of G. Replacing CP_n by DNN_n results in a relaxation of the problem providing a bound on α . This bound ϑ' is called Lovász-Schrijver bound:

$$\vartheta' = \max\{\langle E, X \rangle : \langle I, X \rangle = 1, \ \langle A_G, X \rangle = 0, \ X \in \mathcal{DNN}_n\}.$$
(4)

We consider some instances for which $\vartheta' \neq \alpha$ and aim to get better bounds by adding cuts to the doubly nonnegative relaxation, using our approach.

Application to the stable set problem contd.

Let \bar{X} denote the optimal solution we get by solving (4). If $\vartheta' \neq \alpha$, then $\bar{X} \in DNN_n \setminus CP_n$. We want to find cuts that separate \bar{X} from the feasible set of (3). If $G(\bar{X})$ is triangle-free, we can separate \bar{X} from CP_n . Otherwise, we look for a principal submatrix whose graph is triangle-free and its comparison matrix is not positive semidefinite, construct a cut for this submatrix.

Application to the stable set problem contd.

Let *Y* denote such a submatrix. In general, diag $(Y) \neq e$ as in (1). Therefore, we consider the scaled matrix *DYD*, where *D* is a diagonal matrix with $D_{ii} = \frac{1}{\sqrt{Y_{ii}}}$. Since *Y* is a doubly nonnegative matrix having a triangle-free graph, the same holds for *DYD*. Furthermore, *DYD* can be written as DYD = I + C, where *C* is a matrix with zero diagonal and G(C) a triangle-free graph. Let ρ denote the spectral radius of *C* and let *u* be the eigenvector of *C* corresponding to the eigenvalue ρ . Furthermore, let *A* be If $\rho > 1$, then we have

$$0 > \langle A \circ uu^T, DYD \rangle = \langle D(A \circ uu^T)D, Y \rangle.$$

Therefore, $D(A \circ uu^T)D$ defines a cut that separates Y from the completely positive cone.

Numerical results for some stable set problems

As test instances, we consider the 5-cycle C_5 and the graphs G_8 , G_{11} , G_{14} and G_{17} from [Pena, Vera and Zuluaga (2007)]. In each case we determine all submatrices as described above. It turns out that for these instances the biggest order of such a submatrix is 5×5 . The matrix A we use is therefore the Horn matrix. We then solve the doubly nonnegative relaxation after adding each of these cuts and after adding all computed cuts. The results are shown in the Table below. We denote by ϑ_{\min}^{K} and ϑ_{\max}^{K} the minimal respectively maximal bound we get by adding a single cut to the doubly nonnegative relaxation (4), and ϑ_{all}^{K} denotes the bound we get after adding all computed cuts. The last column indicates the reduction of the optimality gap $\vartheta' - \alpha$ when all cuts are added.

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Numerical results for some stable set problems

Graph	α	ϑ'	ϑ_{min}^{K}	ϑ_{\max}^K	ϑ_{all}^{K}	# cuts	reduction
C_5	2	2.236	2.0000	2.0000	2.0000	1	100%
G_8	3	3.468	3.3992	3.3992	3.2163	4	54%
G_{11}	4	4.694	4.6273	4.6672	4.4307	10	38%
G_{14}	5	5.916	5.8533	5.8977	5.6460	20	29%
G_{17}	6	7.134	7.0745	7.1227	6.8615	35	24%

Table : Results on different stable set problems

Happy Birthday Bob!

CP, COP matrices & Optimization

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Happy Birthday Bob!

Based on:

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