PSD factorizations of nonnegative matrices and lower bounds on semidefinite representations

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Based on joint work with Hamza Fawzi (MIT), João Gouveia (U. Coimbra) and Rekha Thomas (U. Washington).
Given a nonnegative matrix \( A \in \mathbb{R}^{n \times m} \), a factorization

\[
A = UV
\]

where \( U \in \mathbb{R}^{n \times k} \), \( V \in \mathbb{R}^{k \times m} \) are also nonnegative.

- The smallest such \( k \) is the \textit{nonnegative rank} of the matrix \( A \).
- Very difficult problem, many heuristics exist.
Factorizations and hidden variables

Let $X$, $Y$ be discrete random variables, with joint distribution

$$P[X = i, Y = j] = P_{ij}.$$  

The nonnegative rank of $P$ is the smallest support of a random variable $Z$, such that $X$ and $Y$ are *conditionally independent* given $Z$ (i.e., $X \perp Z \perp Y$ is Markov):

$$P[X = i, Y = j] = \sum_{s=1}^{k} P[Z = s] \cdot P[X = i|Z = s] \cdot P[Y = j|Z = s].$$

- Relations with information theory, “correlation generation,”
  communication complexity, etc.
- Quantum versions are also of interest.

As we’ll see, fundamental in optimization . . .
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Motivating example

The crosspolytope $C_n$ is the unit ball of the $\ell_1$ ball:

$$C_n := \{ x \in \mathbb{R}^n : \sum_{i=1}^{n} |x_i| \leq 1 \}.$$

It is a polytope defined by $2^n$ linear inequalities:

$$\pm x_1 \pm x_2 \pm \cdots \pm x_n \leq 1$$

The “obvious” linear program is exponentially large!
A better representation

By introducing *slack* or *auxiliary* variables, the set $C_n$ can be represented more conveniently:

$$
C_n := \{ \mathbf{x} \in \mathbb{R}^n : \exists \mathbf{y} \in \mathbb{R}^n, \quad -y_i \leq x_i \leq y_i, \quad \sum_{i=1}^{n} y_i = 1 \}.
$$

This has only $2n$ variables ($x_1, y_1, \ldots, x_n, y_n$) and $2n + 1$ constraints. A “small” linear program. Much better!

What is going on in here?
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Geometric viewpoint

Geometrically, we are representing our polytope as a *projection* of a higher-dimensional polytope.

The number of *vertices* does not increase, but the number of *facets* can grow exponentially!

“Complicated” objects are sometimes easily described as “projections” of “simpler” ones.

A general theme: algebraic varieties, graphical models, …
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Extended formulations

These representations are usually called *extended formulations*. Particularly relevant in combinatorial optimization (e.g., TSP).

Seminal work by Yannakakis (1991), who used them to disprove the existence of a “symmetric” LP formulation for the TSP polytope. Nice recent survey by Conforti-Cornuéjols-Zambelli (2010).

Our goal: to understand this phenomenon for convex optimization, not just LP.
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“Extended formulations” in SDP

Many convex sets and functions can be modeled by SDP or SOCP in nontrivial ways. Among others:

- Sums of eigenvalues of symmetric matrices
- Convex envelope of univariate polynomials
- Multivariate polynomials that are sums of squares
- Unit ball of matrix operator and nuclear norms
- Geometric and harmonic means
- (Some) orbitopes – convex hulls of group orbits

E.g., Nesterov/Nemirovski, Boyd/Vandenberghe, Ben-Tal/Nemirovski, Sanyal/Sottile/Sturmfels, etc.

Often, clever and non-obvious reformulations.
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Our questions

Existence and efficiency:
- When is a convex set representable by conic optimization?
- How to quantify the number of additional variables that are needed?

Given a convex set $C$, is it possible to represent it as

$$C = \pi(K \cap L)$$

where $K$ is a cone, $L$ is an affine subspace, and $\pi$ is a linear map?
When do such representations exist?
Even ignoring complexity aspects, this question is not well understood.

- Why a sphere is not a polytope?
- Can every basic closed semialgebraic set be represented using semidefinite programming?

What are “obstructions” for cone representability?
What happens in the case of polytopes?

\[ P = \{ x \in \mathbb{R}^n : f_i^T x \leq 1 \} \]

(WLOG, compact with 0 \( \in \) int \( P \)).

Polytopes have a finite number of facets \( f_i \) and vertices \( v_j \).

Define a nonnegative matrix, called the \textit{slack matrix} of the polytope:

\[
[S_P]_{ij} = 1 - f_i^T v_j, \quad i = 1, \ldots, |F| \quad j = 1, \ldots, |V|
\]
This talk: polytopes

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Example: hexagon (I)

Consider a regular hexagon in the plane.

It has 6 vertices, and 6 facets. Its slack matrix is

\[
S_H = \begin{pmatrix}
0 & 0 & 1 & 2 & 2 & 1 \\
1 & 0 & 0 & 1 & 2 & 2 \\
2 & 1 & 0 & 0 & 1 & 2 \\
2 & 2 & 1 & 0 & 0 & 1 \\
1 & 2 & 2 & 1 & 0 & 0 \\
0 & 1 & 2 & 2 & 1 & 0
\end{pmatrix}
\]

“Trivial” representation requires 6 facets. Can we do better?
“Geometric” LP formulations exactly correspond to “algebraic” factorizations of the slack matrix.

For polytopes, this amounts to a *nonnegative factorization* of the slack matrix:

\[ S_{ij} = \langle a_i, b_j \rangle, \quad i = 1, \ldots, v, \quad j = 1, \ldots, f \]

where \(a_i, b_i\) are nonnegative vectors.

Yannakakis (1991) showed that the minimal lifting dimension is equal to the nonnegative rank of the slack matrix.
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Example: hexagon (II)

Regular hexagon in the plane.

Its slack matrix is

\[
S_H = \begin{pmatrix}
0 & 0 & 1 & 2 & 2 & 1 \\
1 & 0 & 0 & 1 & 2 & 2 \\
2 & 1 & 0 & 0 & 1 & 2 \\
2 & 2 & 1 & 0 & 0 & 1 \\
1 & 2 & 2 & 1 & 0 & 0 \\
0 & 1 & 2 & 2 & 1 & 0 \\
\end{pmatrix}.
\]

Nonnegative rank is 5.
Example: hexagon (II)

Regular hexagon in the plane.

Its slack matrix is

\[ S_H = \begin{pmatrix}
0 & 0 & 1 & 2 & 2 & 1 \\
1 & 0 & 0 & 1 & 2 & 2 \\
2 & 1 & 0 & 0 & 1 & 2 \\
2 & 2 & 1 & 0 & 0 & 1 \\
1 & 2 & 2 & 1 & 0 & 0 \\
0 & 1 & 2 & 2 & 1 & 0 \\
\end{pmatrix} . \]

Nonnegative rank is 5.
Beyond LPs and nonnegative factorizations

LPs are nice, but what about broader representability questions?

In [GPT11], a generalization of Yannakakis’ theorem to the general convex case. General theme:

“Geometric” extended formulations exactly correspond to “algebraic” factorizations of a slack operator.

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Polytopes and PSD factorizations

Even for polytopes, PSD factorizations can be interesting.

Well-known example: the *stable set* or *independent set* polytope. For perfect graphs, we have efficient SDP representations, but no known subexponential LP.

Natural notion: *positive semidefinite rank* ([GPT 11]). Exactly captures the complexity of SDP-representability.
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Well-known example: the stable set or independent set polytope. For perfect graphs, we have efficient SDP representations, but no known subexponential LP.

Natural notion: positive semidefinite rank ([GPT 11]). Exactly captures the complexity of SDP-representability.
Let $M \in \mathbb{R}^{m \times n}$ be a nonnegative matrix.

The *PSD rank* of $M$, denoted $\text{rank}_\text{psd}$, is the smallest $r$ for which there exists $r \times r$ PSD matrices $\{A_1, \ldots, A_m\}$ and $\{B_1, \ldots, B_n\}$ such that

$$M_{ij} = \text{trace } A_i B_j, \quad i = 1, \ldots, m \quad j = 1, \ldots, n.$$
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M_{ij} = \text{trace} \ A_i B_j, \quad i = 1, \ldots, m \quad j = 1, \ldots, n.
\]

Natural generalization of nonnegative rank.

The PSD rank determines the “best” semidefinite lifting.
Some inequalities

- For any nonnegative matrix $M$
  \[
  \frac{1}{2} \sqrt{1 + 8 \text{rank}(M)} - \frac{1}{2} \leq \text{rank}_{psd}(M) \leq \text{rank}_+(M).
  \]

- Gap between $\text{rank}_+(M)$ and $\text{rank}_{psd}(M)$ can be arbitrarily large:
  \[
  M_{ij} = (i - j)^2 = \left\langle \begin{pmatrix} i^2 & -i \\ -i & 1 \end{pmatrix}, \begin{pmatrix} 1 & j \\ j & j^2 \end{pmatrix} \right\rangle
  \]
  has $\text{rank}_{psd}(M) = 2$, but $\text{rank}_+(M) = \Omega(\log n)$.

Arbitrarily large gaps between all pairs of ranks ($\text{rank}$, $\text{rank}_+$ and $\text{rank}_{psd}$). For slack matrices of polytopes, arbitrarily large gaps between rank and $\text{rank}_+$, and rank and $\text{rank}_{psd}$. 
Bounding nonnegative rank

Want techniques to *lower bound* the nonnegative rank of a matrix.

In applications, these bounds may yield:

- Minimal size of latent variables
- Complexity lower bounds on extended representations

Known bounds exist (e.g. rank bound, combinatorial bounds, etc.).

Good lower bounds using “nonnegative nuclear norm” (Fawzi-P. 2012). Improved SOS/SDP techniques (Fawzi-P. 2013), also extend to other “product cone” ranks (e.g., NN tensor rank, CP-rank, etc).
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Lower bounding PSD rank?

Currently extending our bounds to PSD rank, since combinatorial methods (based on sparsity patterns) don’t quite work.

But, a few unexpected difficulties...

- In the PSD case, the underlying norm is non-atomic, and the corresponding “obvious” inequalities do not hold...
- “Noncommutative” trace positivity, quite complicated structure...

Nice links between rank$_{\text{psd}}$ and quantum communication complexity, mirroring the situation between rank$_{+}$ and classical communication complexity (e.g., Fiorini et al. (2011), Jain et al. (2011), Zhang (2012)).

Nevertheless, in some cases one can get nice strong results...
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Lifts with product cones

Let $d$ fixed. We are interested in lifts over the cone:

$$S^d_+ \times \cdots \times S^d_+ = (S^d_+)^r$$

$r$ copies

Why?

- $d = 1 \rightarrow$ LP lifts
- $d = 2 \rightarrow$ SOCP lifts: ice-cream cone is affinely isomorphic to $S^2_+$:

$$\sqrt{x^2 + y^2} \leq t \iff \begin{bmatrix} t + x & y \\ y & t - x \end{bmatrix} \succeq 0.$$ 

In practice, these are SDPs we can solve efficiently ($d$ small)
Factorization theorem

Factorization theorem [GPT] applied to \((S^d_+)^r\) lifts:

Theorem

*Polytope \(P\) has a \((S^d_+)^r\) lift iff slack matrix \(S_P\) can be written as the sum of \(r\) matrices of psd rank \(\leq d\).*

- Define \(\text{rank}_{S^d_+}(A)\) as:

  \[
  \text{rank}_{S^d_+}(A) = \min r \text{ s.t. } A \text{ can be written as the sum of } r \text{ matrices of psd rank } \leq d
  \]

- \(\text{rank}_{S^d_+}\) is atomic rank

- Interesting in quantum information: *classical-quantum* states (a.k.a., cq-states) where the dimension of the quantum part is \(\leq d\).
**Correlation polytope**

- **Correlation polytope**

  \[
  \text{COR}(n) = \text{conv} \left( bb^T : b \in \{0, 1\}^n \right).
  \]

- **COR}(n) is affinely isomorphic to cut polytope of \(K_{n+1}\).**

  Fiorini et al. 2012, and subsequent papers, showed that any LP lift of \(\text{COR}(n)\) has exponential size.
  → Proof based on analysis of a submatrix of slack matrix of \(\text{COR}(n)\), known as *unique-disjointness* matrix.

- What about \((S^d_+)^r\) lifts?
(\mathcal{S}^d_+)^r \text{ lifts of } \text{COR}(n)

Theorem (Fawzi-P. 2013)

If \text{COR}(n) has a \((\mathcal{S}^d_+)^r\)-lift then necessarily \(r \geq \kappa(d) \cdot c(d)^n\) where \(c(d) > 1\) and \(\kappa(d) > 0\) explicit constants:

\[
c(d) = (1 - 3^{-d})^{-1/d} > 1 \quad \kappa(d) = (3^d - 1)^{-\frac{1-1/d}{d}}
\]

Implications:

- No small LP representations (case \(d = 1\), c.f. Fiorini et. al)
- No small SOCP representations (case \(d = 2\))
- For any constant \(d\), exponentially many LMIs...

Results are \textit{unconditional} (no P/NP assumptions, not about specific constructions)
Exponential lower bounds for psd rank

$(S^d_+)^r$ lifts of $\text{COR}(n)$

Theorem (Fawzi-P. 2013)

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$$c(d) = (1 - 3^{-d})^{-1/d} > 1 \quad \kappa(d) = (3^d - 1)^{(1-1/d)}$$

Proof by showing that $\text{rank}_{S^d_+}(\text{UDISJ}(n))$ is exponentially large.

Main ingredients:

- Analysis of sparsity pattern of certain matrices of small psd rank
- + induction argument inspired from Kaibel and Weltge [KW13].
Unique disjointness matrix

- $2^n \times 2^n$ matrix indexed by $n$-bit strings:

$$UDISJ(n)_{a,b} = (1 - a^T b)^2 \quad \forall a \in \{0, 1\}^n, b \in \{0, 1\}^n$$

- Submatrix of slack matrix of $COR(n)$

- Two key facts about $UDISJ$:
  - if $a^T b = 0$ then $UDISJ_{a,b} = 1$
  - if $a^T b = 1$ then $UDISJ_{a,b} = 0$

- $UDISJ$ for $n = 1$ and $n = 2$:
Atoms

\[ A_{S^d}(n) = \{ M \in \mathbb{R}^{2n \times 2n}_+ : \text{rank}_{psd}(M) \leq d \text{ and } M_{a,b} = 0 \text{ for } a^T b = 1 \}. \]

- In any \((S^d)^r\)-factorization of \( UDISJ \), all terms must be in \( A_{S^d} \).
- To prove lower bound on \( \text{rank}_{S^d}(UDISJ) \), we show that matrices in \( A_{S^d}(n) \) must be very sparse, and thus \( \text{rank}_{S^d}(UDISJ) \) has to be large to be able to fill up the \( > 0 \) entries of \( UDISJ \).

Precisely, let

\[ \text{val}(M) = \text{card} \left\{ (a, b) \in (\{0, 1\}^n)^2 : a^T b = 0 \text{ and } M_{a,b} > 0 \right\}. \]

Lower bound on \( \text{rank}_{S^d}(UDISJ) \) follows from two facts:

\( \rightarrow \) Fact 1: \( \text{val}(UDISJ) = 3^n \) (simple calculation)

\( \rightarrow \) Fact 2 (main part): Any \( M \in A_{S^d} \) has \( \text{val}(M) \leq t(d)^n \) where \( t(d) < 3 \)
Atoms

\[ A_{S^d_+}(n) = \{ M \in \mathbb{R}^{2^n \times 2^n}_+: \text{rank}_{psd}(M) \leq d \text{ and } M_{a,b} = 0 \text{ for } a^T b = 1 \}. \]

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Induction argument of Kaibel and Weltge for $d = 1$ (I)

- Quantity $\text{val}(M)$ introduced by Kaibel and Weltge [2013] for LP-lifts ($d = 1$). They give elementary induction proof that $\text{val}(M) \leq 2^n$ for all $M \in \mathcal{A}(n)$
- Proof relies on a simple fact about $2 \times 2$ matrices in $\mathcal{A}(n = 1)$:
  Consider rectangles $R_1 = \{0\} \times \{0, 1\}$ and $R_2 = \{0, 1\} \times \{0\}$.

Let $M$ be a $2 \times 2$ rank-one matrix with $M_{1,1} = 0$. Then $M$ has at most 2 nonzero entries and these can be associated in a one-to-one way to the rectangles $R_1$ and $R_2$:

Two possible sparsity patterns: $\begin{bmatrix} 1 & \ \ \\ 2 & \end{bmatrix}$ or $\begin{bmatrix} 2 & 1 \end{bmatrix}$
Bootstrap the previous observation, to show that for any $n \geq 1$ and any $M \in \mathcal{A}(n)$

$$\text{val}(M) \leq \text{val}(M_{0,0}^0 + M_{0,1}^0) + \text{val}(M_{0,0}^0 + M_{1,0}^1)$$

where $M_{x,y}^{x,y}$ blocks of $M$:

$$M = \begin{bmatrix} M_{0,0}^0 & M_{0,1}^0 \\ M_{1,0}^1 & M_{1,1}^1 \end{bmatrix}$$

By induction this gives $\text{val}(M) \leq 2^n$
Generalize the induction argument to arbitrary $d$ using the notion of a uniform covering with rectangles.

**Theorem**

Let $K = S_+^d$. If $A_K(d')$ has a uniform-covering with $k$ rectangles then any $M \in A_K(n)$ for $n \geq d'$ satisfies:

\[
\text{val}(M) \leq k\left\lceil \frac{(n-1)}{d'} \right\rceil + 1
\]

- Kaibel and Weltge [2013] correspond to $d = d' = 1$. The two rectangles $R_1$ and $R_2$ from before give a uniform covering of $A(1)$ with 2 rectangles.
Constructing uniform coverings (I)

- To finish the proof we will show that $\mathcal{A}_{S^d_+}(d)$ has a uniform covering with $k < 3^d$ rectangles.
- We need to understand the sparsity pattern of elements in $\mathcal{A}_{S^d_+}(d)$.
- For $d = 2$ we can do things by hand:

**Lemma**

*Any $4 \times 4$ matrix $M \in \mathcal{A}_{S^2_+}(2)$ has one of the following six sparsity patterns below:*

\[
\begin{align*}
(1) & \quad \begin{bmatrix}
\times & \times & \times & \times \\
\times & 0 & 0 & 0 \\
\times & 0 & 0 & 0 \\
\times & 0 & 0 & ?
\end{bmatrix} & \quad \text{or} & \quad (2) & \quad \begin{bmatrix}
\times & \times & \times & 0 \\
\times & 0 & 0 & 0 \\
\times & 0 & 0 & 0 \\
0 & 0 & 0 & ?
\end{bmatrix} & \quad \text{or} & \quad (3) & \quad \begin{bmatrix}
\times & \times & \times & \times \\
0 & 0 & 0 & 0 \\
\times & \times & 0 & 0 \\
\times & 0 & 0 & ?
\end{bmatrix} \\
\text{or} & \quad (4) & \quad \begin{bmatrix}
\times & \times & \times & \times \\
\times & 0 & 0 & 0 \\
\times & 0 & 0 & 0 \\
0 & 0 & 0 & ?
\end{bmatrix} & \quad \text{or} & \quad (5) & \quad \begin{bmatrix}
\times & \times & \times & \times \\
\times & 0 & 0 & 0 \\
\times & 0 & 0 & 0 \\
\times & 0 & 0 & ?
\end{bmatrix} & \quad \text{or} & \quad (6) & \quad \begin{bmatrix}
\times & \times & \times & \times \\
\times & 0 & 0 & 0 \\
\times & 0 & 0 & 0 \\
\times & 0 & 0 & ?
\end{bmatrix}
\end{align*}
\]

*In particular $\text{val}(M) \leq 7$.*
For $d = 2$ one can construct a uniform covering with $k = 7$ rectangles by hand.

What about general $d$? A detailed analysis of sparsity pattern seems difficult, but one can show the following fact, which will turn out to be enough:

**Lemma**

If $M$ is a $2^d \times 2^d$ matrix with $M_{a,b} = 0$ when $a^T b = 1$ and $\text{rank}_{psd}(M) \leq d$, then $M$ has at least one zero on the antidiagonal, i.e., $M_{\alpha,\bar{\alpha}} = 0$ for some $\alpha \in \{0, 1\}^d$.

Using this lemma, one can use a recursive construction to show that $\mathcal{A}_{S^d}(d')$ has a uniform covering with $k = 3^d - 1 < 3^d$ rectangles.
Recap

Using uniform coverings we showed that for any $M \in A_{S^d}(n)$

$$\text{val}(M) \leq t(d)^n$$

where $t(d) < 3$. Thus we get the following exponential lower bound:

$$\text{rank}_{S^d}(UDISJ) \geq \frac{\text{val}(UDISJ)}{t(d)^n} = \left(\frac{3}{t(d)}\right)^n.$$
The End

Thank You!

Want to know more?


Example: hexagon (III)

A nonnegative factorization:

\[
S_H = \begin{pmatrix}
1 & 0 & 1 & 0 & 0 \\
1 & 0 & 0 & 0 & 1 \\
0 & 0 & 0 & 1 & 2 \\
0 & 1 & 0 & 0 & 1 \\
0 & 1 & 1 & 0 & 0 \\
0 & 0 & 2 & 1 & 0
\end{pmatrix}
\begin{pmatrix}
0 & 0 & 0 & 1 & 2 & 1 \\
1 & 2 & 1 & 0 & 0 & 0 \\
0 & 0 & 1 & 1 & 0 & 0 \\
0 & 1 & 0 & 0 & 1 & 0 \\
1 & 0 & 0 & 0 & 0 & 1
\end{pmatrix},
\]