PSD factorizations of nonnegative matrices and lower bounds on semidefinite representations

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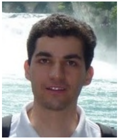

Based on joint work with **Hamza Fawzi** (MIT),
João Gouveia (U. Coimbra) and **Rekha Thomas** (U. Washington).

Nonnegative factorizations

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 *nonnegative rank* of the matrix A.
- Many applications: statistics, factor models, machine learning, ...
- Very difficult problem, many heuristics exist.

Factorizations and hidden variables

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

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

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., $X - Z - Y$ is Markov):

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

- 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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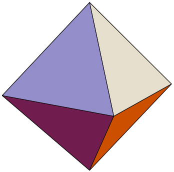
Motivating example

The *crosspolytope* $\mathcal{C}_n$ is the unit ball of the ℓ_1 ball:

$$\mathcal{C}_n := \{x \in \mathbb{R}^n \,:\, \sum_{i=1}^{n} |x_i| \leq 1\}.$$



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 $\mathcal{C}_n$ can be represented more conveniently:

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

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

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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

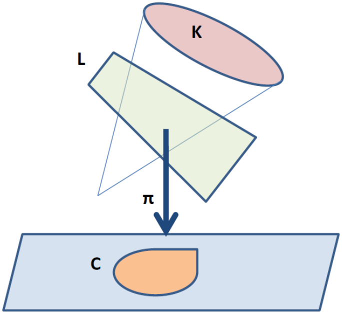
Existence and efficiency:

- 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 π is a linear map?



Cone lifts of convex bodies

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?

This talk: polytopes

What happens in the case of polytopes?

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

(WLOG, compact with $0 \in \operatorname{int} P$).

Polytopes have a finite number of facets f_i and vertices v_j.
Define a nonnegative matrix, called the *slack matrix* of the polytope:

$$[S_P]_{ij} = 1 - f_i^T v_j, \qquad i = 1, \ldots, |F| \quad j = 1, \ldots, |V|$$

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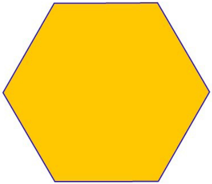
Example: hexagon (I)

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?

Cone factorizations and representability

"Geometric" LP formulations exactly correspond to "algebraic" factorizations of the slack matrix.

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

$$S_{ij} = \langle a_i, b_j \rangle, \qquad i = 1, \ldots, v, \qquad j = 1, \ldots, f$$

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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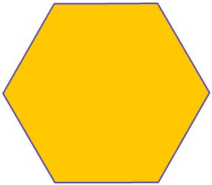

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Nonnegative rank is 5.

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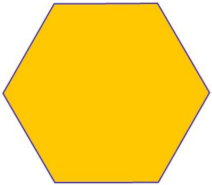

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Nonnegative rank is 5.

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.

polytopes/LP	convex sets/convex cones
slack matrix	slack operators
vertices	extreme points of C
facets	extreme points of polar C°
nonnegative factorizations	conic factorizations
$S_{ij} = \langle a_i, b_j \rangle, \quad a_i \geq, b_j \geq 0$	$S_{ij} = \langle a_i, b_j \rangle, \quad a_i \in K, b_j \in K^*$

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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Exactly captures the complexity of SDP-representability.

PSD rank of a nonnegative matrix

Let $M \in \mathbb{R}^{m \times n}$ be a nonnegative matrix.

The *PSD rank* of M, denoted rank_{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

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

Natural generalization of nonnegative rank.

The PSD rank determines the “best” semidefinite lifting.

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Some inequalities

- For any nonnegative matrix M

$$\frac{1}{2}\sqrt{1 + 8\,\mathrm{rank}(M)} - \frac{1}{2} \leq \mathrm{rank}_{psd}(M) \leq \mathrm{rank}_{+}(M).$$

- Gap between $\mathrm{rank}_{+}(M)$ and $\mathrm{rank}_{psd}(M)$ 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 $\mathrm{rank}_{psd}(M) = 2$, but $\mathrm{rank}_{+}(M) = \Omega(\log n)$.

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

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_{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:

$$\underbrace{\mathcal{S}_+^d \times \cdots \times \mathcal{S}_+^d}_{r \text{ copies}} = (\mathcal{S}_+^d)^r$$

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

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

  - In practice, these are SDPs we can solve efficiently (d small)

Factorization theorem

Factorization theorem [GPT] applied to $(\mathcal{S}_+^d)^r$ lifts:

Theorem

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

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

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

- $\text{rank}_{\mathcal{S}_+^d}$ 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

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

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

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

- What about $(\mathcal{S}_+^d)^r$ lifts?

$(\mathcal{S}_+^d)^r$ lifts of $COR(n)$

Theorem (Fawzi-P. 2013)

If $COR(n)$ 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:

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

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 *unconditional* (no P/NP assumptions, not about specific constructions)

$(\mathcal{S}_+^d)^r$ lifts of $COR(n)$

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Proof by showing that $\text{rank}_{\mathcal{S}_+^d}(UDISJ(n))$ 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 $n = 2$:

$$\begin{array}{c} \\ 0 \\ 1 \end{array} \begin{array}{c} \begin{array}{cc} 0 & 1 \end{array} \\ \begin{bmatrix} 1 & 1 \\ 1 & 0 \end{bmatrix} \end{array} \qquad \begin{array}{c} \\ 00 \\ 01 \\ 10 \\ 11 \end{array} \begin{array}{c} \begin{array}{cccc} 00 & 01 & 10 & 11 \end{array} \\ \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} \end{array}$$

Atoms

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

- In any $(\mathcal{S}_+^d)^r$-factorization of *UDISJ*, all terms must be in $\mathcal{A}_{\mathcal{S}_+^d}$
- To prove lower bound on $\text{rank}_{\mathcal{S}_+^d}(UDISJ)$, we show that matrices in $\mathcal{A}_{\mathcal{S}_+^d}(n)$ must be very sparse, and thus $\text{rank}_{\mathcal{S}_+^d}(UDISJ)$ 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 $\text{rank}_{\mathcal{S}_+^d}(UDISJ)$ follows from two facts:
→ Fact 1: $\text{val}(UDISJ) = 3^n$ (simple calculation)
→ Fact 2 (main part): Any $M \in \mathcal{A}_{\mathcal{S}_+^d}$ has $\text{val}(M) \leq t(d)^n$ where $t(d) < 3$

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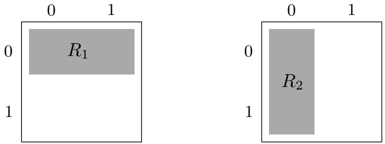
Induction argument of Kaibel and Weltge for $d = 1$ (I)

- 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 2×2 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 2×2 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 $\begin{bmatrix} 2 & 1 \\ & \end{bmatrix}$

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

- Bootstrap the previous observation, to show that for any $n \geq 1$ and any $M \in \mathcal{A}(n)$

$$\mathrm{val}(M) \leq \mathrm{val}(\underbrace{M^{0,0} + M^{0,1}}_{\in \mathcal{A}(n-1)}) + \mathrm{val}(\underbrace{M^{0,0} + M^{1,0}}_{\in \mathcal{A}(n-1)})$$

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

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

- By induction this gives $\mathrm{val}(M) \leq 2^n$

Generalize the induction argument to arbitrary d

Generalize this induction argument to arbitrary d using the notion of a *uniform covering* with rectangles.

Theorem

Let $K = \mathcal{S}^d_+$. If $\mathcal{A}_K(d')$ has a uniform-covering with k rectangles then any $M \in \mathcal{A}_K(n)$ for $n \geq d'$ satisfies:

$$val(M) \leq k^{\lfloor (n-1)/d' \rfloor + 1}$$

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

Constructing uniform coverings (I)

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

Lemma

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

$$(1) \begin{bmatrix} \times & \times & \times & \times \\ \times & 0 & 0 & 0 \\ \times & 0 & 0 & 0 \\ \times & 0 & 0 & ? \end{bmatrix} \text{ or } (2) \begin{bmatrix} \times & \times & \times & 0 \\ \times & 0 & \times & 0 \\ \times & \times & 0 & 0 \\ 0 & 0 & 0 & ? \end{bmatrix} \text{ or } (3) \begin{bmatrix} \times & \times & \times & \times \\ 0 & 0 & 0 & 0 \\ \times & \times & 0 & 0 \\ \times & 0 & 0 & ? \end{bmatrix}$$

$$\text{or } (4) \begin{bmatrix} \times & \times & \times & \times \\ \times & 0 & \times & 0 \\ 0 & 0 & 0 & 0 \\ \times & 0 & 0 & ? \end{bmatrix} \text{ or } (5) \begin{bmatrix} \times & 0 & \times & \times \\ \times & 0 & \times & 0 \\ \times & 0 & 0 & 0 \\ \times & 0 & 0 & ? \end{bmatrix} \text{ or } (6) \begin{bmatrix} \times & \times & 0 & \times \\ \times & 0 & 0 & 0 \\ \times & \times & 0 & 0 \\ \times & 0 & 0 & ? \end{bmatrix}$$

In particular $val(M) \leq 7$.

Constructing uniform coverings (II)

- 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 $\mathrm{rank}_{psd}(M) \leq d$, 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 $\mathcal{A}_{\mathcal{S}^d_+}(d)$ has a uniform covering with $k = 3^d - 1 < 3^d$ rectangles.

Recap

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

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

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

$$\text{rank}_{\mathcal{S}_+^d}(UDISJ) \geq \frac{\text{val}(UDISJ)}{t(d)^n} = (3/t(d))^n.$$

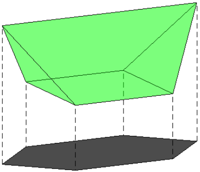
The End

Thank You!

Want to know more?

- J. Gouveia, P.A. Parrilo, R. Thomas, Lifts of convex sets and cone factorizations, *Mathematics of Operations Research*, 38:2, 2013. `arXiv:1111.3164`.
- H. Fawzi, P.A. Parrilo, New lower bounds on nonnegative rank using conic programming, `arXiv:1210.6970`.
- H. Fawzi, P.A. Parrilo, Exponential lower bounds on fixed-size psd rank and semidefinite extension complexity, `arXiv:1311.2571`.

Example: hexagon (III)



A nonnegative factorization:

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