Convex sets, conic matrix factorizations and conic rank lower bounds

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Based on joint work with **João Gouveia** (U. Coimbra),
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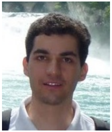

Nonnegative factorizations

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 W, such that X and Y are conditionally independent given W (i.e., $X - W - Y$ 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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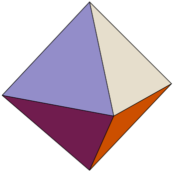
Motivating example



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:

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

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).

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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

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

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Our questions

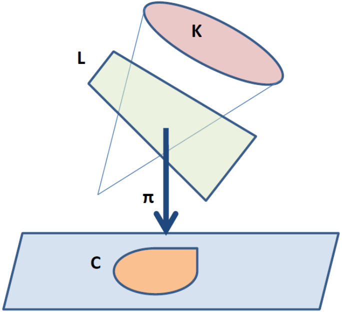
Existence and efficiency:

- 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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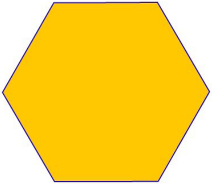
Example: hexagon (I)

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:

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

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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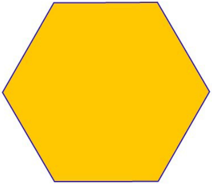
Example: hexagon (II)



Regular hexagon in the plane.

Its slack matrix is

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Nonnegative rank is 5.

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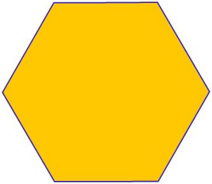

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Bounding nonnegative rank

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.).
Want to do better, using convex optimization...

Two convex cones

Two important and well-known convex cones of symmetric matrices:

- Copositive matrices:

$$\mathcal{C} := \{M \in \mathcal{S}^n : x^T M x \geq 0, \quad \forall x \geq 0\}$$

- Completely positive matrices:

$$\mathcal{B} := \operatorname{conv}\{xx^T : x \geq 0\}$$

These are proper cones (convex, closed, proper and solid), and they are dual to each other:

$$\mathcal{C}^* = \mathcal{B}, \qquad \mathcal{B}^* = \mathcal{C}.$$

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A convex bound for nonnegative rank

Let $A \in \mathbb{R}_+^{m \times n}$ be a nonnegative matrix, and define

$$\nu_+(A) := \max_{W \in \mathbb{R}^{m \times n}} \left\{ \langle A, W \rangle \ : \ \begin{bmatrix} I & -W \\ -W^T & I \end{bmatrix} \text{ copositive } \right\}.$$

Then,

$$\operatorname{rank}_+(A) \geq \left(\frac{\nu_+(A)}{\|A\|_F} \right)^2,$$

where $\|A\|_F := \sqrt{\sum_{i,j} A_{i,j}^2}$ is the Frobenius norm of A.

- Essentially, a kind of “nonnegative nuclear norm”
- Convex, but hard... (membership in $\mathcal{B}$ and $\mathcal{C}$ is NP-hard!)

But, we know how to approximate them...

Proof

If $A = \sum_{i=1}^r u_i v_i^T$, a scaling argument show that wlog we can take $\|u_i\| = \|v_i\|$ for all i. By Cauchy-Schwarz,

$$\frac{\sum_{i=1}^r \|u_i\|\|v_i\|}{\sqrt{\sum_{i=1}^r \|u_i\|^2\|v_i\|^2}} \leq \sqrt{r} = \sqrt{\text{rank}_+(A)}$$

We can then bound the numerator and denominator:

- Numerator: if W is feasible, then $u_i^T W v_i \leq \|u_i\|\|v_i\|$, and thus $\langle A, W\rangle \leq \sum_{i=1}^r \|u_i\|\|v_i\|$.
- Denominator:

$$\|A\|_F^2 = \sum_{i,j=1}^r \langle u_i v_i^T, u_j v_j^T\rangle \geq \sum_{i=1}^r \|u_i\|^2\|v_i\|^2.$$

SOS Approximation

Can approximate the cones $\mathcal{C}$ and $\mathcal{B}$ using sum of squares and semidefinite programming (P. 2000). We can write $\mathcal{C}$ as

$$\mathcal{C} = \left\{ M \in \mathcal{S}^n \;:\; \text{the polynomial } \sum_{i,j=1}^{n} M_{i,j} x_i^2 x_j^2 \text{ is nonnegative} \right\}.$$

The kth order relaxation is defined as:

$$\mathcal{C}^{[k]} = \left\{ M \in \mathcal{S}^n \;:\; \left(\sum_{i=1}^{n} x_i^2 \right)^k \left(\sum_{i,j=1}^{n} M_{i,j} x_i^2 x_j^2 \right) \text{ is a sums-of-squares} \right\}.$$

Clearly, $\mathcal{C}^{[k]} \subseteq \mathcal{C}$ and also $\mathcal{C}^{[k]} \subseteq \mathcal{C}^{[k+1]}$. Furthermore, each $\mathcal{C}^{[k]}$ is computable via SDP.

Simplest case ($k = 0$)

The case $k = 0$ is the simple sufficient condition for copositivity

$$M = P + N, \qquad P \succeq 0, \quad N_{ij} \geq 0.$$

Thus, the quantity $\nu_+^{[0]}(A)$ takes the more explicit form:

$$\nu_+^{[0]}(A) = \max \left\{ \langle A, W \rangle \ : \ \begin{bmatrix} I & -W \\ -W^T & I \end{bmatrix} \in \mathcal{N}^{n+m} + \mathcal{S}_+^{n+m} \right\}$$

For any $k \geq 0$:

$$\nu(A) \leq \nu_+^{[0]}(A) \leq \nu_+^{[k]}(A) \leq \nu_+(A) \leq \sqrt{\mathrm{rank}_+(A)}\|A\|_F$$

where $\nu(A)$ is the standard nuclear norm.

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Comparison: Rank bound

Trivially, $\text{rank}(A) \leq \text{rank}_+(A)$. Can our bound improve on this?

Consider

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

It is known that $\text{rank}(A) = 3$ and $\text{rank}_+(A) = 4$.

We have $\nu_+^{[0]}(A) = 4\sqrt{2}$, and thus our lower bound is sharp:

$$4 = \text{rank}_+(A) \geq \left(\frac{\nu_+^{[0]}(A)}{\|A\|_F} \right)^2 = \left(\frac{4\sqrt{2}}{\sqrt{8}} \right)^2 = 4.$$

Comparison: Boolean rank (rectangle covering)

A lower bound used in communication complexity. Relies only on sparsity pattern of matrix.

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

The rectangle covering number of A is 2 since $\operatorname{supp}(A)$ can be covered with the two rectangles $\{1,2\} \times \{2,3,4\}$ and $\{2,3,4\} \times \{1,2\}$.

Our bound yields $\operatorname{rank}_+(A) \geq \lceil (\nu_+^{[0]}(A)/\|A\|_F)^2 \rceil = 3$. In fact $\operatorname{rank}_+(A)$ is exactly equal to 3:

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

Example: hypercube

What is the extension complexity of the *n*-dimensional hypercube? Is there a better representation than the “obvious” $2n$ inequalities?

Notice that the slack matrix is exponentially large ($2n \times 2^n$).

Rank bound is $n+1$. Goemans’ face-counting lower bound gives $\approx \sqrt{3}n$... Perhaps something nontrivial can be done?

Proposition: Let $C_n = [0,1]^n$ be the hypercube in n dimensions and let $S(C_n) \in \mathbb{R}^{2n \times 2^n}$ be its slack matrix. Then

$$\operatorname{rank}_+(S(C_n)) = \left(\frac{\nu_+^{[0]}(S(C_n))}{\|S(C_n)\|_F} \right)^2 = 2n.$$

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Applications

Yields computable approximations to an “atomic norm” for nonnegative factorization (e.g., Chandrasekaran-Recht-P.-Willsky 2010).

Can use as regularizer for model selection problems (e.g., to identify “near independent” or “most conditionally independent” models).

Q: In a statistical setting, tradeoffs between sample and computational complexity? (Srebro et al., Chandrasekaran-Jordan, etc).

In particular, sample estimates in terms of *Gaussian widths*?

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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.
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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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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Lower bounding PSD rank?

Currently extending our bound to PSD rank, since combinatorial methods (based on sparsity patterns) cannot possibly 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” versions of $\mathcal{C}$ and $\mathcal{B}$, 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)).

Computation

Even for nonnegative factorization, non-convex and very difficult.

A simple approach: alternating convex minimization.

For instance, for PSD factorizations of a nonnegative matrix $M = AB$, we can alternate between minimizing over $A = [A_1, \dots, A_m]^T$ and $B = [B_1, \dots, B_n]$:

$$\underset{A_i \succeq 0}{\text{minimize}} \, \|M - AB\| \qquad\qquad \underset{B_i \succeq 0}{\text{minimize}} \, \|M - AB\|$$

These subproblems are SDPs (and if $\|\cdot\|$ is the Euclidean norm, they are decoupled). However, no global guarantees.

Ongoing work of F. Glineur (UCL).

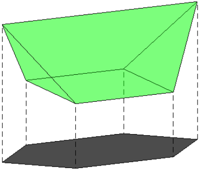
The End

Thank You!

Want to know more?

- J. Gouveia, P.A. Parrilo, R. Thomas, Lifts of convex sets and cone factorizations, *Mathematics of Operations Research*, to appear, 2013. `arXiv:1111.3164`.
- H. Fawzi, P.A. Parrilo, New lower bounds on nonnegative rank using conic programming, `arXiv:1210.6970`.

Example: hexagon (III)



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