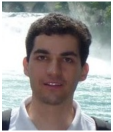
Convex sets, matrix factorizations and positive semidefinite rank

Pablo A. Parrilo

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Based on joint work with
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Question: representability of convex sets

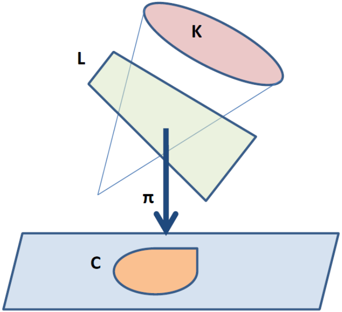
Existence and efficiency:

- 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?



Outline

1. Factorizations
   - Conic factorizations
   - Positive semidefinite rank
2. Representations of convex sets
   - Extended formulations
   - Slack operators
   - Factorizations and representability
3. Positive semidefinite rank
   - Basic properties
   - Bounds and extensions

Matrix factorizations

Given a matrix $M \in \mathbb{R}^{m \times n}$, can factorize it as $M = AB$, i.e.,

$$\mathbb{R}^n \xrightarrow{B} \mathbb{R}^k \xrightarrow{A} \mathbb{R}^m$$

Ideally, k is small (matrix M is low-rank), so we're factorizing through a "small subspace."

Why is this useful?

- Principal component analysis (e.g., factorization of covariance matrix of a Gaussian process)
- System realization theory (e.g., factorization of the Hankel matrix)

And many others... Standard notion in linear algebra.

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More Factorizations...

However, often we impose further conditions on $M = AB$...

- Norm conditions on the factors A, B:
  - Want factors A, B to be "small" in some norm
  - Well-studied topic in Banach space theory, through the notion of *factorization norms*
  - E.g., the *nuclear norm* $\|M\|_\star := \sum_k \sigma_k(M)$ has the variational characterization

$$\|M\|_\star = \min_{A,B\,:\,M=AB} \frac{1}{2}(\|A\|_F^2 + \|B\|_F^2)$$

- Nonnegativity conditions:
  - Matrix M is (componentwise) nonnegative, and so must be the factors.
  - This is the *nonnegative factorization* problem (e.g., Berman-Plemmons '74, Cohen-Rothblum '93)
  - Let's see this in more detail...

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Nonnegative factorizations and nonnegative rank

Given a nonnegative matrix $M \in \mathbb{R}^{m \times n}$, a factorization

$$M = AB$$

where $A \in \mathbb{R}^{m \times k}$, $B \in \mathbb{R}^{k \times n}$ are also *nonnegative*.

- The smallest such k is the nonnegative rank of the matrix M.
- Can interpret as

$$M_{ij} = e_i^T M e_j = (A^T e_i)^T (B e_j) = \langle a_i, b_j \rangle,$$

  where $a_i := (A^T e_i) \in \mathbb{R}_+^k$, $b_j := (B e_j) \in \mathbb{R}_+^k$.
- Many applications: probability/statistics, information theory, machine learning, communication complexity, . . .
- Very difficult problem, many heuristics exist.

Conic factorizations

We're interested in a different class: conic factorizations [GPT11]

Let $M \in \mathbb{R}_+^{m \times n}$ be a nonnegative matrix, and $\mathcal{K}$ be a convex cone in $\mathbb{R}^k$. Then, we want $M = AB$, where

$$\mathbb{R}_+^n \xrightarrow{B} \mathcal{K} \xrightarrow{A} \mathbb{R}_+^m$$

- M maps the nonnegative orthant into the nonnegative orthant.
- For $\mathcal{K} = \mathbb{R}_+^k$, this is a standard nonnegative factorization.
- In general, factorize a linear map through a "small cone"

Important special case: $\mathcal{K}$ is the cone of psd matrices...

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PSD rank of a nonnegative matrix

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

Definition [GPT11]: The PSD rank of M, denoted rank_{psd}, is the smallest integer r for which there exists $r \times r$ PSD matrices $\{A_1, \ldots, A_m\}$ and $\{B_1, \ldots, B_n\}$ such that

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

(The maps are then given by $x \mapsto \sum_i x_i A_i$, and $Y \mapsto \operatorname{trace} Y B_j$.)

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Example (I)

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

M admits a psd factorization of size 2:

$$A_1 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \quad A_2 = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \quad A_3 = \begin{bmatrix} 1 & -1 \\ -1 & 1 \end{bmatrix}$$

$$B_1 = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \quad B_2 = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \quad B_3 = \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}.$$

One can easily check that the matrices A_i and B_j are positive semidefinite, and that $M_{ij} = \langle A_i, B_j \rangle$. This factorization shows that $\text{rank}_{\text{psd}}(M) \le 2$, and in fact $\text{rank}_{\text{psd}}(M) = 2$.

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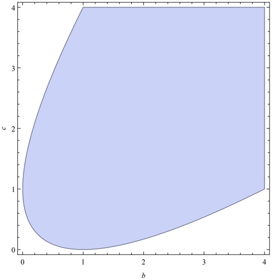
Example (II)

Consider the matrix

$$M(a,b,c) = \begin{bmatrix} a & b & c \\ c & a & b \\ b & c & a \end{bmatrix}.$$



- Usual rank of $M(a,b,c)$ is 3, unless $a = b = c$ (then, rank is 1).
- One can show that

$$\text{rank}_{\text{psd}}\left(M(a,b,c)\right) \leq 2 \quad \Longleftrightarrow \quad a^2 + b^2 + c^2 \leq 2(ab + bc + ac).$$

Back to representability...

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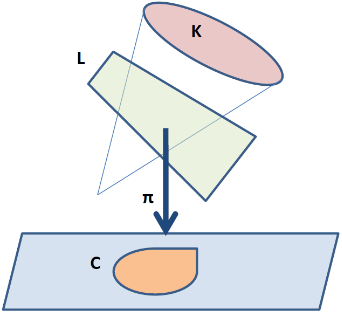


Question: representability of convex sets

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

A general theme: algebraic varieties, unitaries/contractions, . . .

Extended formulations

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

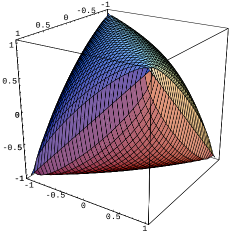
Seminal work by Yannakakis (1991). He gave a beautiful characterization (for LP) in terms of *nonnegative factorizations*, and used it to disprove the existence of "symmetric" LPs for the TSP polytope.
Nice recent survey by Conforti-Cornuéjols-Zambelli (2010).

Our goal: to understand this phenomenon for convex optimization (SDP), not just LP.

"Extended formulations" in semidefinite programming

Many convex sets can be modeled by SDP. 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



How to produce extended formulations?

- Clever, non-obvious constructions
  - E.g., the KYP (Kalman-Yakubovich-Popov) lemma, LMI solution of interpolation problems (e.g., AAK, Ball-Gohberg-Rodman), ...
  - Work of Nesterov/Nemirovski, Boyd/Vandenberghe, Scherer, Gahinet/Apkarian, Ben-Tal/Nemirovski, Sanyal/Sottile/Sturmfels, etc.
- Systematic "lifting" techniques
  - Reformulation/linearization (Sherali-Adams, Lovasz-Schrijver)
  - Sum of squares (or moments), Positivstellensatz, (Lasserre, Putinar, P.)
  - Determinantal representations (Helton/Vinnikov, Nie)
  - Hyperbolic polynomials (Renegar)

Much research in this area. More recently, efforts towards understanding the general case (not just specific constructions).

Polytopes

What happens in the case of polytopes?

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

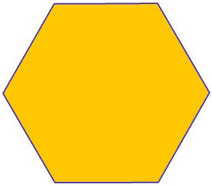
(WLOG, compact with $0 \in \operatorname{int} P$).

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

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

Example: hexagon (I)

Consider a regular hexagon in the plane.



It has 6 vertices, and 6 facets. Its slack matrix has rank 3, and 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:

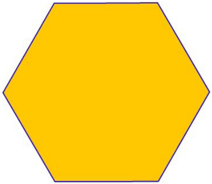
$$S_{ij} = \langle a_i, b_j \rangle, \qquad i = 1, \ldots, v, \qquad j = 1, \ldots, f$$

where a_i, b_i are nonnegative vectors.

Theorem (Yannakakis 1991): The minimal lifting dimension of a polytope is equal to the *nonnegative rank* of its slack matrix.

Example: hexagon (II)

Regular hexagon in the plane.



Its slack matrix is

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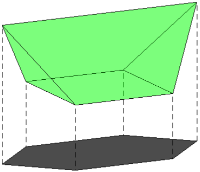
Nonnegative rank is 5.

Example: hexagon (III)



A nonnegative factorization:

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

Beyond LPs and nonnegative factorizations

LPs are nice, but what about broader representability questions?

In [GPT11], a generalization of Yannakakis' theorem to the full 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
$S_{ij} = \langle a_i, b_j \rangle, \quad a_i \geq 0, b_j \geq 0$	$S_{ij} = \langle a_i, b_j \rangle, \quad a_i \in K, b_j \in K^*$

Polytopes, semidefinite programming, and factorizations

Even for polytopes, SDP representations can be interesting.

(Example: the *stable set* or *independent set* polytope of a graph. For *perfect graphs*, efficient SDP representations exist, but no known subexponential LP.)

Thm: ([GPT 11]) Positive semidefinite rank of slack matrix exactly characterizes the complexity of SDP-representability.

PSD factorizations of slack matrix $\Longleftrightarrow$ SDP extended formulations

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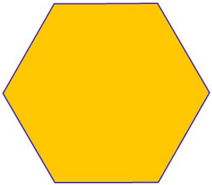
SDP representation of hexagon

A regular hexagon in the plane.

PSD rank of its slack matrix is 4.



Hexagon is the projection onto (x, y) of a 4×4 spectrahedron:

$$\begin{bmatrix} 1 & x & y & t \\ x & (1+r)/2 & s/2 & r \\ y & s/2 & (1-r)/2 & -s \\ t & r & -s & 1 \end{bmatrix} \succeq 0$$

Representation has nice symmetry properties (equivariance, [FSP14/15]).

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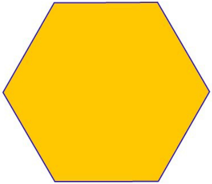

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Towards understanding psd rank

Generally difficult, since it's semialgebraic (inequalities matter), and symmetry group is "small".

- Basic properties
- Dependence on field and topology of factorizations
- Lower bounds on cone ranks
- Special cases and extensions

Basic 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 $\mathrm{rank}_{\mathrm{psd}}$.

Real and rational ranks can be different

If the matrix M has rational entries, sometimes it is natural to consider only factors A_i, B_i that are rational.

In general we have

$$\mathrm{rank}_{\mathrm{psd}}(M) \leq \mathrm{rank}_{\mathrm{psd}\,\mathbb{Q}}(M).$$

and inequality *can be strict*. Explicit examples (Fawzi-Gouveia-Robinson `arXiv:1404.4864`).

Same question for nonnegative rank was open (since Cohen-Rothblum 93). Finally settled a few weeks ago! (Chistikov *et al.*, `arXiv:1605.06848`; Shitov, `arXiv:1605.07173`). Furthermore, *universality* results!

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Bounding nonnegative/SDP rank

Factorization methods (e.g., local search) give *upper bounds* on ranks.

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

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A convex lower bound for nonnegative rank [FP13]

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,

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

- Essentially, a kind of "nonnegative nuclear norm"
- Convex, but hard... (membership in copositive cone is NP-hard!)

Approximate them using SDP!

Can be improved by "self-scaled" techniques (Fawzi-P. 2013), and extends to other product-cone ranks (e.g., NN tensor rank, CP-rank, etc).

Lower bounding PSD rank?

Bounds on PSD rank are of high interest, 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)).

In complexity-theoretic settings, recent strong results, see e.g. Lee-Raghavendra-Steurer (2015).

The symmetric case

Given a symmetric $M \in \mathbb{R}^{n \times n}$, do there exist $A_i \succeq 0$ such that

$$M_{ij} = \langle A_i, A_j \rangle \qquad i, j = 1, \ldots, n.$$

Equivalently, is M the Gram matrix of a set of psd matrices?

- Dual to *trace positivity* of noncommutative polynomials (e.g., Klep, Burgdorf, etc.)
- Of interest in quantum information (tomorrow's talk by M. Laurent)
- Many open questions; related to outstanding conjectures of Connes and Tsirelson

Many open questions!

- Computation, computation, computation!
- Efficient/practical lower/upper bounds?
- Approximate factorizations?
- Topology of space of factorizations?
- Structured matrices? PSD-rank preservers?
- Are current constructive methods (e.g., SOS) far from optimal?

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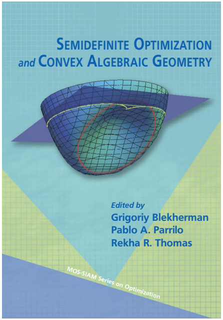
Summary

- Interesting new class of factorization problems
- Interplay of algebraic and geometric aspects
- Many open questions, lots to do!



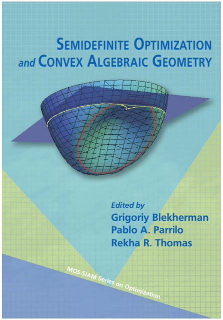
If you want to know more:

- H. Fawzi, J. Gouveia, P.A. Parrilo, R. Robinson, R. Thomas, Positive semidefinite rank, *Mathematical Programming*, 153:1, 2015. `arXiv:1407.4095`.
- J. Gouveia, P.A. Parrilo, R. Thomas, Lifts of convex sets and cone factorizations, *Mathematics of Operations Research*, 38:2, 2013. `arXiv:1111.3164`.
- SIAM book SDP and convex algebraic geometry (Helton/P./Nie/Sturmfels/Thomas NSF FRG), available online.

Thanks for your attention!

Summary

- Interesting new class of factorization problems
- Interplay of algebraic and geometric aspects
- Many open questions, lots to do!



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