Positive semidefinite rank

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Question: representability of convex sets

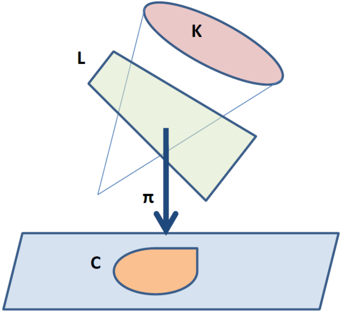
Existence and efficiency:

- 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?



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?

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

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

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More Factorizations...

However, often we need 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*
  - For instance, the nuclear norm $\|M\|_\star := \min_{A,B\,:\,M=AB} \frac{1}{2}(\|A\|_F^2 + \|B\|_F^2)$
- Nonnegativity conditions:
  - Matrix M is (componentwise) nonnegative, and so must be the factors.
  - This is the *nonnegative factorization* problem.
  - Many applications, e.g., in probability (conditional independence) and machine learning (additive features).

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Nonnegative factorization 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.

As we'll see, also fundamental in optimization ...

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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 r for which there exists $r \times r$ PSD matrices $\{A_1, \ldots, A_m\}$ and $\{B_1, \ldots, B_n\}$ such that

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

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

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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 $\text{rank}_{\text{psd}}(M) \leq 2$, and in fact $\text{rank}_{\text{psd}}(M) = 2$.

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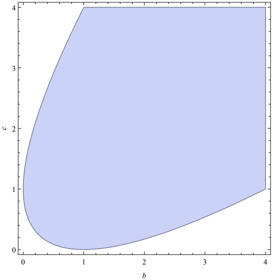
Example (II)

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

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

Back to representability...

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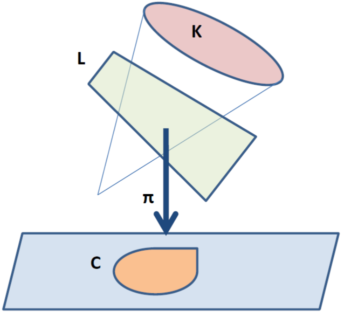


Question: representability of convex sets

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

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

Extended formulations

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

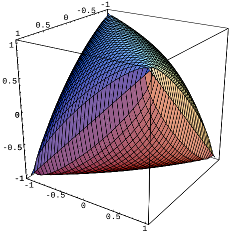
Seminal work by Yannakakis (1991). He gave a beautiful characterization (for LP) in terms of *nonnegative factorizations*, and used it to disprove the existence of "symmetric" LPs for the TSP polytope.
Nice recent survey by Conforti-Cornuéjols-Zambelli (2010).

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 and LMIs. 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 (Guler, 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?

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

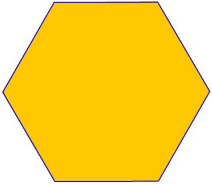
(WLOG, compact with $0 \in \operatorname{int} P$).

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:

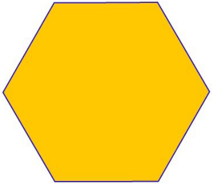
$$S_{ij} = \langle a_i, b_j \rangle, \qquad i = 1, \ldots, v, \qquad j = 1, \ldots, f$$

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.

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.

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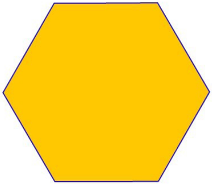
SDP representation of hexagon

A regular hexagon in the plane.



Projection onto (x, y) of a 5-dimensional 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).

Towards understanding psd rank

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

- Basic properties
- Other interpretations (e.g., information-theoretic)
- Dependence on field and topology of factorizations
- 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 PSD rank 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

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

and inequality can be strict. Explicit examples (Fawzi-Gouveia-Robinson).

Same question for nonnegative rank is open (since Cohen-Rothblum 93).

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Computing and bounding PSD rank

Computing PSD rank seems to be quite hard, both in theory and practice. Are there situations where it is easy?

- $k = 1$ easy, since $\text{rank}_{\text{psd}}(M) = 1$ if and only if $\text{rank}(M) = 1$.
- $k = 2$ also easy, since it is reducible to semidefinite programming (e.g., via S-lemma).

What about for fixed psd rank (even $k = 3$)? Analogue of Arora-Ge-Kannan-Moitra polynomiality result for nonnegative rank?

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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

Many known bounds (e.g. rank, combinatorial, information-theoretic, etc.).

New "self-scaled bounds" via SOS (Fawzi-P., `arXiv:1404.3240`), that extend to other "product cone" ranks (e.g., NN tensor rank, CP-rank, etc). We describe these next...

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Lower bound

- Main observation: Assume
$$M = X_1 + \cdots + X_r \tag{1}$$
nonnegative factorization of M where $X_i \geq 0$ and rank-one.
Then $X_i \leq M$ (componentwise) for all $i = 1, \ldots, r$.

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- Define

$$\mathcal{A}(M) = \left\{ X \in \mathbb{R}^{p \times q} \ : \ X \text{ rank-one and } 0 \leq X \leq M \right\}$$

Each X_i from Equation (1) belongs to $\mathcal{A}(M)$.

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Proposition

Assume $L : \mathbb{R}^{p \times q} \to \mathbb{R}$ linear function such that $L(X) \leq 1$ for all $X \in \mathcal{A}(M)$. Then $L(M) \leq \operatorname{rank}_+(M)$.

Proof.

$$L(M) = L(X_1) + \cdots + L(X_r) \leq 1 + \cdots + 1 = r = \operatorname{rank}_+(M).$$

□

Lower bound

- Look for the linear function L which gives the best lower bound (call the resulting quantity $\tau(M)$):

$$\begin{aligned} \tau(M) := \quad & \max_{L} \quad L(M) \\ & \text{s.t.} \quad L : \mathbb{R}^{p \times q} \to \mathbb{R} \text{ linear} \\ & \qquad\;\; L \leq 1 \text{ on } \mathcal{A}(M) \end{aligned}$$

- From previous proposition, $\tau(M)$ satisfies:

$$\tau(M) \leq \text{rank}_+(M)$$

- Computing $\tau(M)$ is a convex optimization problem (but feasible set may be complicated to represent)

Duality

$$\tau(M) := \max_{L \text{ linear}} \quad L(M) \quad \text{s.t.} \quad L \leq 1 \text{ on } \mathcal{A}(M)$$

$$= \quad \min \quad t \quad \text{s.t.} \quad M \in t\,\text{conv}(\mathcal{A}(M))$$

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- $\tau(M)$ is Minkowski gauge function of conv($\mathcal{A}(M)$), evaluated at M.
- "*Self-scaled*": the atoms $\mathcal{A}(M)$ *depend* on the matrix M

Example: diagonal matrices

$$M = \begin{bmatrix} a_1 & 0 \\ 0 & a_2 \end{bmatrix}$$

$$\mathcal{A}(M) = \left\{ X \in \mathbb{R}^{2\times 2} \ : \ \text{rank}\, X \leq 1 \text{ and } 0 \leq X \leq \begin{bmatrix} a_1 & 0 \\ 0 & a_2 \end{bmatrix} \right\} \tag{2}$$

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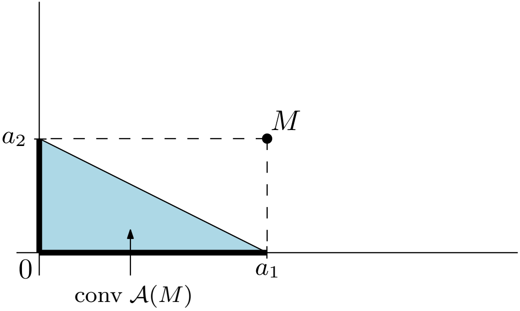

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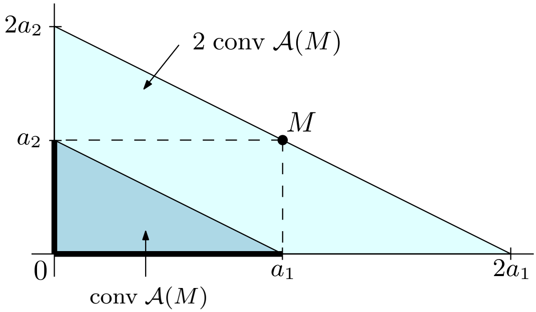

Computing the lower bound

$$\tau(M) = \max_{L \text{ linear}} \quad L(M) \quad \text{s.t.} \quad L \leq 1 \text{ on } \mathcal{A}(M)$$

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SOS relaxation

- Define:

$$\tau^{\text{sos}}(M) := \max_{L} \quad L(M)$$
$$\text{s.t.} \quad L \text{ linear and has SOS representation}$$

- Quantity $\tau^{\text{sos}}(M)$ can be computed using semidefinite programming. Satisfies:

$$\tau^{\text{sos}}(M) \leq \tau(M) \leq \text{rank}_+(M)$$

Structural properties of τ and τ^{sos}

- Invariant under scaling:

$$\tau(D_1 M D_2) = \tau(M)$$

  for any D_1, D_2 diagonal matrices with positive diagonal elements.

- Block-diagonal matrices: $\tau(\text{blockdiag}(M_1, M_2)) = \tau(M_1) + \tau(M_2)$
- Subadditivity: $\tau(M + N) \leq \tau(M) + \tau(N)$
- Product: $\tau(MN) \leq \min(\tau(M), \tau(N))$
- Monotonicity: If P submatrix of M then $\tau(P) \leq \tau(M)$.

Comparison with combinatorial bounds

- Combinatorial bounds on $\text{rank}_+(M)$ are bounds that only depend on sparsity pattern of M. Can be expressed in terms of the *rectangle graph* G_M of M:

$$\underbrace{\omega(G_M)}_{\text{fooling set bound}} \leq \overline{\vartheta}(G_M) \leq \chi_{\text{frac}}(G_M) \leq \underbrace{\chi(G_M)}_{\text{rect. cover number}} \leq \text{rank}_+(M)$$

- The quantities $\tau(M)$ and $\tau^{sos}(M)$ can be shown to be *non-combinatorial* counterparts of *fractional rectangle cover number* and of $\overline{\vartheta}(G_M)$:

Theorem

$$\tau(M) \geq \chi_{frac}(G_M) \qquad \tau^{sos}(M) \geq \overline{\vartheta}(G_M)$$

General "atomic cone ranks"

- General framework: K convex cone and V is some set

$$M = \sum_{i=1}^{r} X_i \quad \text{where} \quad X_i \in K \cap V$$

Define $\text{rank}_{K,V}(M)$ to be the size of the smallest such decomposition.

$$\mathcal{A}(M) = \{X \ : \ 0 \preceq_K X \preceq_K M\}$$

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- Examples:
    - Completely positive matrices: $M = \sum_{i=1}^{r} u_i u_i^T \quad \text{where} \quad u_i \geq 0.$
    - Quadrature formulae:

$$\int_{\Omega} p(x)dx = \sum_{i=1}^{r} w_i p(x_i) \quad w_i \geq 0.$$

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...

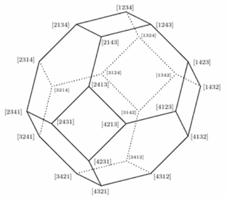
Nice links between rank_{psd} and quantum communication complexity, mirroring the situation between rank_+ and classical communication complexity (e.g., Fiorini *et al.* (2011), Jain *et al.* (2011), Zhang (2012)).

Orbitopes and equivariant lifts

Special class of convex bodies: regular orbitopes

$$C = \{\mathrm{conv}(g \cdot x_0) \;:\; g \in G\},$$

where G is a compact group.



Many important examples: hypercubes, hyperspheres, Grassmannians, Birkhoff polytope, parity polytope, cut polytope, etc..

(More about this in tomorrow's talk.)

Symmetric PSD factorizations

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 (e.g., Piovesan-Laurent)
- Many open questions; related to outstanding conjectures of Connes and Tsirelson

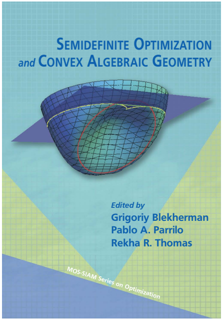
Many questions

Many open aspects of positive semidefinite rank:

- Computation of lower/upper bounds?
- Approximate factorizations?
- Topology of space of factorizations?
- For polytopes, separations between rank_+ and rank_{psd} for slack matrices?
- Are current constructions (e.g., SOS) far from optimal?

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, arXiv:1407.4095.
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Thanks for your attention!

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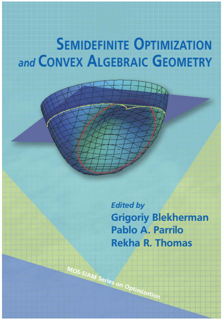

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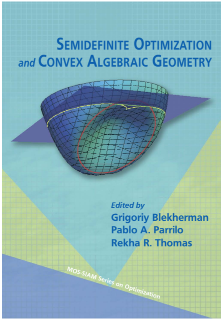

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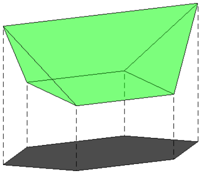
Example: hexagon (III)



A nonnegative factorization:

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