

Sum of squares optimization

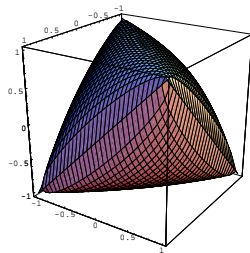
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Laboratory for Information and Decision Systems
Massachusetts Institute of Technology

Summer School on
Numerical Computing in Algebraic Geometry
MPI Leipzig - August 2018

Topics

- Convexity, non-convexity, and tractability
- Convex sets with algebraic descriptions
- Semidefinite programming and sums of squares
- Unifying idea: convex hull of algebraic varieties
- Examples and applications throughout
- Discuss results, but also open questions
- Computational considerations
- Connections with other areas of mathematics



Outline

- Part I
 - Motivation, Basic notions
 - Convexity vs. non-convexity
 - Linear and Semidefinite programming
- Part II
 - Sums of squares
 - Convex hull of algebraic varieties
 - General constructions and approximation guarantees
- Part III
 - Applications and extensions
 - Rank minimization via nuclear norm
 - Estimation and synchronization over $SO(n)$
 - Algorithmic aspects
 - Recap and conclusions

Motivation: what problems can we solve efficiently?

Many questions in applied mathematics can be formulated in terms of polynomials (sometimes, after nontrivial modeling!)

- Global optimization (e.g., binary, constrained, etc.)
- Stability of dynamical systems (e.g., Lyapunov analysis)
- Quantum information (e.g., entanglement)

Some have “nice” solutions.

Others, we are still struggling with after many years...

Why this difference?

What are the underlying mathematical reasons?

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A (rough) first classification: **convex** vs. **non-convex**

Extremely valuable insights! (e.g., Boyd-Vandenberghe)

But, the full answer is a bit more subtle...

- Convexity is “relative,” may depend on modeling/parameterization
- If not convex, may perhaps be tractable (e.g., PCA, deep learning)
- Even if convex, may not be efficiently tractable! (e.g., nonnegative polynomials)

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“Geometric” vs. “computational” convexity

Need to enrich convexity theory with a **computational** twist.

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Convex sets: geometry vs. algebra

The geometric theory of convex sets (e.g., Minkowski, Carathéodory, Fenchel) is very rich and well-understood.

Enormous importance in applied mathematics and engineering, in particular in optimization.

But, what if we are concerned with the *representation* of these geometric objects? For instance, basic semialgebraic sets?

How do the *algebraic*, *geometric*, and *computational* aspects interact?

Ex: Convex optimization is not always “easy”.

The polyhedral case

Consider first the case of *polyhedra*, which are described by finitely many *linear* inequalities $\{x \in \mathbb{R}^n : a_i^T x \leq b_i\}$.

- Behave well under projections (Fourier-Motzkin)
- Farkas' lemma (or duality) gives emptiness certificates
- Good associated computational techniques
- Optimization over polyhedra is linear programming (LP)

Great. But how to move away from linearity? For instance, if we want convex sets described by polynomial inequalities?

Claim: semidefinite programming is an essential tool.

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Linear programming

LP in standard (primal) form:

$$\min c^T x \quad \text{s.t.} \quad Ax = b, \quad x \geq 0.$$

A geometric view: if \mathcal{L} is an affine subspace of \mathbb{R}^n ,

$$\min c^T x \quad \text{s.t.} \quad x \in \mathcal{L} \cap \mathbb{R}_+^n$$

Minimize a linear function, over the intersection of an **affine subspace** and a **polyhedral cone** (nonnegative orthant).

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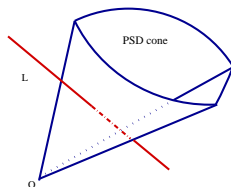
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Semidefinite programming (SDP, LMIs)

A broad generalization of LP to symmetric matrices

$$\min \text{Tr } CX \quad \text{s.t.} \quad X \in \mathcal{L} \cap \mathcal{S}_+^n$$



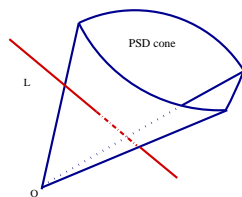
- Intersection of an affine subspace \mathcal{L} and the cone of positive semidefinite matrices.
- Feasible set is called *spectrahedron*
- Lots of applications. A true “revolution” in computational methods for engineering applications
- Convex finite dimensional optimization. Nice duality theory.
- Essentially, solvable in **polynomial time** (interior point, etc.)

SDPs in standard form

Standard (primal) form of a semidefinite program:

$$\min \operatorname{Tr} CX \quad \text{s.t.} \quad \begin{cases} \operatorname{Tr} A_i X = b_i \\ X \succeq 0, \end{cases}$$

where $X \in \mathbb{R}^{n \times n}$ is the (matrix) decision variable and $A_1, \dots, A_m \in \mathbb{R}^{n \times n}$ are given symmetric matrices.



The inequality $A \succeq 0$ means that A is **positive semidefinite** (psd):

$$A \succeq 0 \quad \Leftrightarrow \quad z^T A z \geq 0 \quad \forall z \in \mathbb{R}^n \quad \Leftrightarrow \quad \lambda_i(A) \geq 0 \quad i = 1, \dots, n.$$

By Sylvester's criterion, also equivalent to nonnegativity of all principal minors:

$$\det A_{S,S} \geq 0 \quad \forall S \subset \{1, \dots, n\}.$$

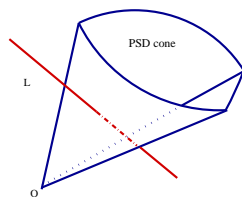
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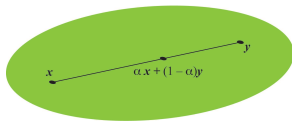
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Convexity

Recall that a set S is **convex** if

$$x, y \in S \Rightarrow \alpha x + (1 - \alpha)y \in S$$

for all $\alpha \in [0, 1]$.



Lemma: The cone of positive semidefinite matrices is **convex**.

Let A and B be psd, and $C = \alpha A + (1 - \alpha)B$ with $\alpha \in [0, 1]$.
Then, for all $z \in \mathbb{R}^n$,

$$z^T C z = z^T (\alpha A + (1 - \alpha)B) z = \alpha \underbrace{z^T A z}_{\geq 0} + (1 - \alpha) \underbrace{z^T B z}_{\geq 0} \geq 0,$$

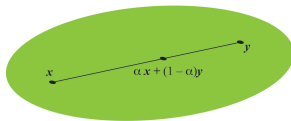
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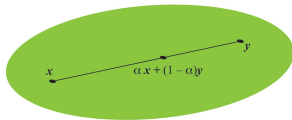
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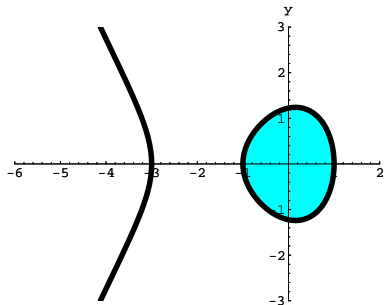
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Example (I)

Consider the spectrahedron given by the SDP:

$$\begin{bmatrix} x & 0 & y \\ 0 & 1 & -x \\ y & -x & 1 \end{bmatrix} \succeq 0.$$



- Convex, but not necessarily polyhedral
- In general, boundary is piecewise-smooth
- Determinant vanishes on the boundary

In this example, the determinant is the elliptic curve $x - x^3 = y^2$.

Example (II)

Consider the spectrahedron:

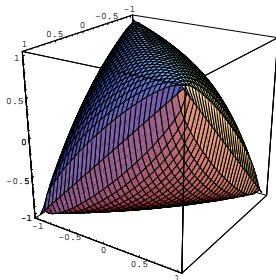
$$X_{ii} = 1 \quad X \succeq 0$$

- PSD matrices of unit diagonal
- Interpretation: set of correlation matrices
- Known as the **elliptope**.

$$M = \begin{bmatrix} 1 & a & b \\ a & 1 & c \\ b & c & 1 \end{bmatrix} \succeq 0$$

Boundary is the Cayley cubic

$$\det M = 1 - (a^2 + b^2 + c^2) + 2abc$$



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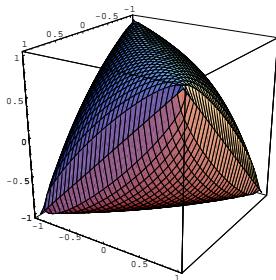
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Symbolic vs. numerical computation

An ongoing discussion. Clearly, both have advantages/disadvantages.

- “Exact solutions” vs. “approximations”
- “Input data often inexact”
- “Global” vs. “local”. One vs. all solutions.
- Computational models: bits vs. reals. Encoding of solutions.

“Best” method depends on the context. Hybrid symbolic-numeric methods are an interesting possibility.

SDP bring some interesting new twists.

- For LP, “numerical” algorithms (ellipsoid, interior-point) are polytime, while “symbolic” or “combinatorial” ones (e.g. simplex) are not.
- Worse for SDP.

Algebraic aspects of SDP

In LPs with rational data, the optimal solution is rational. Not so for SDP.

- Optimal solutions of relatively small SDPs generically have minimum defining polynomials of very high degree.
- Example (von Bothmer and Ranestad): For $n = 20$, $m = 105$, the algebraic degree of the optimal solution is $\approx 1.67 \times 10^{41}$.
- Explicit algebraic representations are absolutely impossible to compute (even without worrying about coefficient size!).
- Nevertheless, interior point methods yield arbitrary precision numerical approximations!

SDP provides an efficient, and numerically convenient *encoding*. Representation does not pay the price of high algebraic complexity.

Application: binary quadratic optimization

Consider the maximization problem

$$\max_x x^T Q x \quad \text{s.t.} \quad x_i \in \{-1, 1\}.$$

A quadratic function, on the vertices of the hypercube. Difficult in theory (NP-hard), and also in practice. Very important in applications.

Can we produce “strong” upper bounds on the optimal value q^* ? (e.g., for branch and bound)

Let γ_* be the optimal value of the SDP:

$$\min \text{Tr } D \quad Q \preceq D, \quad D \text{ diagonal}.$$

Then, for any $x \in \{-1, 1\}^n$, and any feasible D we have:

$$x^T Q x \leq x^T D x = \sum_{i=1}^n D_{ii} x_i^2 = \text{Tr } D$$

and thus $q^* \leq \gamma_*$. The upper bound γ_* can be efficiently computed.

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Application: binary quadratic optimization (II)

How good is this upper bound? How to quantify this?

Different cases, depending on properties of the cost function Q :

- Q is **diagonally dominant** ($Q_{ii} \geq \sum_{i \neq j} Q_{ij}$). This is the case of MAX-CUT, where Q is the Laplacian of a graph. Goemans and Williamson showed that

$$0.878 \gamma_{\star} \leq f^* \leq \gamma_{\star}$$

- Q is **positive semidefinite** ($Q \succeq 0$). By results of Nesterov (and earlier, in very different form, Grothendieck)

$$\frac{2}{\pi} \gamma_{\star} \leq f^* \leq \gamma_{\star}$$

- Q has a **bipartite** structure. Then, Grothendieck's inequality (and Krivine's bound) yields

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Semidefinite representations

Natural question in convex optimization:

What sets can be represented using semidefinite programming?

Equivalently, can I solve this problem using SDP?

In the LP case, well-understood question: finite number of extreme points/rays (polyhedral sets, Minkowski-Weyl)

Are there “obstructions” to SDP representability?

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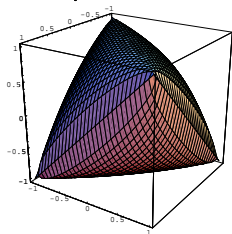
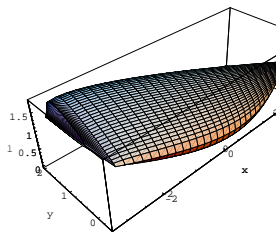
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Known SDP-representable sets

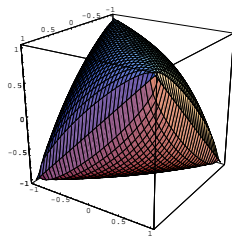
- Many interesting sets are known to be SDP-representable (e.g., polyhedra, convex quadratics, matrix norms, etc.)
- Preserved by “natural” properties: affine transformations, convex hull, polarity, etc.
- Several known structural results (e.g., facial exposedness)

Work of Nesterov-Nemirovski, Ben-Tal, Ramana, Tunçel, Güler, Renegar, Chua, etc.



A few examples of SDP-representable sets

- 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
- Lyapunov functions of (non)linear systems
- Optimal decentralized controllers (under certain information structures)



Often, clever and non-obvious reformulations.

Existing results

Obvious necessary conditions: \mathcal{S} must be convex and semialgebraic.

Several versions of the problem:

- *Exact vs. approximate* representations.
- “Direct” (non-lifted) representations: no additional variables.

$$x \in \mathcal{S} \iff A_0 + \sum_i x_i A_i \succeq 0$$

- “Lifted” representations: can use extra variables (projection)

$$x \in \mathcal{S} \iff \exists y \text{ s.t. } A_0 + \sum_i x_i A_i + \sum_j y_j B_j \succeq 0$$

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Liftings and projections

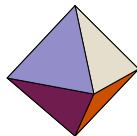
Often, “simpler” descriptions of convex sets from higher-dimensions.

Ex: The n -dimensional crosspolytope (ℓ_1 unit ball). Requires 2^n linear inequalities, of the form

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

However, can efficiently represent it as a *projection*:

$$\{(x, y) \in \mathbb{R}^{2n}, \quad \sum_{i=1}^n y_i = 1, \quad -y_i \leq x_i \leq y_i \quad i = 1, \dots, n\}$$



Only $2n$ variables, and $2n + 1$ constraints!

In convexity, elimination is *not* always a good idea.

Quite the opposite, it is often advantageous to go to higher-dimensional spaces, where descriptions (can) become simpler.

Liftings and projections

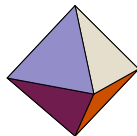
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$$\pm x_1 \pm x_2 \pm \cdots \pm x_n \leq 1.$$

However, can efficiently represent it as a *projection*:

$$\{(x, y) \in \mathbb{R}^{2n}, \quad \sum_{i=1}^n y_i = 1, \quad -y_i \leq x_i \leq y_i \quad i = 1, \dots, n\}$$



Only $2n$ variables, and $2n + 1$ constraints!

In convexity, elimination is *not* always a good idea.

Quite the opposite, it is often advantageous to go to higher-dimensional spaces, where descriptions (can) become simpler.

Aside: representability of convex sets

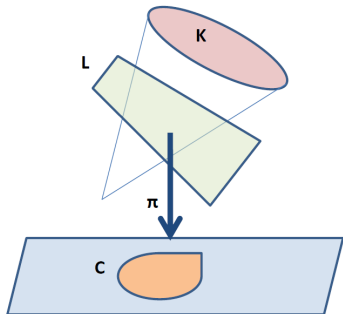
Existence and efficiency:

- 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?



A beautiful story, much of it in progress. But not today...

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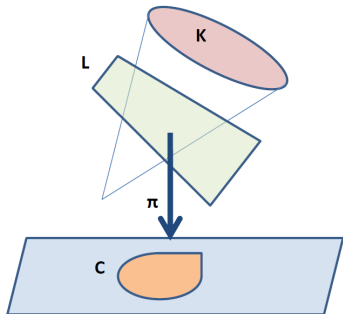
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Example: facility location and k -ellipses

Consider the *facility location* problem: given k customer locations $(u_i, v_i) \in \mathbb{R}^2$, decide where to build a new facility in such a way that total shipping costs are minimized:

$$\min_{(x,y)} \sum_{i=1}^k f((x,y), (u_i, v_i)),$$

where $f(\cdot, \cdot)$ models the shipping costs.

If f is the Euclidean distance, this is the classical Fermat-Weber problem.

Simple and natural SOCP/SDP representation (w/extra variables):

$$\min \sum_{i=1}^k d_i \quad \text{s.t.} \quad \begin{bmatrix} x - u_i + d_i & y - v_i \\ y - v_i & x - u_i - d_i \end{bmatrix} \succeq 0$$

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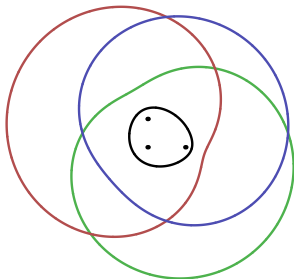
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Example: k -ellipse

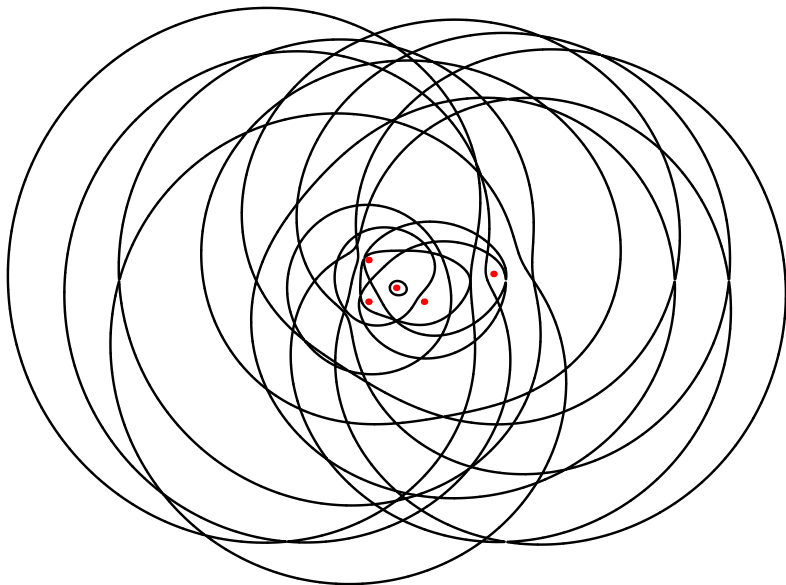
Fix a positive real number d and fix k distinct points (u_i, v_i) in \mathbb{R}^2 . The k -ellipse with foci (u_i, v_i) and radius d is the following curve in the plane:

$$\left\{ (x, y) \in \mathbb{R}^2 : \sum_{i=1}^k \sqrt{(x - u_i)^2 + (y - v_i)^2} = d \right\}.$$



Thm:(Nie-P.-Sturmfels 07) The k -ellipse has degree 2^k if k is odd and degree $2^k - \binom{k}{k/2}$ if k is even. It has an explicit $2^k \times 2^k$ SDP representation.

5-ellipse



Results on exact SDP representations

- Direct representations:

- Necessary condition: **rigid convexity**. Helton & Vinnikov (2004) showed that in \mathbb{R}^2 , rigid convexity is also sufficient.
- Related to hyperbolic polynomials and the Lax conjecture (Güler, Renegar, Lewis-P.-Ramana 2005)
- For higher dimensions the problem is open.

- Lifted representations:

- Does every convex basic SA set have a lifted exact SDP representation?
- (Helton & Nie 2007): Under strict positive curvature assumptions on the boundary, this is true.
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$$x \in \mathcal{S} \quad \Leftrightarrow \quad A_0 + \sum_i x_i A_i \succeq 0$$

Necessary condition: “rigid convexity.” Every line through the set must intersect the Zariski closure of the boundary a constant number of times (equal to the degree of the curve).

[Assume $A_0 \succ 0$, and let $x_i = t\beta_i$. Then the univariate polynomial $q(t) := \det(A_0 + \sum x_i A_i) = \det(A_0 + t \cdot \sum \beta_i A_i)$ has all its d roots real.]

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Exact representations: lifted case

Very active research topic, both in qualitative and quantitative flavors.
Recent exciting progress, on several fronts!

- Gouveia-P.-Thomas (arXiv:1111.3164): PSD rank of a convex set, extension of Yannakakis' LP theory to SDP extension complexity.
- Lee-Raghavendra-Steurer (arXiv:1411.6317, STOC2015): exponential lower bounds on SDP relaxations of cut polytope.
- Fawzi (arXiv:1610.04901): S_+^3 is **not** SOCP-representable.
SOCP-rank + Turán's theorem
- Scheiderer (arXiv:1612.07048): nonnegative polynomials (for $d \geq 4$, $n \geq 2$) are **not** SDP-representable. Real algebraic-geometric tools (real spectrum, Tarski's transfer principle, ...)

Summary

- SDP is a natural generalization of linear programming
- Rich algebraic-geometric structure
- Many applications, efficient numerical solvers
- Some fundamental aspects not fully understood yet



End of Part I

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Part II

Recap

- Motivation: convexity, with computational content
- SDP as a natural generalization of LP
- Understanding the power and limitations of SDP

Lyapunov stability analysis

- A linear system $\dot{x} = Ax$, quadratic Lyapunov function $V(x) = x^T P x$

$$P \succ 0, \quad A^T P + P A \prec 0$$

- More generally, for a nonlinear system $\dot{x} = f(x)$,

$$V(x) > 0 \quad x \neq 0, \quad \dot{V}(x) = \left(\frac{\partial V}{\partial x}\right)^T f(x) < 0, \quad x \neq 0$$

(locally, or globally if V is radially unbounded).

- Many variations: \mathcal{H}_2 and/or \mathcal{H}_∞ analysis, parameter-dependent Lyapunov functions, etc.
- The problem is clearly convex in $V(x)$. But, how to solve this?

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Nonnegativity is hard

What is the issue?

- Structure of V is unclear in general. Differentiable? Algebraic? Polynomial?
- More importantly, even if we nicely parameterize $V(x)$ (e.g., polynomials), how to verify the nonnegativity conditions?

$$V(x) > 0 \quad x \neq 0, \quad \dot{V}(x) = \left(\frac{\partial V}{\partial x} \right)^T f(x) < 0, \quad x \neq 0$$

- Unfortunately, given a polynomial $p(x_1, \dots, x_n)$, verifying if

$$p(x_1, \dots, x_n) \geq 0 \quad \forall \mathbf{x} \in \mathbb{R}^n$$

is **NP-hard** (and also difficult in practice)

What to do about this?

Sum of squares

A multivariate polynomial $p(x)$ is a sum of squares (SOS) if

$$p(x) = \sum_i q_i^2(x), \quad q_i(x) \in \mathbb{R}[x].$$

- If $p(x)$ is SOS, then clearly $p(x) \geq 0$ for all $x \in \mathbb{R}^n$.
- Converse not true, in general (Hilbert). Counterexamples exist.
- For univariate or quadratics, nonnegativity is equivalent to SOS.

Let $P_{n,2d}$ be the set of nonnegative polynomials in n variables of degree less than or equal to $2d$, and $\Sigma_{n,2d}$ the corresponding set of SOS. Clearly,

$$\Sigma_{n,2d} \subseteq P_{n,2d}$$

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Nonnegativity and sum of squares

In 1888, Hilbert showed that $P_{n,2d} = \Sigma_{n,2d}$ iff:

- $2d = 2$. Quadratic forms. SOS decomposition follows from eigenvalue/eigenvector, square root, or Cholesky decomposition.
- $n = 2$. Equivalent to polynomials in one variable.
- $2d = 4, n = 3$. Quartic forms in three variables.

Also, a nonconstructive proof of the nonequivalence in all other cases.

Years later, Motzkin gave an explicit counterexample:

$$M(x, y, z) = x^2y^4 + x^4y^2 + z^6 - 3x^2y^2z^2$$

- Is positive semidefinite. Apply the AGI to (x^2y^4, x^4y^2, z^6) .
- Is *not* a sum of squares.

How do we check the sums of squares condition?

Checking the SOS condition

Basic “Gram matrix” method (Shor 87, Choi-Lam-Reznick 95, Powers-Wörmann 98, Nesterov, Lasserre, P., etc.)

A polynomial $F(x)$ is SOS if and only if

$$F(x) = w(x)^T Q w(x),$$

where $w(x)$ is a vector of monomials, and $Q \succeq 0$.

(If $F \in \mathbb{R}[x]_{n,2d}$, it is sufficient to choose for $w(x)$ all $\binom{n+d}{d}$ monomials of degree less than or equal to d .)

This is a semidefinite program!

Let's see an example, and then the general formulation...

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SOS Example

$$\begin{aligned} F(x, y) &= 2x^4 + 5y^4 - x^2y^2 + 2x^3y \\ &= \begin{bmatrix} x^2 \\ y^2 \\ xy \end{bmatrix}^T \begin{bmatrix} q_{11} & q_{12} & q_{13} \\ q_{12} & q_{22} & q_{23} \\ q_{13} & q_{23} & q_{33} \end{bmatrix} \begin{bmatrix} x^2 \\ y^2 \\ xy \end{bmatrix} \\ &= q_{11}x^4 + q_{22}y^4 + (q_{33} + 2q_{12})x^2y^2 + 2q_{13}x^3y + 2q_{23}xy^3 \end{aligned}$$

An SDP with equality constraints. Solving, we obtain:

$$Q = \begin{bmatrix} 2 & -3 & 1 \\ -3 & 5 & 0 \\ 1 & 0 & 5 \end{bmatrix} = L^T L, \quad L = \frac{1}{\sqrt{2}} \begin{bmatrix} 2 & -3 & 1 \\ 0 & 1 & 3 \end{bmatrix}$$

And therefore $F(x, y) = \frac{1}{2}(2x^2 - 3y^2 + xy)^2 + \frac{1}{2}(y^2 + 3xy)^2$

Checking SOS via SDP

Let $F(x) = \sum f_\alpha x^\alpha$. Index rows and columns of Q by monomials. Then,

$$F(x) = w(x)^T Q w(x) \quad \Leftrightarrow \quad f_\alpha = \sum_{\beta+\gamma=\alpha} Q_{\beta\gamma}$$

Thus, we have the SDP feasibility problem

$$f_\alpha = \sum_{\beta+\gamma=\alpha} Q_{\beta\gamma}, \quad Q \succeq 0$$

- Factorize $Q = L^T L$. The SOS is given by $F(x) = \|Lw(x)\|^2$.

(Can exploit sparsity, symmetry, etc. — more on this later).

And, we can actually **search** over such polynomials!

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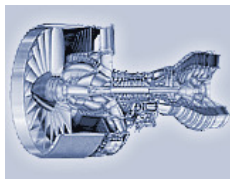
Nonlinear Lyapunov

For $\dot{x} = f(x)$, a Lyapunov function must satisfy

$$V(x) \geq 0, \quad \left(\frac{\partial V}{\partial x} \right)^T f(x) \leq 0$$

Jet engine model (derived from Moore-Greitzer), with controller:

$$\begin{aligned}\dot{x} &= -y + \frac{3}{2}x^2 - \frac{1}{2}x^3 \\ \dot{y} &= 3x - y\end{aligned}$$



Postulate a generic 4th order polynomial Lyapunov function:

$$V(x, y) = \sum_{0 \leq j+k \leq 4} c_{jk} x^j y^k$$

Find a $V(x, y)$ by solving the SOS program:

$$V(x, y) \text{ is SOS}, \quad -\nabla V(x, y) \cdot f(x, y) \text{ is SOS.}$$

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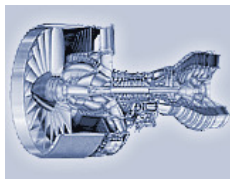
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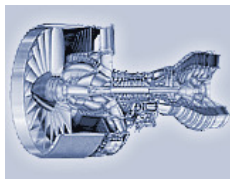
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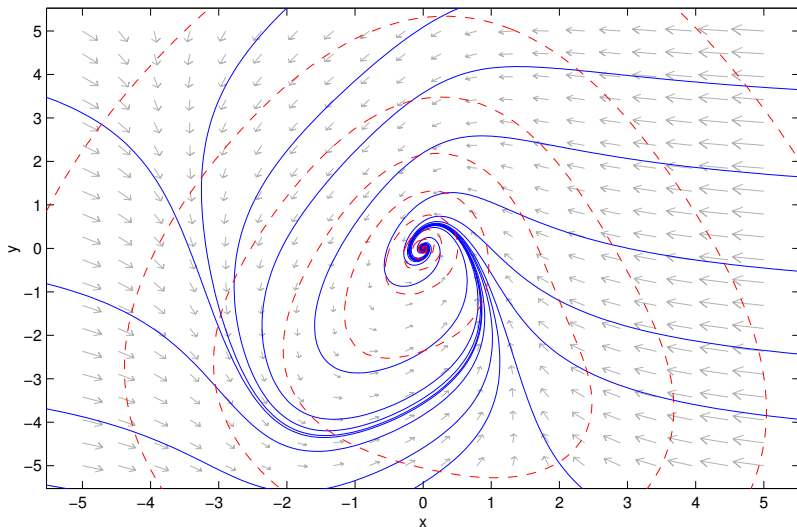
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Lyapunov example (cont.)

After solving, we obtain a Lyapunov function.

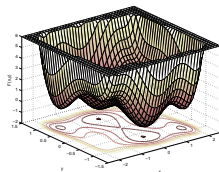


From feasibility to optimization

SOS directly yields lower bounds for optimization!

$$F(x) - \gamma \text{ is SOS} \quad \Rightarrow \quad F(x) \geq \gamma \text{ for all } x$$

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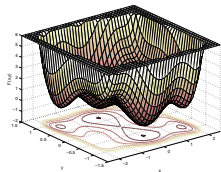


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Polynomial systems over \mathbb{R}

- When do equations and inequalities have real solutions?
- A remarkable answer: the **Positivstellensatz**.
- Centerpiece of real algebraic geometry (Stengle 1974).
- Common generalization of Hilbert's Nullstellensatz and LP duality.
- Guarantees the existence of algebraic **infeasibility certificates** for real solutions of systems of polynomial equations.
- Sums of squares are a fundamental ingredient.

How does it work?

P-satz and SOS

Given $\{x \in \mathbb{R}^n \mid f_i(x) \geq 0, \quad h_i(x) = 0\}$, want to *prove* that it is empty.

Define:

$$\text{Cone}(f_i) = \sum s_i \cdot (\prod_j f_j), \quad \text{Ideal}(h_i) = \sum t_i \cdot h_i,$$

where the $s_i, t_i \in \mathbb{R}[x]$ and the s_i are sums of squares.

What is this? What's the idea?

Want to capture the **algebraic structure** of the allowable operations among constraints (alternatively, how to generate new constraints from old ones):

- If $f_i(x) \geq 0, f_j(x) \geq 0$, then $f_i(x)f_j(x) \geq 0$.
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Describes *all* valid constraints that can be “easily” generated.

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Describes *all* valid constraints that can be “easily” generated.

P-satz and SOS

Given $\{x \in \mathbb{R}^n \mid f_i(x) \geq 0, \quad h_i(x) = 0\}$, want to *prove* that it is empty.
Define:

$$\text{Cone}(f_i) = \sum s_i \cdot (\prod_j f_j), \quad \text{Ideal}(h_i) = \sum t_i \cdot h_i,$$

where the $s_i, t_i \in \mathbb{R}[x]$ and the s_i are sums of squares.

What is this? What's the idea?

Want to capture the **algebraic structure** of the allowable operations among constraints (alternatively, how to generate new constraints from old ones):

- If $f_i(x) \geq 0, f_j(x) \geq 0$, then $f_i(x)f_j(x) \geq 0$.
- If $f_i(x) \geq 0$, then $s(x)f_i(x) \geq 0$, where $s(x)$ is SOS.
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$$f + h = -1.$$

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- Complete SOS hierarchy, by certificate degree (P. 2000).
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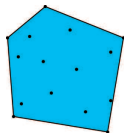
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Convex hulls of algebraic varieties

Back to SDP representations...

Focus here on a specific, but very important case.



Given a set $S \subset \mathbb{R}^n$, we can define its *convex hull*

$$\text{conv} S := \left\{ \sum_i \lambda_i x_i : x_i \in S, \sum_i \lambda_i = 1, \lambda_i \geq 0 \right\}$$

Our interest: S is a real algebraic variety and the approximation is an SDP-representable set.



Convex hulls of algebraic varieties

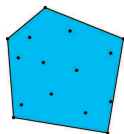
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Why?

Many interesting problems require or boil down *exactly* to understanding and describing convex hulls of algebraic varieties.

- Nonnegative polynomials and optimization
- Polynomial games
- Convex relaxations for minimum-rank
- Convex hull of rotation matrices

We'll discuss some of these in detail...

Polynomial optimization

Consider the unconstrained minimization of a multivariate polynomial

$$p(x) = \sum_{\alpha \in S} p_{\alpha} x^{\alpha},$$

where $x \in \mathbb{R}^n$ and S is a given set of monomials (e.g., all monomials of total degree less than or equal to $2d$, in the dense case).

Define the (real, toric) algebraic variety $V_S \subset \mathbb{R}^{|S|}$:

$$V_S := \{(x^{\alpha_1}, \dots, x^{\alpha_{|S|}}) : x \in \mathbb{R}^n\}.$$

This is the image of \mathbb{R}^n under the monomial map (e.g., in the homogeneous case, the Veronese embedding).

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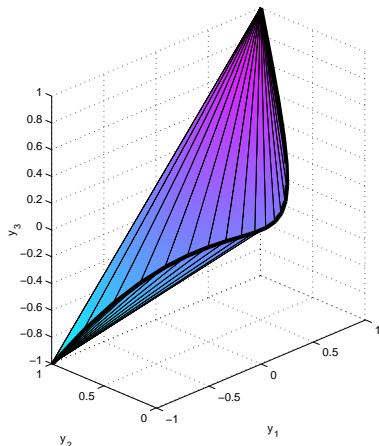
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Univariate case

Convex hull of the rational normal curve
 $(1, t, \dots, t^d)$.

Not polyhedral.

Known geometry (Karlin-Shapley)



“Simplicial”: every supporting hyperplane yields a simplex.
Related to cyclic polytopes.

Polynomial optimization

We have then (almost trivially):

$$\inf_{x \in \mathbb{R}^n} p(x) = \inf\{p^T y : y \in \text{conv } V_S\}$$

Optimizing a nonconvex polynomial is equivalent to linear optimization over a convex set (!)

Unfortunately, in general, it is NP-hard to check membership in $\text{conv } V_S$. Nevertheless, we can turn this around, and use SOS relaxations to obtain “good” approximate SDP descriptions of the convex hull V_S .

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A geometric interlude

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Convexity is *relative*. Every problem can be trivially “lifted” to a convex setting (in general, infinite dimensional).

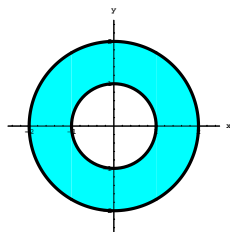
Ex: mixed strategies in games, “relaxed” controls, Fokker-Planck, etc. Interestingly, however, often a finite (and small) dimension is enough.

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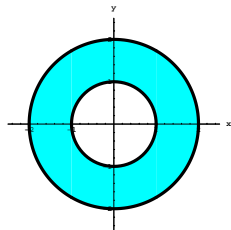
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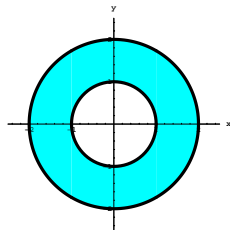
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Geometric interpretation

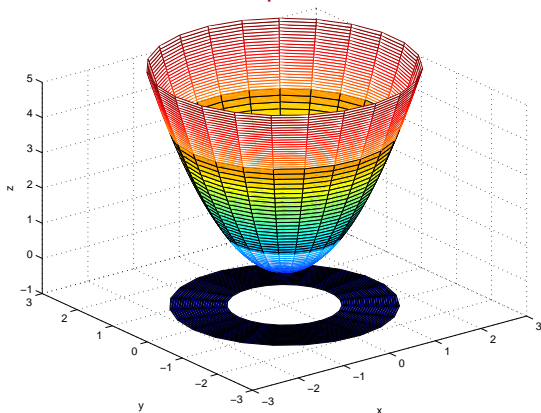
A polynomial “lifting” to a higher dimensional space:

$$(x, y) \mapsto (x, y, x^2 + y^2)$$

The nonconvex set is the **projection** of the **extreme points** of a convex set.

In particular, the convex set defined by

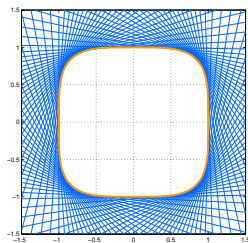
$$\begin{aligned} x^2 + y^2 &\leq z \\ 1 &\leq z \leq 4 \end{aligned}$$



Convex hull of varieties: a “polar” viewpoint

How to describe a convex hull?

Any convex set \mathcal{S} is uniquely defined by its supporting hyperplanes.



Thus, if we can optimize a *linear function* over a set using SDP, we effectively have an SDP representation.

Need to solve (or approximate)

$$\min c^T x \quad \text{s.t. } x \in \mathcal{S}$$

If \mathcal{S} is defined by polynomial equations/inequalities, can use SOS.

Theta bodies

We define the k -th *theta body* of a real variety (Gouveia-P.-Thomas 08).

Let V be an algebraic variety, and $I = I(V) \subseteq \mathbb{R}[x_1, \dots, x_n]$ the associated polynomial ideal. The polynomial f is **k -sos modulo the ideal I** if

$$f = \sum_i q_i^2 \quad \forall x \in V, \quad \deg(q_i) \leq k.$$

If f is k -sos mod I , then clearly f is nonnegative on V .

Recall the characterization of the (closed) convex hull of a set S as the intersection of all half-spaces that contain S :

$$\overline{\text{conv}(S)} = \{\mathbf{p} \in \mathbb{R}^n : f(\mathbf{p}) \geq 0 \text{ for all } f \text{ affine and nonnegative on } S\}$$

Next, we will do the same, but replacing nonnegativity with k -sos.

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Replace all halfspaces with “ k -sos certifiable” halfspaces.

Since

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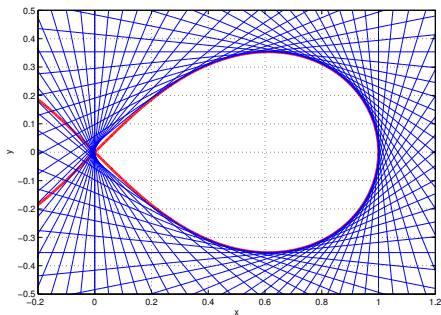
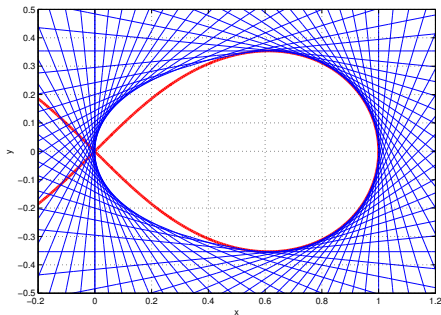
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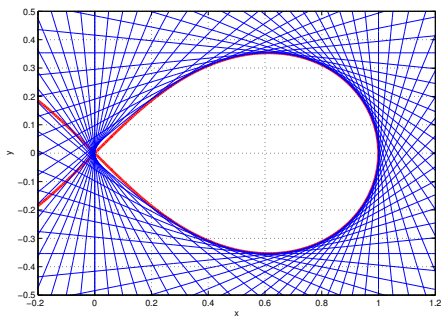
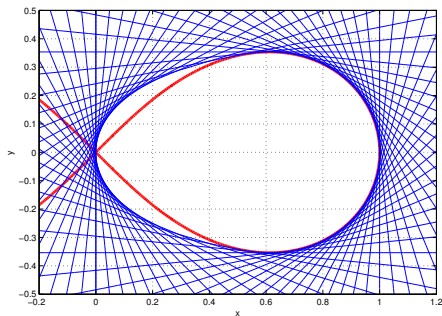
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Summary

- Sum of squares allows the use of SDP for polynomial problems
- Through the P-satz, extend to constrained problems
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Part III

Example: orthogonal matrices

Consider $O(3)$, the group of 3×3 orthogonal matrices. It has two connected components (determinant is ± 1). Rotation matrices have *determinant one* (preserve orientation).

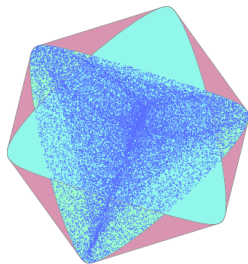
Can use the double-cover of $SO(3)$ with $SU(2)$ (equivalently, quaternions) to provide an exact SDP representation of the convex hull of $SO(3)$:

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This is a convex set in \mathbb{R}^9 .

Here is a two-dimensional projection.

Generalizations to $SO(n)$ via Clifford algebras
(Saunderson-P.-Willsky, arXiv:1403.4914,
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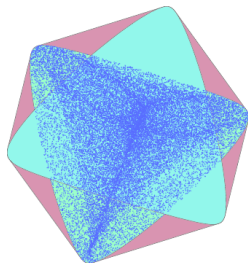
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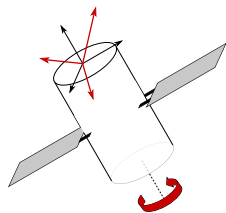
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Joint spin-rate and attitude estimation



- unknown initial 'attitude' Q
- spinning at unknown rate ω around known (in body frame) axis

Data: sequence of noisy measurements (in body frame) of reference directions (sun, stars, magnetic field, etc) known in inertial frame

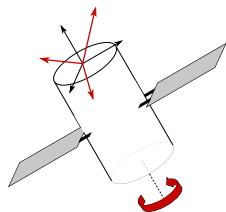
Problem: Estimate initial attitude Q and spin-rate ω from data.

$$\max_{\substack{Q \in SO(3) \\ \omega \in [-\pi, \pi)}} \sum_{n=0}^N [\langle A_n, Q \cos(n\omega) \rangle + \langle B_n, Q \sin(n\omega) \rangle]$$

Representation allow us to exactly solve this problem with SDP!

(arXiv:1410.2841, J. Guidance, Control, and Dynamics, 39:1, 118-127, 2016.)

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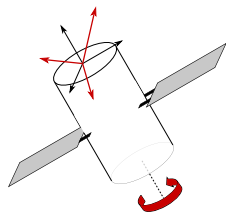
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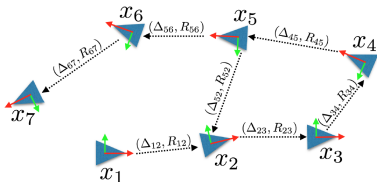
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Pose graph optimization

e.g., Bandeira-Kennedy-Singer, Carlone-Rosen-Calafiore-Leonard-Dellaert, ...

- Collection of rigid bodies (e.g., drones w/cameras, SLAM)
- (Few) measurements of pairwise relative positions M_{ij}
- Estimate the position of *all* bodies



(figure from Calafiore *et al.*)

$$\min_{\{R_i\} \in SO(3)} \sum_{(ij) \in \mathcal{M}} \|M_{ij} - R_i R_j^T\|^2$$

Natural semidefinite relaxation:

$$\min \sum_{(ij) \in \mathcal{M}} \|M_{ij} - R_{ij}\|^2 \quad \text{s.t.} \quad \begin{bmatrix} I_3 & R_{12} & \dots & R_{1n} \\ R_{12}^T & I_3 & \dots & R_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ R_{1n}^T & R_{2n}^T & \dots & I_3 \end{bmatrix} \succeq 0, \quad R_{ij} \in \text{conv}SO(3).$$

Minimum rank and convex relaxations

Consider the rank minimization problem

$$\text{minimize } \text{rank } X \quad \text{subject to } \mathcal{A}(X) = b,$$

where $\mathcal{A} : \mathbb{R}^{m \times n} \rightarrow \mathbb{R}^p$ is a linear map.

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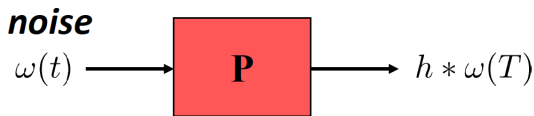
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Application: System identification



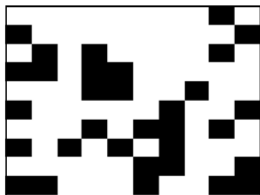
- Measure response at time T (e.g., for random input)
- Response at time T is linear in impulse response h .

$$\text{hank}(h) := \begin{bmatrix} h(0) & h(1) & \cdots & h(N) \\ h(1) & h(2) & \cdots & h(N+1) \\ \vdots & \vdots & \ddots & \vdots \\ h(N) & h(N+1) & \cdots & h(2N) \end{bmatrix}$$

- Complexity of $P \approx \text{rank}(\text{hank}(h))$.

Application: Matrix completion

$M =$



M_{ij} known for black cells

M_{ij} unknown for white cells

- Partially specified matrix, known pattern
- Often, random sampling of entries
- Applications:
 - Partially specified covariances (PSD case)
 - Collaborative prediction (e.g., Rennie-Srebro'05, "Netflix problem", Candès-Recht'09)

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Convex hulls and nuclear norm

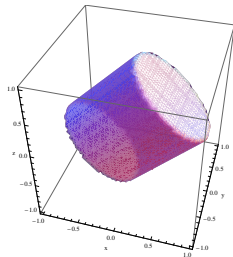
Nuclear norm ball is convex hull of rank one matrices:

$$\begin{aligned} B &= \{X \in \mathbb{R}^{m \times n} : \|X\|_* \leq 1\} \\ &= \text{conv}\{uv^T : u \in \mathbb{R}^m, v \in \mathbb{R}^n, \|u\|^2 = 1, \|v\|^2 = 1\} \end{aligned}$$

Exactly SDP-characterizable!

$$B = \left\{ X \in \mathbb{R}^{m \times n} : \begin{bmatrix} W_1 & X \\ X^T & W_2 \end{bmatrix} \succeq 0, \quad \text{Tr } W_1 + \text{Tr } W_2 = 2 \right\}$$

Under certain conditions (e.g., if subspace defined by \mathcal{A} is “random”), optimizing the nuclear norm yields the *true minimum rank solution*.



For details, see Recht-Fazel-P., “Guaranteed minimum-rank solutions of linear matrix equations via nuclear norm minimization,” *SIAM Review*, 2010.

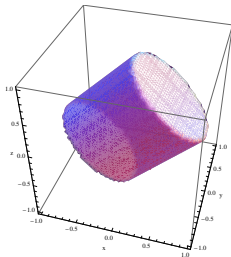
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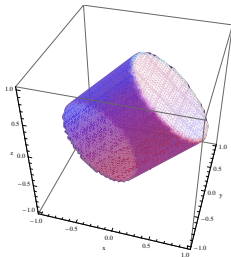
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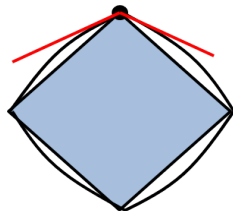
Rank, sparsity, and beyond: atomic norms

Exactly the same constructions can be applied to more general situations: **atomic norms**.

Structure-inducing regularizer is convex hull of atom set, e.g., low-rank matrices/tensors, permutation matrices, cut matrices, etc.

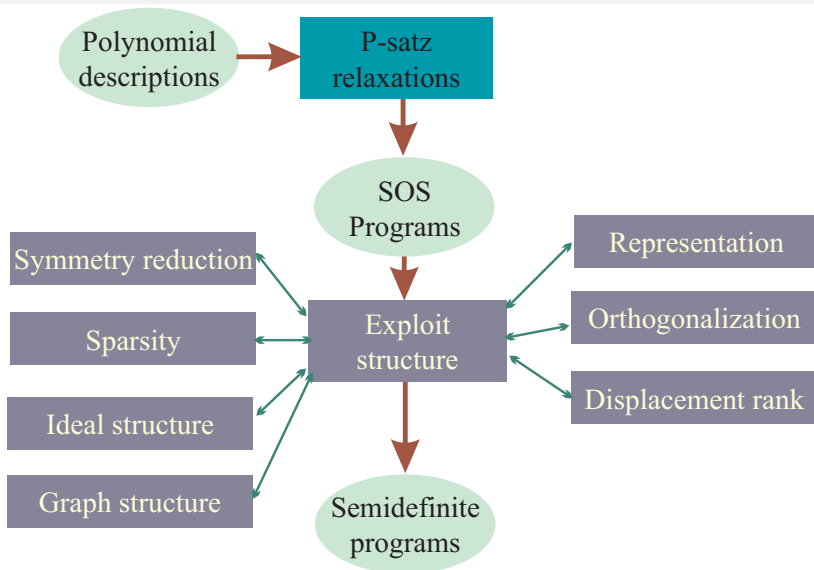
Generally NP-hard to compute, but good SDP approximations.

Statistical guarantees for recovery based on *Gaussian width of tangent cones*. Interesting interplay between computational and sample complexities.



For details, see Chandrasekaran-Recht-P.-Willsky, "The convex geometry of linear inverse problems," *Found. Comp. Math.*, 2012.

Exploiting structure



Algebraic structure

- **Algebraic sparsity:** polynomials with few nonzero coefficients.
 - Newton polytopes techniques.
- **Ideal structure:** equality constraints.
 - SOS on *quotient rings* $\mathbb{R}[x]/I$.
 - Compute in the coordinate ring. Quotient bases.
- **Graphical structure:**
 - Dependency graph among the variables
 - Chordality/treewidth techniques
- **Symmetries:** invariance under a group
 - SOS on *invariant rings*
 - Representation theory and invariant-theoretic methods.
 - Enabling factor in applications (e.g., Markov chains)

Numerical structure

- Rank one SDPs.
 - Dual coordinate change makes all constraints rank one
 - Efficient computation of Hessians and gradients
- Representations
 - Interpolation representation
 - Orthogonalization
- Displacement rank
 - Fast solvers for search direction
- Alternatives to interior-point methods?
 - E.g., factorization approaches (Burer-Monteiro)?

Related work

(very incomplete/partial list!)

- Related basic work: N.Z. Shor, Nesterov, Lasserre, etc.
- Systems and control (Prajna, Rantzer, Hol-Scherer, Henrion, etc.)
- Sparse optimization (Waki-Kim-Kojima-Muramatsu, Lasserre, Nie-Demmel, etc.)
- Approximation algorithms (de Klerk-Laurent-P.)
- Filter design (Alkire-Vandenberghe, Hachez-Nesterov, etc.)
- Stability number of graphs (Laurent, Peña, Rendl)
- Quantum information theory (Doherty-Spedalieri-P., Childs-Landahl-P.)
- Joint spectral radius (P.-Jadbabaie, Legat-Jungers)
- Game theory (Stein-Ozdaglar-P.)
- Theoretical computer science (Barak, Kelner, Steurer, Lee, Raghavendra)

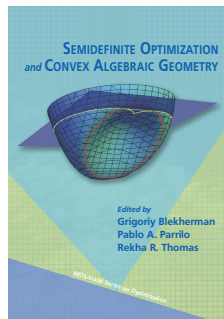
Connections

Many fascinating links to other areas of mathematics:

- Probability (moments, exchangeability and de Finetti, etc)
- Operator theory (via Gelfand-Neimark-Segal)
- Harmonic analysis on semigroups
- Noncommutative probability and quantum information
- Complexity and proof theory (degrees of certificates)
- Graph theory (perfect graphs)
- Tropical geometry (SDP over more general fields)

Summary

- A very rich class of optimization problems
- Methods have enabled many new applications
- Interplay of many branches of mathematics
- Structure must be exploited for reliability and efficiency
- Combination of numerical and algebraic techniques.



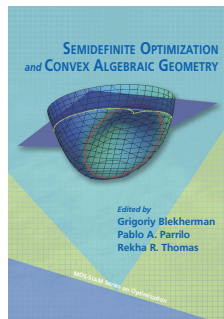
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Thanks for your attention!

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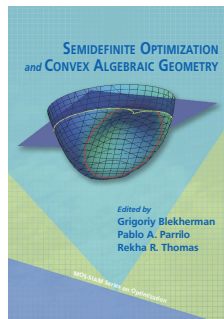
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