Sum of Squares Optimization

in the Analysis and Synthesis of Control Systems

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Outline

- Motivating examples: problems we want to solve
  - Analysis and synthesis for nonlinear systems
  - Partial differential inequalities
  - Polynomial systems and semialgebraic games.
- Sum of squares programs
  - Convexity, relationships with semidefinite programming
  - Interpretations
- Exploiting structure for efficiency
  - Algebraic and Numerical techniques.
- Perspectives, limitations, and challenges

Control problems

How to provide "satisfactory" computational solutions? For instance:

- How to prove stability of a nonlinear dynamical system?
- Region of attraction of a given equilibrium?
- What about performance guarantees?
- If uncertain/robust, how to compute stability margins?
- What changes (if anything) for switched/hybrid systems?

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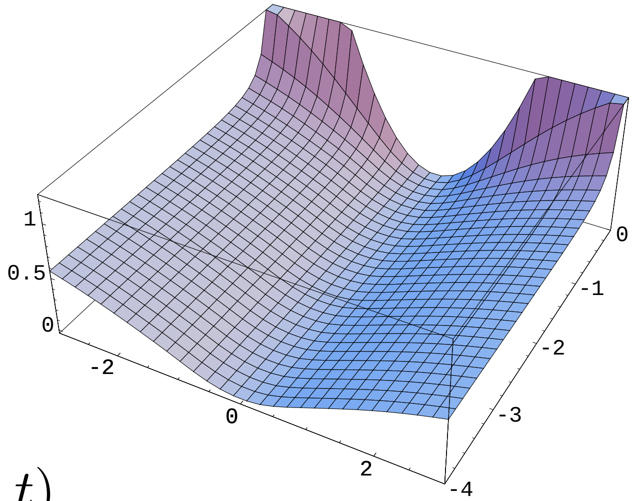
"Good" bounds can be obtained by considering associated convex optimization problems (e.g., linearization, D-scales, IQCs, etc)

Partial diff inequalities

- Solutions for linear PDIs:
  - Lyapunov:

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



  - Hamilton-Jacobi:

$$V(x,t) \geq 0, \quad -\frac{\partial V}{\partial t} + \mathcal{H}(x, \frac{\partial V}{\partial x}) \leq 0, \quad \forall (x,u,t)$$

- Very difficult in three or higher dimensions.
- Many approaches: approximation, discretizations, level set methods, etc.

How to find certified solutions?

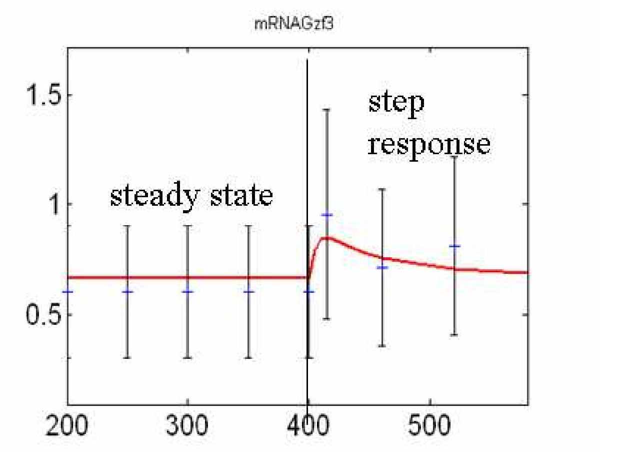
Can we obtain bounds on linear functionals of the solutions?

Data consistency

Elementary reaction models for gene expression in yeast

$$
\begin{aligned}
\frac{d[TF]}{dt} &= -K_{A,1}\cdot[TF]\cdot[GENE] + K_{D,1}\cdot[TF\bullet GENE]\\
\frac{d[GENE]}{dt} &= -K_{A,1}\cdot[TF]\cdot[GENE] + K_{D,1}\cdot[TF\bullet GENE]\\
\frac{d[TF\bullet GENE]}{dt} &= K_{A,1}\cdot[TF]\cdot[GENE] - K_{D,1}\cdot[TF\bullet GENE] -\\
&\quad -K_{A,2}\cdot[TF\bullet GENE]\cdot[RNAPol] + K_{D,2}\cdot[TF\bullet GENE\bullet RNAPol] +\\
&\quad +K_{TC}\cdot[TF\bullet GENE\bullet RNAPol]
\end{aligned}
$$

- Nonlinear dynamics
- Microarray data of wildtype and mutants
- Steady state + dynamic measurements
- Extract as much information as possible



What parameter/rate values are consistent with measurements?

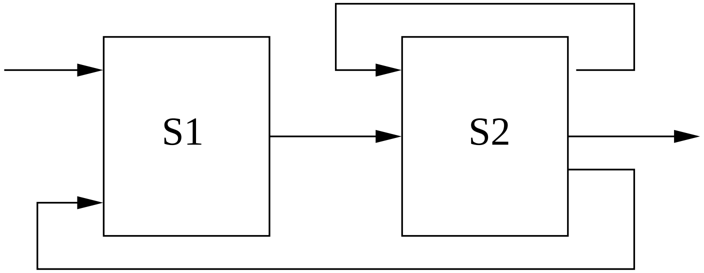
Joint work with L. Küpfer and U. Sauer (ETH Zürich)

Queueing networks and copositivity

Open re-entrant line.

Arrival and service rates λ, μ_i.

How to analyze performance?



Def: A matrix Q is *copositive* if $x \geq 0$ implies $x^T Q x \geq 0$.

Stability/performance analysis is possible using a Lyapunov-like function

$$E[x^T(\tau_n) Q x(\tau_n)],$$

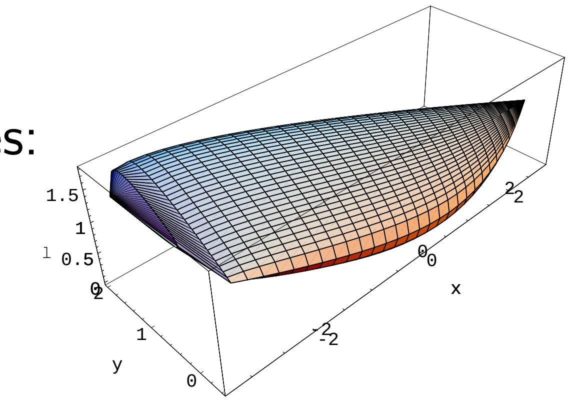
where $x(\tau)$ are the queue lenghts at time τ (Kumar-Meyn).

But how to characterize copositive matrices? (coNP-complete)

Polynomial systems

General systems of polynomial equations/inequalities:

$$\{x \in \mathbb{R}^n, \quad f_i(x) \geq 0, \quad h_i(x) = 0\}$$



- Define *semialgebraic* sets
- In general, nonconvex and difficult (NP-hard)
- Includes continuous and combinatorial aspects
- Natural representation for many problems

How to optimize, or decide and certify infeasibility?

Motivation

All very different problems, that share common properties.

- Can be expressed/approximated with polynomials and/or rational functions
- Include nonnegativity constraints (perhaps implicitly)
- Provably difficult (NP-complete, or worse)

These constitute a very significant class of problems in Control: quantified polynomial inequalities or semialgebraic problems.

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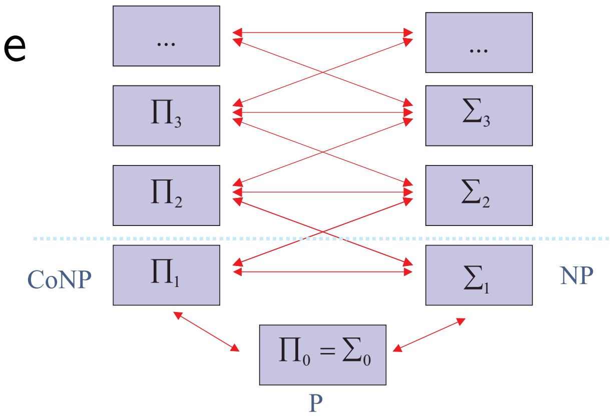
Fundamental importance recognized many years ago (e.g., Anderson-Bose-Jury, Dorato-Yang-Abdallah, Glad-Jirstrand, etc.).

Aside: quantifiers and alternation

To analyze structural features, need to understand the underlying first-order formula:

$$(Q_1 x_1)(Q_2 x_2) \ldots (Q_n x_n)\, P(x_1, x_2, \ldots, x_n),$$

where $Q_i \in \{\forall, \exists\}$ (e.g., Tierno-Doyle)



Usually defined for discrete problems (e.g., SAT, QBF), extends to reals.

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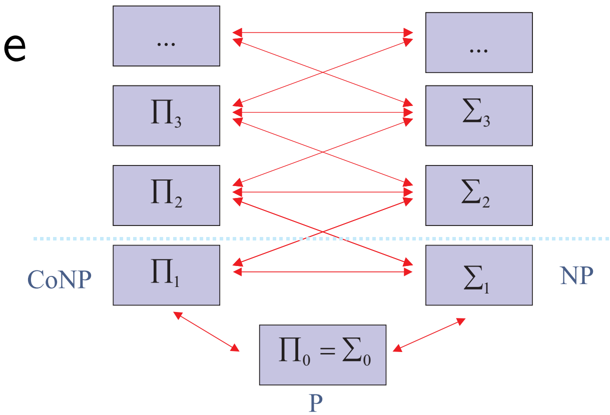

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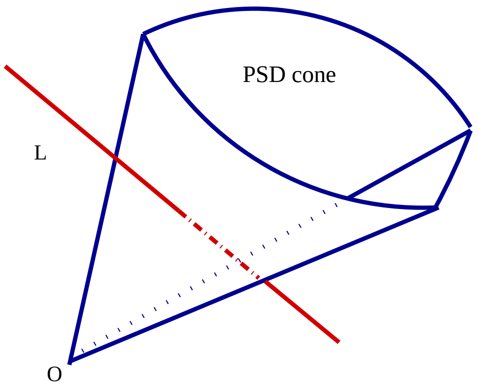
Many different approaches, quality/performance tradeoffs:

- Tarski-Seidenberg, quantifier elimination
- Explicit discretization and enumeration
- Bounding/abstraction (e.g., interval arithmetic, etc)
- Sampling and statistical learning

Semidefinite programming (LMIs)

A broad generalization of LP to symmetric matrices

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



- The intersection of an affine subspace $\mathcal{L}$ and the cone of positive semidefinite matrices.
- *Lots* of applications. A true "revolution" in computational methods for engineering applications
- Originated in control theory (Boyd *et al.*, etc) and combinatorial optimization (e.g., Lovász). Nowadays, applied everywhere.
- Convex finite dimensional optimization. Nice duality theory.
- Essentially, solvable in polynomial time (interior point, etc.)

Why are LMIs so appealing?

In coordinates, we have $A_0 + \sum_i A_i x_i \succeq 0$, i.e.,

$$\exists x \forall y \; P(x, y) \geq 0,$$

where $P(x, y) := y^T (A_0 + \sum_i A_i x_i) y$ is *affine* in x and *quadratic* in y.

This should be really hard (Σ_2), but it's actually in P!

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In other words, LMIs are:

quadratic forms, that are *nonnegative*.

We want to generalize this as much as possible, while keeping tractability.

For this, we introduce the notion of sum of squares.

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 $p(x) \geq 0 \; \forall x \in \mathbb{R}^n$.
- *Convex* condition: p_1, p_2 SOS $\Rightarrow \lambda p_1 + (1-\lambda) p_2$ SOS for $0 \leq \lambda \leq 1$.
- SOS polynomials form a convex cone

For univariate or quadratic polynomials, SOS and nonnegativity are equivalent.

From LMIs to SOS

LMI optimization problems:

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An SOS program is an optimization problem with SOS constraints:

$$\begin{array}{ll} \min_{u_i} & c_1 u_1 + \cdots + c_n u_n \\ \text{s.t} & P_i(x,u) := A_{i0}(x) + A_{i1}(x) u_1 + \cdots + A_{in}(x) u_n \quad \text{are SOS} \end{array}$$

This is a finite-dimensional, convex optimization problem.

SOS programs: questions

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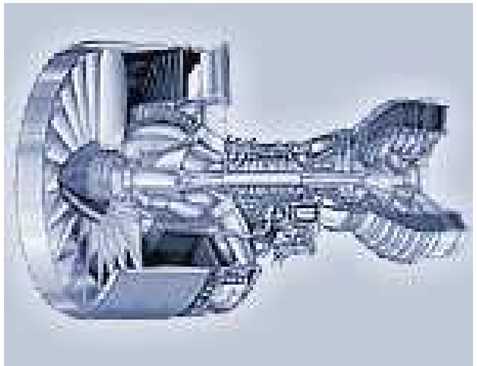
- How? And how do you solve them?

OK, I'll tell you. But first, examples!

Lyapunov

For $\dot{x} = f(x)$, a Lyapunov function must satisfy
$V(x) \geq 0, \quad \left(\frac{\partial V}{\partial x}\right)^T f(x) \leq 0$. Inequalities are *linear* in V.

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



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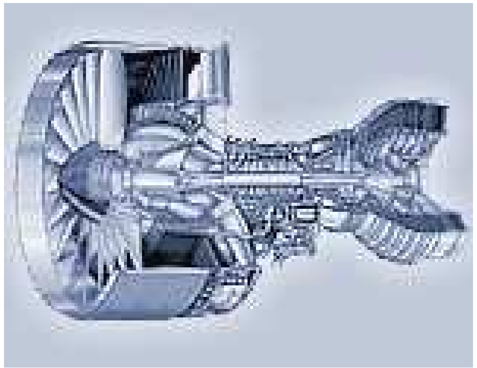

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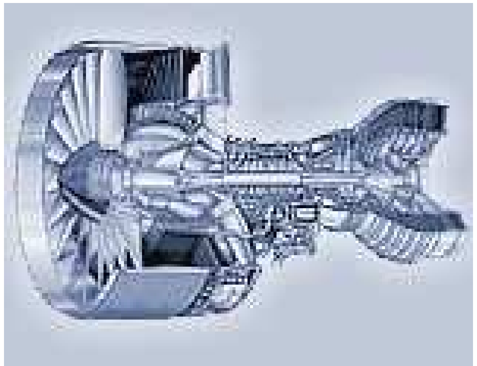

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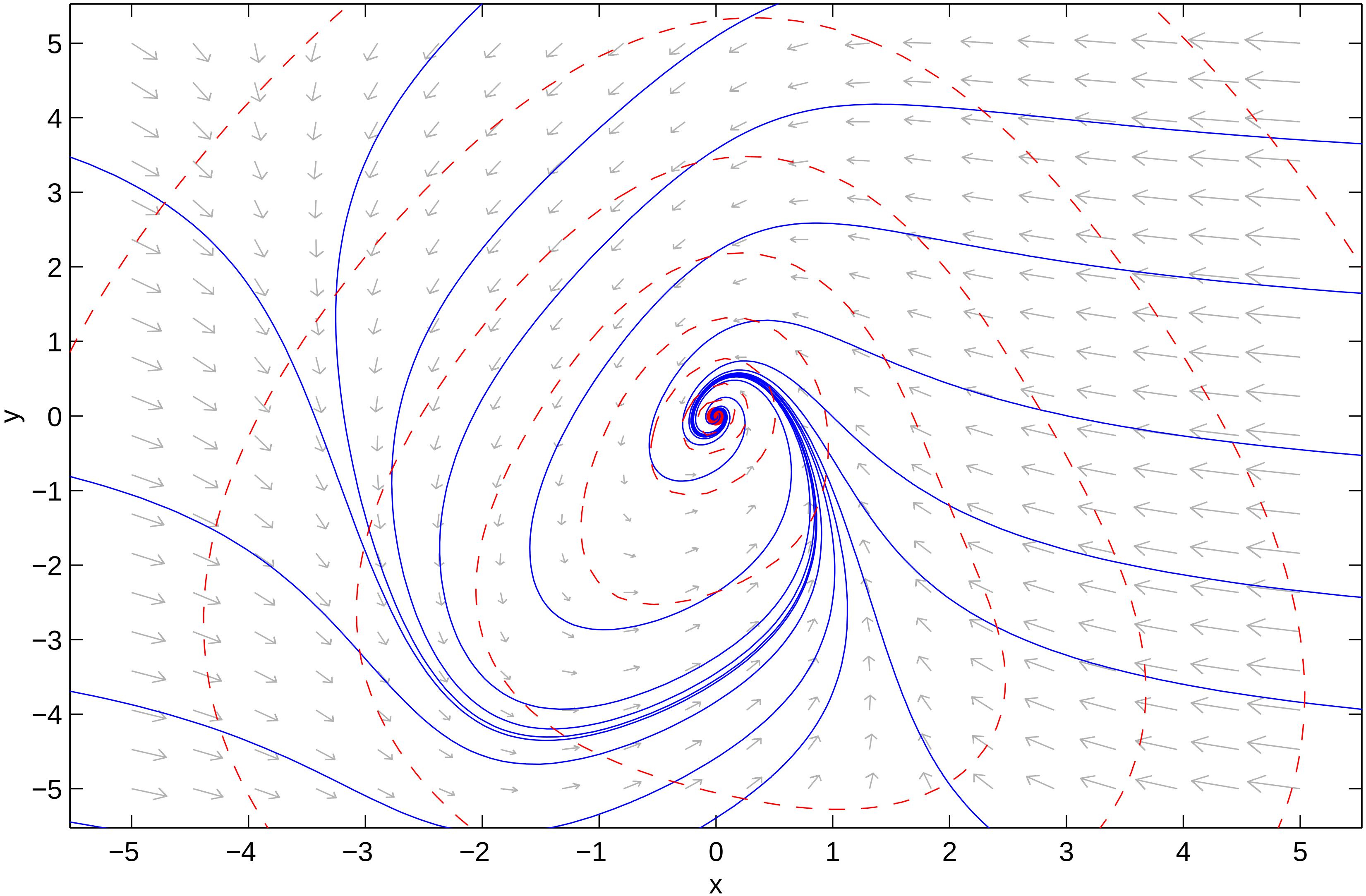
Find a $V(x,y)$ by solving the SOS program:

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

Lyapunov example (cont.)

After solving, we obtain a Lyapunov function.



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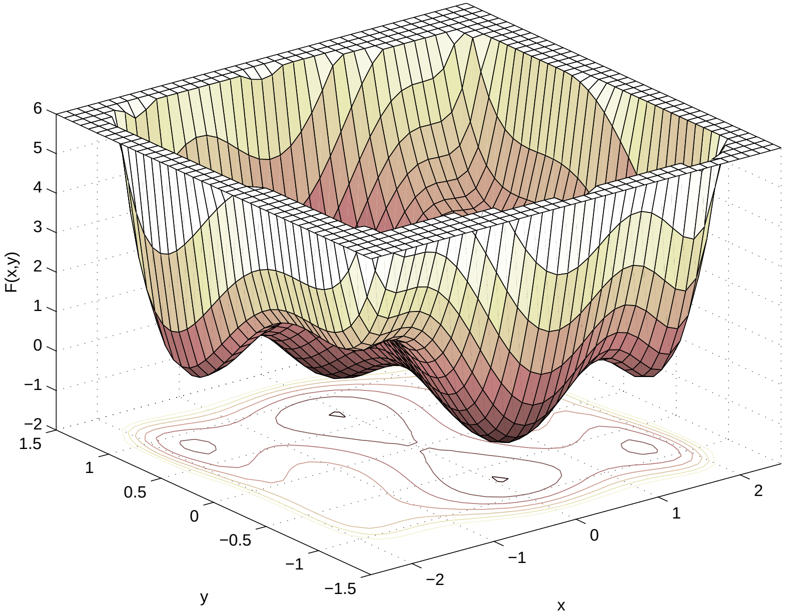
Global optimization

Consider $\min_{x,y} F(x,y)$, with
$F(x,y) := 4x^2 - \frac{21}{10}x^4 + \frac{1}{3}x^6 + xy - 4y^2 + 4y^4.$

Not convex. Many local minima. NP-hard. How to find good lower bounds?



- Find the largest γ s.t.

$$F(x,y) - \gamma \text{ is SOS.}$$

- If exact, can recover optimal solution.
- Surprisingly effective.

Solving, the maximum γ is -1.0316. Exact bound.
Details in (P. & Sturmfels, 2001).

Direct extensions to constrained case.

Constrained problems

What if we are interested in $p(x) \geq 0$, on the set defined by $\{g_i(x) \geq 0\}$?

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$$[1+q(x)]p(x) = s_0(x) + \sum_i s_i(x) g_i(x) + \sum_{ij} s_{ij}(x) g_i(x) g_j(x) \qquad q, s_i, s_{ij} \text{ SOS}$$

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Any of these is a valid sufficient condition, and is an SOS program.

What is the most general case? Are there "converse" results?

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 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:

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

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

To prove infeasibility, find $f \in \text{Cone}(f_i), h \in \text{Ideal}(h_i)$ such that

$$f + h = -1.$$

- Can find certificates by solving SOS programs!
- Complete SOS hierarchy, by certificate degree (P. 2000).
- Directly provides hierarchies of bounds for optimization.

SOS constraints are SDPs

"Gram matrix" method: $F(x)$ is SOS iff $F(x) = w(x)^T Q w(x)$, where $w(x)$ is a vector of monomials, and $Q \succeq 0$.

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

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

Thus, we have the SDP feasibility problem

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

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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:

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

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

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A geometric interlude

How is this possible?

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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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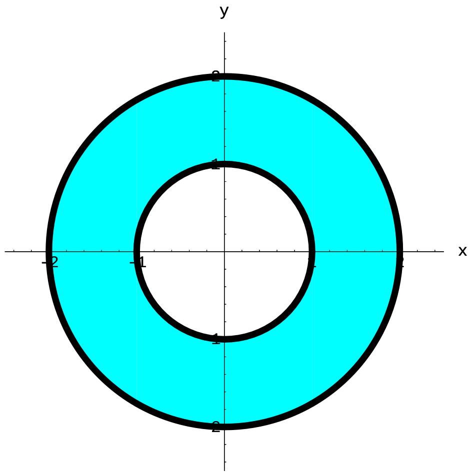
Interestingly, however, often a finite (and small) dimension is enough.

Consider the set defined by

$$1 \leq x^2 + y^2 \leq 2$$

Clearly non-convex.

Can we use convex optimization?



Geometric interpretation

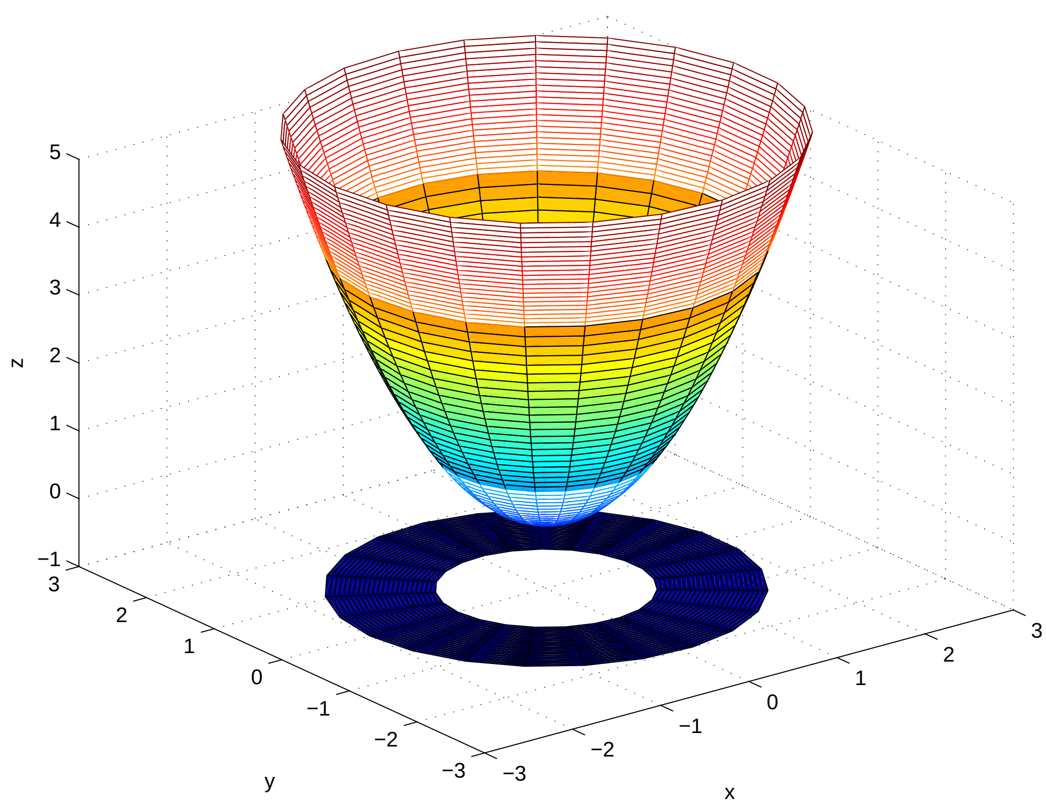
A polynomial "lifting" to a higher dimensional space:

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

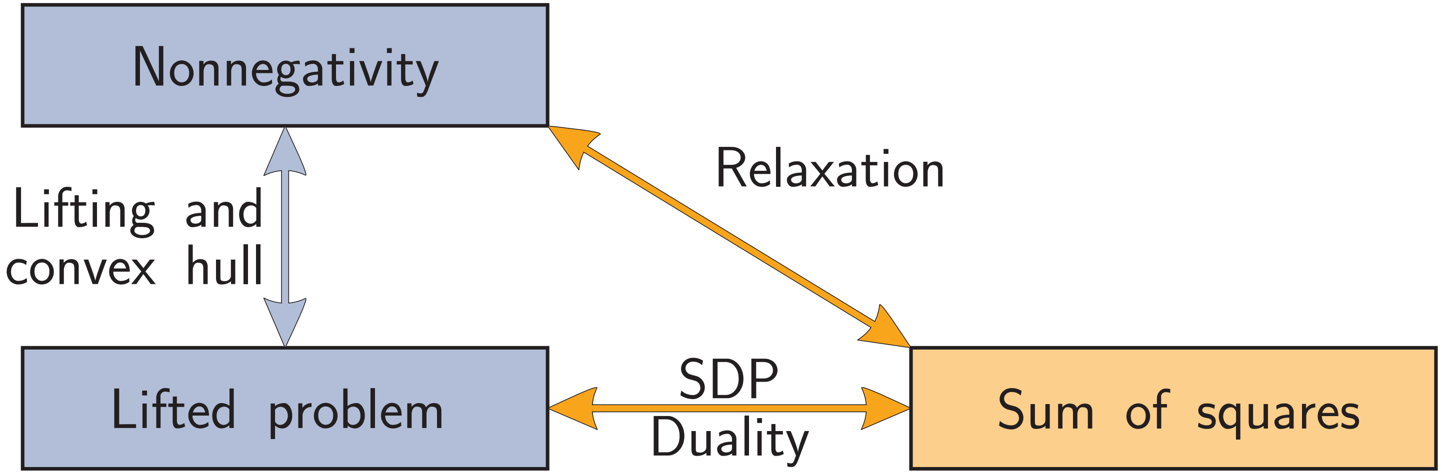
The nonconvex set is the projection of the extreme points of a convex set.

In particular, the convex set defined by

$$x^2 + y^2 \leq z$$
$$1 \leq z \leq 4$$



Relaxation scheme



Many related open questions:

- What sets have "nice" SDP representations?
- Links to "rigid convexity" and hyperbolic polynomials: Helton-Vinnikov, Lewis-P.-Ramana (Lax conjecture), etc.

SOS and SDP

Strong relationship between SOS programs and SDP.

In their full generality, they are equivalent to each other.

- Semidefinite matrices are SOS quadratic forms.
- Conversely, can embed SOS polynomials into PSD cone.

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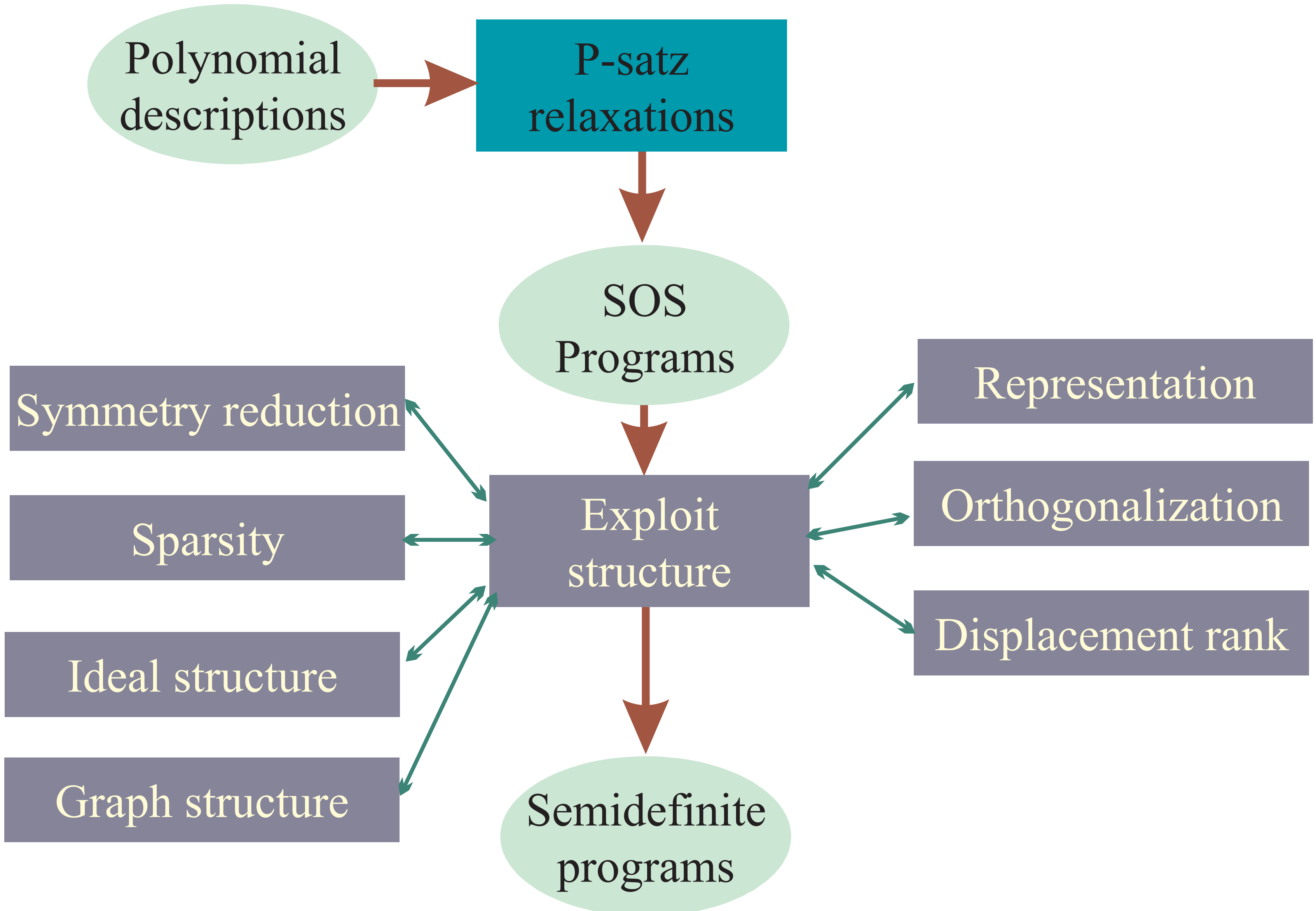
However, they are a *very special* kind of SDP, with very rich algebraic and combinatorial properties.

Exploiting this structure is *crucial* in applications.

Both algebraic and numerical methods are required.

Exploiting structure



Algebraic structure

- Sparseness: few nonzero coefficients.
  - Newton polytopes techniques.
- Ideal structure: equality constraints.
  - SOS on *quotient rings*.
  - Compute in the coordinate ring. Quotient bases.
- Graph structure:
  - Dependency graph among the variables.
- Symmetries: invariance under a group (w/ K. Gatermann)
  - SOS on *invariant rings*
  - Representation theory and invariant-theoretic methods.
  - Enabling factor in applications (e.g., Markov chains)

SOS over everything...

Algebraic tools are *essential* to exploit problem structure:

Standard	**Equality constraints**	**Symmetries**
polynomial ring $\mathbb{R}[x]$	quotient ring $\mathbb{R}[x]/I$	invariant ring $\mathbb{R}[x]^G$
monomials (deg $\leq k$)	*standard* monomials	isotypic components
$\frac{1}{(1-\lambda)^n} = \sum_{k=0}^{\infty} \binom{n+k-1}{k} \cdot \lambda^k$	Hilbert series	Molien series
	Finite convergence for zero dimensional ideals	Block diagonalization

Massachusetts Institute of Technology

Numerical structure

Joint work with J. Löfberg (ETH Zürich), J.-L. Sun (SMA-MIT).

- 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

Let's see some details...

Numerical methods

Recall the SOS representation $p(x) = z(x)^T Q z(x)$

In our earlier discussion, we have implicitly assumed the *monomial basis* in both primal and dual. Bad numerical properties.

But, we are free to choose *any* basis we desire. Particularly good ones: Chebyshev on the primal, Lagrange on the dual.

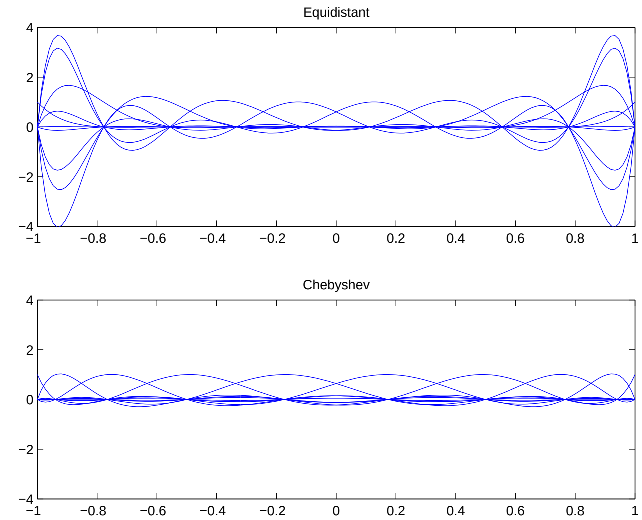
E.g., rather than matching coeffs, force the polynomials to agree on a given set of points. Basis independent notion.

In this basis, SDP constraints have *rank one*:

$$p(x_i) = z(x_i)^T Q z(x_i) = Q \bullet (z(x_i) z^T(x_i))$$

Very good for barrier gradient and Hessians! This low-rank property can be exploited by current SDP solvers (e.g., SDPT3).

Numerical methods



Location of the sampling points:

- Theoretically, weak requirement: *poisedness*
- Distribution strongly affects conditioning

Cf. classical interpolation (spectral methods, Lebesgue constants, etc).

Much improved numerical properties, both in terms of the conditioning of the problem and solution time. In the univariate case, degree 100+ in under a second.

Extensive evaluation upcoming, preliminary results very encouraging.

Applications using SOS

- Related basic work: N.Z. Shor, Nesterov, Lasserre, etc.
- Systems and control.
  - Uncertain system analysis (Papachristodoulou, Prajna)
  - Region of attraction (Tibken, Tan-Packard, P., etc.)
  - Control design (Packard *et al.*, Henrion, Chesi *et al.*, etc.)
  - Time-varying robustness analysis (Hol-Scherer)
  - Density functions (Prajna-Rantzer-P.)
  - Passivity-based synthesis (Ebenbauer-Allgöwer)
  - Contraction analysis for nonlinear systems (Aylward-P.-Slotine)
  - Stochastic reachability analysis (Prajna *et al.*)
  - Hybrid system verification (Prajna-Jadbabaie-Pappas)

SOS applications in other areas

- Matrix copositivity (de Klerk-Pasechnik, Peña, P., etc)
- Sparse optimization (Waki-Kim-Kojima-Muramatsu, etc.)
- Approximation algorithms (de Klerk-Laurent-P.)
- Filter design (Alkire-Vandenberghe, Hachez-Nesterov, etc.)
- Option pricing (Bertsimas-Popescu, Lasserre, Primbs)
- Stability number of graphs (Laurent, Peña, Rendl)
- Geometric theorem proving (P.-Peretz)
- Quantum information theory (Doherty-Spedalieri-P., Childs-Landahl-P.)
- Game theory (Stein-Ozdaglar-P.)

Semialgebraic games

Games with an *infinite* number of pure strategies.

In particular, strategy sets are semialgebraic, defined by polynomial equations and inequalities.

Simplest case (introduced by Dresher-Karlin-Shapley): two players, zero-sum, payoff given by $P(x, y)$, strategy space is a product of intervals.

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Thm: The value of the game, and the corresponding optimal mixed strategies, can be computed by solving a single SOS program.

Perfect generalization of the classical LP for finite games.

Related results for multiplayer games and correlated equilibria (w/ N. Stein and A. Ozdaglar).

Software: SOSTOOLS

$$\begin{array}{ll} \min_{u_i} & c_1 u_1 + \cdots + c_n u_n \\ \text{s.t} & P_i(x,u) := A_{i0}(x) + A_{i1}(x) u_1 + \cdots + A_{in}(x) u_n \quad \text{are SOS} \end{array}$$

- MATLAB toolbox, freely available.
- Uses MATLAB's symbolic toolbox, and SeDuMi (SDP solver).
- Natural syntax, efficient implementation.
- Collaboration w/S. Prajna, A. Papachristodoulou, P. Seiler.
- Includes customized functions for several problems.

Get it from: `www.mit.edu/~parrilo/sostools`
`www.cds.caltech.edu/sostools`

Perspectives, challenges

- Theory:
  - Proof complexity, lower bounds, etc.
  - Approximability properties?
  - What's the right measure of certificate size?
  - Conditioning issues
- Computation and numerical efficiency:
  - Representation issues: straight-line programs?
  - Alternatives to interior point methods?
  - How big are the problems we can reliably solve?
- Many more applications. . .

Summary

- A rich class of optimization problems for engineering
- Methods have enabled many new applications
- Mathematical structure must be exploited for reliability and efficiency
- Combination of numerical and algebraic techniques.
- Fully algorithmic implementations

Finally...

If you want to know more:

- Papers, slides, etc. at website: `www.mit.edu/~parrilo`
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Thank you very much for your attention. Questions?