Sum of squares techniques and polynomial optimization

Pablo A. Parrilo

Laboratory for Information and Decision Systems
Electrical Engineering and Computer Science
Massachusetts Institute of Technology
www.mit.edu/~parrilo

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Massachusetts Institute of Technology

Polynomial problems

We will discuss optimization and decision problems involving *multivariate polynomials*.

Usually, this means a standard optimization problem

$$\min f(x) \qquad \text{s.t.} \quad g_i(x) \leq 0,$$

where the objective and constraints are polynomial expressions.

We may also have (slightly) more complicated *quantified* formulas, and problems where the *variables* are themselves polynomials.

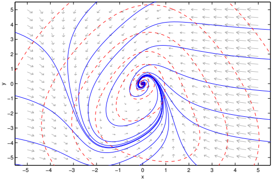
Focus on the basic ideas, emphasizing the geometric and complexity aspects. Much more is known.

Where do these problems appear?

Stability of dynamical systems

- Given a system of ODEs

$$\dot{x}(t) = f(x(t)), \quad x(0) = x_0$$



- Want to prove stability, i.e., that solutions converge to the origin for all initial conditions
- To prove this, need to find an energy-like *Lyapunov function*:

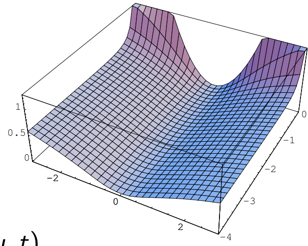
$$V(x) \geq 0, \qquad \dot{V}(x) := \left(\frac{\partial V}{\partial x}\right)^T f(x) \leq 0$$

- Many variations: uncertain parameters, time delays, PDEs, etc.

Partial differential inequalities

- Solutions for linear PDIs:
  - Dissipation or 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, discretization, level-set methods...

How to find certified solutions?
Can we obtain bounds on linear functionals of the solutions?

Motivation

Common properties:

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

These correspond to a very large class of problems:
quantified polynomial inequalities or semialgebraic problems.

Roadmap

- Motivating examples
- Optimization over polynomials
- Sum of squares programs
  - Convexity, relationships with semidefinite programming
  - Geometric interpretations
- Certificates
- Examples: extremal polynomials, joint spectral radius
- Exploiting structure: algebraic and numerical techniques.
- Perspectives, challenges, open questions

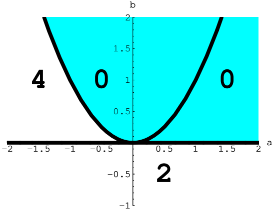
Things get complicated...

The set of nonnegative polynomials is not *basic* semialgebraic.

The set $\{(a_1, \ldots, a_n) \mid \sum_{k=1}^n a_k x^k \geq 0 \ \forall x\}$ *cannot* be described using a *finite* number of unquantified polynomial inequalities $g_i(a_1, \ldots, a_n) \geq 0$.

Ex: Consider the convex set of (a, b) for which

$$x^4 + 2ax^2 + b \geq 0 \quad \forall x \in \mathbb{R}$$



This set *cannot* be defined by $\{g_i(a, b) \geq 0\}$.

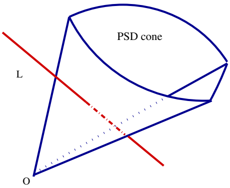
Gets worse in higher dimensions. We need either:

- Boolean set operations (unions of basic SA sets)
- Embed in higher dimensional spaces (lift and project)

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
- First applications in control theory and combinatorial optimization. Nowadays, applied everywhere.
- Convex finite dimensional optimization. Nice duality theory.
- Essentially, solvable in polynomial time (interior point, etc.)

Sum of squares

As we have seen, handling nonnegativity directly is too difficult. Instead. . .

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:

> affine families of *quadratic* forms, that are *nonnegative*.

Instead, for SOS we have:

> affine families of *polynomials*, that are *sums of squares*.

An SOS program is an optimization problem with SOS constraints:

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

This is a finite-dimensional, convex optimization problem.

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SOS programs: questions

- Why not just use nonnegative polynomials?
  While convex, unfortunately it's NP-hard ;(
- And is SOS any better?
  Yes, we can solve SOS programs in polynomial time
- Aren't we losing too much then?
  In several important cases (quadratic, univariate, etc), nonnegativity and SOS is the same thing.
- And in the other cases?
  Low dimension, computations and some theory show small gap.
  Recent negative results in very high dimension, though (Blekherman)
- Isn't it a very special formulation?
  No, we can approximate *any* semialgebraic problem!
- How? And how do you solve them?

OK, I'll tell you. But first, an example!

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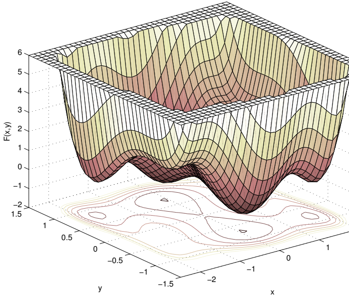
Global optimization

Given a multivariate polynomial, can we find the global minimum? 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.



Often, the optimal γ is the true minimum.
Extensions to constrained case via representation theorems (Putinar/Lasserre) or the Positivstellensatz, yield *hierarchies* of relaxations.

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

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

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

Example 1: range of nonnegativity

For what range of values of a is the polynomial

$$P(x,y) = x^4 + y^2 - 4axy + (2a-3)x^2 + ax + 20$$

a sum of squares? Nonnegative?

For SOS, essentially:

```
sosprogram([x,y]); sosdecvar([a]);
P = x^4 + y^2 - 4*a*x*y + (2*a-3)*x^2 + a*x + 20 ;
sosineq(P); sossetobj(a);
sossolve; sosgetsol(a);
```

The solution: $a \in [-.94823, 1.42413]$ (numerically correct to 8+ digits).

Both are roots of the irreducible polynomial

$1613120 + 545280a - 1234772a^2 + 517544a^3 - 364251a^4 - 410208a^5 + 369408a^6 - 164224a^7 + 82176a^8$.

Interestingly, for SOS the range is the same as that for $P(x,y) \geq 0$.

Example 2: extremal polynomials

Given $n \geq 1$, define $p(x) = \sum_{i=0}^{n} a_i x^i$, and consider the problem:

$$\max_{a_0,\ldots,a_n} a_n \qquad \text{s.t.} \quad |p(x)| < 1 \; \forall x \in [-1, 1],$$

In words:

How large can the leading coefficient of a univariate polynomial be if the polynomial is unit-bounded in the $[-1, 1]$ interval?

What is the optimal value? What does the extreme $p(x)$ look like?

A QE problem with two blocks of quantifiers, in $n + 2$ variables:

$$(\exists a_0)(\exists a_1)\cdots(\exists a_{n-1})(\forall x)[x \geq -1 \wedge x \leq 1] \Rightarrow [a_n x_n + \cdots + a_0 \leq 1 \wedge a_n x_n + \cdots + a_0 \geq -1]$$

Can we solve it? For what values of n?

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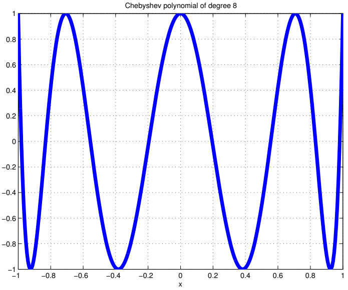
Example 2 (continued)

- By the Markov-Lukacs theorem,

$$p(x) \geq 0, \quad \forall\, x \in [-1,1] \qquad \Longleftrightarrow \qquad p(x) = s(x) + t(x)(1-x^2),$$

  where $s(x)$ and $t(x)$ are SOS.
- The optimal value is $a_n = 2^{n-1}$, and the optimal $p(x)$ are Chebyshev polynomials.

- Highly degenerate solution, $p(x)$ has many global minima.
- For $n \leq 12$, we solve it in ≈ 1 sec.
- For larger n, numerical issues become important.



Example: Joint spectral radius

Given a set of $n \times n$ matrices $\Sigma := \{A_1, \ldots, A_m\}$, what is the maximum "growth rate" that can be achieved by arbitrary switching?

$$\rho(\Sigma) := \limsup_{k \to +\infty} \max_{\sigma \in \{1,\ldots,m\}^k} ||A_{\sigma_k} \cdots A_{\sigma_2} A_{\sigma_1}||^{1/k}$$

Appeared in several different contexts: linear algebra (Rota-Strang 1960), wavelets (Daubechies-Lagarias 1992), switched linear systems, etc.

If $m = 1$, then $\rho(\{A_1\})$ is the *spectral radius* $\max |\lambda(A)|$.
If $m \geq 2$, determining if $\rho(\Sigma) \leq 1$ is undecidable (Blondel-Tsitsiklis 2000).

Upper bounds via polynomials

Thm: Let $p(x)$ be a strictly positive homogeneous multivariate polynomial of degree $2d$, that satisfies

$$\gamma^{2d}\, p(x) \,-\, p(A_i x) \geq 0 \qquad \forall x \in \mathbb{R}^n \quad i = 1, \ldots, m$$

Then, $\rho(\Sigma) \leq \gamma$.

A natural relaxation is obtained by replacing nonnegativity by SOS. Then:

Thm: The SOS relaxation satisfies:

$$\binom{n+d-1}{d}^{-\frac{1}{2d}} \rho_{SOS,2d} \leq \rho(\Sigma) \leq \rho_{SOS,2d}. \qquad (1)$$

Approximation ratio is *independent* of the number of matrices. As $d \to \infty$, the factor converges to 1.

Generalizations to constrained switching (Ahmadi et al. 2012).

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SOS and SDP

Strong relationship between SOS programs and SDP.
In full generality, they are equivalent to each other.

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

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.

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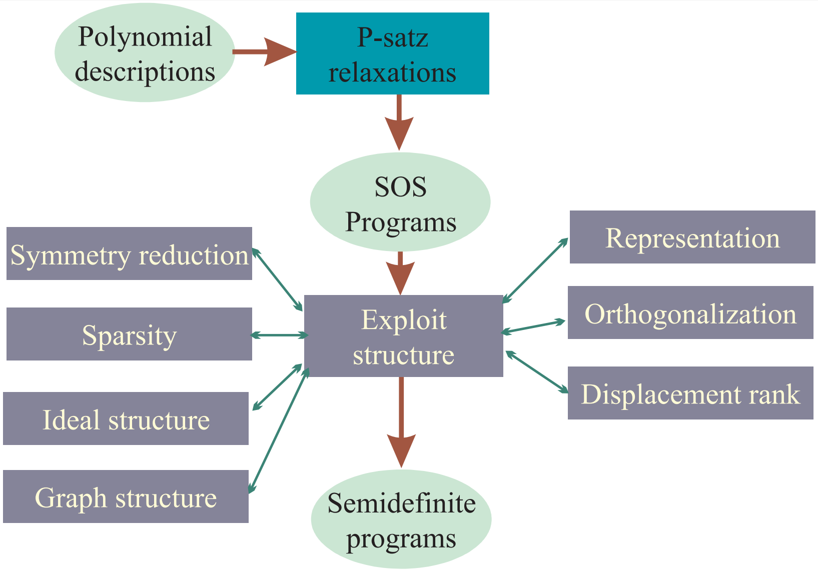
Exploiting structure: algebraic and numerical



Perspectives, challenges, open questions

- Theory:
  - Better understanding of interaction between algebra and convexity ("convex algebraic geometry")
  - Minimum rank decompositions? Low-rank approaches?
  - Proof complexity, lower bounds, etc.
  - Connections with theoretical computer science
- Computation and numerical efficiency:
  - Specialized algorithms, better than SDP
  - Alternatives to interior point methods?
  - Increase numerical stability (better bases, splines, etc)
  - Representation issues: straight-line programs?
- Many more applications. . .

Summary

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

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