Sum of Squares Optimization and Its Applications

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Optimization over nonnegative polynomials

Definition by example: How to pick c_1, c_2, c_3 so to make

$$p(x_1, x_2) = c_1 x_1^4 - 6x_1^3 x_2 - 4x_1^3 + c_2 x_1^2 x_2^2 + 10x_1^2 + 12x_1 x_2^2 + c_3 x_2^4$$

nonnegative over a given basic semialgebraic set?

Basic semialgebraic set: $\{x \in \mathbb{R}^n | g_i(x) \ge 0, h_j(x) = 0\}$

Ex:
$$x_1^3 - 2x_1x_2^4 \ge 0$$

 $x_1^4 + 3x_1x_2 - x_2^6 \ge 0$



-This problem is fundamental to many areas of applied/computational mathematics. -It is the problem that "SOS optimization" is designed to solve.

Why would you want to do this?!

Let's start with five application domains...



1. Polynomial optimization



•Many applications: the optimal power flow problem, low-rank matrix factorization, dictionary learning, training of deep nets with polynomial activation function, sparse regression with nonconvex regularizes, etc.

Intractable in general (includes all NP-complete problem)



2. Optimization under input uncertainty

How to make optimal decisions when input to optimization problem is uncertain/noisy?

Example: The Markowitz portfolio optimization problem



man
$$\&$$

 $x \in \mathbb{R}^n, \& \in \mathbb{R}$
s.t. $\bigwedge^T \chi \xrightarrow{>} \&$ (return)
 $\chi^T \sum \chi \leqslant \&$ (risk)
 $\chi \xrightarrow{>} 0, \sum_{i=1}^n \chi_i = 1$
 $\chi \in \Omega$

 $\mu \in \mathbb{R}^n$: mean vector $\Sigma \in \mathbb{S}^{n \times n}$: covariance of the returns matrix of the returns

In practice estimated from past data/ML model. Optimal portfolio sensitive to this input.



Accounting for uncertainty:

$$\begin{aligned}
U_{\mu} &= \left\{ \begin{array}{l} \int_{0}^{n} + u \in \mathbb{R}^{n} \\ \|u\| \leq R \right\} \\
U_{\Sigma} &= \left\{ \begin{array}{l} \Sigma \in S^{n \times n} \\ \Sigma \in S^{n \times n} \\ \|\Sigma \rangle_{r}^{n} \circ, \\ \Sigma &= \left\{ \begin{array}{l} \Sigma \in S^{n \times n} \\ \Sigma &\in S^{n \times n} \\ \|\Sigma \rangle_{r}^{n} \circ, \\ \Sigma &= \left\{ \begin{array}{l} \sum \\ \kappa \in \mathbb{R}^{n}, \\ \chi \in \mathbb{R}^{n}, \\ \chi \in \mathbb{R}^{n} \\ \\ \chi \in S \end{array} \right\} \\
\end{aligned}$$

$$\begin{aligned}
u_{\Sigma} &= \left\{ \begin{array}{l} \sum \\ \kappa \in S^{n \times n} \\ \chi \in S \\ \\ \chi &= 1 \\ \chi \in S \end{array} \right\} \\
\end{aligned}$$

3. Statistics and machine learning

Shape-constrained regression; e.g., monotone and/or convex regression

Shape constraints act as regularizer, improve test performance, make model more interpretable and trustworthy

Example 1: Shape constraints natural in most applications



5 beds · 4 baths · 2,623 sqft





Monotonicity of a polynomial $p(x_1, ..., x_n)$ with respect to feature $j: \frac{\partial p(x)}{\partial x_j} \ge 0, \forall x \in B$ Example 2: "ML for fast real-time convex optimization"

$$g(b) \coloneqq \min_{x \in \mathbb{R}^n} f_0(x)$$

s.t. $f_i(x) \le b_i \ i = 1, ..., m$
 $x \in \Omega$

 f_0, \ldots, f_m convex functions, Ω a convex set.

PRINCETON UNIVERSITY **Goal:** learn g(b) offline from training set; evaluate it online very fast

$$g: \mathbb{R}^m \to \mathbb{R}$$
 is

- convex

- nonincreasing w.r.t. all arguments

 $y^T \nabla^2 g(b) y \ge 0, \forall b, \forall y \quad \frac{\partial g(b)}{\partial b_i} \le 0, \forall b, \forall j \in C$

Imposing monotonicity

• For what values of *a*, *b* is the following polynomial monotone over [0,1]?

$$p(x) = x^4 + ax^3 + bx^2 - (a+b)x$$





4. Certifying properties of dynamical systems

$$\dot{x} = f(x)$$







Example: certifying stability

 $\dot{x} = f(x)$ $f: \mathbb{R}^n \to \mathbb{R}^n$ **Ex.** $\dot{x}_1 = -x_2 + \frac{3}{2}x_1^2 - \frac{1}{2}x_1^3x_2$ $\dot{x}_2 = 3x_1 - x_1x_2$

Locally asymptotic stability (LAS) of equilibrium points



Lyapunov's theorem (and its converse):

The origin is LAS if and only if there exists a C^1 function $V: \mathbb{R}^n \to \mathbb{R}$ that vanishes at the origin and a scalar $\beta > 0$ such that

V(x) > 0 $V(x) \le \beta \Rightarrow \dot{V}(x) = \nabla V(x)^T f(x) < 0$







(If $\dot{V}(x) < 0$ everywhere, then globally stable.)

Example: certifying collision avoidance



(vector valued polynomial)

- S: needs safety verification
- \mathcal{U} : unsafe (or forbidden) set

(both sets basic semialgebraic)



Safety guaranteed if we find a "Lyapunov function" such that:

$$\begin{array}{ll} B(\mathcal{S}) < 0 \\ B(\mathcal{U}) > 0 \end{array} \quad \dot{B} = \langle \nabla B(x), f(x) \rangle \leq 0 \end{array}$$



5. Automated theorem proving in geometry

• **Kissing number in dimension** *n*: largest number of *n*-dimensional non-overlapping spheres that can simultaneously touch (or "kiss") a common unit sphere.



Newton

Gregory



 $k_3 = 12$ $k_3 = 13$

Discussion/bet in 1694

Newton proved to be correct in 1953!

13 spheres impossible iff the following system is *infeasible*:

$$\begin{aligned} x_i^2 + y_i^2 + z_i^2 &= 4, \ i = 1, \dots, 13 \\ (x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2 \ge 4, \\ i, j \in \{1, \dots, 13\}^2 \\ \end{bmatrix} \begin{cases} \textbf{J}_i(\textbf{x}) \\ \vdots \\ \textbf{J}_{los}(\textbf{x}) \end{cases}$$



 $\exists g_{gg}(\mathbf{x}) \not\ni = g_{boo}(\mathbf{x}) < o$



Outline

- Global nonnegativity
 - Sum of squares (SOS) and semidefinite programming
 - Two applications
 - Hilbert's 17th problem
- Nonnegativity over a region
 - Putinar's Positivstellensat
 - Two applications
- Recap and further reading



How would you prove nonnegativity?

Ex. Decide if the following polynomial is nonnegative:

$$p(x) = x_1^4 - 6x_1^3x_2 + 2x_1^3x_3 + 6x_1^2x_3^2 + 9x_1^2x_2^2 - 6x_1^2x_2x_3 -14x_1x_2x_3^2 + 4x_1x_3^3 + 5x_3^4 - 7x_2^2x_3^2 + 16x_2^4$$

■Not so easy! (In fact, NP-hard for degree ≥ 4)

But what if I told you:

$$p(x) = (x_1^2 - 3x_1x_2 + x_1x_3 + 2x_3^2)^2 + (x_1x_3 - x_2x_3)^2 + (4x_2^2 - x_3^2)^2.$$

Natural questions:

Q1: Is it any easier to test for a sum of squares (SOS) decomposition?
Q2: Is every nonnegative polynomial SOS?



Sum of squares and semidefinite programming



PSD cone

- **Q1:** Is it any easier to decide SOS?
- Yes! Can be reduced to a semidefinite program (SDP)

- Can also efficiently search and optimize over SOS polynomials
- As we will see, this latter property is very important in applications...



Semidefinite programming (SDP)

• A broad generalization of linear programs

• Can be solved to arbitrary accuracy in polynomial time (e.g., using interior point algorithms) [Nesterov, Nemirovski], [Alizadeh]

$$\begin{array}{c} \mbox{min.} & \mbox{Tr} (C X) \\ \chi \in S^{n \times n} \\ st. & \mbox{Tr} (A_i X) = b_i \quad i = 1 \dots, m \\ & X_{i > 0} \\ & & X_{i > 0} \\ & & & X_{i > 0} \\ & & & & X_{i > 0} \\ & & & & & \\ \end{array}$$

$$\begin{array}{c} \mbox{Motes:} & \mbox{Tr} (C X) = \sum_{i > i} C_{i j} \chi_{i j} \\ & X_{i > 0} \\ & & & & \\ \chi_{i > 0} & & & & \\ & & & & \\ \chi_{i > 0} & & & & \\ \end{array}$$

$$\begin{array}{c} \mbox{Motes:} & \mbox{Tr} (C X) = \sum_{i > i} C_{i j} \chi_{i j} \\ & & & & \\ \chi_{i > 0} & & & \\ \chi_{i > 0} & & & & \\ \chi_{i > 0} & & & & \\ \chi_{i > 0} & & & & \\ \end{array}$$

$$\begin{array}{c} \mbox{Motes:} & \mbox{Tr} (C X) = \sum_{i > i} C_{i j} \chi_{i j} \\ & & & & \\ \chi_{i > 0} & & & \\ \chi_{i > 0} & & & & \\ \chi_{i > 0} & & & & \\ \chi_{i > 0} & & & & \\ \end{array}$$

$$\begin{array}{c} \mbox{Motes:} & \mbox{Tr} (C X) = \sum_{i > i} C_{i j} \chi_{i j} \\ & & & \\ \chi_{i > 0} & & & \\ \end{array}$$

SOS→SDP

Thm:

A polynomial p of degree 2d is SOS if and only if $\exists Q \ge 0$ such that $p(x) = z(x)^T Q z(x)$ where $z = [1, x_1, ..., x_n, x_1 x_2, ..., x_n^d]^T$ is the vector of monomials of degree up to d.

(It follows that checking membership or optimizing a linear function over the set of SOS polynomials is an SDP)

Proof: (=) Suppose
$$\exists Q_{z}, s.t. p(x) = Z^{T}(x)Q_{z}(x) \forall x.$$

 $Q_{z}, \Rightarrow Q = V^{T}V \Rightarrow p(x) = Z^{T}(x)V^{T}VZ(x) = ||VZ(x)||^{2} = \sum_{i=1}^{r} (U_{i}^{T}Z(x))^{2}.$
 $r_{x} \binom{n+d}{d}$

$$(\Leftarrow) \text{ Suppose } p(x) \text{ is SOS.}$$

$$\exists v_{1,1} - v_r \in \mathbb{R}^{\binom{n+d}{d}} \text{ s.t. } p(x) = \sum_{i=1}^{r} \left(v_i^T \neq (x) \right)^2 = \sum_{i=1}^{r} \left(\overline{\forall}_i^T \neq (x) \right)^2 = \overline{\forall}_i \left(\overline{\forall}_i^T \neq (x) \right) = \overline{\forall}_i \left(\overline{\begin{pmatrix} v_i & v_i \\ v_i & v_i \end{pmatrix}} \neq (x) \right)^2 = \overline{\forall}_i \left(\overline{\forall}_i^T \neq (x) \right)^2 = \overline{\forall}_i \left(\overline{\forall}_i^T \neq (x) \right)^2 = \overline{\forall}_i \left(\overline{\begin{pmatrix} v_i & v_i \\ v_i & v_i \end{pmatrix}} \neq (x) \right)^2 = \overline{\forall}_i \left(\overline{\forall}_i^T \forall (x) \right)^2 = \overline{\forall}_i \left(\overline{\forall}_i^T \forall$$

Example

$$P(x) = 10 \ x^{4} - 2 \ x^{3} - 7 \ x^{2} + 4 \ x + 4$$

$$Is \ p \ SOS ?$$

$$P(x) = \begin{bmatrix} 1 \\ x \\ x^{4} \end{bmatrix} \begin{bmatrix} 9 \\ u \\ q_{12} \\ q_{12} \\ q_{13} \\ q$$

Let's revisit two of our applications!



Optimization over nonnegative polynomials

Sum of squares (SOS) programming

Semidefinite programming (SDP)



1) Nonconvex unconstrained minimization

Find:
$$p_{sos}^{*} = inf$$
 $4x^{2} - \frac{21}{10}x^{4} + \frac{1}{3}x^{6} + xy - 4y^{2} + 4y^{4} + x^{2}y$ $P(x, y)$
 $(x,y) \in \mathbb{R}^{2}$
 $p_{sos}^{*} = s_{NP} \qquad x$
 $g \in \mathbb{R}$
 $s t \cdot P(x, y) - 8 \qquad sos$
 $p_{sos}^{*} \leq P^{*}$

```
p=4*x^2-2.1*x^4+(1/3)*x^6+1*x*y-4*y^2+4*y^4+x^2*y; solvertime: 0.6 (s)
solvesos(sos(p-gam),-gam,[],[gam])
p_sos=double(gam)
p_sos=double(gam)
```

-2.921560950963582

```
[inf,z,Q]=solvesos(p-p_sos);
sdisplay(z{1})
[v,d]=eig(double(Q{1}));
zxstar=v(:,1)/v(1,1);
xstar=[zxstar(3);zxstar(2)]
p_at_xstar=replace(p,[x,y],[xstar(1),xstar(2)])
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(inf,z,Q]=solvesos(p-p_sos);
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2) Automated proof of global asymptotic stability



Tue 2/9/2021 1:13 PM To: Amir Ali Ahmadi

Hi Amir Ali,

MK

I hope life and career are going well.

.edu> on behalf of

I have a question that I assume might take little more than 5-10 of your time but please feel free to let me know if it would actually take more.



I started constructing a strict one in real time and it quickly got out of hand, necessitating higher and higher powers and many cross terms. I inevitably thought of you and your (and Pablo's) SOS program that would spit out a good strict V within seconds.

If you can plug in this system and let me know what comes out, I'd appreciate it, and my 40-50 students in class would learn a few things (complexity of Lyapunov functions, automated options for finding them, etc.).





Automated proof of global asymptotic stability



sdpvar x y
xdot=-x+y^3; >> sdisplay(clean(double(c)'*m,1e-3))
ydot=-x; 1.00000084865*x^2-0.333330248293*x*y+0.166665124147*y^2+0.500118639025*y^4

$$\begin{bmatrix} V, c, m \end{bmatrix} = \text{polynomial}([x; y], 4, 2); \\ Vdot= \text{jacobian}(V, [x, y]) * [xdot; ydot]; \\ V(\mathcal{X}, \mathcal{Y}) = \mathcal{X}^2 - \frac{1}{3}\mathcal{X}\mathcal{Y} + \frac{1}{6}\mathcal{Y}^2 + \frac{1}{2}\mathcal{Y}^4 \\ \text{FF} = [sos(V), sos(-Vdot)] \\ \text{solvesos}(\text{FF}, [], [], [c]) \\ \end{bmatrix}$$

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$$= (\chi - \frac{1}{6}g)^{2} + \frac{5}{36}g^{2} + \frac{1}{2}g^{4}$$
 (hence positive definite)

$$\gg \frac{1}{36} (\chi^2 + y^2) + \frac{1}{2} y^4$$
 (hence radially unbounded)

 $V(x,y) = -\frac{5}{3} x^2 - \frac{1}{3} y^4$ (hence negative definite)

Hilbert's 1888 Paper Q2: SOS \Leftarrow Nonnegativity

n,d	2	4	≥6
1	yes	yes	yes
2	yes	yes	no
3	yes	no	no
≥4	yes	no	no



Motzkin (1967):

$$M(\pi_{1},\pi_{2}) = \pi_{1}^{4}\pi_{2}^{2} + \pi_{1}^{2}\pi_{2}^{4} - 3\pi_{1}^{2}\pi_{2}^{2} + 1$$
Robinson (1973):

$$R(\pi_{1},\pi_{2},\pi_{3}) = \pi_{1}^{2}(\pi_{1}-1)^{2} + \pi_{2}^{2}(\pi_{2}-1)^{2} + \pi_{3}^{2}(\pi_{3}-1)^{2} + 2\pi_{1}\pi_{2}\pi_{3}(\pi_{1}+\pi_{2}+\pi_{3}-2)$$

$$+ 2\pi_{1}\pi_{2}\pi_{3}(\pi_{1}+\pi_{2}+\pi_{3}-2)$$

The Motzkin polynomial

0.8 - 0.6 - 0.4 - 0.2 -

$$M(x,y) = x^2y^4 + x^4y^2 + 1 - 3x^2y^2$$

How to prove it is nonnegative?

$$\begin{aligned} (x^2 + y^2 + 1) M(x, y) &= (x^2y - y)^2 + (xy^2 - x)^2 + (x^2y^2 - 1)^2 + \frac{1}{4}(xy^3 - x^3y)^2 + \frac{3}{4}(xy^3 + x^3y - 2xy)^2 \\ &+ \frac{1}{4}(xy^3 - x^3y)^2 + \frac{3}{4}(xy^3 + x^3y - 2xy)^2 \end{aligned}$$



Hilbert's 17th Problem (1900)
Q. *p* nonnegative
$$\Rightarrow p = \sum_{i} \left(\frac{g_i}{q_i}\right)^2$$

Artin (1927): Yes!

Implications:

- $p \ge 0 \Rightarrow \exists h \text{ sos such that } p.h \text{ sos}$
- **Reznick:** (under mild conditions) can take $h = (\sum_{i} x_{i}^{2})^{r}$
- Certificates of nonnegativity can *always* be given with sos (i.e., with semidefinite programming)!
- We'll see how the Positivstellensatz generalizes this even further...

Outline of the rest of the talk...

Global nonnegativity

- Sum of squares (SOS) and semidefinite programming
- Two applications
- Hilbert's 17th problem

• Nonnegativity over a region

- Putinar's Positivstellensatz
- Two applications
- Recap and further reading



Positivstellensatz





Putinar's Positivstellensatz (1993)

 $p(x) > 0 \text{ on } S = \{x \in \mathbb{R}^n | g_i(x) \ge 0, i = 1, ..., m\}$

 $\exists \epsilon > 0 \text{ and SOS polynomials } s_0(x), \dots, s_m(x) \text{ such that} \\ p(x) - \epsilon = s_0(x) + \sum_i s_i(x) g_i(x).$

- This is algebraic certificate of positivity
- Leads to an SDP hierarchy for polynomial optimization (the ``Lasserre hierarchy'')
- Degree bounds on SOS multipliers based on the coefficients (though in special cases, better degree bounds possible)



How did I plot this?

• For what values of *a*, *b* is the following polynomial monotone over [0,1]?



Theorem. A polynomial p(x) of degree 2d is monotone on [0,1] if and only if

 $p'(x) = xs_1(x) + (1 - x)s_2(x),$

where $s_1(x)$ and $s_2(x)$ are some SOS polynomials of degree 2d - 2.

Let's end with a couple applications:

- Finance
- Control

Optimization over nonnegative polynomials

Sum of squares (SOS) programming

Semidefinite programming (SDP)



Distributionally robust optimization

What's the probability that Zoom's stock goes bust?



Three months starting Feb 1, 2020 $r_i = \frac{P_i - P_{i-1}}{P_i}, i = 1, ..., 61$ Empirical moments $m_k = \mathbb{E}[r^k]$: $m_1 = 0.0068, m_2 = 0.0034,$ $m_3 = 2 \times 10^{-6}, m_4 = 5 \times 10^{-5}$

The distribution of r is supported on [-0.4,0.4] but is otherwise unknown

What is the probability that Zoom's stock return will be below -0.1 today?

Want the worst-case probability over all distributions whose first 4 moments are within 10% of those computed from data.

Sum of squares optimization can compute this probability!

$$\alpha := \inf_{q,r,s,\gamma} \gamma$$
s.t. $q(x) = \sum_{k=0}^{4} q_k x^k$ is a degree-4 (univariate) polynomial,
 $r(x), s(x)$ are quadratic polynomials that are sos,
 $q_0 + \sum_{k=1}^{4} q_k m'_k \le \gamma \forall m'_k \in [0.9 \ m_k, 1.1 \ m_k]$ for $k = 1, \dots, 4$.
 $q(x) - (0.4^2 - x^2) \ s(x)$ is sos,
 $q(x) \ge 1 \quad \forall x \in [-0.4, 0.4]$
 $q(x) - 1 - (0.4 + x)(-0.1 - x)r(x)$ is sos.

$$\Rightarrow q(x) \ge 0 \quad \forall x \in [-0.4, 0.4]$$

$$\Rightarrow q(x) \ge 1 \quad \forall x \in [-0.4, -0.1]$$

$$\mathbb{P}(r \in [-0.4, -0.1]) = \mathbb{E}[\mathbf{1}_{[-0.4, -0.1]}] \Rightarrow \mathbf{1}_{[-0.4, -0.1]} \le q(x) \ \forall x \in [-0.4, 0.4]$$

$$\Rightarrow \mathbb{E}[\mathbf{1}_{[-0.4, -0.1]}] \le \mathbb{E}[q(x)] = \sum_{k=0}^{4} q_k m_k \le \gamma$$
In fact, we always have
 $\mathbb{P}(r \in [-0.4, -0.1]) = \alpha$

$$\mathbb{P}(r \in [-0.4, -0.1]) = \alpha$$

$$\mathbb{P}(r \in [-0.4, -0.1]) \le \alpha$$

Stabilizing a humanoid robot on one foot





Certifying collision avoidance



Safety guaranteed if we find a "Lyapunov function" such that:

$$\begin{array}{ll} B(\mathcal{S}) < 0 \\ B(\mathcal{U}) > 0 \end{array} \quad \dot{B} = \langle \nabla B(x), f(x) \rangle \leq 0 \end{array}$$



Real-time collision avoidance certificates



(w/ Majumdar)

Dubins car model

Run-time: 20 ms



Recap: "See an inequality? Think SOS!"

Is $p(x) \ge 0$ on $\{g_1(x) \ge 0, \dots, g_m(x) \ge 0\}$?

Automated SOS-based proofs via SDP!

Many applications!



Optimization



Control





Want to learn more?



MONIQUE LAURENT*

Georgina Hall



aaa.princeton.edu