8. Sum of Squares

- Polynomial nonnegativity
- Sum of squares (SOS) decomposition
- Example of SOS decomposition
- Computing SOS using semidefinite programming
- Necessary conditions
- Newton Polytopes and Sparsity
- Positivity in one variable
- Background
- Global optimization
- Optimizing in parameter space
- Lyapunov functions
Polynomial Programming

So far

- Polynomial equations over the complex field

Objectives

- General quantified formulae
- Boolean connectives
- Polynomial equations, inequalities, and inequations over the reals

e.g., does there exist $x$ such that for all $y$

$$\left( f(x, y) \geq 0 \right) \land \left( g(x, y) = 0 \right) \lor \left( h(x, y) \neq 0 \right)$$
Polynomial Nonnegativity

First, consider the case of one inequality; given $f \in \mathbb{R}[x_1, \ldots, x_n]$

Does there exist $x \in \mathbb{R}^n$ such that $f(x) < 0$

- If not, then $f$ is globally non-negative

\[ f(x) \geq 0 \quad \text{for all } x \in \mathbb{R}^n \]

and $f$ is called *positive semidefinite* or *PSD*

- The problem is *NP-hard*, but decidable

- Many applications
Certificates

Primal decision problem

\[
\text{does there exist } x \in \mathbb{R}^n \text{ such that } f(x) < 0
\]

- Answer \textit{yes} is easy to verify; exhibit \( x \) such that \( f(x) < 0 \)

- Answer \textit{no} is hard; we need a \textit{certificate} or a \textit{witness}
  i.e, a proof that there is no feasible point
Sum of Squares Decomposition

If there are polynomials $g_1, \ldots, g_s \in \mathbb{R}[x_1, \ldots, x_n]$ such that

$$f(x) = \sum_{i=1}^{s} g_i^2(x)$$

then $f$ is nonnegative.

A purely syntactic, easily checkable certificate, called a sum-of-squares (SOS) decomposition

- How do we find the $g_i$?
- When does such a certificate exist?
Example

We can write any polynomial as a *quadratic form* on monomials

\[ f = 4x^4 + 4x^3y - 7x^2y^2 - 2xy^3 + 10y^4 \]

\[ = \begin{bmatrix} x^2 \\ xy \\ y^2 \end{bmatrix}^T \begin{bmatrix} 4 & 2 & -\lambda \\ 2 & -7 + 2\lambda & -1 \\ -\lambda & -1 & 10 \end{bmatrix} \begin{bmatrix} x^2 \\ xy \\ y^2 \end{bmatrix} \]

\[ = z^T Q(\lambda) z \]

which holds for all \( \lambda \in \mathbb{R} \)

If for some \( \lambda \) we have \( Q(\lambda) \succeq 0 \), then we can factorize \( Q(\lambda) \)
Example, continued

e.g., with $\lambda = 6$, we have

$$Q(\lambda) = \begin{bmatrix} 4 & 2 & -6 \\ 2 & 5 & -1 \\ -6 & -1 & 10 \end{bmatrix} = \begin{bmatrix} 0 & 2 \\ 2 & 1 \\ 1 & -3 \end{bmatrix} \begin{bmatrix} 0 & 2 & 1 \\ 2 & 1 & -3 \end{bmatrix}$$

so

$$f = \begin{bmatrix} x^2 \\ xy \\ y^2 \end{bmatrix}^T \begin{bmatrix} 0 & 2 \\ 2 & 1 \\ 1 & -3 \end{bmatrix} \begin{bmatrix} 0 & 2 & 1 \\ 2 & 1 & -3 \end{bmatrix} \begin{bmatrix} x^2 \\ xy \\ y^2 \end{bmatrix}$$

$$= \left\| \begin{bmatrix} 2xy + y^2 \\ 2x^2 + xy - 3y^2 \end{bmatrix} \right\|^2$$

$$= (2xy + y^2)^2 + (2x^2 + xy - 3y^2)^2$$

which is an SOS decomposition
Sum of Squares and Semidefinite Programming

Suppose \( f \in \mathbb{R}[x_1, \ldots, x_n] \), of degree \( 2d \)

Let \( z \) be a vector of all monomials of degree less than or equal to \( d \)

\( f \) is SOS if and only if there exists \( Q \) such that

\[
Q \succeq 0 \\
f = z^T Q z
\]

- This is an SDP in standard primal form
- The number of components of \( z \) is \( \binom{n+d}{d} \)
- Comparing terms gives affine constraints on the elements of \( Q \)
Sum of Squares and Semidefinite Programming

If $Q$ is a feasible point of the SDP, then to construct the SOS representation factorize $Q = VV^T$, and write $V = [v_1 \ldots v_r]$, so that

$$f = z^T V V^T z$$

$$= \|V^T z\|^2$$

$$= \sum_{i=1}^{r} (v_i^T z)^2$$

- One can factorize using e.g., Cholesky or eigenvalue decomposition
- The number of squares $r$ equals the rank of $Q$
Example

\[ f = 2x^4 + 2x^3y - x^2y^2 + 5y^4 \]

\[
\begin{bmatrix}
  x^2 \\
  xy \\
  y^2 
\end{bmatrix}^T \begin{bmatrix}
  q_{11} & q_{12} & q_{13} \\
  q_{12} & q_{22} & q_{23} \\
  q_{13} & q_{23} & q_{33}
\end{bmatrix} \begin{bmatrix}
  x^2 \\
  xy \\
  y^2 
\end{bmatrix}
\]

\[ = q_{11}x^4 + 2q_{12}x^3y + (q_{22} + 2q_{13})x^2y^2 + 2q_{23}xy^3 + q_{33}y^4 \]

So \( f \) is SOS if and only if there exists \( Q \) satisfying the SDP

\[
Q \succeq 0 \quad q_{11} = 2 \quad 2q_{12} = 2 \\
2q_{12} + q_{22} = -1 \quad 2q_{23} = 0 \\
q_{33} = 5
\]
Convexity

The sets of PSD and SOS polynomials are *convex cones*; i.e.,

\[ f, g \text{ PSD} \implies \lambda f + \mu g \text{ is PSD for all } \lambda, \mu \geq 0 \]

let \( P_{n,d} \) be the set of PSD polynomials of degree \( \leq d \)
let \( \Sigma_{n,d} \) be the set of SOS polynomials of degree \( \leq d \)

- Both \( P_{n,d} \) and \( \Sigma_{n,d} \) are *convex cones* in \( \mathbb{R}^N \) where \( N = \binom{n+d}{d} \)
- We know \( \Sigma_{n,d} \subseteq P_{n,d} \), and testing if \( f \in P_{n,d} \) is NP-hard
- But testing if \( f \in \Sigma_{n,d} \) is an SDP
Polynomials in One Variable

If $f \in \mathbb{R}[x]$, then $f$ is SOS if and only if $f$ is PSD

Example

All real roots must have even multiplicity, and highest coeff. is positive

\[
f = x^6 - 10x^5 + 51x^4 - 166x^3 + 342x^2 - 400x + 200
\]

\[
= (x - 2)^2(x - (2 + i))(x - (2 - i))(x - (1 + 3i))(x - (1 - 3i))
\]

Now reorder complex conjugate roots

\[
= (x - 2)^2(x - (2 + i))(x - (1 + 3i))(x - (2 - i))(x - (1 - 3i))
\]

\[
= (x - 2)^2((x^2 - 3x - 1) - i(4x - 7))((x^2 - 3x - 1) + i(4x - 7))
\]

\[
= (x - 2)^2((x^2 - 3x - 1)^2 + (4x - 7)^2)
\]

So every PSD scalar polynomial is the sum of two squares
**Quadratic Polynomials**

A quadratic polynomial in \( n \) variables is PSD if and only if it is SOS

Because it is PSD if and only if

\[
f = x^T Q x
\]

where \( Q \geq 0 \)

And it is SOS if and only if

\[
f = \sum_i (v_i^T x)^2 = x^T \left( \sum_i v_i v_i^T \right) x
\]
Some Background

In 1888, Hilbert showed that PSD=SOS if and only if

- $d = 2$, i.e., quadratic polynomials
- $n = 1$, i.e., univariate polynomials
- $d = 4$, $n = 2$, i.e., quartic polynomials in two variables

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- In general $f$ is PSD does not imply $f$ is SOS
Some Background

- Connections with Hilbert’s 17th problem, solved by Artin: every PSD polynomial is a SOS of *rational functions*.

- If $f$ is not SOS, then can try with $gf$, for some $g$.
  - For fixed $f$, can optimize over $g$ too
  - Otherwise, can use a “universal” construction of Pólya-Reznick.

More about this later.
The Motzkin Polynomial

A positive semidefinite polynomial, that is not a sum of squares.

\[ M(x, y) = x^2 y^4 + x^4 y^2 + 1 - 3x^2 y^2 \]

- Nonnegativity follows from the arithmetic-geometric inequality applied to \( (x^2 y^4, x^4 y^2, 1) \)
- Introduce a nonnegative factor \( x^2 + y^2 + 1 \)
- Solving the SDPs we obtain the decomposition:

\[
(x^2 + y^2 + 1) M(x, y) = (x^2 y - y)^2 + (xy^2 - x)^2 + (x^2 y^2 - 1)^2 + \\
+ \frac{1}{4}(xy^3 - x^3 y)^2 + \frac{3}{4}(xy^3 + x^3 y - 2xy)^2
\]
The Univariate Case

\[ f(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots + a_{2d} x^{2d} \]

\[
= \begin{bmatrix} 1 \\ x \\ \vdots \\ x^d \end{bmatrix}^T \begin{bmatrix} q_{00} & q_{01} & \cdots & q_{0d} \\ q_{01} & q_{11} & \cdots & q_{1d} \\ \vdots & \vdots & \ddots & \vdots \\ q_{0d} & q_{1d} & \cdots & q_{dd} \end{bmatrix} \begin{bmatrix} 1 \\ x \\ \vdots \\ x^d \end{bmatrix}
\]

\[ = \sum_{i=0}^{d} \left( \sum_{j+k=i} q_{jk} \right) x^i \]

- In the univariate case, the SOS condition is exactly equivalent to nonnegativity.
- The matrices \( A_i \) in the SDP have a Hankel structure. We will see how this can be exploited for efficient computation.
Necessary Conditions

Suppose $f = c_d x^d + c_{d-1} x^{d-1} + \cdots + c_1 x + c_0$; then

$$f \text{ is PSD} \quad \iff \quad d \text{ is even, } c_d > 0 \text{ and } c_0 \geq 0$$

What is the analogue in $n$ variables?
The Newton Polytope

Suppose

\[ f = \sum_{\alpha \in M} c_{\alpha} x^{\alpha} \]

The set of monomials \( M \subset \mathbb{N}^n \) is called the frame of \( f \)

The Newton polytope of \( f \) is its convex hull

\[ \text{new}(f) = \text{co}(\text{frame}(f)) \]

The example shows

\[ f = 7x^4y + x^3y + x^2y^4 + x^2 + 3x \]
Necessary Conditions for Nonnegativity

If \( f \in \mathbb{R}[x_1, \ldots, x_n] \) is PSD, then every vertex of \( \text{new}(f) \) has even coordinates, and a positive coefficient

- \( f = 7x^4y + x^3y + x^2y^4 + x^2 + 3xy \)
  is not PSD, since term \( 3xy \) has coords \((1, 1)\)

- \( f = 7x^4y + x^3y - x^2y^4 + x^2 + 3y^2 \)
  is not PSD, since term \( -x^2y^4 \) has a negative coefficient
Properties of Newton Polytopes

- Products: \( \text{new}(fg) = \text{new}(f) + \text{new}(g) \)

- Consequently \( \text{new}(f^n) = n \text{new}(f) \)

- If \( f \) and \( g \) are PSD polynomials then

\[
f(x) \leq g(x) \text{ for all } x \in \mathbb{R}^n \implies \text{new}(f) \subseteq \text{new}(g)
\]

- This tells us which monomials we have in an SOS decomposition

\[
f = \sum_{i=1}^{t} g_i^2 \implies \text{new}(g_i) \subseteq \frac{1}{2} \text{new}(f)
\]
Example of Sparse SOS Decomposition

Find an SOS representation for

\[ f = 4x^4y^6 + x^2 - xy^2 + y^2 \]

The squares in an SOS decomposition can only contain the monomials

\[ \text{new} \left( \frac{1}{2} f \right) \cap \mathbb{N}^n = \{ x^2y^3, xy^2, xy, x, y \} \]

Without using sparsity, we would include all 21 monomials of degree < 5 in the SDP

With sparsity, we only need 5 monomials
About SOS/SDP

- The resulting SDP problem is polynomially sized (in $n$, for fixed $d$).

- By properly choosing the monomials, we can exploit structure (sparsity, symmetries, ideal structure).

- An important feature: the problem is still a SDP if the coefficients of $F$ are variable, and the dependence is affine.

- Can optimize over SOS polynomials in affinely described families.
  For instance, if we have $p(x) = p_0(x) + \alpha p_1(x) + \beta p_2(x)$, we can “easily” find values of $\alpha, \beta$ for which $p(x)$ is SOS.

This fact will be crucial in everything that follows...
Global Optimization

Consider the problem

\[
\min_{x,y} f(x, y)
\]

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.
- Find the largest \( \gamma \) s.t. \( f(x, y) - \gamma \) is SOS
- A semidefinite program (convex!).
- If exact, can recover optimal solution.
- \textbf{Surprisingly} effective.

Solving, the maximum \( \gamma \) is -1.0316. Exact value.
Why Does This Work?

Three *independent* facts, theoretical and experimental:

- The existence of efficient algorithms for SDP.
- The size of the SDPs grows much slower than the Bézout number $\mu$.
  - A bound on the number of (complex) critical points.
  - A reasonable estimate of complexity.
  - The bad news: $\mu = (2d - 1)^n$ (for dense polynomials).
  - Almost all (exact) algebraic techniques scale as $\mu$.
- The lower bound $f^{SOS}$ very often coincides with $f^*$. (Why? what does *often* mean?)

SOS provides *short proofs*, even though they’re not guaranteed to exist.
Coefficient Space

Let \( f_{\alpha \beta}(x) = x^4 + (\alpha + 3\beta)x^3 + 2\beta x^2 - \alpha x + 1 \).

What is the set of values of \((\alpha, \beta) \in \mathbb{R}^2\) for which \( f_{\alpha \beta} \) is PSD? SOS?

To find a SOS decomposition:

\[
f_{\alpha, \beta}(x) = 1 - \alpha x + 2\beta x^2 + (\alpha + 3\beta)x^3 + x^4
= \begin{bmatrix} 1 \\ x \\ x^2 \end{bmatrix}^T \begin{bmatrix} q_{11} & q_{12} & q_{13} \\ q_{12} & q_{22} & q_{23} \\ q_{13} & q_{23} & q_{33} \end{bmatrix} \begin{bmatrix} 1 \\ x \\ x^2 \end{bmatrix}
= q_{11} + 2q_{12}x + (q_{22} + 2q_{13})x^2 + 2q_{23}x^3 + q_{33}x^4
\]

The matrix \( Q \) should be PSD and satisfy the affine constraints.
The feasible set is given by:

\[
\begin{align*}
\left\{ (\alpha, \beta) \mid \exists \lambda \text{ s.t.} \begin{bmatrix} 1 & -\frac{1}{2} \alpha & \beta - \lambda \\ -\frac{1}{2} \alpha & 2\lambda & \frac{1}{2} (\alpha + 3\beta) \\ \beta - \lambda & \frac{1}{2} (\alpha + 3\beta) & 1 \end{bmatrix} \succeq 0 \right\}
\end{align*}
\]
What is the set of values of \((\alpha, \beta) \in \mathbb{R}^2\) for which \(f_{\alpha \beta}\) PSD? SOS? Recall: in the univariate case PSD=SOS, so here the sets are the same.

- Convex and semialgebraic.
- It is the projection of a spectrahedron in \(\mathbb{R}^3\).
- We can easily test membership, or even optimize over it!

Defined by the curve: 
\[
288\beta^5 - 36\alpha^2 \beta^4 + 1164\alpha \beta^4 + 1931\beta^4 - 132\alpha^3 \beta^3 + 1036\alpha^2 \beta^3 + 1956\alpha \beta^3 - 2592\beta^3 - 112\alpha^4 \beta^2 + 432\alpha^3 \beta^2 + 1192\alpha^2 \beta^2 - 1728\alpha \beta^2 + 512\beta^2 - 36\alpha^5 \beta + 72\alpha^4 \beta + 360\alpha^3 \beta - 576\alpha^2 \beta - 576\alpha \beta - 4\alpha^6 + 60\alpha^4 - 192\alpha^2 - 256 = 0
\]
Lyapunov Stability Analysis

To prove asymptotic stability of $\dot{x} = f(x)$,

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

- For linear systems $\dot{x} = Ax$, quadratic Lyapunov functions $V(x) = x^T P x$
  $$P > 0, \quad A^T P + PA < 0.$$
- With an affine family of candidate polynomial $V$, $\dot{V}$ is also affine.
- Instead of checking nonnegativity, use a SOS condition.
- Therefore, for polynomial vector fields and Lyapunov functions, we can check the conditions using the theory described before.
Lyapunov Example

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

\[
\begin{align*}
\dot{x} &= -y - \frac{3}{2}x^2 - \frac{1}{2}x^3 \\
y &= 3x - y
\end{align*}
\]

Try a generic 4th order polynomial Lyapunov function.

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

Find a \(V(x, y)\) that satisfies the conditions:

- \(V(x, y)\) is SOS.
- \(-\dot{V}(x, y)\) is SOS.

Both conditions are affine in the \(c_{j,k}\). Can do this directly using SOS/SDP!
Lyapunov Example

After solving the SDPs, we obtain a Lyapunov function.

\[ V = 4.5819x^2 - 1.5786xy + 1.7834y^2 - 0.12739x^3 + 2.5189x^2y - 0.34069xy^2 \\
+ 0.61188y^3 + 0.47537x^4 - 0.052424x^3y + 0.44289x^2y^2 + 0.0000018868xy^3 + 0.090723y^4 \]
Lyapunov Example

(M. Krstić) Find a Lyapunov function for

\[
\begin{align*}
\dot{x} &= -x + (1 + x) y \\
\dot{y} &= -(1 + x) x.
\end{align*}
\]

we easily find a quartic polynomial

\[
V(x, y) = 6x^2 - 2xy + 8y^2 - 2y^3 + 3x^4 + 6x^2y^2 + 3y^4.
\]

Both \(V(x, y)\) and \((-\dot{V}(x, y))\) are SOS:

\[
V(x, y) = \begin{bmatrix} x \\ y \\ x^2 \\ xy \\ y^2 \end{bmatrix}^T \begin{bmatrix} 6 & -1 & 0 & 0 & 0 \\ -1 & 8 & 0 & 0 & -1 \\ 0 & 0 & 3 & 0 & 0 \\ 0 & 0 & 0 & 6 & 0 \\ 0 & -1 & 0 & 0 & 3 \end{bmatrix} \begin{bmatrix} x \\ y \\ x^2 \\ xy \\ y^2 \end{bmatrix}, \quad -\dot{V}(x, y) = \begin{bmatrix} x \\ y \\ x^2 \\ xy \\ y^2 \end{bmatrix}^T \begin{bmatrix} 10 & 1 & -1 & 1 \\ 1 & 2 & 1 & -2 \\ -1 & 1 & 12 & 0 \\ 1 & -2 & 0 & 6 \end{bmatrix} \begin{bmatrix} x \\ y \\ x^2 \\ xy \end{bmatrix}
\]

The matrices are positive definite, so this proves asymptotic stability.
Extensions

- Other linear differential inequalities (e.g. Hamilton-Jacobi).

- Many possible variations: nonlinear $H_\infty$ analysis, parameter dependent Lyapunov functions, etc.

- Can also do local results (for instance, on compact domains).

- Polynomial and rational vector fields, or functions with an underlying algebraic structure.

- Natural extension of the LMIs for the linear case.

- Only for analysis. Proper synthesis is trickier…
**Nonlinear Control Synthesis**

Recently, Rantzer provided an alternative stability criterion, in some sense “dual” to the standard Lyapunov one.

\[ \nabla \cdot (\rho f) > 0 \]

- The *synthesis* problem is now **convex** in \((\rho, u\rho)\).

\[ \nabla \cdot [\rho(f + gu)] > 0 \]

- Parametrizing \((\rho, u\rho)\), can apply SOS methods.

**Example:**

\[
\begin{align*}
\dot{x} &= y - x^3 + x^2 \\
\dot{y} &= u
\end{align*}
\]

A stabilizing controller is:

\[ u(x, y) = -1.22x - 0.57y - 0.129y^3 \]