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

$$\big(f(x,y) \geq 0\big) \wedge \big(g(x,y) = 0\big) \vee \big(h(x,y) \neq 0\big)$$

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

  $f(x) \geq 0$ 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

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

- Answer *yes* is easy to verify; exhibit x such that $f(x) < 0$
- Answer *no* is hard; we need a *certificate* or a *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

$$\begin{aligned} f &= 4x^4 + 4x^3y - 7x^2y^2 - 2xy^3 + 10y^4 \\ &= \begin{bmatrix} x^2 \\ xy \\ y^2 \end{bmatrix}^T \begin{bmatrix} 4 & 2 & -\lambda \\ 2 & -7+2\lambda & -1 \\ -\lambda & -1 & 10 \end{bmatrix} \begin{bmatrix} x^2 \\ xy \\ y^2 \end{bmatrix} \\ &= z^T Q(\lambda) z \end{aligned}$$

which holds for all $\lambda \in \mathbb{R}$

If for some λ 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

$$\begin{aligned} f &= \begin{bmatrix} x^2 \\ xy \\ y^2 \end{bmatrix}^T \begin{bmatrix} 0 & 2 \\ 2 & 1 \\ 1 & -3 \end{bmatrix} \begin{bmatrix} 0 & 2 & 1 \\ 2 & 1 & -3 \end{bmatrix} \begin{bmatrix} x^2 \\ xy \\ y^2 \end{bmatrix} \\ &= \left\| \begin{bmatrix} 2xy + y^2 \\ 2x^2 + xy - 3y^2 \end{bmatrix} \right\|^2 \\ &= \left(2xy + y^2\right)^2 + \left(2x^2 + xy - 3y^2\right)^2 \end{aligned}$$

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

$$\boxed{\begin{aligned} Q &\succeq 0 \\ f &= z^T Q z \end{aligned}}$$

- 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 $V = \begin{bmatrix} v_1 & \dots & v_r \end{bmatrix}$, so that

$$\begin{aligned} f &= z^T V V^T z \\ &= \|V^T z\|^2 \\ &= \sum_{i=1}^{r} (v_i^T z)^2 \end{aligned}$$

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

Example

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

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

$$
Q \succeq 0 \qquad
\begin{aligned}
q_{11} &= 2 & 2q_{12} &= 2 \\
2q_{12} + q_{22} &= -1 & 2q_{23} &= 0 \\
q_{33} &= 5
\end{aligned}
$$

Convexity

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

$$f, g \text{ PSD} \qquad \Longrightarrow \qquad \lambda f + \mu g \text{ is PSD for all } \lambda, \mu \geq 0$$

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

$$\begin{aligned} f &= x^6 - 10x^5 + 51x^4 - 166x^3 + 342x^2 - 400x + 200 \\ &= (x-2)^2\big(x-(2+i)\big)\big(x-(2-i)\big)\big(x-(1+3i)\big)\big(x-(1-3i)\big) \end{aligned}$$

Now reorder complex conjugate roots

$$\begin{aligned} &= (x-2)^2\big(x-(2+i)\big)\big(x-(1+3i)\big)\big(x-(2-i)\big)\big(x-(1-3i)\big) \\ &= (x-2)^2\big((x^2-3x-1)-i(4x-7)\big)\big((x^2-3x-1)+i(4x-7)\big) \\ &= (x-2)^2\big((x^2-3x-1)^2+(4x-7)^2\big) \end{aligned}$$

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

$$\begin{aligned} f &= \sum_i (v_i^T x)^2 \\ &= x^T \Big(\sum_i v_i v_i^T \Big) x \end{aligned}$$

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

$n \backslash d$	2	4	6	8
1	yes	yes	yes	yes
2	yes	*yes*	no	no
3	yes	no	no	no
4	yes	no	no	no

- 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*.

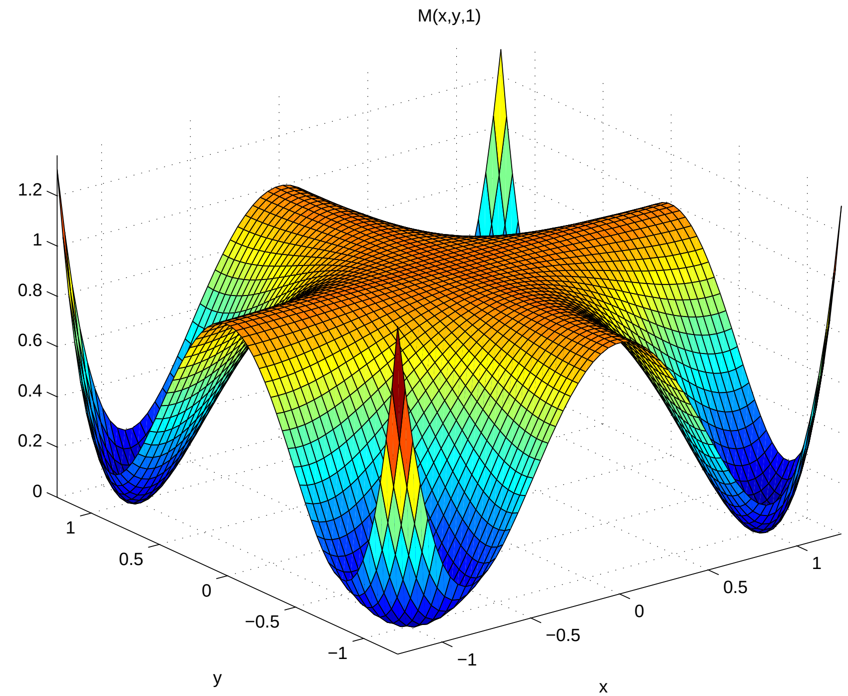
- If f is not SOS, then can try with gf, for some g.
  - For fixed f, can optimize over g too
  - Otherwise, can use a "universal" construction of Pólya-Reznick.

More about this later.

The Motzkin Polynomial

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

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



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

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

The Univariate Case

$$\begin{aligned}
f(x) &= a_0 + a_1 x + a_2 x^2 + a_3 x^3 + \cdots + a_{2d} x^{2d} \\
&= \begin{bmatrix} 1 \\ x \\ \vdots \\ x^d \end{bmatrix}^T \begin{bmatrix} q_{00} & q_{01} & \cdots & q_{0d} \\ q_{01} & q_{11} & \cdots & q_{1d} \\ \vdots & \vdots & \ddots & \vdots \\ q_{0d} & q_{1d} & \cdots & q_{dd} \end{bmatrix} \begin{bmatrix} 1 \\ x \\ \vdots \\ x^d \end{bmatrix} \\
&= \sum_{i=0}^{d} \Big(\sum_{j+k=i} q_{jk} \Big) x^i
\end{aligned}$$

- 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

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

What is the analogue in n variables?

The Newton Polytope

Suppose

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

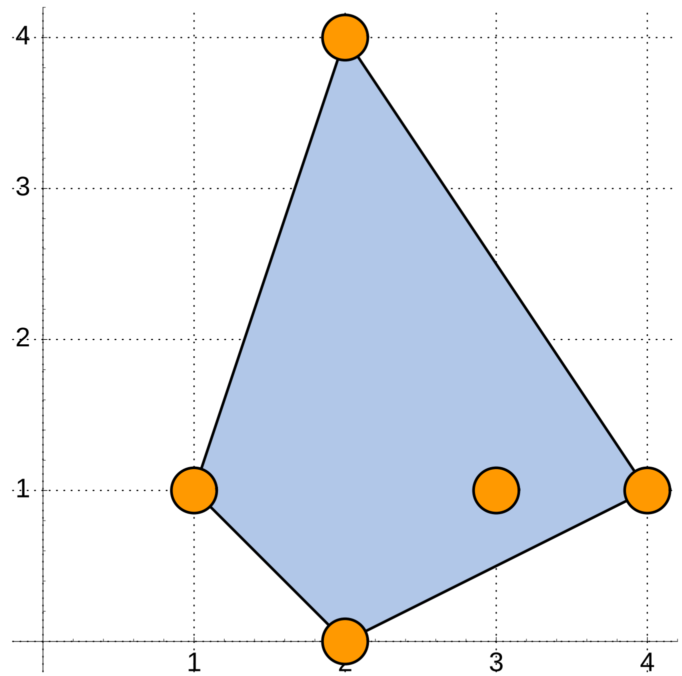
The set of monomials $M \subset \mathbb{N}^n$ is called the *frame* of f

The *Newton polytope* of f is its convex hull

$$\mathbf{new}(f) = \mathbf{co}\big(\mathbf{frame}(f)\big)$$

The example shows

$$f = 7\,x^4\,y + x^3\,y + x^2\,y^4 + x^2 + 3\,x\,y$$



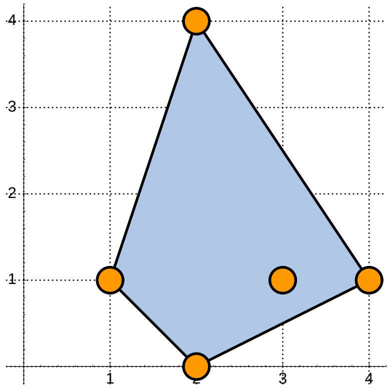
Necessary Conditions for Nonnegativity

If $f \in \mathbb{R}[x_1, \ldots, x_n]$ is PSD, then

every vertex of $\mathbf{new}(f)$ has even coordinates, and a positive coefficient

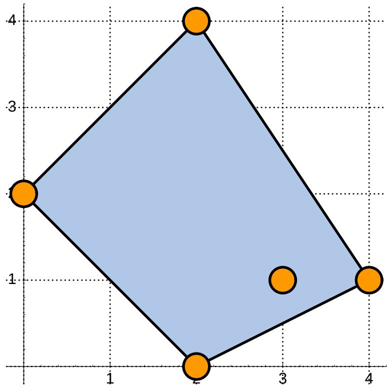
- $f = 7\,x^4\,y + x^3\,y + x^2\,y^4 + x^2 + 3\,x\,y$

  is not PSD, since term $3xy$ has coords $(1, 1)$



- $f = 7\,x^4\,y + x^3\,y - x^2\,y^4 + x^2 + 3\,y^2$

  is not PSD, since term $-x^2\,y^4$ has a negative coefficient



Properties of Newton Polytopes

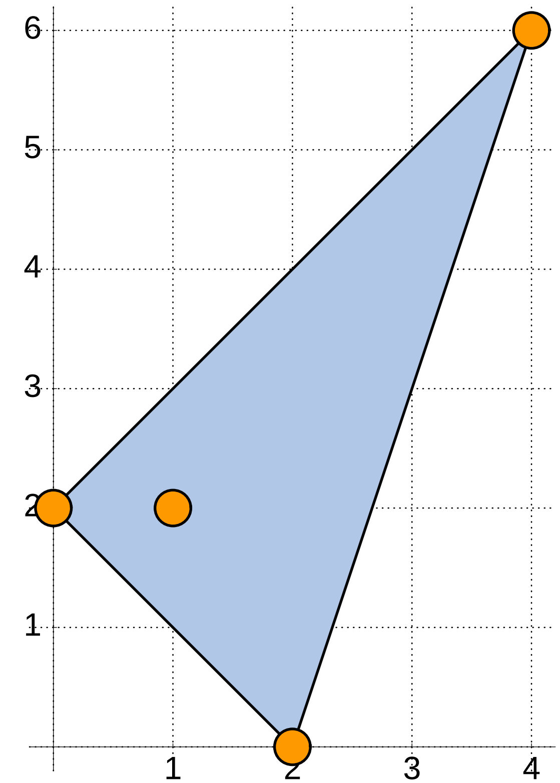
- Products: $\mathbf{new}(fg) = \mathbf{new}(f) + \mathbf{new}(g)$
- Consequently $\mathbf{new}(f^n) = n\,\mathbf{new}(f)$
- If f and g are PSD polynomials then

$$f(x) \leq g(x) \text{ for all } x \in \mathbb{R}^n \qquad \Longrightarrow \qquad \mathbf{new}(f) \subseteq \mathbf{new}(g)$$

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

$$f = \sum_{i=1}^{t} g_i^2 \qquad \Longrightarrow \qquad \mathbf{new}(g_i) \subseteq \frac{1}{2}\mathbf{new}(f)$$

Example of Sparse SOS Decomposition

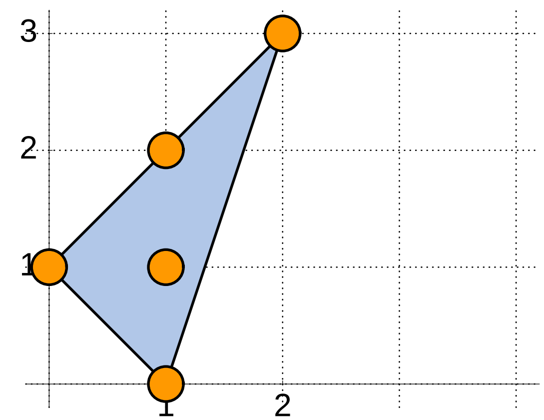


Find an SOS representation for

$$f = 4\,x^4\,y^6 + x^2 - x\,y^2 + y^2$$

The squares in an SOS decomposition can only contain the monomials

$$\mathbf{new}(\frac{1}{2}f) \cap \mathbb{N}^n = \{x^2y^3, xy^2, xy, x, y\}$$



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 α, β for which $p(x)$ is SOS.

This fact will be *crucial* in everything that follows...

Global Optimization

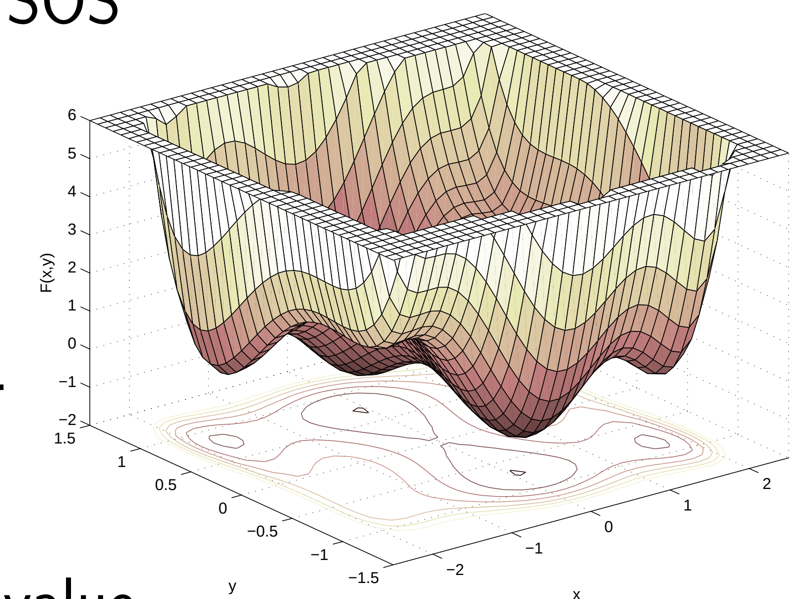
Consider the problem

$$\min_{x,y} f(x,y)$$

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 γ s.t. $f(x,y) - \gamma$ is SOS
- Essentially due to Shor (1987).
- A semidefinite program (convex!).
- If exact, can recover optimal solution.
- *Surprisingly* effective.



Solving, the maximum γ 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 μ.
  - 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 μ.
- 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?

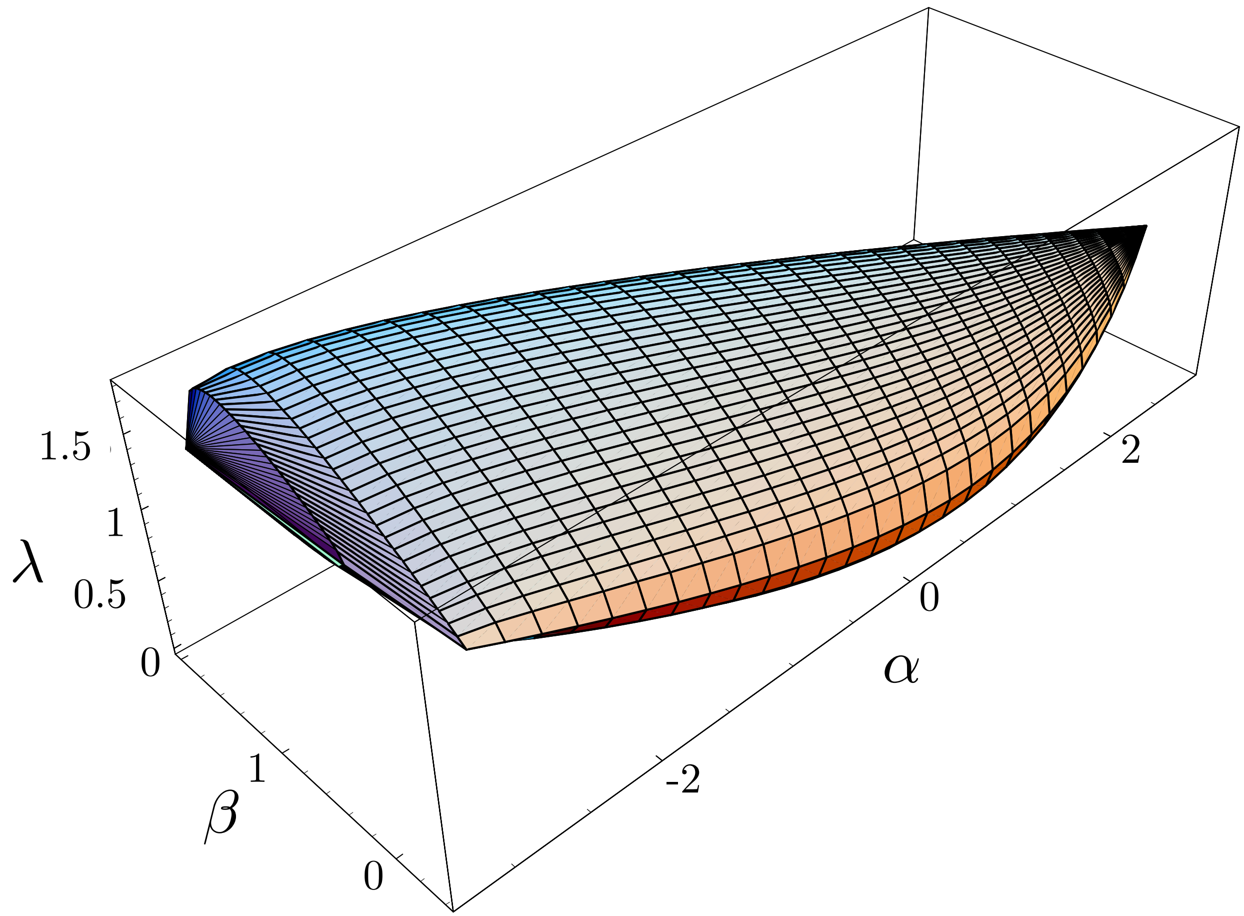
To find a SOS decomposition:

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

The matrix Q should be PSD and satisfy the affine constraints.

The feasible set is given by:

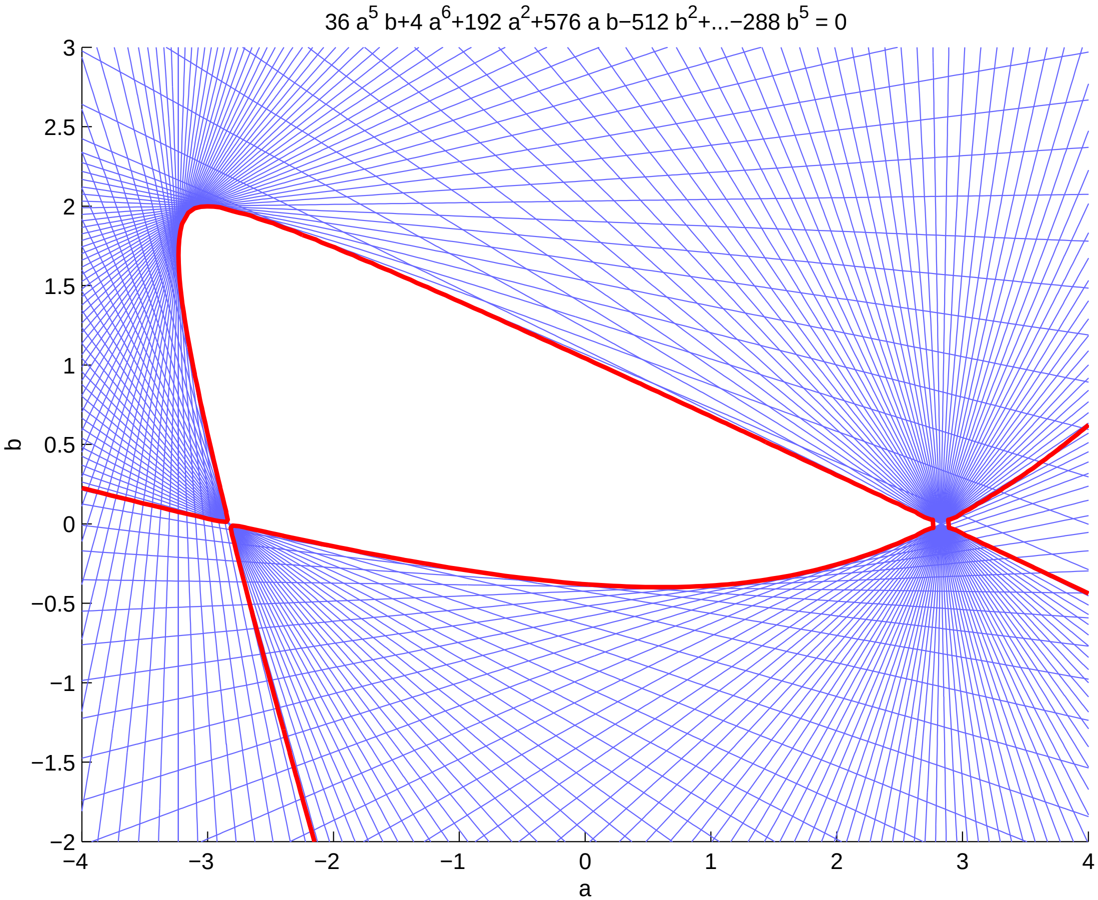
$$\left\{ (\alpha, \beta) \quad \middle| \quad \exists \lambda \text{ s.t. } \begin{bmatrix} 1 & -\frac{1}{2}\alpha & \beta - \lambda \\ -\frac{1}{2}\alpha & 2\lambda & \frac{1}{2}(\alpha + 3\beta) \\ \beta - \lambda & \frac{1}{2}(\alpha + 3\beta) & 1 \end{bmatrix} \succeq 0 \right\}$$



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!



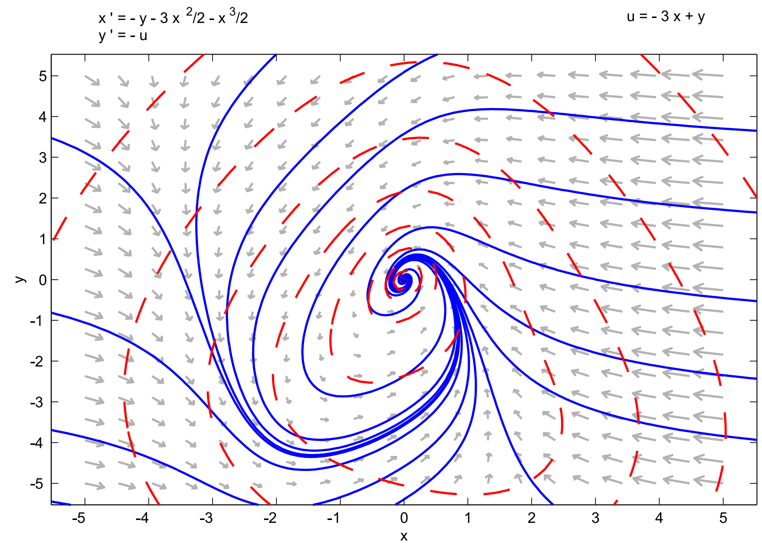
Defined by the curve: $288\beta^5 - 36\alpha^2\beta^4 + 1164\alpha\beta^4 + 1931\beta^4 - 132\alpha^3\beta^3 + 1036\alpha^2\beta^3 + 1956\alpha\beta^3 - 2592\beta^3 - 112\alpha^4\beta^2 + 432\alpha^3\beta^2 + 1192\alpha^2\beta^2 - 1728\alpha\beta^2 + 512\beta^2 - 36\alpha^5\beta + 72\alpha^4\beta + 360\alpha^3\beta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

Lyapunov Stability Analysis

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

$$V(x) > 0 \quad x \neq 0$$

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



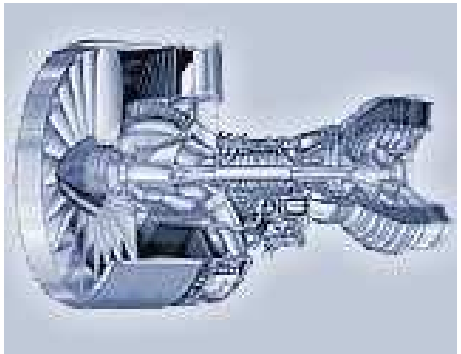
- For linear systems $\dot{x} = Ax$, quadratic Lyapunov functions $V(x) = x^T P x$

$$P > 0, \qquad A^T P + PA < 0.$$

- 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:



$$\dot{x} = -y - \frac{3}{2}x^2 - \frac{1}{2}x^3$$
$$\dot{y} = 3x - y$$

Try a generic 4th order polynomial Lyapunov function.

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

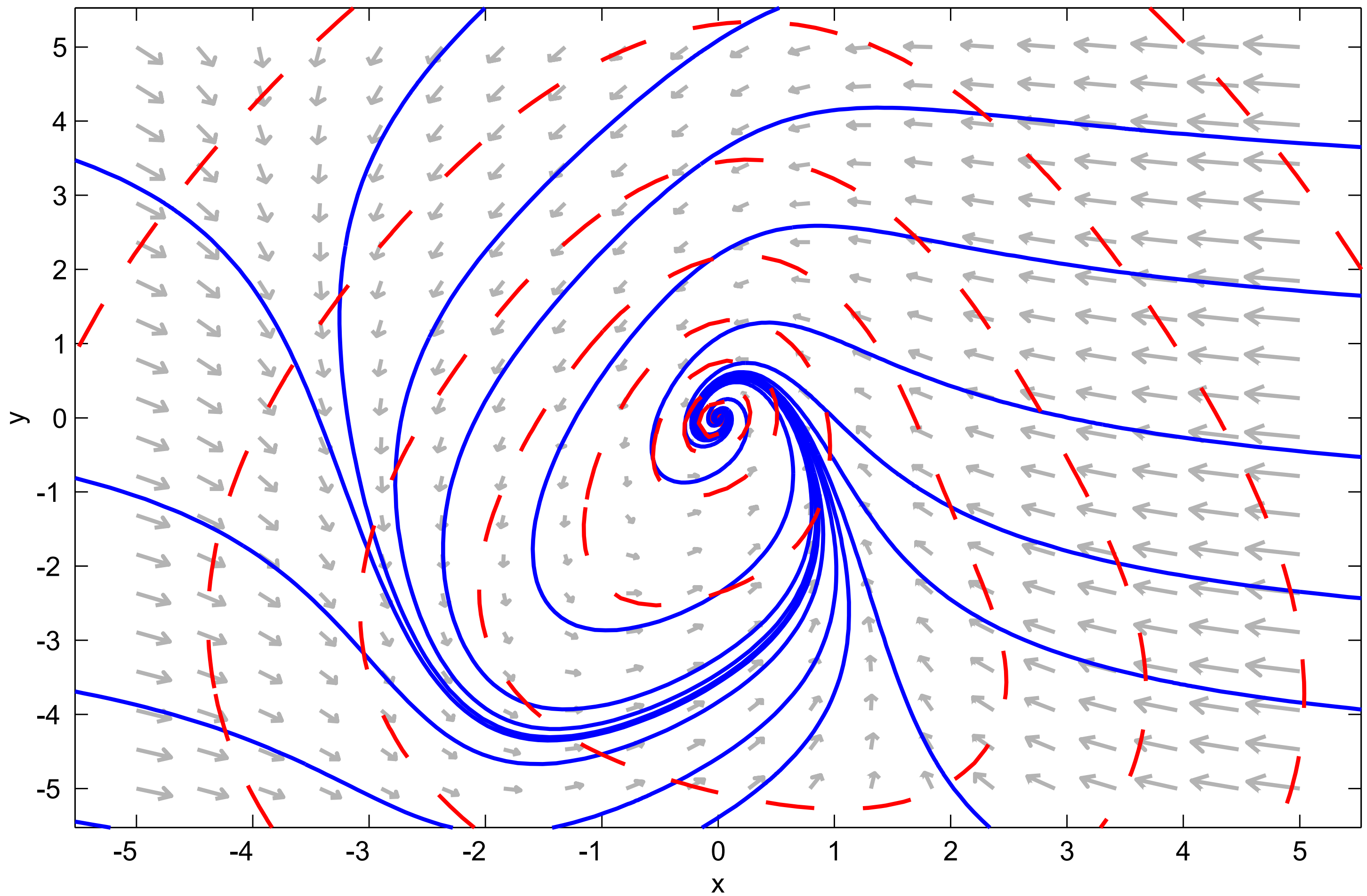
Find a $V(x, y)$ that satisfies the conditions:

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

Both conditions are affine in the c_{jk}. 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

$$\dot{x} = -x + (1+x)\,y$$
$$\dot{y} = -(1+x)\,x.$$

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:

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

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

Extensions

- Other linear differential inequalities (e.g. Hamilton-Jacobi).
- Many possible variations: nonlinear $\mathcal{H}_\infty$ 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:

$$\dot{x} = y - x^3 + x^2$$
$$\dot{y} = u$$

A stabilizing controller is:

$$u(x, y) = -1.22x - 0.57y - 0.129y^3$$