Sum of Squares Optimization and Its Applications

Amir Ali Ahmadi
Princeton University
Dept. of Operations Research and Financial Engineering (ORFE)

ORF 523

Optimization over nonnegative polynomials

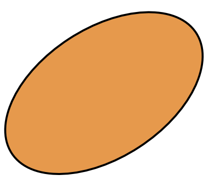
Definition by example: How to pick c_1, c_2, c_3 so to make

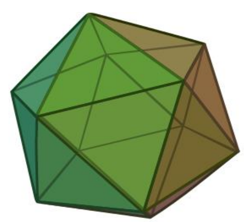
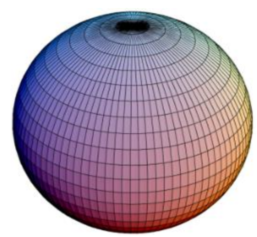
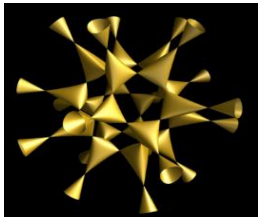
$$p(x_1,x_2) = c_1 x_1^4 - 6x_1^3 x_2 - 4x_1^3 + c_2 x_1^2 x_2^2 + 10x_1^2 + 12x_1 x_2^2 + c_3 x_2^4$$

nonnegative over a given basic semialgebraic set?

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

Ex: $x_1^3 - 2x_1 x_2^4 \geq 0$
$x_1^4 + 3x_1 x_2 - x_2^6 \geq 0$



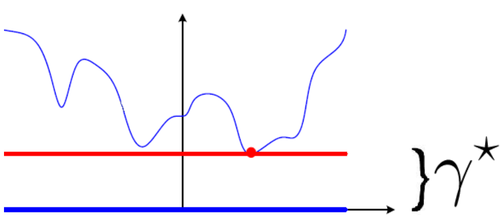
-This problem is fundamental to many areas of applied/computational mathematics.
-It is the problem that "SOS optimization" is designed to solve.

Why would you want to do this?!

- Let's start with five application domains…

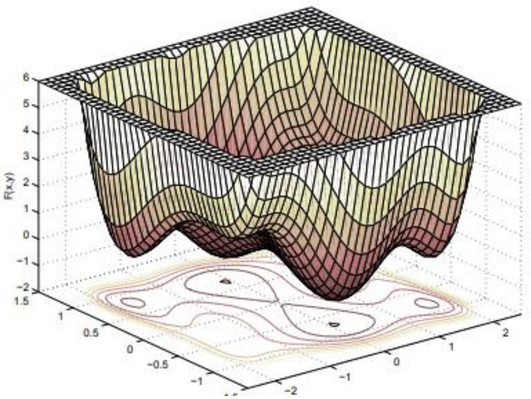
1. Polynomial optimization

$$\left[\begin{array}{ll} \min\limits_{x \in \mathbb{R}^n} & p(x) \\ \text{s.t.} & g_i(x) \geq 0 \\ & h_j(x) = 0 \end{array}\right] \longleftrightarrow \left[\begin{array}{ll} \max\limits_{\gamma \in \mathbb{R}} & \gamma \\ \text{s.t.} & p(x) - \gamma \geq 0 \quad \forall x \in K \end{array}\right]$$



$p, g_i, h_j : \mathbb{R}^n \to \mathbb{R}$ polynomials

Feasible set $K := \{x \in \mathbb{R}^n \mid g_i(x) \geq 0, h_j(x) = 0\}$



- **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 your favorite 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

$$
\begin{aligned}
\max_{x\in\mathbb{R}^n,\ \gamma\in\mathbb{R}} \quad & \gamma \\
\text{s.t.} \quad & \mu^T x \geq \gamma \quad \text{(return)} \\
& x^T \Sigma x \leq \delta \quad \text{(risk)} \\
& x \geq 0, \ \sum_{i=1}^{n} x_i = 1 \\
& x \in \Omega
\end{aligned}
$$

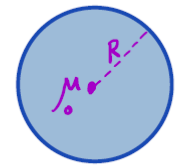
$\mu \in \mathbb{R}^n$: mean vector of the returns

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

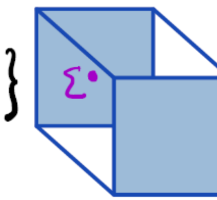
In practice estimated from past data/ML model. Optimal portfolio sensitive to this input.

Accounting for uncertainty:

$$U_\mu = \{ \mu_0 + u \in \mathbb{R}^n \mid \|u\| \leq R \}$$



$$U_\Sigma = \{ \Sigma \in S^{n\times n} \mid \Sigma \succeq 0, \ \Sigma^l_{ij} \leq \Sigma_{ij} \leq \Sigma^u_{ij} \}$$

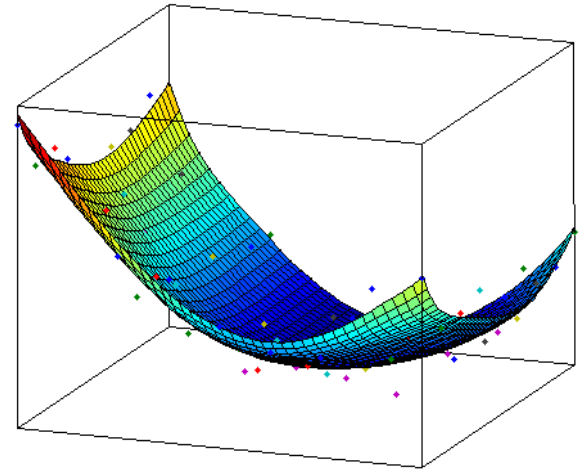


$$
\begin{aligned}
\max_{x\in\mathbb{R}^n,\ \gamma\in\mathbb{R}} \quad & \gamma \\
\text{s.t.} \quad & \mu^T x \geq \gamma \quad \forall \mu \in U_\mu \\
& x^T \Sigma x \leq \delta \quad \forall \Sigma \in U_\Sigma \\
& x \geq 0, \ \sum_{i=1}^{n} x_i = 1 \\
& x \in \Omega
\end{aligned}
$$

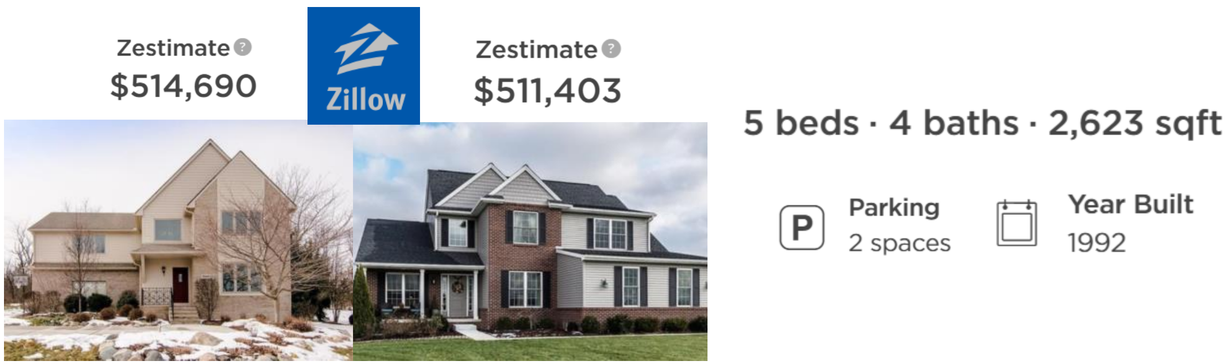
3. Statistics and machine learning

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



Monotonicity of a polynomial $p(x_1, \dots, x_n)$ with respect to feature j: $\dfrac{\partial p(x)}{\partial x_j} \geq 0, \forall x \in B$

Example 2: "ML for fast real-time convex optimization"

$$
\begin{aligned}
g(b) := \min_{x \in \mathbb{R}^n} \; & f_0(x) \\
\text{s.t.} \; & f_i(x) \leq b_i \; i = 1, \dots, m \\
& x \in \Omega
\end{aligned}
$$

$f_0, \dots, f_m$ convex functions, Ω a convex set.

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

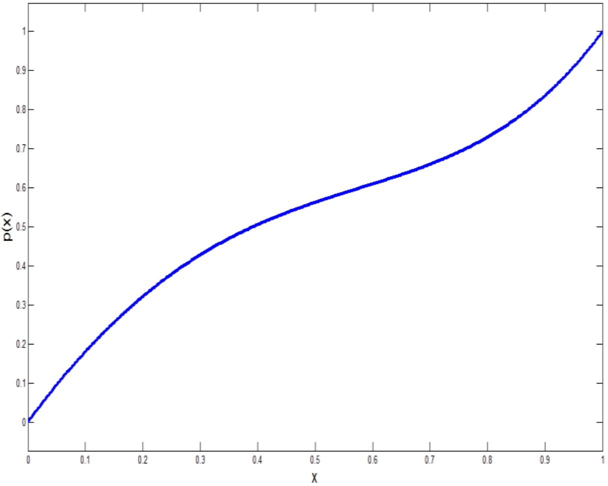
$g: \mathbb{R}^m \to \mathbb{R}$ is
- convex
- nonincreasing w.r.t. all arguments

$y^T \nabla^2 g(b) y \geq 0, \forall b, \forall y$ $\quad \dfrac{\partial g(b)}{\partial b_j} \leq 0, \forall b, \forall j$

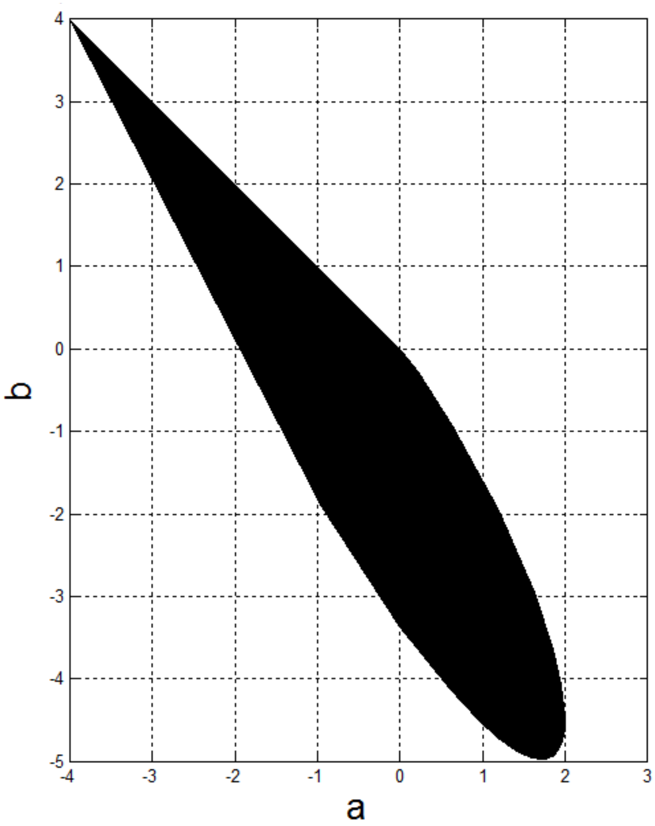
Imposing monotonicity

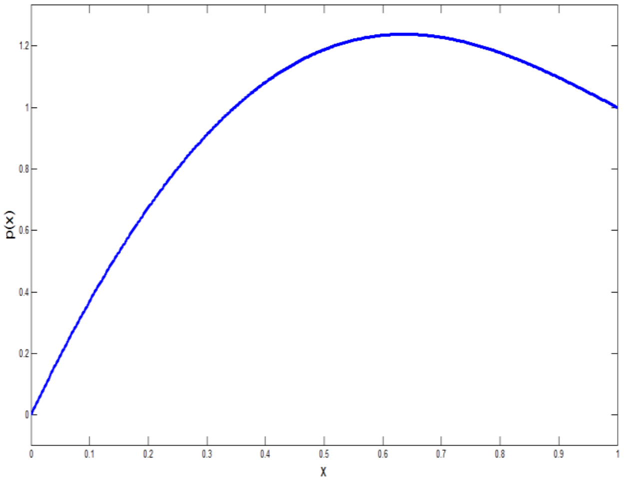
- For what values of a, b is the following polynomial monotone over $[0,1]$?

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



$a = 0, b = -2$

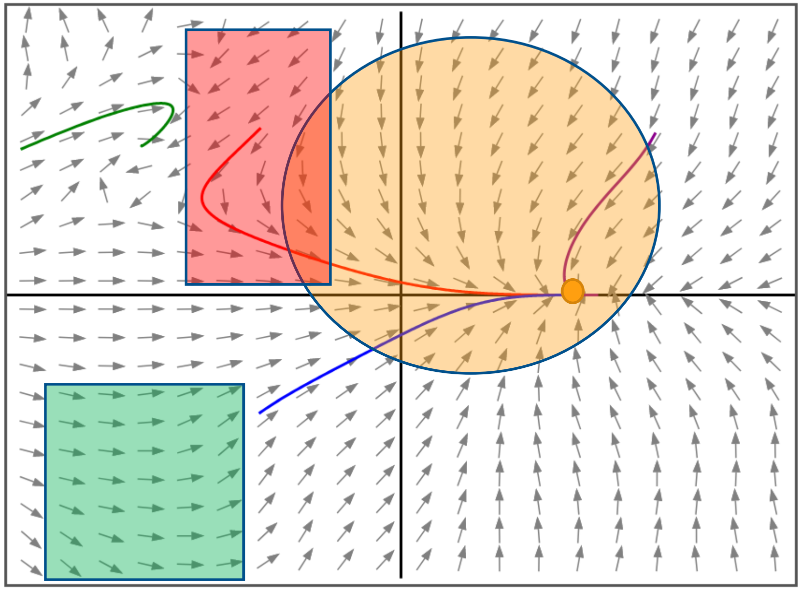




$a = -1, b = -3$

4. Certifying properties of dynamical systems

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



Questions about properties of dynamical systems (e.g., stability, safety)

Lyapunov theory →

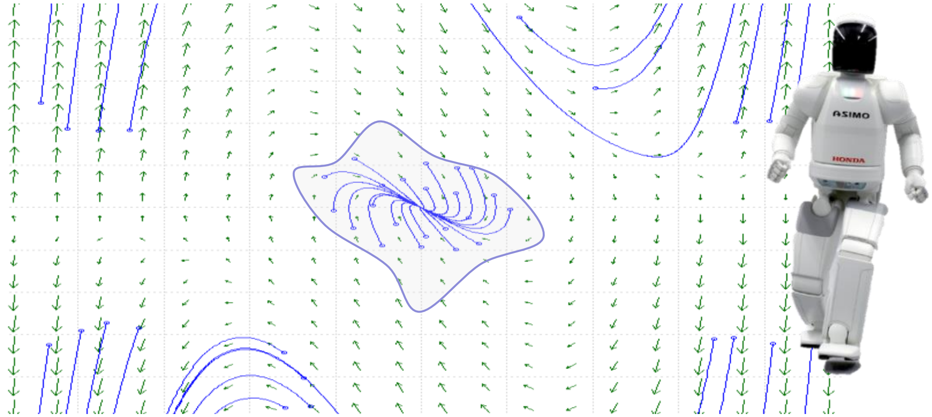
Search for functions satisfying nonnegativity constraints

Semialgebraic parametrization →

Polynomial inequalities

Example: certifying stability

$$\dot{x} = f(x) \quad f : \mathbb{R}^n \to \mathbb{R}^n$$

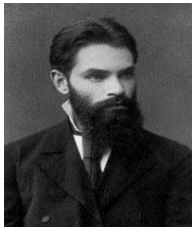


Ex. $\dot{x}_1 = -x_2 + \frac{3}{2}x_1^2 - \frac{1}{2}x_1^3 x_2$

$\dot{x}_2 = 3x_1 - x_1 x_2$

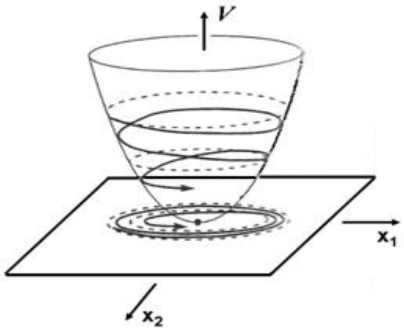
Locally asymptotic stability (LAS) of equilibrium points

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

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

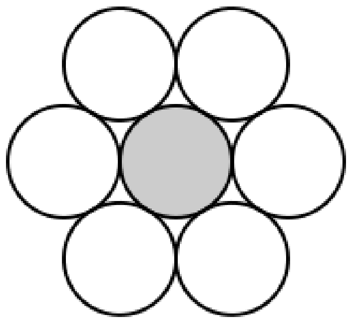


(If $\dot{V}(x) < 0$ everywhere, then globally stable.)

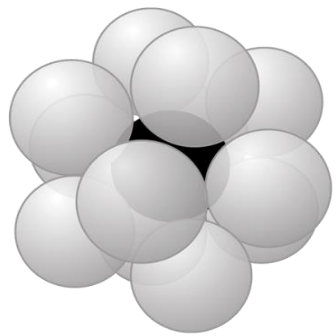
5. Automated theorem proving in geometry

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

$k_2 = 6$



$k_3 = ?$



$k_3 \geq 12$

Newton

$k_3 = 12$

Gregory

$k_3 = 13$

Discussion/bet in 1694

Newton proved to be correct in 1953!

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

$$x_i^2 + y_i^2 + z_i^2 = 4, \;\; i = 1, \ldots, 13$$
$$(x_i - x_j)^2 + (y_i - y_j)^2 + (z_i - z_j)^2 \geq 4,$$
$$i, j \in \{1, \ldots, 13\}^2$$

$$\boxed{\left\{\begin{array}{l} g_1(x) \geq 0 \\ \vdots \\ g_{100}(x) \geq 0 \end{array}\right\} \text{ infeasible}} \Leftrightarrow \boxed{\begin{bmatrix} g_1(x) \geq 0 \\ \vdots \\ g_{99}(x) \geq 0 \end{bmatrix} \Rightarrow g_{100}(x) < 0}$$

Outline of the rest of the talk…

- **Global nonnegativity**
  - Sum of squares (SOS) and semidefinite programming
  - Two applications
  - Hilbert's 17^{th} problem
- **Nonnegativity over a region**
  - Positivstellensatze of Stengle and Putinar
  - Three applications
- **Recap and further reading**

How would you prove nonnegativity?

Ex. Decide if the following polynomial is nonnegative:

$$\begin{aligned} p(x) &= x_1^4 - 6x_1^3x_2 + 2x_1^3x_3 + 6x_1^2x_3^2 + 9x_1^2x_2^2 - 6x_1^2x_2x_3 \\ &\quad -14x_1x_2x_3^2 + 4x_1x_3^3 + 5x_3^4 - 7x_2^2x_3^2 + 16x_2^4 \end{aligned}$$

- Not so easy! (In fact, **NP-hard for degree ≥ 4**)
- But what if I told you:

$$\begin{aligned} p(x) &= (x_1^2 - 3x_1x_2 + x_1x_3 + 2x_3^2)^2 + (x_1x_3 - x_2x_3)^2 \\ &\quad +(4x_2^2 - x_3^2)^2. \end{aligned}$$

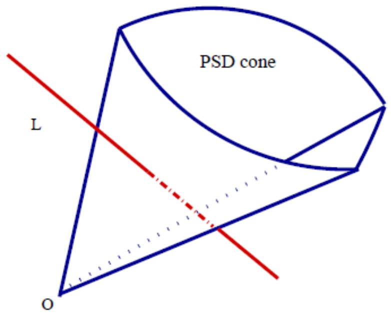
Natural questions:

- **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

[Lasserre], [Nesterov], [Parrilo]

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 $LP \subseteq (\text{Convex})\ QP \subseteq SOCP \subseteq SDP$
- Can be solved to arbitrary accuracy in polynomial time (e.g., using interior point algorithms) **[Nesterov, Nemirovski], [Alizadeh]**

$$\boxed{\begin{aligned} \min_{X \in S^{n\times n}} \quad & Tr(CX) \\ \text{s.t.} \quad & Tr(A_i X) = b_i \quad i=1,\dots,m \\ & X \succeq 0 \ \leftarrow \text{"psd"} \end{aligned}}$$

Data to SDP: $C, A_1, \dots, A_m \in S^{n\times n}, b_1, \dots, b_m \in \mathbb{R}$

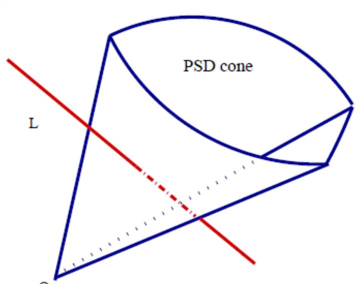
Notes: $Tr(CX) = \sum_{i,j} C_{ij} X_{ij}$

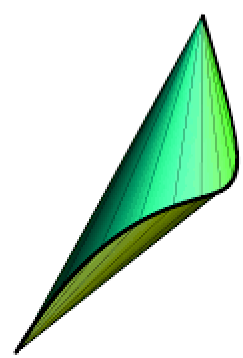
$X \succeq 0: \quad y^T X y \geq 0 \quad \forall y \in \mathbb{R}^n$

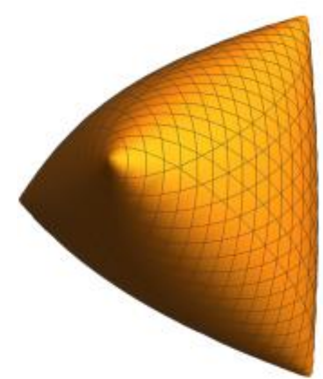
$\Updownarrow$

Eigenvalues of X are ≥ 0.

Feasible set called a "spectrahedron":







SOS→SDP

Thm:

A polynomial p of degree $2d$ is SOS if and only if $\exists Q \succcurlyeq 0$ such that

$$p(x) = z(x)^T Q z(x)$$

where $z = [1, x_1, \dots, x_n, x_1x_2, \dots, x_n^d]^T$ 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: $(\Rightarrow)$ Suppose $\exists Q \succcurlyeq 0$ s.t. $p(x) = z^T(x) Q z(x)$ $\forall x$.

$$Q \succcurlyeq 0 \Rightarrow Q = \underbrace{V^T V}_{V:\ r \times \binom{n+d}{d}} \Rightarrow p(x) = z^T(x) V^T V z(x) = \| V z(x) \|^2 = \sum_{i=1}^{r} (v_i^T z(x))^2.$$

$(\Leftarrow)$ Suppose $p(x)$ is SOS.

$\exists v_1, \dots, v_r \in \mathbb{R}^{\binom{n+d}{d}}$ s.t. $p(x) = \sum_{i=1}^{r} (v_i^T z(x))^2 = \sum_{i=1}^{r} (z^T(x) v_i)(v_i^T z(x)) = z^T(x) \overbrace{\left(\sum_{i=1}^{r} v_i v_i^T \right)}^{:= Q} z(x).$

Example

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

Is p SOS ?

SDP feasibility problem

$$p(x) = \underbrace{\begin{bmatrix} 1 \\ x \\ x^2 \end{bmatrix}^T}_{z^T(x)} \underbrace{\begin{bmatrix} q_{11} & q_{12} & q_{13} \\ q_{12} & q_{22} & q_{23} \\ q_{13} & q_{23} & q_{33} \end{bmatrix}}_{Q} \underbrace{\begin{bmatrix} 1 \\ x \\ x^2 \end{bmatrix}}_{z(x)}$$

$\forall x$

Find $Q \succeq 0$ s.t.

$q_{33} = 10$, $2q_{23} = -2$

$q_{22} + 2q_{13} = -7$

$2q_{12} = 4$, $q_{11} = 4$

SDP solver output:

$$Q = \begin{bmatrix} 4 & 2 & -6 \\ 2 & 5 & -1 \\ -6 & -1 & 10 \end{bmatrix} \overset{\text{e.g. Cholesky}}{=} \underbrace{\begin{bmatrix} 0 & 2 \\ 2 & 1 \\ 1 & -3 \end{bmatrix}}_{V^T} \underbrace{\begin{bmatrix} 0 & 2 & 1 \\ 2 & 1 & -3 \end{bmatrix}}_{V}$$

$$\Rightarrow p(x) = z^T(x) V^T V z(x) = \| V z(x) \|^2 = \left\| \begin{bmatrix} 0 & 2 & 1 \\ 2 & 1 & -3 \end{bmatrix} \begin{bmatrix} 1 \\ x \\ x^2 \end{bmatrix} \right\|^2$$

$$\boxed{p(x) = (2x + x^2)^2 + (2 + x - 3x^2)^2}$$

Let's revisit two of our applications!

Optimization over nonnegative polynomials

↑

Sum of squares (SOS) programming

↑

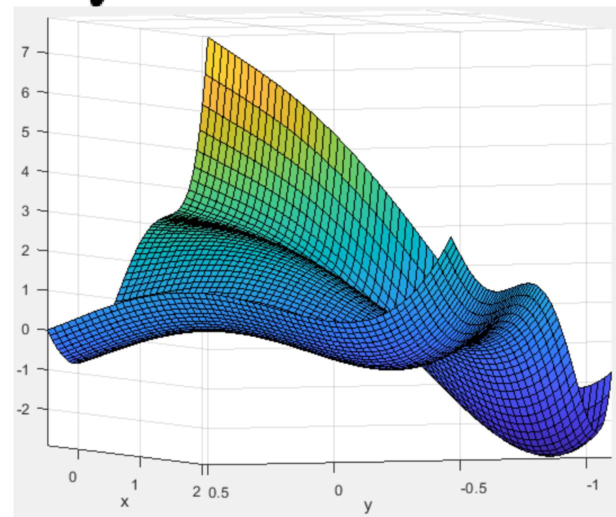
Semidefinite programming (SDP)

1) Nonconvex unconstrained minimization

Find: $$p^* := \inf_{(x,y)\in\mathbb{R}^2} \; 4x^2 - \frac{21}{10}x^4 + \frac{1}{3}x^6 + xy - 4y^2 + 4y^4 + x^2y \;\longleftarrow\; p(x,y)$$

$$\boxed{\begin{array}{lll} p_{sos} := & \sup\limits_{\gamma\in\mathbb{R}} & \gamma \\ & \text{s.t.} & p(x,y) - \gamma \quad \text{sos} \end{array}} \rightarrow \text{SDP!}$$

$$p_{sos} \leq p^*$$




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

solvertime: 0.6 (s)

p_sos =

-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)])
```

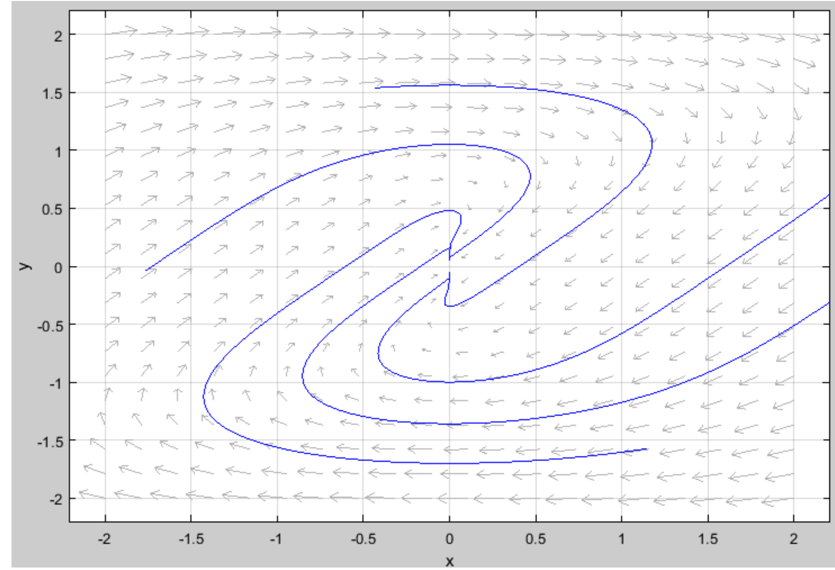
```
xstar =

   1.83299614475561
  -0.922931478421273

p_at_xstar =

  -2.921559422066406
```

2) Automated proof of global asymptotic stability



MK [redacted].edu> on behalf of [redacted]

Tue 2/9/2021 1:13 PM

To: Amir Ali Ahmadi

Hi Amir Ali,

I hope life and career are going well.

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.

> Today in class we got into an interesting discussion with students about what a strict Lyapunov function would be for the system
>
> dx/dt = -x +y^3
> dy/dt = -x
>
> A non-strict L.f.. is easy, V = x^2/2 + y^4/4, with dV/dt = - x^2. One could then deduce g.a.s. by a Barbashin-Krasovskii/Lasalle argument, but that's not satisfactory.
>
> 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.

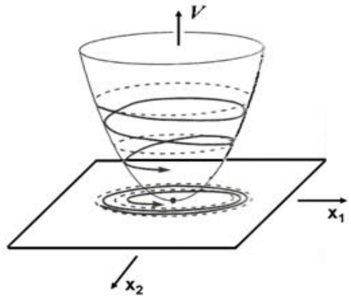
If you can plug in this system and let me know what comes out, I'd appreciate it, and my 40-50 students in class would learn a few things (complexity of Lyapunov functions, automated options for finding them, etc.).

Best regards,

[redacted]

Automated proof of global asymptotic stability

$$\begin{bmatrix} \dot{x} = -x + y^3 \\ \dot{y} = -x \end{bmatrix}$$



Find $V(x,y)$ of degree 4 s.t.

$V(x,y)$ SOS

$-\dot{V}(x,y) = -\left\langle \nabla V(x,y), \begin{pmatrix} -x+y^3 \\ -x \end{pmatrix} \right\rangle$ SOS

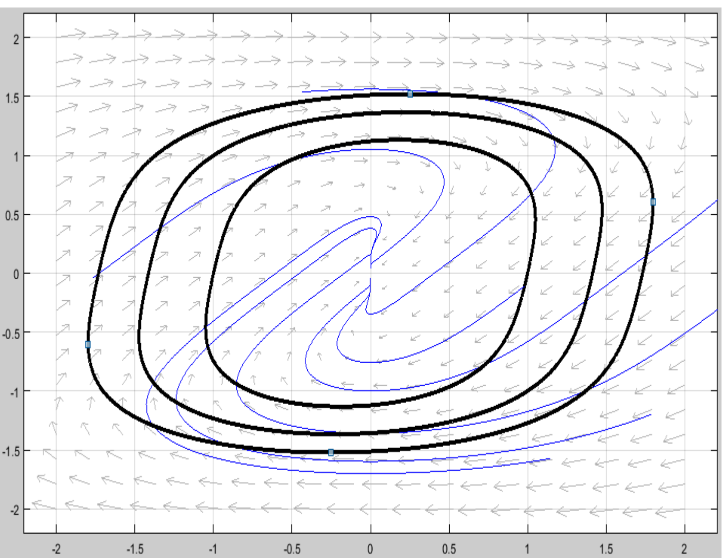
$\rightarrow$ SDP!

```
sdpvar x y
xdot=-x+y^3;
ydot=-x;

[V,c,m]=polynomial([x;y],4,2);
Vdot=jacobian(V,[x,y])*[xdot;ydot];
FF=[sos(V),sos(-Vdot)]
solvesos(FF,[],[],[c])
```

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

$$V(x,y) = x^2 - \frac{1}{3}xy + \frac{1}{6}y^2 + \frac{1}{2}y^4$$



$$= \left(x - \frac{1}{6}y\right)^2 + \frac{5}{36}y^2 + \frac{1}{2}y^4 \quad \text{(hence positive definite)}$$

$$\geq \frac{1}{36}(x^2+y^2) + \frac{1}{2}y^4 \quad \text{(hence radially unbounded)}$$

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

Hilbert's 1888 Paper

Q2: SOS $\overset{?}{\Leftarrow}$ Nonnegativity

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

From Logicomix

Motzkin (1967):

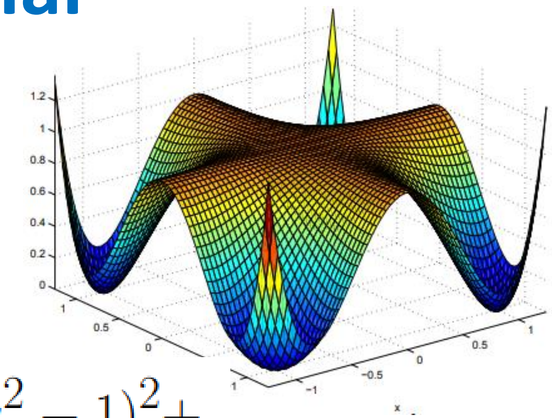
$$M(x_1,x_2) = x_1^4 x_2^2 + x_1^2 x_2^4 - 3x_1^2 x_2^2 + 1$$

Robinson (1973):

$$R(x_1,x_2,x_3) = x_1^2(x_1-1)^2 + x_2^2(x_2-1)^2 + x_3^2(x_3-1)^2 + 2x_1x_2x_3(x_1+x_2+x_3-2)$$

The Motzkin polynomial

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

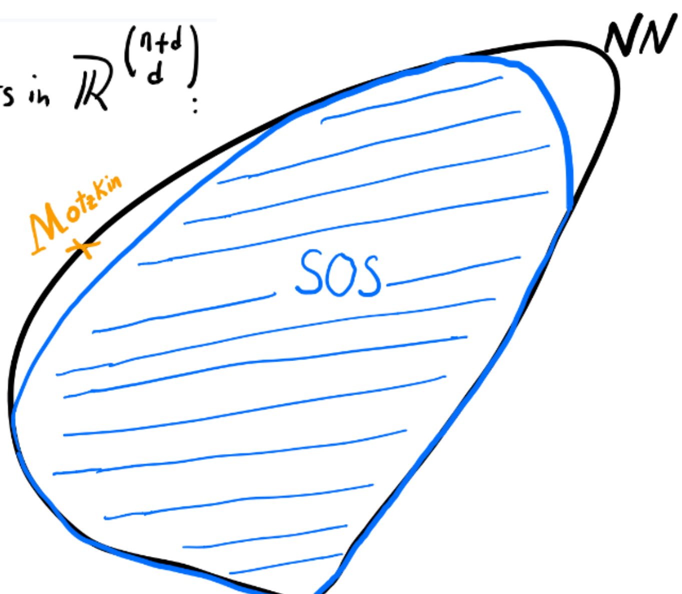


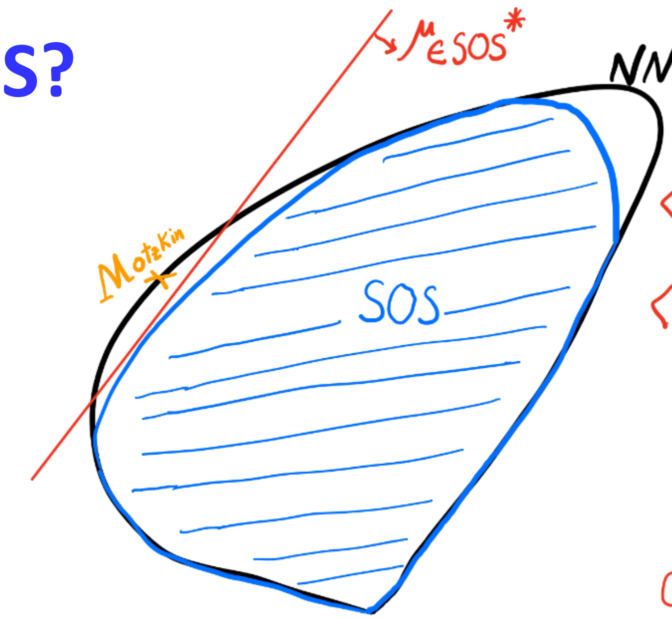
How to prove it is nonnegative?

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

How to prove it is not SOS?

Two sets in $\mathbb{R}^{\binom{n+d}{d}}$:





$\langle \mu, \mathrm{coeff}(M) \rangle < 0$

$\langle \mu, \mathrm{coeff}(q) \rangle \geq 0 \;\; \forall q \in SOS$

$\Updownarrow$

$\left[z(x) z(x)^T \right] \Big|_{\mu} \succeq 0$

Can find μ with SDP.

$NN^* \subseteq SOS^*$

Hilbert's 17th Problem (1900)

Q. $\boldsymbol{p}$ **nonnegative** $\overset{?}{\Rightarrow}$ $$p = \sum_i \left(\frac{g_i}{q_i}\right)^2$$

- Artin (1927): **Yes!**

- Implications:
  - $p \geq 0 \Rightarrow \exists \boldsymbol{h}$ **sos** such that $\boldsymbol{p}.\boldsymbol{h}$ **sos**
  - **Reznick:** (under mild conditions) can take $\boldsymbol{h} = \left(\sum_i \boldsymbol{x}_i^2\right)^{\boldsymbol{r}}$
  - 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**
  - Positivstellensatze of Stengle and Putinar
  - Three applications
- **Recap and further reading**

Positivstellensatz

$p(x) > 0, \forall x \in \mathbb{R}^n$

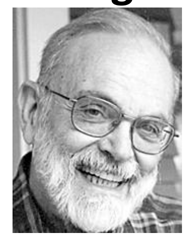
Artin

If $p(x) \geq 0, \forall x \in \mathbb{R}^n$,
then $\exists$ sos q s.t. $p \cdot q$ sos.

1927

20th century

Stengle



1974

1991

1993

$p(x) > 0,$
$\forall x \in S = \{x \mid g_i(x) \geq 0\}$

Schmudgen

Putinar

Positivstellensatz: a complete algebraic proof system

- Let's motivate it with a toy example:

Consider the task of proving the statement:

$$\forall a, b, c, x, \;\; ax^2 + bx + c = 0 \Rightarrow b^2 - 4ac \geq 0$$

Short algebraic proof (certificate):

$$b^2 - 4ac = (2ax + b)^2 - 4a(ax^2 + bx + c)$$

- The Positivstellensatz vastly generalizes what happened here:
  - Algebraic certificates of infeasibility of any system of polynomial inequalities (or algebraic implications among them)
  - **Automated** proof system (via semidefinite programming)

Positivstellensatz: a generalization of Farkas lemma

Farkas lemma (1902):

$Ax = b$ and $x \geq 0$ is infeasible

$$\Updownarrow$$

There exists a y such that $y^T A \geq 0$ and $y^T b < 0$.

(The S-lemma is also a theorem of this type for quadratics)

Stengle's Positivstellensatz (1974)

$$S = \{x \in \mathbb{R}^n \mid g_1(x) \geq 0, \ldots, g_m(x) \geq 0\} \quad \textit{is empty}$$

if and only if

there exist sum of squares polynomials $s_0(x), s_1(x), \ldots, s_m(x), s_{12}(x), s_{13}(x), \ldots, s_{123\ldots m}(x)$

such that

$$-1 = s_0(x) + \sum_i s_i(x)g_i(x) + \sum_{\{i,j\}} s_{ij}(x)g_i(x)g_j(x) + \ldots + s_{123\ldots m}(x)g_1(x)\ldots g_m(x).$$

- This is algebraic certificate of emptiness of *S*
- Works in full generality (no assumptions on *S)*
- Degree bounds on SOS multipliers based on $n, m, \deg(g_i)$ only
- Artin's solution to Hilbert's 17th problem is a corollary
- Leads to an SDP hierarchy for polynomial optimization (the ``Parrilo hierarchy'')

Putinar's Positivstellensatz (1993)

$$\boldsymbol{p(x) > 0 \text{ on } S = \{x \in \mathbb{R}^n \mid g_i(x) \geq 0, i = 1, \dots, m\}}$$

easy direction $\Uparrow$ $\Downarrow$ under the "Archimedean condition"
(slightly stronger than compactness of S)

$\exists \epsilon > 0$ and SOS polynomials $s_0(x), \dots, s_m(x)$ such that

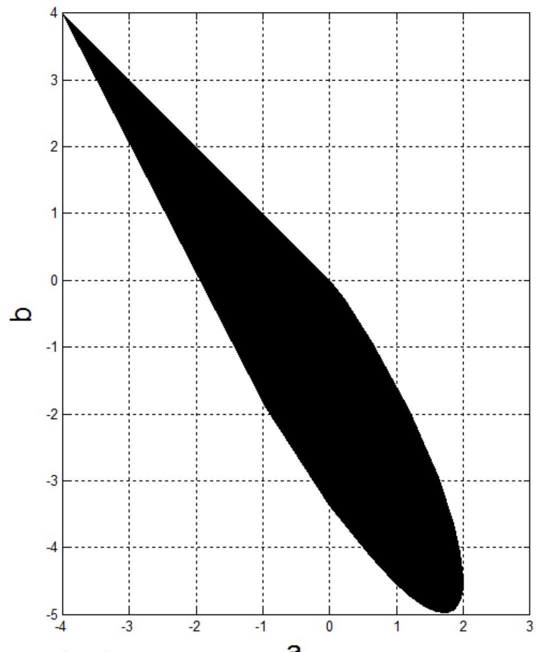
$$\boldsymbol{p(x) - \epsilon = s_0(x) + \textstyle\sum_i s_i(x) g_i(x).}$$

- 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 $[0,1]$?

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



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 3 applications:

- **Finance**
- **Control**
- **Learning dynamical systems**

Optimization over nonnegative polynomials

↑

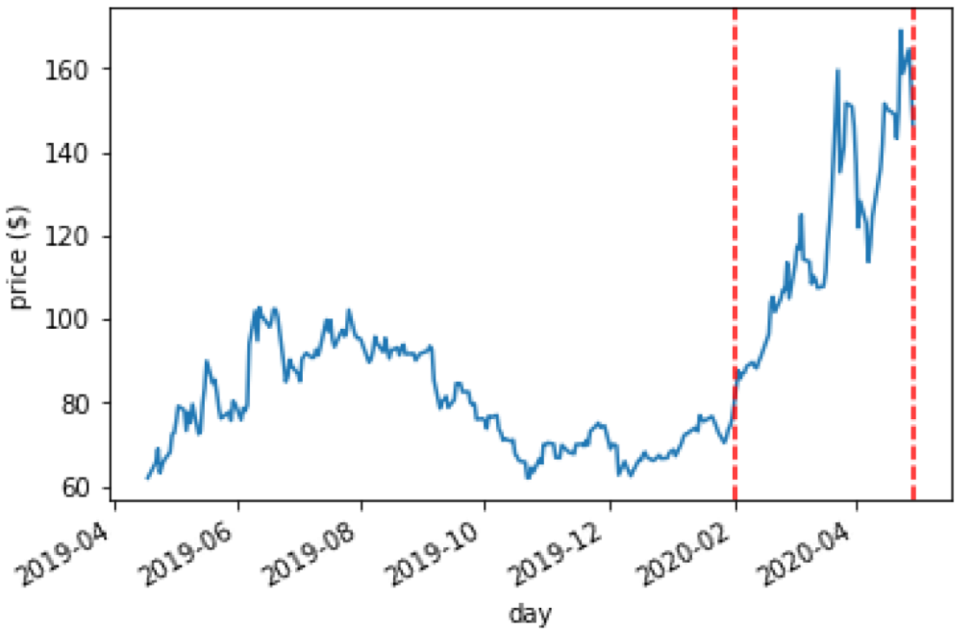
Sum of squares (SOS) programming

↑

Semidefinite programming (SDP)

Distributionally robust optimization

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



- Three months starting Feb 1, 2020

$$r_i = \frac{P_i - P_{i-1}}{P_i}, \quad i = 1, \ldots, 61$$

- Empirical moments $m_k = \mathbb{E}[r^k]$:

$$m_1 = 0.0068, m_2 = 0.0034,$$
$$m_3 = 2 \times 10^{-6}, m_4 = 5 \times 10^{-5}$$

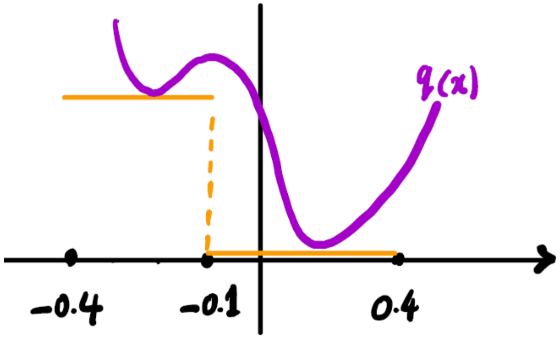
- The distribution of r is supported on [-0.4,0.4] but is otherwise unknown
- What is the probability that Zoom's stock return will be below -0.1 today?
- Want the worst-case probability over all distributions whose first 4 moments are within 10% of those computed from data.

Sum of squares optimization can compute this probability!

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

$$\Longrightarrow q(x) \geq 0 \quad \forall x \in [-0.4, 0.4]$$

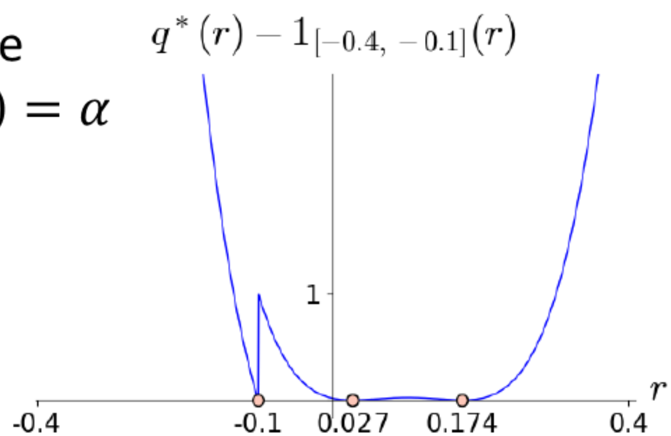
$$\Longrightarrow q(x) \geq 1 \quad \forall x \in [-0.4, -0.1]$$



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

$$\Rightarrow \mathbb{E}\left[1_{[-0.4,-0.1]}\right] \leq \mathbb{E}[q(x)] = \sum_{k=0}^{4} q_k m_k \leq \gamma$$

In fact, we always have
$\mathbb{P}(r \in [-0.4, -0.1]) = \alpha$



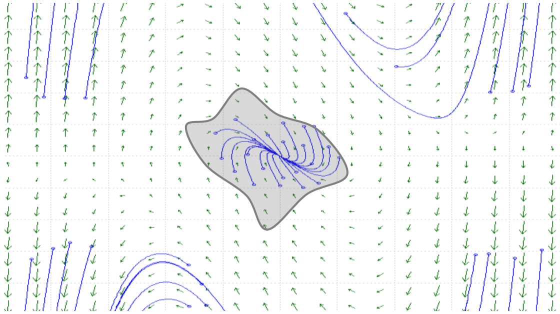
$$\mathbb{P}(r \in [-0.4, -0.1]) \leq \alpha$$

```
Optimizer terminated. Time: 0.17
alpha =

    0.2073
```

SOS proofs of local asymptotic stability (LAS)

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

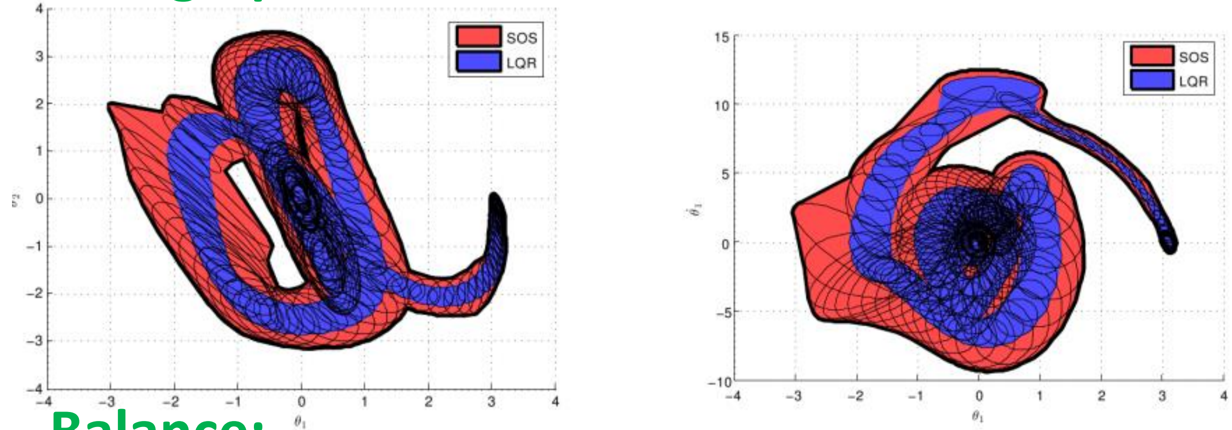


$$V(x) > 0$$
$$V(x) \leq \beta \Rightarrow \dot{V}(x) = \nabla V(x)^T f(x, u) < 0$$

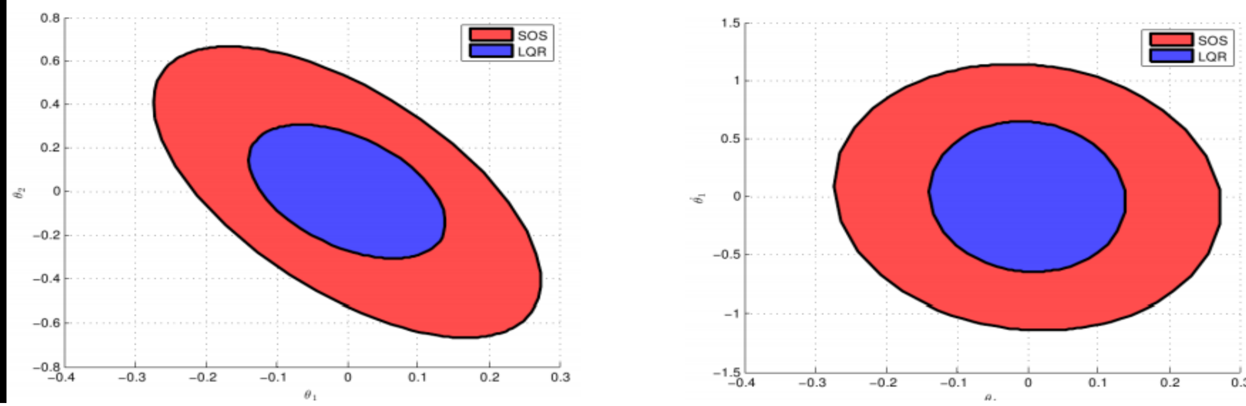
- Deals with nonlinear systems directly.
- Gives easily-verifiable proofs of stability in a fully-automated fashion.

Local stability – SOS on the Acrobot

Swing-up:



Balance:

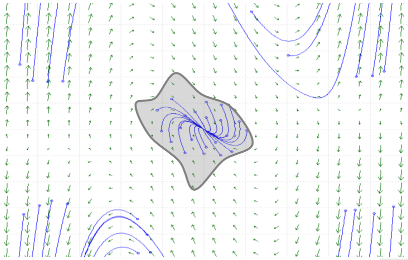


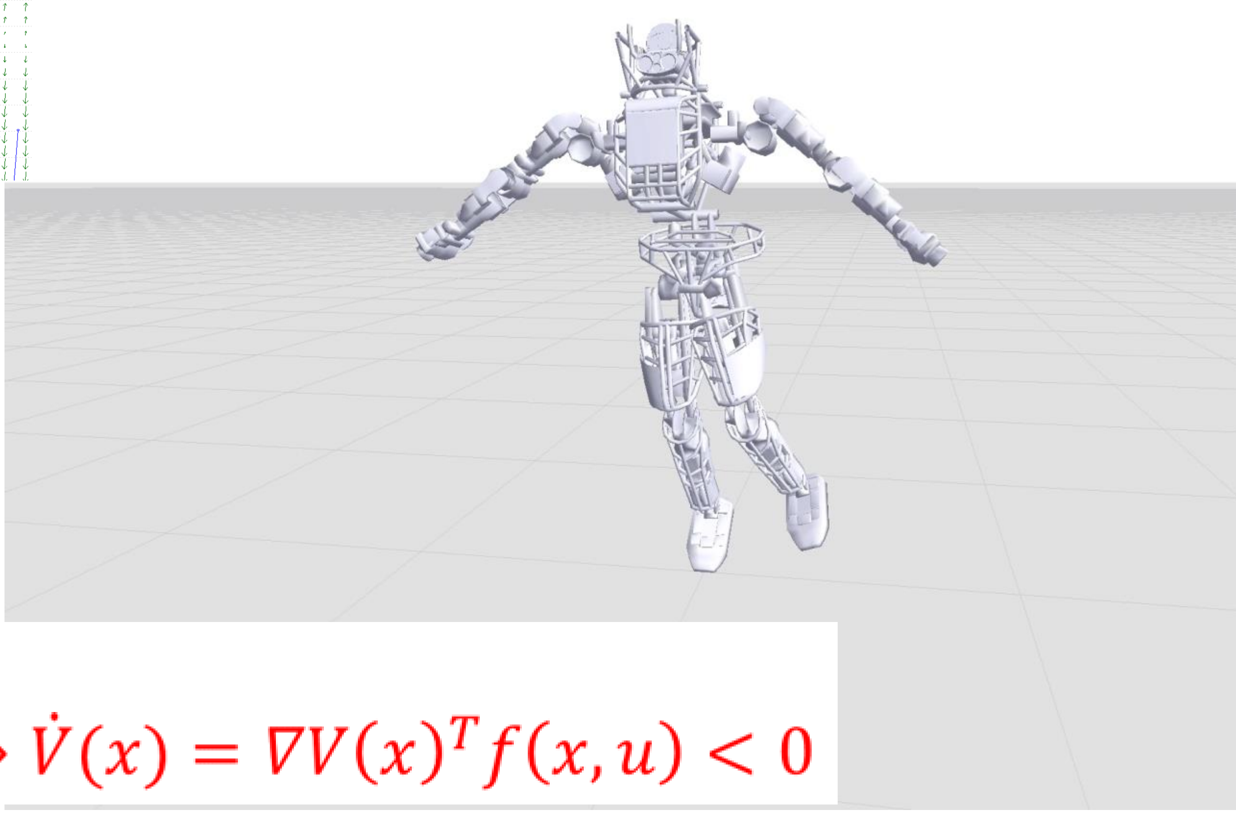
Controller designed by SOS

(w/ Majumdar and Tedrake)

Stabilizing a humanoid robot on one foot

$\dot{x} = f(x,u)$ 30 states 14 control inputs Cubic dynamics





$V(x) > 0$

$V(x) \leq \beta \Rightarrow \dot{V}(x) = \nabla V(x)^T f(x,u) < 0$

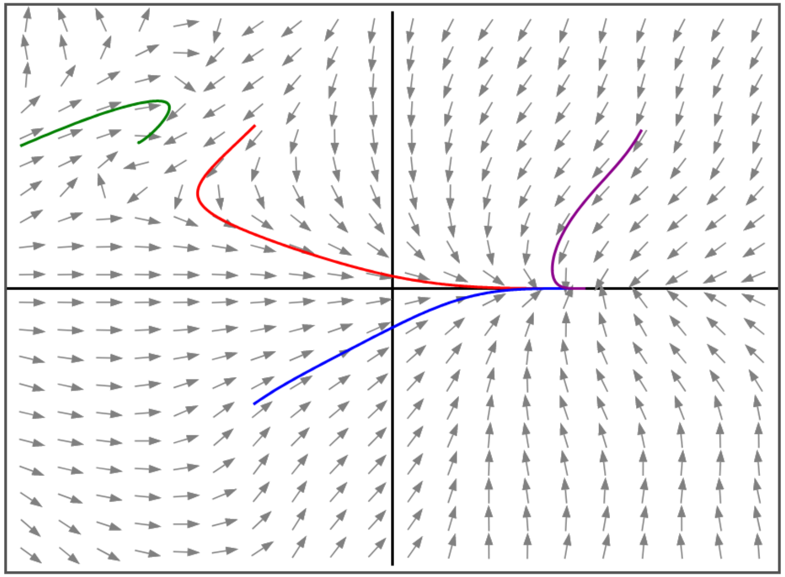
(w/ Majumdar and Tedrake)

Learning dynamical systems with side information

- Goal is to learn a dynamical system

  $$\dot{x} = f(x) \quad (\text{where } f\colon \mathbb{R}^n \to \mathbb{R}^n)$$

  from a *limited* number of *noisy* measurements of its trajectories.



Examples of "side information":

- Equilibrium points (and their stability)
- Invariance of certain sets
- Decrease of certain energy functions
- Sign conditions on derivatives of states
- Having gradient structure
- Monotonicity conditions
- Incremental stability
- (Non)reachability of a set B from a set A, …

- Parametrize a polynomial vector field $p\colon \mathbb{R}^n \to \mathbb{R}^n$.
- Use SOS optimization to impose side information as constraints on p.
- Pick the p that best explains the data.

An epidemiology example

A model from the epidemiology literature for spread of Gonorrhea in a heterosexual population:

$$\dot{x} = f_1(x, y) = -a_1 x + b_1(1 - x)y$$

$$\dot{y} = f_2(x, y) = -a_2 y + b_2(1 - y)x$$

$x(t)$: fraction of infected males at time t

$y(t)$: fraction of infected females at time t

a_1: recovery rate of males

a_2: recovery rate of females

b_1: infection rate of males

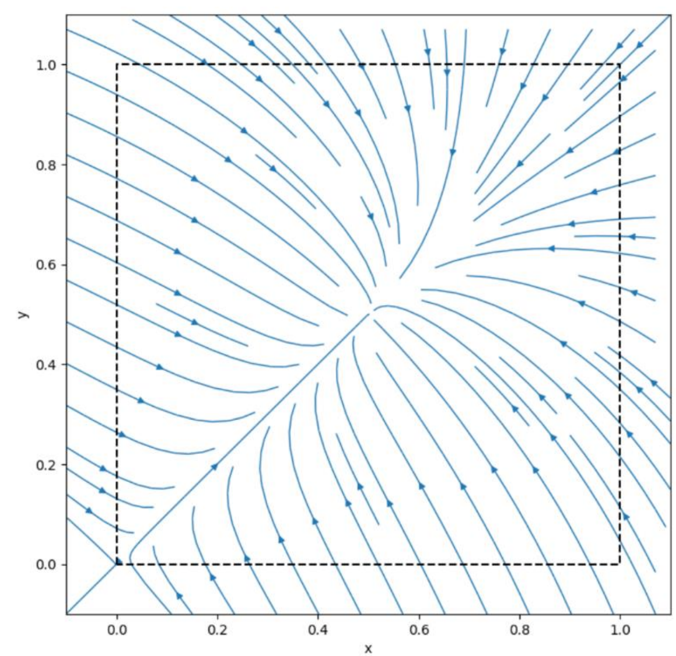
b_2: infection rate of females

For our experiments:

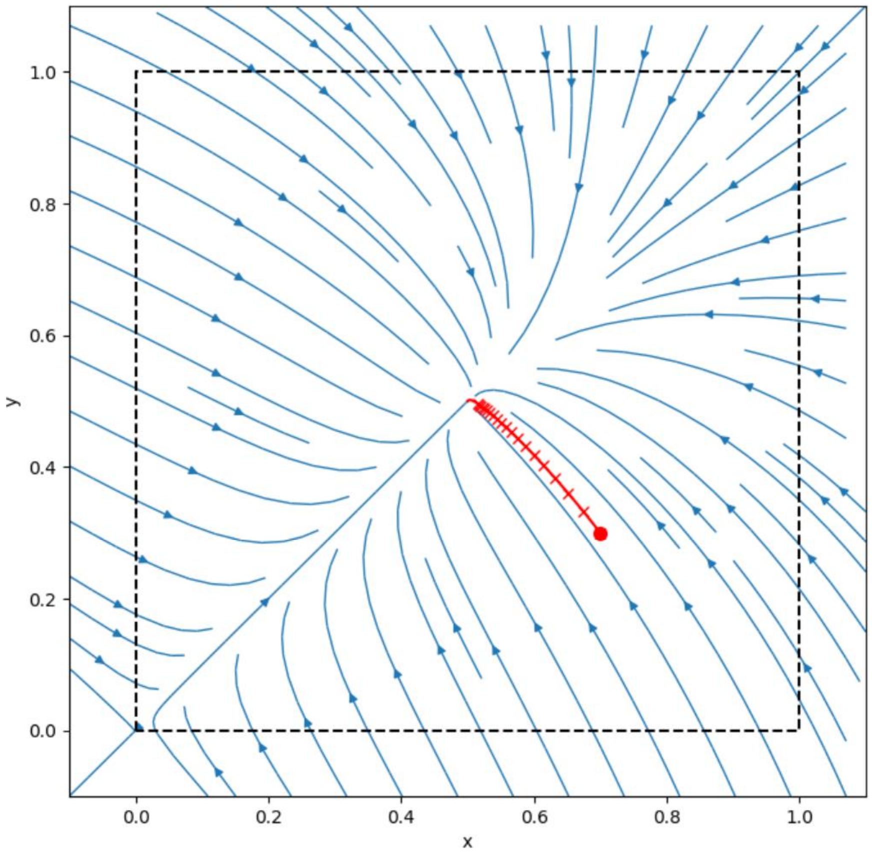
$a_1 = a_2 = .1; b_1 = b_2 = .05.$

This is taken to be "the ground truth".

- The dynamics (both its parameters and its special structure) is unknown to us.
- We only get to observe noisy trajectories of this dynamical system.



The setup



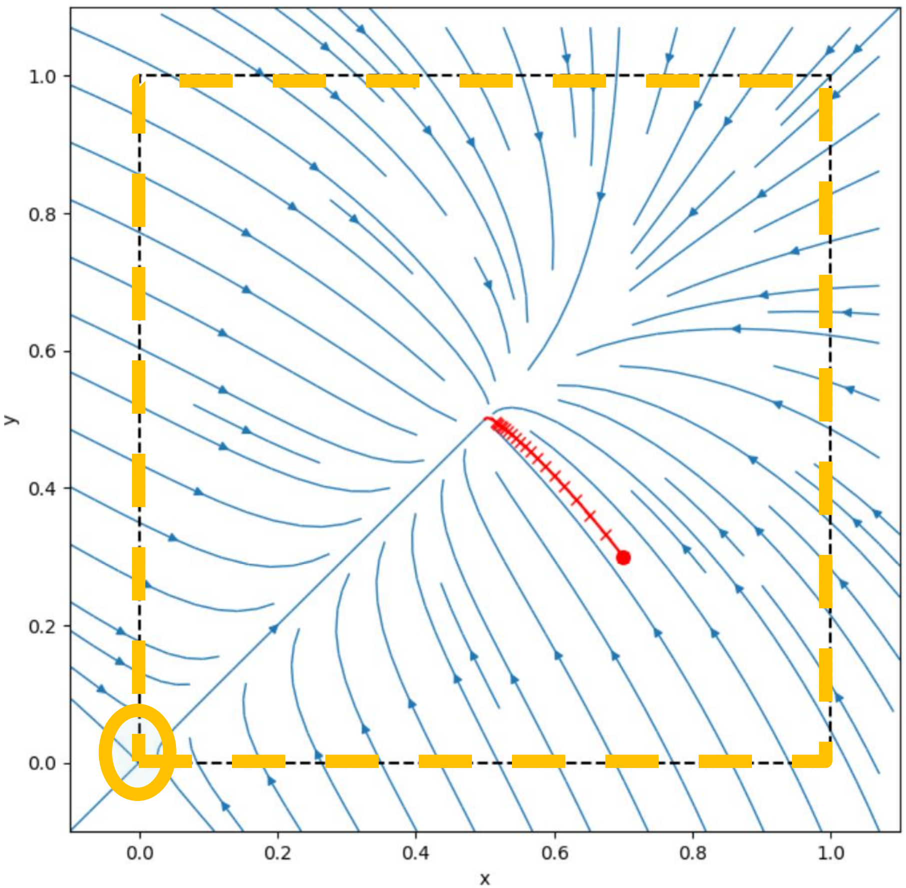
- The true dynamics f is unknown

- **What we observe:**
  Noisy measurements of the vector field on 20 points from a single trajectory starting from [0.7;0.3]

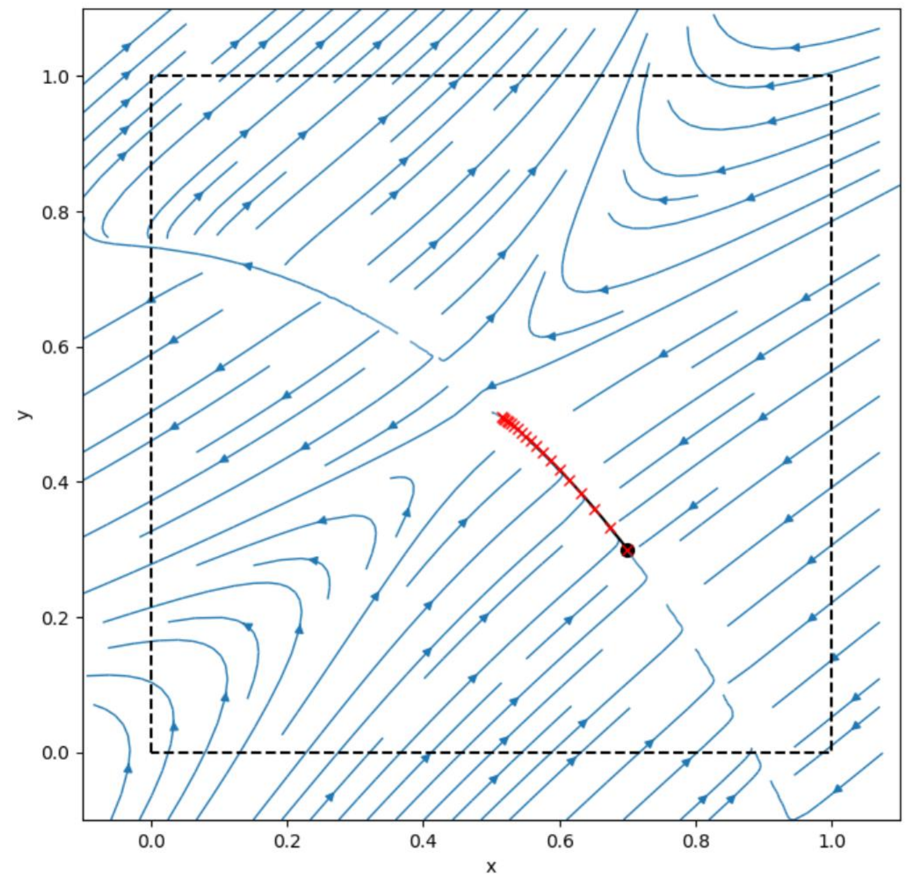
- **Goal:**
  - Learn a polynomial vector field p that best agrees with the observed trajectory
  - Incorporate side information to generalize better to unobserved trajectories

Learning p of degree 3

The true dynamics f (unknown)



Least squares solution



f(0)=0

- Good performance on the observed trajectory. Terrible elsewhere.

Fraction of infected individuals cannot go negative or more than one!

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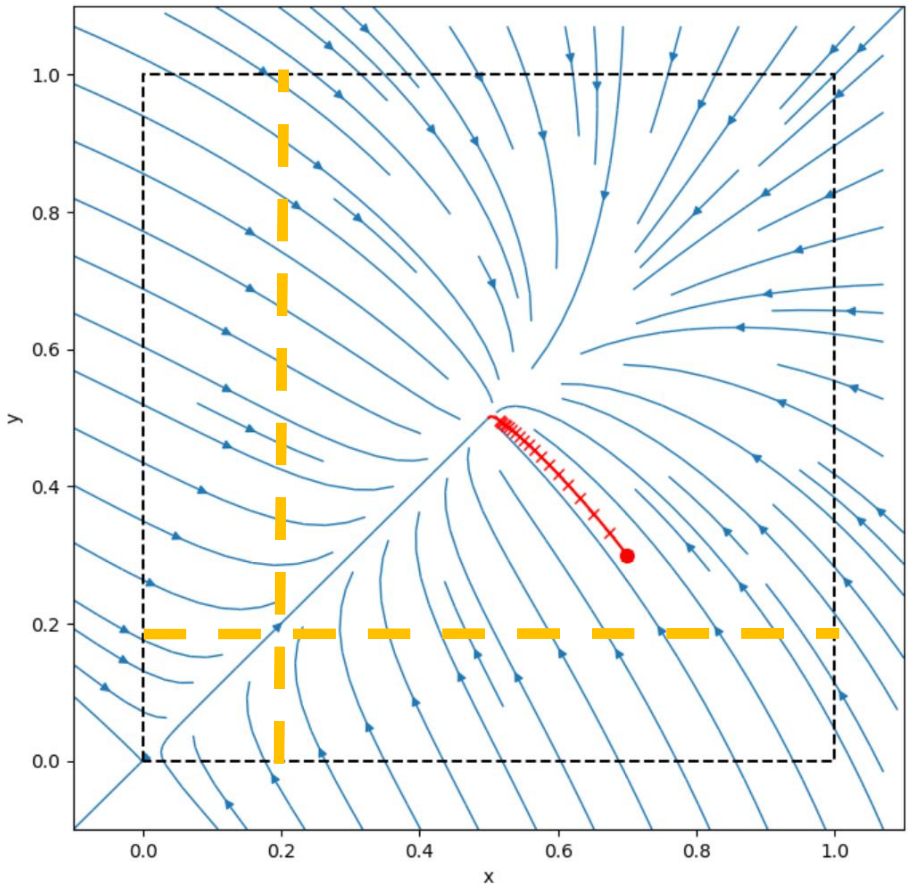
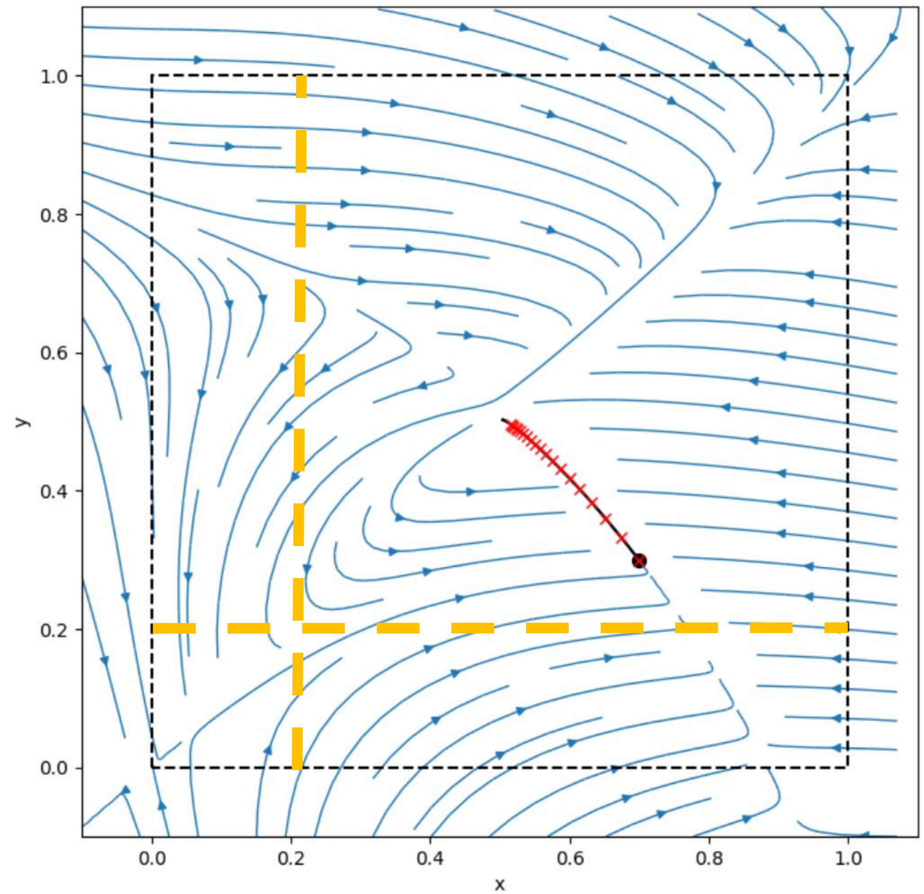
The unit square must be an invariant set!!

Learning p of degree 3

The true dynamics f (unknown)



Least squares solution subject to $p(0) = 0$, unit square invariant



- Better, but not perfect. What other side information can you think of?

More infected females should imply higher infection rate for males! (and vice versa)

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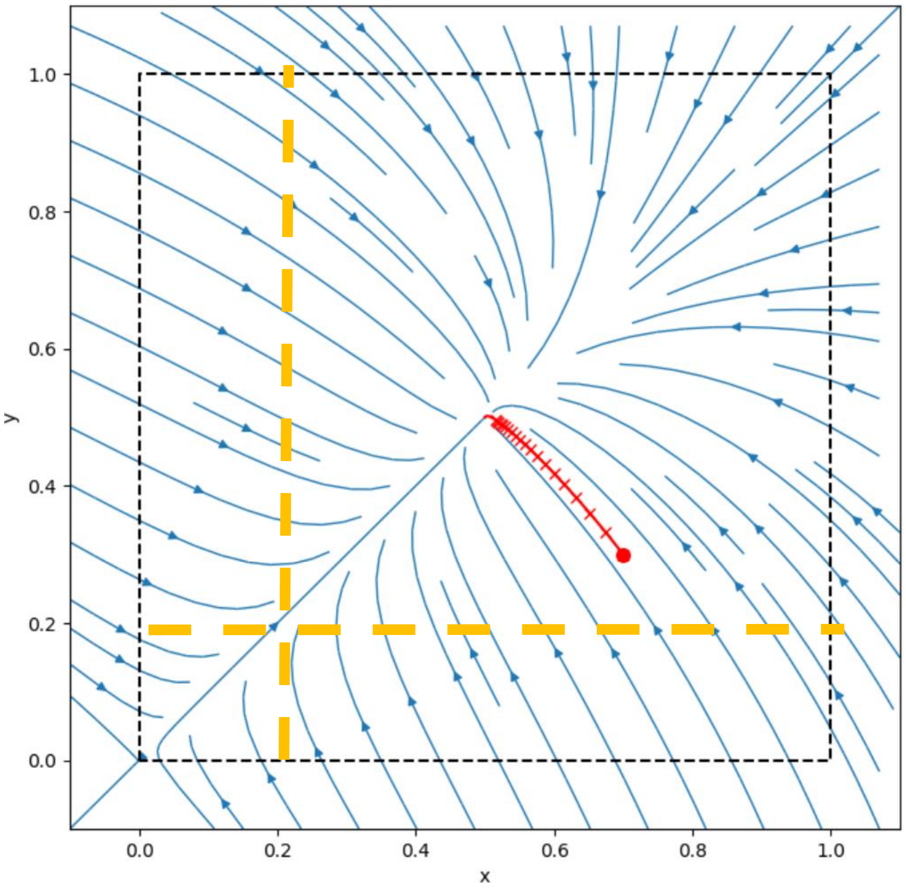
Side information: directional monotonicity

The true dynamics f (unknown)



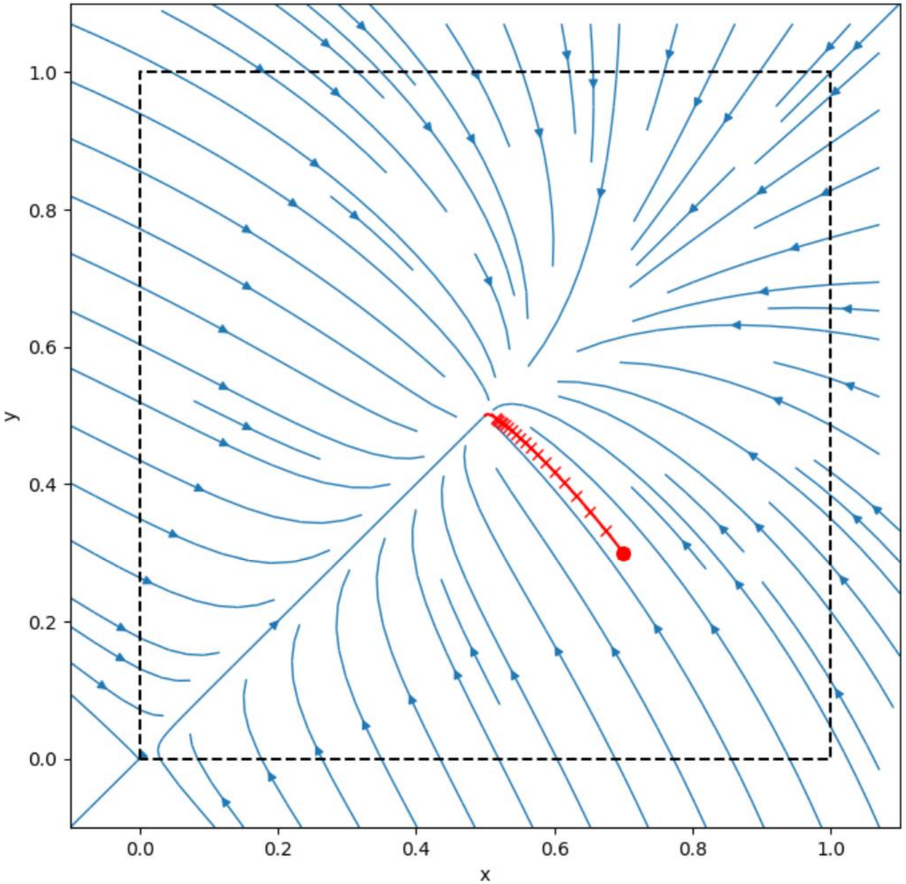
$$\frac{\partial f_1(x,y)}{\partial y} \geq 0, \forall (x,y) \in [0,1]^2$$

$$\frac{\partial f_2(x,y)}{\partial x} \geq 0, \forall (x,y) \in [0,1]^2$$

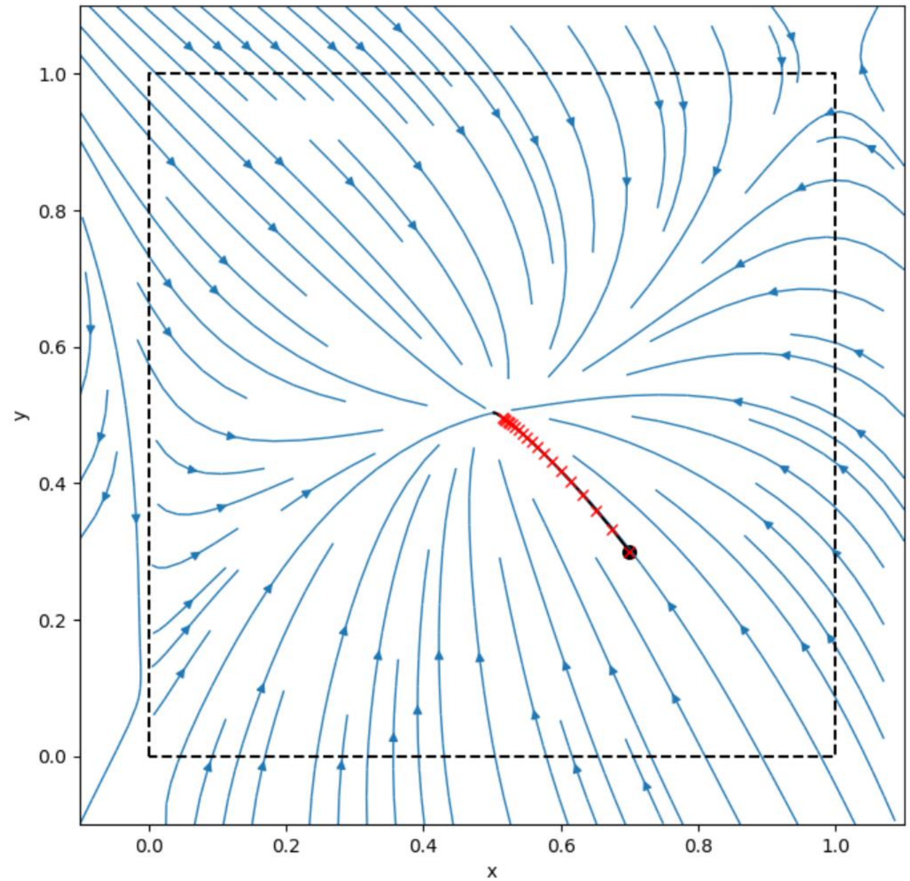
We want p to satisfy the same constraints!

Learning p of degree 3

The true dynamics f (unknown)



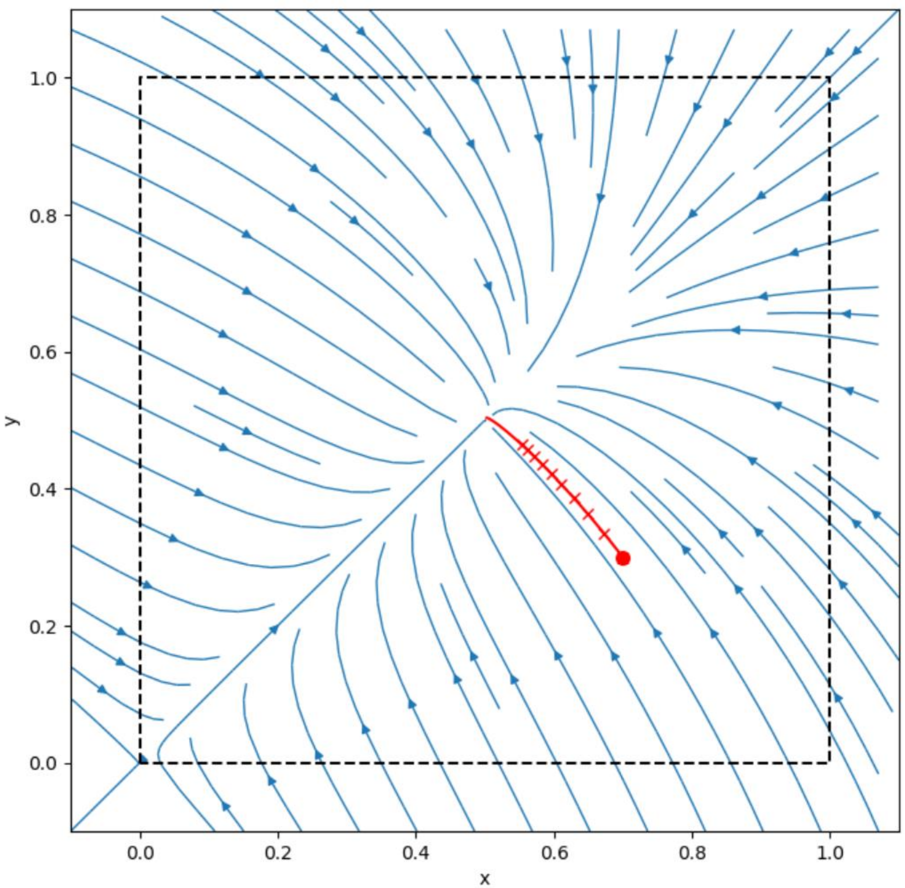
Least squares solution subject to $p(0) = 0$, unit square invariant, directional monotonicity



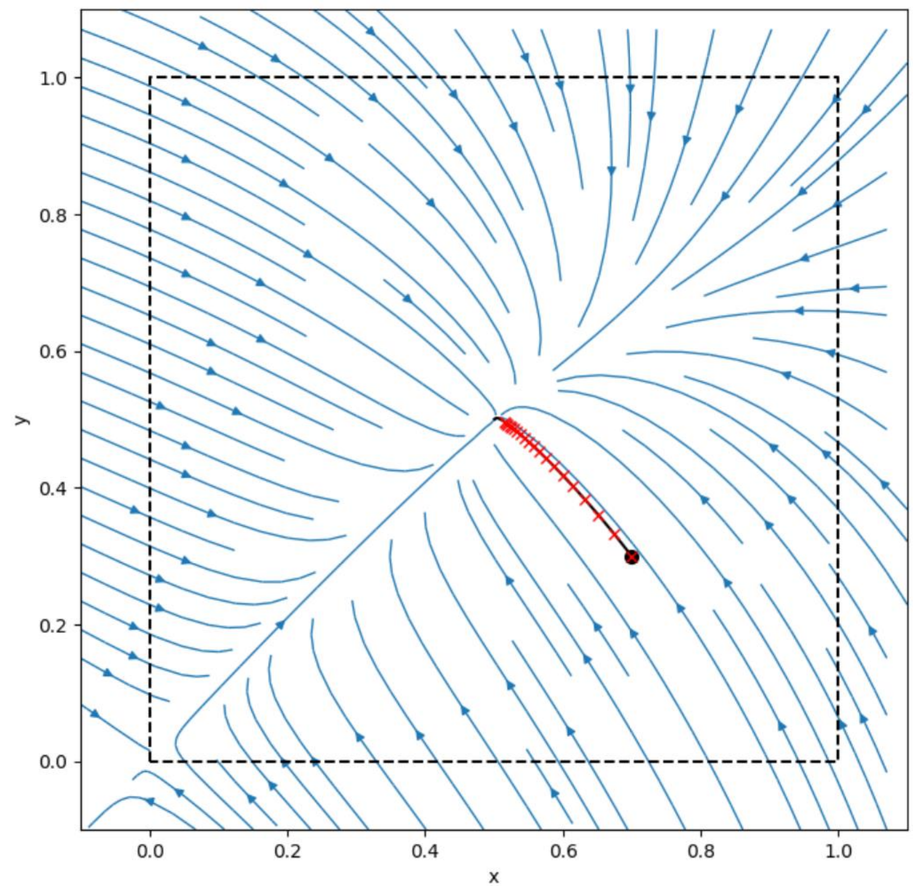
- Now we are getting the qualitative behavior correct everywhere!

Let's learn p of degree 2

The true dynamics f (unknown)



Least squares solution subject to $p(0) = 0$, unit square invariant, directional monotonicity

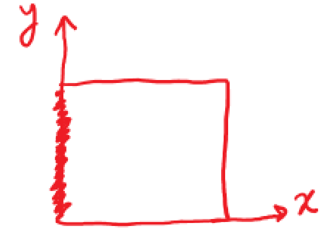


- p is pretty much dead on everywhere even though it was trained on a single trajectory!

The SDP that is being solved in the background

$$\min_{\substack{P=\begin{pmatrix}P_1\\P_2\end{pmatrix},\ \deg(P)\leq 3\\ \sigma_0,\sigma_1,\ \deg(\sigma_i)\leq 2\\ \hat\sigma_0,\hat\sigma_1,\hat\sigma_2\\ \deg(\hat\sigma_0)\leq 2}} \quad \sum_{i=1}^{20} \left(p(x^i,y^i) - \hat{f}(x^i,y^i) \right)^2$$

s.t. $P_1(0,0)=0, \quad P_2(0,0)=0$



$$\left.\begin{aligned} &P_1(0,y) = y\,\sigma_0(y) + (1-y)\,\sigma_1(y) \\ &\sigma_0,\ \sigma_1 \ \text{SOS} \end{aligned}\right\} \Rightarrow \left[x=0,\ 0\leq y\leq 1 \Rightarrow \dot{x} \geq 0\right]$$

(+ three similar constraints)

$$\left.\begin{aligned} &\frac{\partial P_1}{\partial y}(x,y) = \hat\sigma_0(x,y) + \hat\sigma_1(1-x)x + \hat\sigma_2(1-y)y \\ &\hat\sigma_0 \ \text{SOS},\ \hat\sigma_1 \geq 0,\ \hat\sigma_2 \geq 0 \end{aligned}\right\}$$

$$\Rightarrow \left[0\leq x\leq 1,\ 0\leq y\leq 1 \Rightarrow \frac{\partial P_1}{\partial y}(x,y) \geq 0\right]$$

(similarly for $\frac{\partial P_2}{\partial x}(x,y)$)

Output of SDP solver:

p1=0.2681*x^3 - 0.0361*x^2*y - 0.095*x*y^2 + 0.1409*y^3 - 0.4399*x^2 + 0.0956*x*y - 0.0805*y^2 + 0.1232*x + 0.0201*y

p2=0.1188*x^3 + 0.2606*x^2*y + 0.2070*x*y^2 + 0.0005*y^3 - 0.3037*x^2 - 0.4809*x*y -0.099*y^2+ 0.2794*x+0.01689*y

Existence of constrained polynomial dynamics close to f

Thm [AAA, El Khadir]. For any continuously differentiable vector field $f: \mathbb{R}^n \to \mathbb{R}^n$, any $T > 0, \epsilon > 0$, and any compact set $\Omega \subseteq \mathbb{R}^n$,

there exists a polynomial vector field $p: \mathbb{R}^n \to \mathbb{R}^n$ such that

1) **trajectories of $\boldsymbol{f}$ and $\boldsymbol{p}$ starting from any initial conditions $\boldsymbol{x_0} \in \boldsymbol{\Omega}$ remain within $\boldsymbol{\epsilon}$ for all time $\boldsymbol{t} \in [\boldsymbol{0}, \boldsymbol{T}]$** (as long as they stay in Ω),

2) **$\boldsymbol{p}$ satisfies any combination of the following constraints if $\boldsymbol{f}$ does:**

a. equilibria at a given finite set of points $(p(v_i) = 0)$,
b. invariance of a basic semialgebraic set $B = \{x \in \mathbb{R}^n | g_i(x) \geq 0\}$, where each g_i is concave (assumption can be relaxed),
c. directional monotonicity on a compact set $\left(\frac{\partial p_i(x)}{\partial x_j} \geq 0, \forall x \in C\right)$,
d. nonnegativity on a compact set $(p_i(x) \geq 0, \forall x \in D)$.

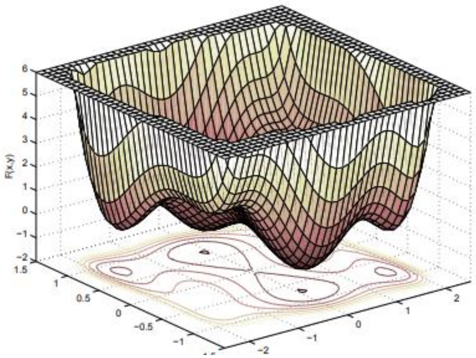
Moreover, all such properties of p come with an **SOS certificate**.

Recap: "See an inequality? Think SOS!"

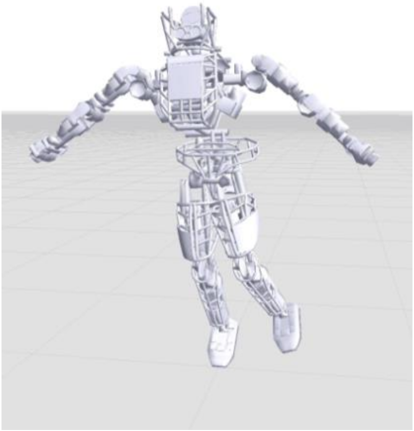
Is $p(x) \geq 0$ on $\{g_1(x) \geq 0, \ldots, g_m(x) \geq 0\}$?

Automated SOS-based proofs via SDP!

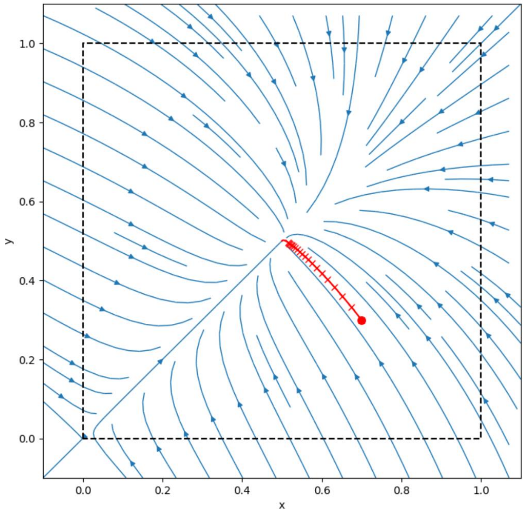
Many applications!



Optimization

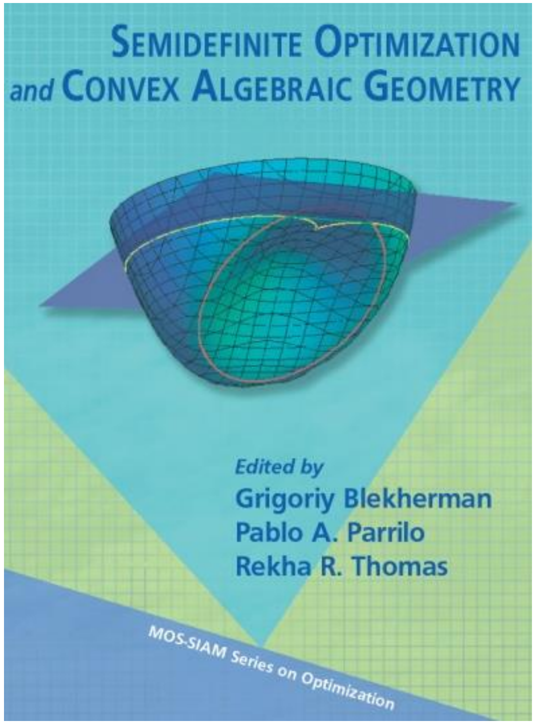


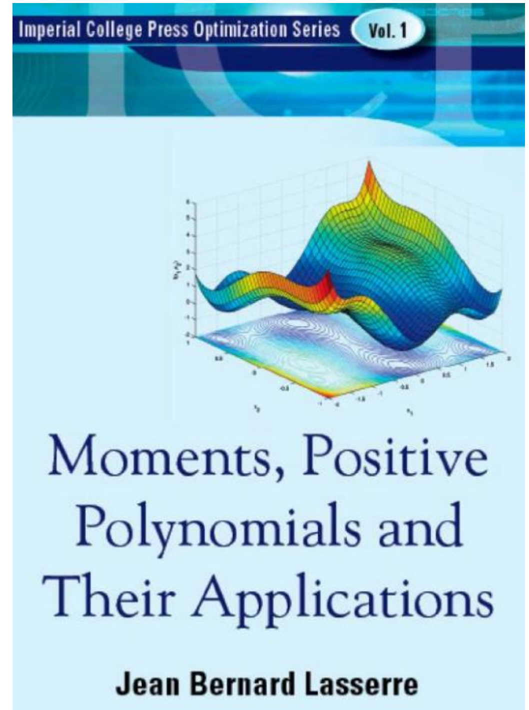
Control



Learning

Want to learn more?





SUMS OF SQUARES, MOMENT MATRICES AND OPTIMIZATION OVER POLYNOMIALS

MONIQUE LAURENT*

Applications of sums of squares

Georgina Hall