Learning Dynamical Systems with Side Information

Bachir El Khadir (bachirelkhadir.com), Amir Ali Ahmadi (aaa.princeton.edu)

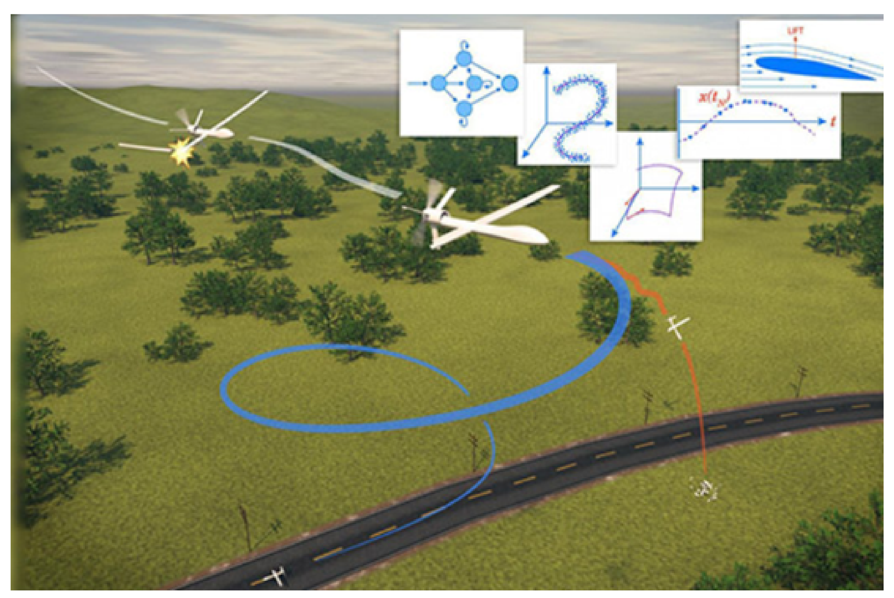
Princeton University

Motivation

Our goal is to learn a dynamical system from a **limited** number of **noisy** measurements of its trajectories.

Imagine, e.g., a passenger airplane that has gone through sudden structural damage. Can we learn the new dynamics on the fly so to autonomously land the plane? Since data is scarce, side information (e.g., physical laws/contextual knowledge) must be exploited.

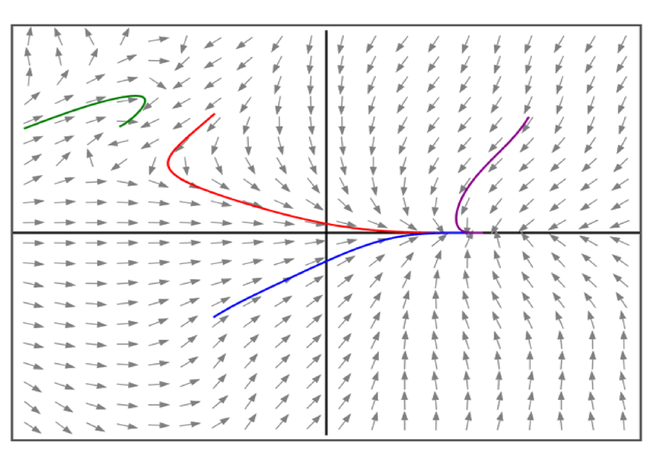
MURI (2019-2024)



For instance, we may know:

- When the engines are off, the plane cannot accelerate upwards.
- Some bounds on the velocities of all the states.

A mathematical formulation



We are given (noisy) samples $(x_i, f(x_i))$ of a smooth vector field

$$f : \mathbb{R}^n \to \mathbb{R}^n$$

that is unknown to us, but on which we have some side information:

- Invariance of given regions
- Decrease of certain energy functions
- Equilibrium points (and their stability)
- Sign conditions on derivatives of states
- Monotonicity conditions
- Incremental stability
- (Non)reachability of a set B from a set A
- ...

Our goal is to learn a vector field which is close to f on observed trajectories and respects side information.

Our plan of action

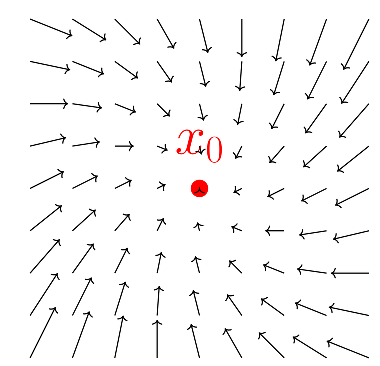
Parametrize a polynomial vector field $p : \mathbb{R}^n \to \mathbb{R}^n$ of fixed degree.

Pick the p that best explains the data, e.g. minimizes the quantity

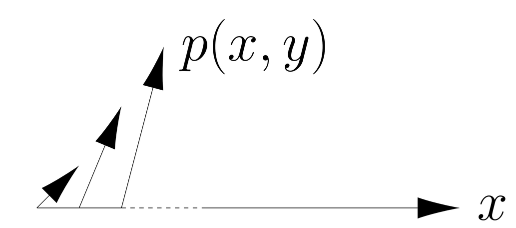
$$\sum_i \|p(x_i) - f(x_i)\|^2.$$

Use sum of squares optimization to impose side information on p.

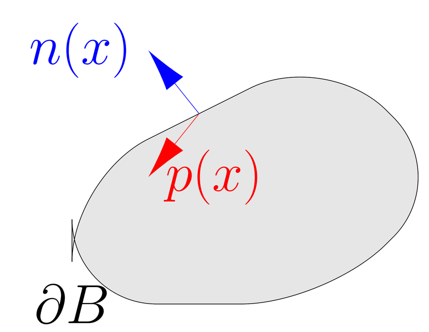
Imposing side information



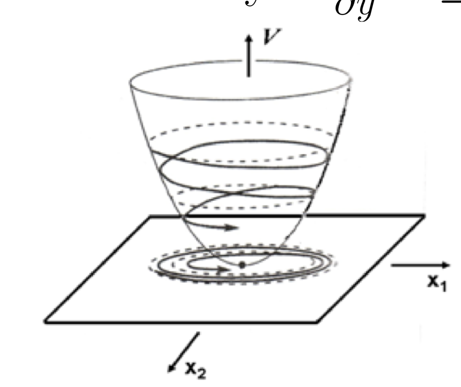
Equilibirum $p(x_0) = 0$



Monotonicity $\frac{\partial p_i(x,y)}{\partial y} \geq 0$



Invariance of a basic semialgebraic set B



Decrease of some scalar-valued polynomial V

$\langle p(x), \nabla V(x) \rangle \leq 0 \quad \forall x$

. . .

Takeaway: Imposing some side information on a polynomial vector fields amounts to imposing nonnegativity of certain polynomials over certain basic semialgebraic sets.

A gentle introduction to SOS optimization

A polynomial p is *nonnegative* if $p(x) \geq 0$ for all $x \in \mathbb{R}^n$.
A polynomial p is a *sum of squares* (SOS) if $p = \sum_i q_i^2$ for some polynomials q_i.
Obviously, all SOS polynomials are nonnegative. While checking nonnegativity of a polynomial is NP-hard, testing (or imposing) the SOS property is a semidefinite program (SDP). Indeed,

$$p \text{ is SOS} \iff \exists Q \succeq 0 \quad p(x) = z^T(x) Q z(x),$$

where $z(x) := (1, x_1, x_2, \ldots, x_1 x_2, \ldots, x_n^{\frac{deg(p)}{2}})^T$.

Takeaway: Searching over the set of SOS polynomials is a semidefinite program!

Putinar's Positivstellensatz (1993)

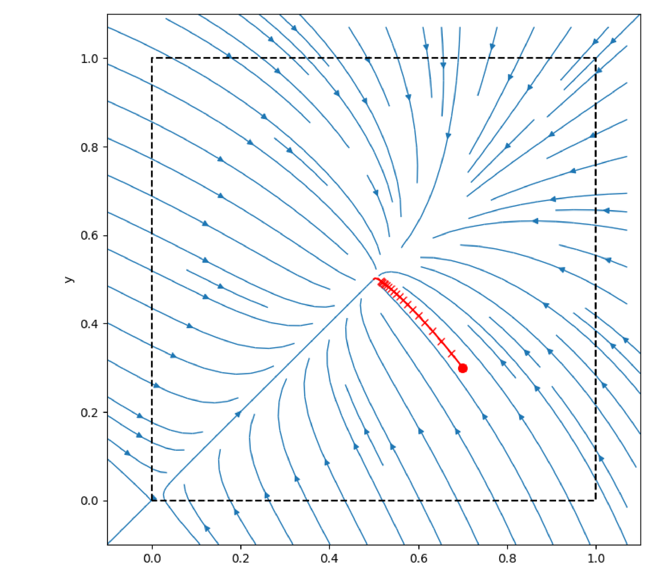
Q: How to impose nonnegativity over a basic semialgebraic set? Let $B := \{x \in \mathbb{R}^n \mid g_1(x) \geq 0, \ldots, g_m(x) \geq 0\}$ for some polynomial g_i. Under mild assumptions (slightly stronger than compactness of B), if a polynomial p is positive on B, then

$$p(x) = \sigma_0(x) + \sum_i \sigma_i(x) g_i(x) \text{ for some SOS polynomials } \sigma_i(x).$$

Search for σ_i of bounded degree is an SDP!

A concrete epidemiology example...

...for spread of Gonorrhea in a heterosexual population:



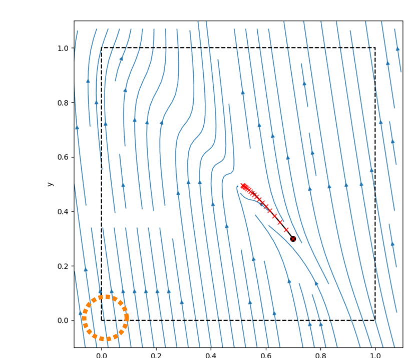
The (unknown) vector field f

$$\dot{x} = f_1(x, y) = -a_1 x + b_1(1 - x)y$$
$$\dot{y} = f_2(x, y) = -a_2 y + b_2(1 - y)x$$

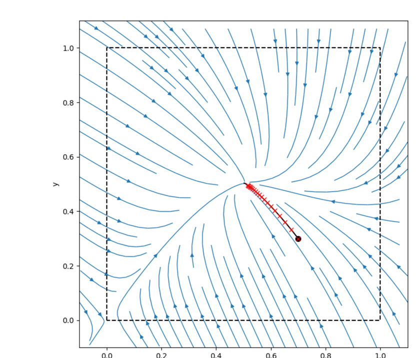
$x(t)$: fraction of infected males at time t
$y(t)$: fraction of infected females at time t
a_1: recovery rate of males
a_2: recovery rate of females
b_1: infection rate of males
b_2: infection rate of females

Setup: The dynamics above is unknown to us. We only get to observe noisy measurements of the vector field on 20 points from a single trajectory starting from $(0.7, 0.3)^T$.

Learning $p(x)$ of degree 2

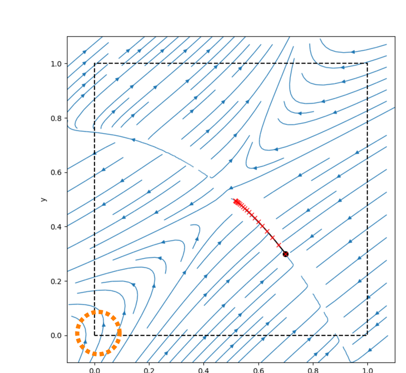


Least square solution

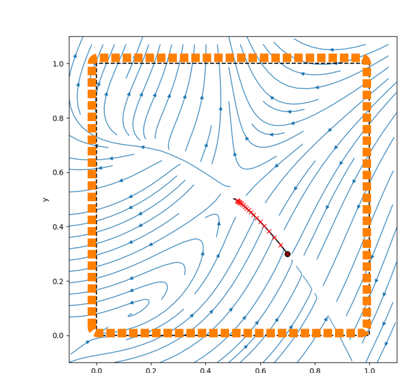


Least square solution + Imposing an eq. at 0

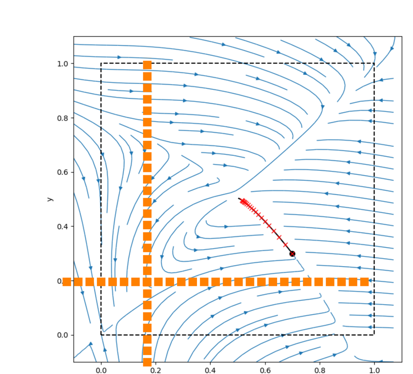
How about degree 3?



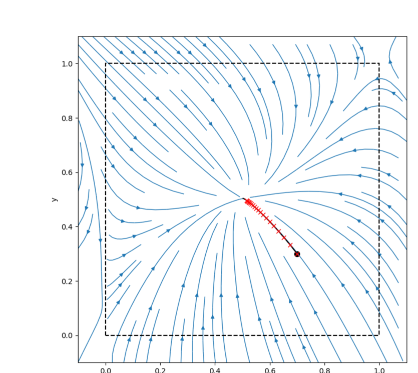
Least square solution



Least square solution + Imposing an eq. at 0



Least square solution + Imposing an eq. at 0+ Invariance of $[0, 1]^2$



Least square solution + Imposing an eq. at 0+ Invariance of $[0, 1]^2$ + Monotonicity

Theorem: density of polynomial vector fields

For any smooth vector field f, any scalars $T > 0$, $\varepsilon > 0$, and any compact set $\Omega \subseteq \mathbb{R}^n$, there exists a polynomial vector field p such that:

1) trajectories of f and p starting from any initial condition $x_0 \in \Omega$ remain within ε for all time $t \in [0, T]$ (as long as they stay in Ω),
2) p satisfies any combination of the following constraints if f does: (a) equilibria at a given finite set of points, (b) invariance of a convex basic semialgebraic set, (c) directional monotonicity, (d) nonnegativity.

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