## Topics

Today (Topcu, Buzi)

- "Breaking" SOStools-based method
- Robustness and verification

Not today:

- Hybrid foundations (Lamperski)
  - Bisimulation
  - Zeno phenomena (+Ames)
- Architecture and verification (many)
- Unified fundamental limits (many)

## Can we "break" SOS tools?

Sharpening our view of what is hard.

## Glycolysis

**3BP** 



Reaction

**Error/flow** 

Level

- Ultimate cyberphysical network
- >3B years of evolution
- >10<sup>30</sup> systems deployed
- Heavily studied, modeled
- Interesting dynamics, bifurcations
- Tunable "complexity"

Oxa

TCA

- Start of "layering" for the cell
- Motivates unified limits

## 2D Model

- build intuition and illustrate concepts easily explainable in 2D (using pictures and simple plots),
- develop ideas and analysis techniques that are generalizable to higher dimensional models.



## Fixed points, stability, and bifurcations

Number of fixed points determined by the solutions to  $f(y) = g_y(y)$ .

Most systems topologicaly equivalent to one of the three instances



Pathway is consuming ATP faster than it can produce. The origin is globally asymptotically stable. Pathway crashes (all concentrations go to zero)

1 nonzero fixed point. It's either globally asymptotically stable or there exists a limit cycle that is globally asymptotically stable

2 nonzero fixed points, a saddle point and a node. Stable manifold of the saddle separates the RoA of the two nodes.

#### **Global Behavior**



$$\dot{x} = f(y) - g_x(x)$$
  

$$\dot{y} = 2g_x(x) - f(y) - g_y(y)$$
  

$$f(y) = \frac{Vy^{q}}{1 + \gamma y^{h}}$$

Using the level sets of the function

$$U(x, y) = \begin{cases} 2x + y - \beta_0 & y > \beta_0 \\ 2x & y \le \beta_0 \end{cases}$$
$$\beta_0 := \inf \left\{ y_0 \mid g_y(y) - f(y) > \varepsilon, \forall y > y_0 \right\}$$

We can show that the trajectories of the system are bounded



#### Region of Attraction (RoA) Estimation

If the vector field

$$\dot{x} = F(x)$$
$$x \in \mathbb{R}^n$$

is rational, we can estimate RoA of the origin using Lyapunov functions and Sum of Squares (SOS) programming.

Given a positive definite function  $\varphi$  with compact level sets, we search for a polynomial Lyapunov function U and  $\alpha$  such that

$$U(x) - \varepsilon x^{T} x + s_{1}(x)(\varphi(x) - \alpha) \text{ is SOS}$$
  

$$d(x) \left\{ \frac{\partial}{\partial x} U(x) \cdot F(x) - \varepsilon x^{T} x + s_{2}(x)(\varphi(x) - \alpha) \right\} \text{ is SOS}$$
  

$$s_{1}(x), s_{2}(x) \text{ are SOS polynomials}$$
  

$$d(x) \text{ is the denominator of the vector field}$$

The sublevel set  $\Omega_{\varphi,\alpha}$ ,

$$\Omega_{\varphi,\alpha} = \left\{ x \, | \, \varphi(x) \leq \alpha \right\}$$

is an invariant subset of the RoA of the origin

## **RoA Estimation**

Estimate RoA of the origin by sublevel sets of Lyapunov functions

For rational vector fields, use Sum of Squares (SOS) programming to search for polynomial Lyapunov function in a neighborhood  $N_0$  of the fixed point.

Sublevel sets which are entirely contained in  $N_0$  are invariant subsets of the RoA.

Next we examine how estimating the RoA is connected to the concepts of complexity and robustness











## **General Decomposition**



 $S_1$  is a well behaved "simple" SISO (single-input single-output) system in  $\mathbb{R}^k$  $S_2$  is SISO system in  $\mathbb{R}^{l+1}$ , l+k=n, that captures most of the nonlinearity.

We will call this an (k, l+1)-decomposition

## **Dissipation Inequalities**

Similarly, we look to for positive definite storage functions  $U_1(x_{l+1}, ..., x_{l+k}) > 0$  and  $U_2(y, x_1, ..., x_l) > 0$ , such that



$$\begin{split} &\frac{d}{dt}U_1(x_{l+1},\ldots,x_{l+k}) \leq z^2 + 2\,\delta\,wz - \kappa\,w^2, \quad \forall \big(x,z\big) \\ &\frac{d}{dt}U_2(y,x_1,\ldots,x_l) < \kappa\,w^2 - 2\,\delta\,wz - z^2, \quad \forall w,\forall (y,x_1,\ldots,x_l) \in B(0) \end{split}$$

where B(0) is a neighborhood of the origin.

Then  $U = U_1 + U_2$  is a Lyapunov function for the full system *S*. The estimate of the RoA is the largest sublevel set of U(x,y) contained in  $R^k \times B(0)$ 

Problem reduces to solving 2 SOS programs in

- 1. Many variables but low degree of polynomials
- 2. Few variables but high degree of polynomials

## Example

How much benefit do we get from the general decomposition?



Here is an example of a 7D pathway using  $(7-n_2,n_2)$ -decomposition

- As the size  $n_2$  of the system  $S_2$ increases, we are able to construct Lyapunov functions for systems with higher gains
- As  $n_2$  increases, so does the computational complexity.

Stability Diagram f or 7D System



## **Complexity and Performance**

If a storage function  $U_1$  exists for  $S_1$ , then a *diagonal* storage function for  $S_1$  also exists



# Size of $S_2$ determines the complexity of the full system.

So, fragile systems (high gains) require large  $S_2$  to construct Lyapunov functions (i.e., computationally complex).

## **Complexity and Pathway Size**

As the pathway size increases, decompositions with large size S2 are required to construct Lyapunov function for smaller gains.





## Old punchline revisited

- 1. Robust instances are easily verified to be so
- 2. Robust instances can be computed exactly
- (Fragile problems cannot)
- 2 is more subtle point
- If it holds in general then robust designs need not be conservatively so to be verifiable
- If "robust?" is easy, then "fragile?" is too approximately

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#### The "simplest" hard problem

NPP (Number partitioning problem)

Given 
$$a_1 \ge a_2 \ge \dots \ge a_n \ge 0$$
  
Compute  

$$\min_{\substack{x_i^2 = 1 \\ x_i = \pm 1}} \left| \sum_{i=1}^{\infty} a_i x_i \right|$$

$$= \min_{\substack{x_i = \pm 1 \\ \pm}} \left| \sum_{i=1}^{\infty} a_i x_i \right|$$

A "classic" NP complete problem

But there are subtle issues with reals, quasi-polynomial

## Old punchline revisited

- 1. Robust instances are easily verified to be so
- 2. Robust instances can be computed exactly

• Proof of robust instance works for nearby (robust) instances?



- Given: a line in the plane  $a_0 + a_1 x + a_2 y = 0$
- Question: does it hit a corner of the square?

 $x^2=1, y^2=1$ 



## Is there a crash?

- Given: a line in the plane  $a_0x + a_1y = 0$
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  - $x^2=1, y^2=1$
- Crash = hits a corner



## Fragile = near miss

- Given: a line in the plane  $a_0 + a_1x + a_2y = 0$
- Question: does it hit a corner of the square?
   x<sup>2</sup>=1, y<sup>2</sup>=1
- Crash = hits a corner
- Fragile = near miss

# $_{0}/a_{1}$ $y = -a_0 / a_2$ $|a_0 + a_1x + a_2y|$ $(-a_0 - a_1 x)/a_2 = y$

## Fragile = near miss

- Given: a line in the plane  $a_0 + a_1 x + a_2 y = 0$
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#### (1/2, 1/4, 1/4)



 $|a_0 + a_1x + a_2y|$ (-a\_0 - a\_1x)/ a\_2=y

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   x<sup>2</sup>=1, y<sup>2</sup>=1
- Crash = hits a corner
- Fragile = near miss

 $x = -a_0 / a_1$ 

(2/3, 1/6, 1/6)



- Given: a line in the plane  $a_0 + a_1 x + a_2 y = 0$
- Question: does it hit a corner of the square?
   x<sup>2</sup>=1, y<sup>2</sup>=1
- Crash = hits a corner
- Fragile = near miss

 $y = -a_0 / a_2$ 

 $x = -a_0 / a_1$ 

(1/3,1/3,1/3)



$$R_{3} = \left\{ \min \delta \quad \left| \begin{array}{c} \min \\ ||x_{i}| - 1| \le \delta \end{array} \right| \sum a_{i} x_{i} || = 0 \right\}$$

- Given: a line in the plane  $a_0 + a_1x + a_2y = 0$
- Question: does it hit a corner of the square?
   x<sup>2</sup>=1, y<sup>2</sup>=1
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- Given: a line in the plane  $a_0 + a_1x + a_2y = 0$
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Compute  

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A "classic" NP complete problem





## Karmakar – Karp heuristics:

$$a_1 \ge a_2 \ge \ldots \ge a_{n-1} \ge a_n$$

$$a_1 \ge a_2 + \dots + a_{n-1} + a_n$$

then the optimal solution is

lf

$$a_1 - a_2 - \dots - a_{n-1} - a_n$$

#### Can also be derived using SOS/SDP.




$$\sum a_i = 1$$

0.2116 0.1677 0.1358 0.1312 0.1307 0.1079 0.0892 0.0259

n=8







#### Still exponentially bad.

#### n=16

0.11874666798309 0.11211512926647 0.11169327453340 0.11095064177068 0.09412186438521 0.08685317462754 0.08118017281551 0.06766995122518 0.05718523360114 0.03754549903682 0.03586488042322 0.03254947795691 0.01521112174069 0.01506074475625 0.01423812298937 0.00901404288853



n=10

0.16212567898594 0.14166406741328 0.13672813657519 0.13542304261100 0.11591869442981 0.11370146803691 0.06062893005904 0.05985800729769 0.04919688814988 0.02475508644126



n=10, uniformly random coefficients

$$\left|\sum a_i x_i\right|$$
 for  $x_i = \pm 1$   
looks roughly like IID uniform random variable



"worst" problem?

$$n = 2m + 1, \ a_i = \frac{1}{n}$$

$$R = \frac{1}{n}$$
$$\left|\sum \pm a_{i}\right| = \frac{1}{n}\left|1 \pm 1 \pm 1 \dots \pm 1\right|$$
$$\binom{2m+1}{m}$$
local optima

Answer is obvious, KK proof length is exponentially bad.

# Why start here

- Easily visualized and explained
- Theorems have short proofs
- Complexity and fragility notions are both clear and easy to understand
- Worst case problems are exponentially bad

# Potential confusion

- Mix of reals and booleans is confusing (but typical in hybrid systems models)
- Complexity theory details are murky
- Problem is clearly "hard" in worst case so these nuances are less important

#### Various levels of paranoia



Theorem: 
$$R = R_2 = R_3$$

# This is the "punchline"



## Let's compare

$$L = \text{tree depth} \\ \# = \text{operation count} \} \implies \# \le n 2^{L}$$
$$L \le \frac{1}{R} \implies \# \le O\left(n 2^{\frac{1}{R}}\right)$$

NPP

Linear  
Program 
$$\Rightarrow \# \le O\left(n^2 \log\left(\frac{1}{R}\right)\right)$$

## Why is NPP "harder"?

Random NPP instances (e.g. physics)

$$\begin{split} \min_{x_i^2 = 1} \left| \sum a_i x_i \right| &\approx \frac{2^{-n}}{\sqrt{n}} \\ \text{This is true "almost surely," but has} \\ \text{proof length of } \# = O\left(2^n\right) \end{split}$$

Also holds in the worst case (e.g. CS).

Robust NPP instances are easy!

$$\# \le O\left(n2^{\frac{1}{R}}\right)$$

R big.

# Rethinking "complexity"

Random & worst case

$$\# = O\left(2^n\right)$$

Ill-conditioning is less "fundamental"?

$$\begin{array}{l} \text{Linear} \\ \text{Program} \end{array} \Rightarrow \quad \# \le O\left(n^2 \log\left(\frac{1}{R}\right)\right) \end{array}$$

$$\# \leq O\left(n2^{\frac{1}{R}}\right)$$



$$n = 2m + 1, \ a_i = \frac{1}{n}$$

$$R = \frac{1}{n}$$
$$\left|\sum \pm a_{i}\right| = \frac{1}{n} \left|1 \pm 1 \pm 1 \dots \pm 1\right|$$
$$\binom{2m+1}{m}$$
local optima

Answer is obvious, KK proof length is exponentially bad.

Bound is exponentially bad.

$$\# \le O\left(n2^{\frac{1}{R}}\right) = O\left(n2^n\right)$$

# Proof Idea

Robust problems have a few big numbers dominating the rest.



#### Less robust....



And so on....

Robustness of the problem bounds the size of the tree.

Robust problems are rare and highly structured





# Punchline revisited

- 1. Robust problems are easily verified to be so
- 2. Robust problems can be computed exactly
- (Fragile problems cannot)
- 2 is more subtle point
- If it holds in general then robust designs need not be conservatively so to be verifiable
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# Simple questionUndecidable

• Chaos

• Fractals

Mandelbrot

It's easy to *prove* that this disk is in *M*.

Other points in *M* are fragile to the definition of the map.  $z_{k+1} = (c + \delta) z_k (1 - z_k)$ 

Merely stating the obvious.

e.g. the boundary moves.

T.C.

Points near the boundary are "fragile."

Merely stating the obvious in this case.

But illustrates general principle that can be exploited by the right algorithms.

#### # iterations



#### Points not in M.

#### # iterations



Color indicates number of iterations of simulation to show point is not in *M*. But simulation cannot show that points are in *M*.





But simulation is fundamentally limited

- Gridding is not scalable
- Finite simulation inconclusive

It's easy to *prove* that this disk is in *M*.

Other points in *M* are fragile to the definition of the map.  $z_{k+1} = (c + \delta) z_k (1 - z_k)$ 

Merely stating the obvious.



**Short proof**  $Z_{k+1} = CZ_k \left(1 - Z_k\right)$  $V(z) = |z|^2$  $V(z_k) \ge V(z_{k+1})$ 

 $\Leftrightarrow \left|z_{k}\right|^{2} - \left|cz_{k}\left(1 - z_{k}\right)\right|^{2} \ge 0$ 

c plane

 $V(z) = |z|^2 \text{ decreases}$  $\Leftarrow 1 \ge |c|(1+|z|)$ 

 $\Leftrightarrow 1 \ge |c(1-z_k)|$ 

Sufficient condition

# Proof method (general) 7 - 67 (1

- Reduce (undecidable) problem in hybrid dynamical systems to
- 2. (NP-hard) problem in *real* semi-algebraic sets
- 3. Prove emptiness of algebraic problem using
- Systematic (P) relaxations
- Positivstellinsatz (Psatz)
- Sum of Squares (SOS)

#### **CDS-SOSTOOLS**

$$\begin{aligned} \mathcal{L}_{k+1} - \mathcal{L}_{k} \left( 1 - \mathcal{L}_{k} \right) \\ V(z) &= \left| z \right|^{2} \\ V(z_{k}) &\geq V(z_{k+1}) \\ \Leftrightarrow \left| z_{k} \right|^{2} - \left| c z_{k} \left( 1 - z_{k} \right) \right|^{2} &\geq 0 \\ \Leftrightarrow \left| z \right| &\leq \left| c \left( 1 - z_{k} \right) \right|^{2} \end{aligned}$$

\_ )

$$V(z) = |z|^2 \text{ decreases}$$
$$\Leftarrow 1 \ge |c|(1+|z|)$$

 $r \ge |c|(1-2_k)|$ 



$$Z_{k+1} = CZ_k \left(1 - Z_k\right)$$

 $|\mathcal{C}| \leq \mathcal{E}_2$ 

$$\left\{ \left| c \right| \le 1 \right\} \subset Mset$$

$$V(z) = |z|^2 \text{ decreases}$$
$$\Leftarrow 1 \ge |c|(1+|z|)$$



Trivial to prove that these points are in Mandelbrot set.

The proof of this region is a bit longer (using SOSTOOLS)

The longer the proof, the more fragile the remaining regions.

Proof even longer.

And so on...


#### Easy to prove these points are in *Mset*.









What's left gets more fragile.

#### This is robustly and provably *not* in *M*.



#### Using SOSTOOLS

#### This is robustly and provably in *M*.



#### Also using SOSTOOLS

### What's left is fragile.









# Next

- Architecture/protocols/layering
- SAT? Coloring? (pure discrete)
- More hybrid foundations
- Unified theories of complexity/limits
- Security and adversaries

## Details

#### A Simple Decomposition

$$\dot{x}_{1} = f(y) - g_{1}(x_{1}) 
 \dot{x}_{2} = g_{1}(x_{1}) - g_{2}(x_{2}) 
 \vdots \vdots \\
 \dot{x}_{n} = g_{n-1}(x_{n-1}) - g_{n}(x_{n}) 
 \dot{y} = 2g_{n}(x_{n}) - f(y) - g_{y}(y)$$

 $g_i$  are continuous monotone increasing functions with  $g_i(0)=0$ 

 $S_1$ 

 $S_1$  is a well behaved "simple" SISO (single-input single-output) system in R<sup>n</sup>  $S_2$  is 1-d SISO system that captures most of the nonlinearity.

The feedback interconnection between  $S_1$  and  $S_2$  is equivalent to the full system S

#### A Simple Decomposition

Given the decomposition, we look to for positive definite storage functions  $U_1(x) > 0$  and  $U_2(y) > 0$ ,  $\forall y \in B(0)$  such that

$$\begin{aligned} &\frac{d}{dt}U_1(x) \le z^2 + 2\,\delta\,wz - \kappa\,w^2, \quad \forall (x,z) \\ &\frac{d}{dt}U_2(y) < \kappa\,w^2 - 2\,\delta\,wz - z^2, \quad \forall w, \forall y \in B(0) \end{aligned}$$



where B(0) is a neighborhood of the origin.

Then  $U(x,y) = U_1(x) + U_2(y)$  is a Lyapunov function for the full system S.

The estimate of the RoA is the largest sublevel set of U(x,y) contained in  $R^n \times B(0)$ 

#### Local Small-Gain Type Condition

$$\frac{d}{dt}U_1(x) \le z^2 - w^2, \quad \forall (x, z)$$
$$\frac{d}{dt}U_2(y) < w^2 - z^2, \quad \forall w, \forall y \in B(0)$$



For  $\hat{h}_s < \hat{h} < \hat{h}_r$ , using this decomposition we can show that

$$U(x,y) = 2\sum_{i=1}^{n} \int_{0}^{x_{i}} g_{i}(\xi) d\xi + \frac{1}{2} \int_{0}^{y} (f(\xi) + g_{y}(\xi)) d\xi$$

is a Lyapunov function for the full system.

#### Local Small-Gain Example

$$\dot{x}_{1} = f(y) - g_{1}(x_{1}) \dot{x}_{2} = g_{1}(x_{1}) - g_{2}(x_{2}) \vdots \vdots \\ \dot{x}_{n} = g_{n-1}(x_{n-1}) - g_{n}(x_{n}) \dot{y} = 2g_{n}(x_{n}) - f(y) - g_{y}(y)$$



#### Let

$$g_i(x_i) = k_i x_i$$
  
 $h = 2$ 
 $q = 1$ 
 $g_y(y) = y$   
 $\gamma = \frac{3}{2}$ 

Then

$$U(x,y) = \sum_{1}^{n} k_{i} x_{i}^{2} + \frac{5}{12} \log(5 + 6y + 3y^{2}) + \frac{1}{4} y^{2} - \frac{1}{2} y - \frac{5}{12} \log 5$$

is a Lyapunov function



#### Local Dissipation Inequalities

$$\begin{aligned} &\frac{d}{dt}U_1(x) \le z^2 + 2\,\delta\,wz, \quad \forall (x,z) \\ &\frac{d}{dt}U_2(y) < -z^2 - 2\,\delta\,wz, \quad \forall w, \forall y \in B(0) \end{aligned}$$



For  $q < \hat{h} < \hat{h}_d(n)$ , using this decomposition we can show that

$$U(x, y) = \sum_{i=1}^{n} d_i \int_{0}^{x_i} g_i(\xi) d\xi - \delta \int_{0}^{y} f(\xi) d\xi$$

for some constants  $d_i > 0$ , is a Lyapunov function for the full system.

### **Block Diagonal Lyapunov Functions**

This decomposition provides a convenient way of searching for block diagonal Lyapunov functions

$$U(x,y) = U_1(x) + U_2(y)$$



#### **Proposition 3**

If there exists a block diagonal quadratic Lyapunov function for the linearization of the full system S, then there exist storage functions  $U_1$  and  $U_2$  satisfying (localy) the dissipation inequality and therefore  $U(x,y) = U_1(x) + U_2(y)$  is a Lyapunov function for the system S.

Proposition states that the dissipation inequalities are sufficient for constructing block diagonal Lyapunov functions for the system

## Limitations of the Decomposition

Let us assume that the intermediate reactions rates have the same slope at the fixed point and let  $\hat{a} = \hat{a}$ 

 $\hat{h} > \hat{h}_d(n)$ 



#### **Proposition 4**

There exists no block diagonal quadratic Lyapunov function for the linearization of the full system S

Proposition implies that this decomposition is not useful for high gains



#### **General Decomposition**



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where B(0) is a neighborhood of the origin.

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Here is an example of a 7D pathway using  $(7-n_2,n_2)$ -decomposition

- As the size  $n_2$  of the system  $S_2$ increases, we are able to construct Lyapunov functions for systems with higher gains
- As  $n_2$  increases, so does the computational complexity.

Stability Diagram f or 7D System



#### **Complexity and Performance**

If a storage function  $U_1$  exists for  $S_1$ , then a *diagonal* storage function for  $S_1$  also exists



# Size of $S_2$ determines the complexity of the full system.

So, fragile systems (high gains) require large  $S_2$  to construct Lyapunov functions (i.e., computationally complex).

#### **Complexity and Pathway Size**

As the pathway size increases, decompositions with large size S2 are required to construct Lyapunov function for smaller gains.





#### **Decomposition for General Pathways**



- Similar decomposition to the precious case
- Presence of reversible reactions means that the two subsystems are not SISO anymore