Mixed Monotone Reachability in Dynamical Systems

with application to safety of learning-enabled systems

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University of Colorado Boulder

March 20, 2025

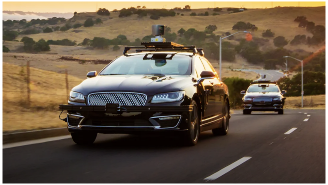
Safety-critical Autonomous Systems

Introduction

Energy/power systems

Air mobility

Autonomous driving



Manufacturing

Transportation systems

Agriculture

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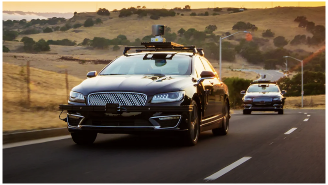

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Many autonomous systems operate in safety-critical environments

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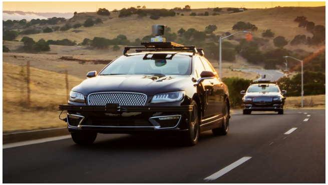

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Many autonomous systems operate in safety-critical environments

An important goal

Perform their tasks while ensuring **safety** and **robustness** of the system.

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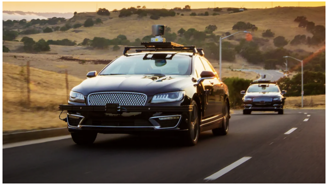

Manufacturing

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Many autonomous systems operate in safety-critical environments

Provide **guarantees** for safety and robustness of autonomous systems

Tools: Dynamical systems, Control theory, Operator theory, Optimization theory

- **Queen's University**

  Research areas: Geometric control, Functional analysis, Differential geometry

  Applications: Controllability of nonlinear systems

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- **University of Colorado Boulder**

  Research areas: Reachability of dynamical systems

  Applications: learning-enabled systems

In this talk: safety of learning-enabled autonomous system

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Significant progress: wide availability of data and computational advances

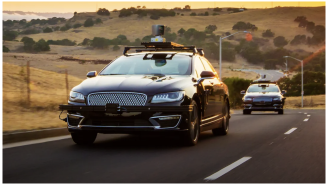
Safety-critical Autonomous Systems

Learning-enabled systems

In this talk: safety of learning-enabled autonomous system

Significant progress: wide availability of data and computational advances

Self-driving vehicles



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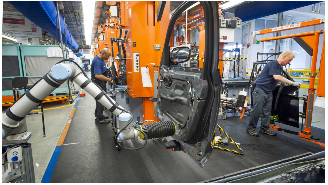

Fulfillment center

In this talk: safety of learning-enabled autonomous system

Significant progress: wide availability of data and computational advances

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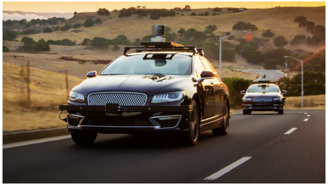

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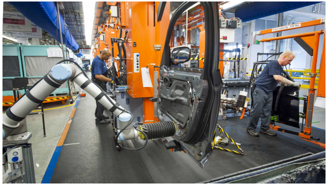

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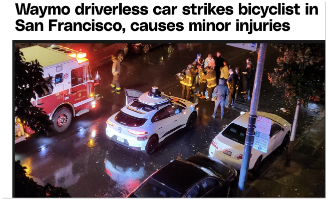
But can we ensure their safety?

In this talk: safety of learning-enabled autonomous system

Significant progress: wide availability of data and computational advances



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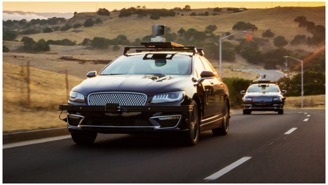

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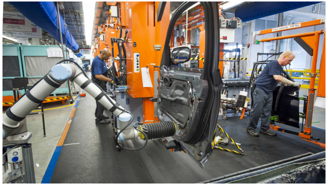

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Challenges

1. large number of parameters
2. complicated and highly nonlinear
3. operate in uncertain environments

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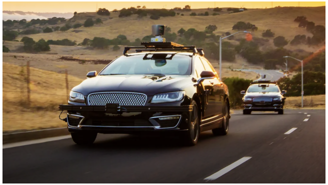

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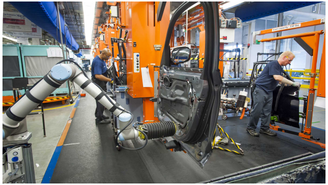

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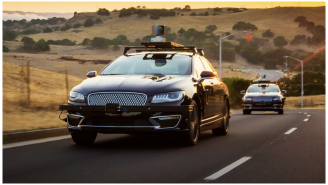

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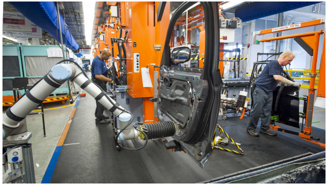

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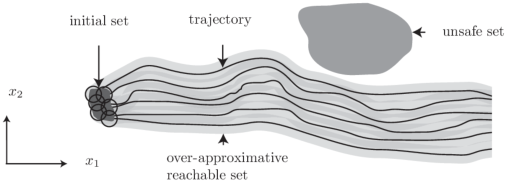
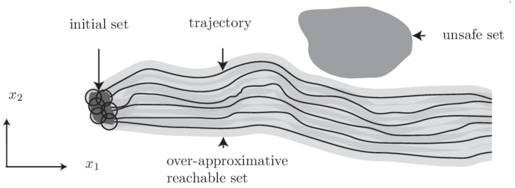


Reachability analysis estimates the evolution of the autonomous system

Safety of autonomous systems using **reachability analysis**



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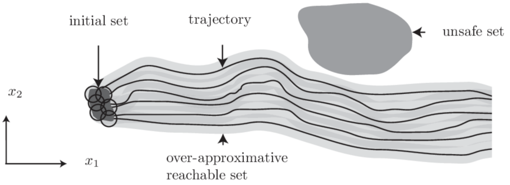
In this talk:

1. Reachability analysis = a mathematical framework for safety assurance

Safety of autonomous systems using **reachability analysis**



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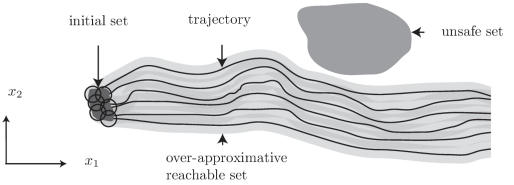
2. Efficient and scalable methods for reachability of dynamical systems

Safety of autonomous systems using **reachability analysis**



Reachability analysis estimates the evolution of the autonomous system

In this talk:

1. Reachability analysis = a mathematical framework for safety assurance
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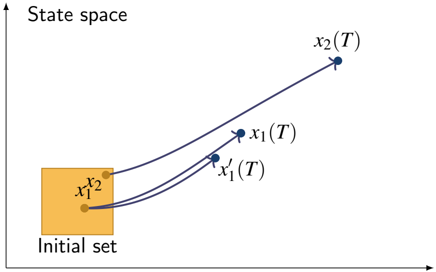
3. Application to safety verification of learning-enabled systems

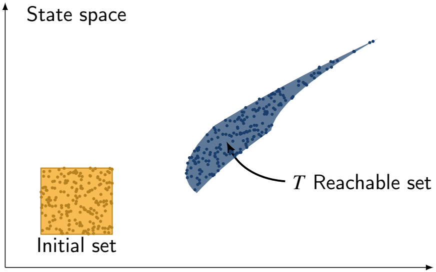
- **Reachability Analysis**
- Mixed Monotone Reachability
- Safety of Learning-enabled Systems
- Future Research Directions

Reachability Analysis

A systematic approach for safety assurance

System : $\dot{x} = f(x, w)$ **State** : $x \in \mathbb{R}^n$ **Uncertainty** : $w \in \mathcal{W} \subseteq \mathbb{R}^m$





What are the possible states of the system at time T?

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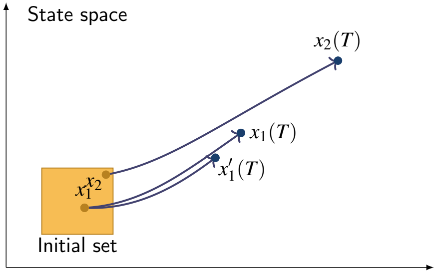

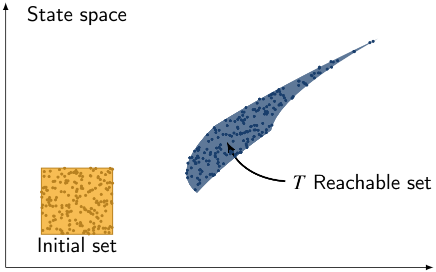

What are the possible states of the system at time T?

- **t-reachable sets** characterize evolution of the system

$$\mathcal{R}_f(t, \mathcal{X}_0, \mathcal{W}) = \{x_w(t) \mid x_w(\cdot) \text{ is a traj for some } w(\cdot) \in \mathcal{W} \text{ with } x_0 \in \mathcal{X}_0\}$$

Reachability Analysis

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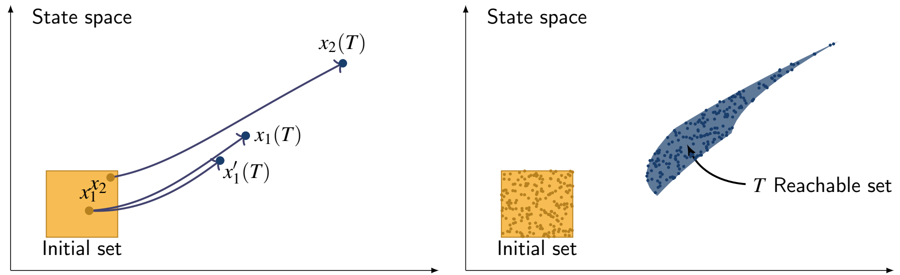

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A large number of **safety specifications** can be represented using t-reachable sets

Definition (Reach-avoid safety)

For an unsafe set $\mathcal{U} \subseteq \mathbb{R}^n$ and a target set $\mathcal{G} \subseteq \mathbb{R}^n$, system is **reach-avoid safe** if

$$\mathcal{R}_f(t, \mathcal{X}_0, \mathcal{W}) \cap \mathcal{U} = \emptyset, \qquad \text{for all } t \in [0, T_{\text{final}}] \qquad \text{(avoid)}$$

$$\mathcal{R}_f(T_{\text{final}}, \mathcal{X}_0, \mathcal{W}) \subseteq \mathcal{G}, \qquad \text{(reach)}$$

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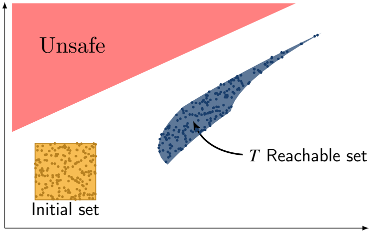

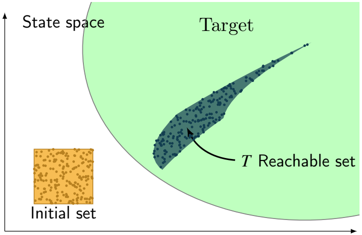

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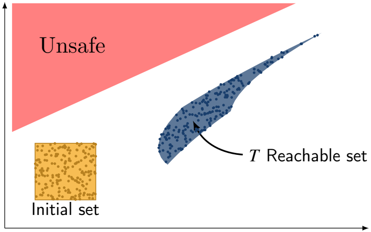

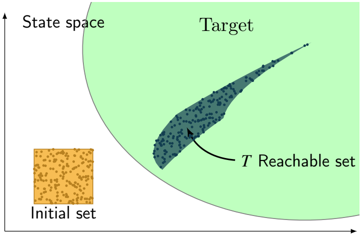

Combining different instantiation of Reach-avoid safety $\Longrightarrow$
diverse range of safety specifications
(complex planning using logics, invariance, stability)

Checking if a point belong to t-reachable sets is undecidable[1]

[1] C. Moore, Unpredictability and undecidability in dynamical systems, 1991

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Solution: over-approximations of reachable sets

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Definition: over-approximation

A set $\overline{\mathcal{R}}_f(t, \mathcal{X}_0, \mathcal{W}) \subseteq \mathbb{R}^n$ is over-approximations of t-reachable sets if

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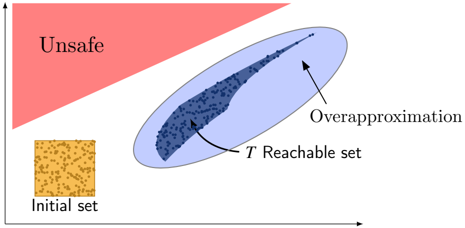
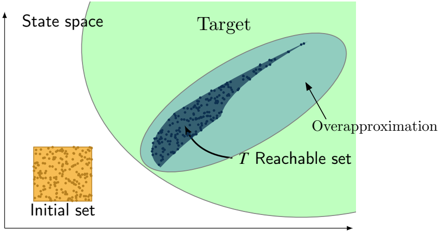


$$\overline{\mathcal{R}}_f(T, \mathcal{X}_0, \mathcal{W}) \cap \text{Unsafe set} = \emptyset$$



$$\overline{\mathcal{R}}_f(T_{\text{final}}, \mathcal{X}_0, \mathcal{W}) \subseteq \text{Target set}$$

[1] C. Moore, Unpredictability and undecidability in dynamical systems, 1991

Reachability of dynamical systems is an old problem

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Properties of reachable sets

- Skolem-Pisot problem (Skolem, 1934)
- Dynamic programing and HJB (Bellman, 1957)
- Geometric control (Sussmann and Jurdjevic, 1972)

Approximating reachable sets

- Numerical method for HJB (Mitchell et al., 2002, Bansal et al., 2017)
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In this talk: develop computationally efficient methods for over-approximating t-reachable sets

Outline of this talk

- Reachability Analysis

- **Mixed Monotonicity Reachability**

- Safety of Learning-enabled Systems

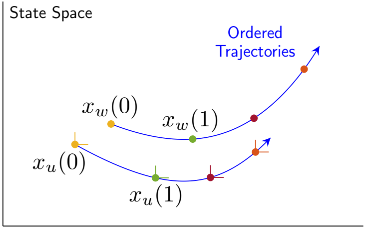
- Future Research Directions

Definition: Monotone systems

A dynamical system $\dot{x} = f(x, w)$ is monotone if

$$x_u(0) \leq y_w(0) \quad \text{and} \quad u \leq w \quad \Longrightarrow \quad x_u(t) \leq y_w(t) \quad \text{for all time}$$

where $\leq$ is the component-wise partial order.



[2] D. Angeli and E. Sontag, Monotone control systems, 2003

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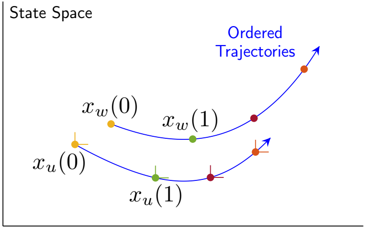
Kamke–Müller condition[2]

A dynamical system $\dot{x} = f(x, w)$ is monotone iff

1. $\frac{\partial f}{\partial x}(x, w)$ is Metzler (off-diag ≥ 0) for all x, w
2. $\frac{\partial f}{\partial w}(x, w) \geq \mathbb{0}_{n\times m}$ for all x, w



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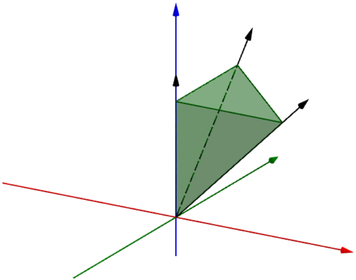
$$x_u(0) \preceq_K y_w(0) \quad \text{and} \quad u \preceq_C w \quad \implies \quad x_u(t) \preceq_K y_w(t) \quad \text{for all time}$$

where $\preceq_K$ ($\preceq_C$) is the partial order with induced by the cone K (C).

Proper pointed cone

A proper pointed cone $K \subseteq \mathbb{R}^n$ satisfies

1. $c \cdot K \subseteq K$ for every $c \geq 0$
2. K is closed and convex
3. K is pointed $(K \cap (-K) = \emptyset)$
4. K is proper $\mathrm{int}(K) \neq \emptyset$



$x \preceq_K y$ if and only if $y - x \in K$

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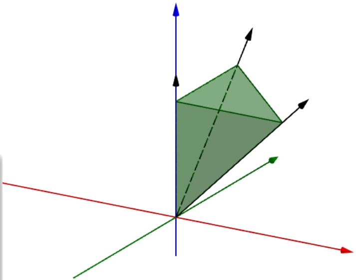
A **polyhedral cone** has the form

$$K = \underbrace{\{y \in \mathbb{R}^n \mid H_K y \geq \mathbb{0}_p\}}_{\text{halfspace rep}} = \underbrace{\{V_K y \mid y \geq \mathbb{0}_p\}}_{\text{vertex rep}}$$



Kamke–Müller condition[3]

1. $H_K(\frac{\partial f}{\partial x}(x, w) + \alpha(x, w) I_n) V_K \geq \mathbb{0}_p$ for some $\alpha(x, w)$
2. $H_K \frac{\partial f}{\partial w}(x, w) V_C \geq \mathbb{0}_q$

[c] **SJ** and S. Coogan, Monotonicity and Contraction on Polyhedral Cones, 2024.

Theorem (classical)[4]

For a monotone system with $\mathcal{W} = [\underline{w}, \overline{w}]$

$$\mathcal{R}_f(t, [\underline{x}_0, \overline{x}_0], [\underline{w}, \overline{w}]) \subseteq [x_{\underline{w}}(t), x_{\overline{w}}(t)]$$

where $x_{\underline{w}}(\cdot)$ (resp. $x_{\overline{w}}(\cdot)$) is the trajectory with disturbance $\underline{w}(\cdot)$ (resp. $\overline{w}(\cdot)$) starting at $\underline{x}_0$ (resp. $\overline{x}_0$)

[4] MW Hirsch, H Smith. Monotone dynamical systems, 2006 [Book]

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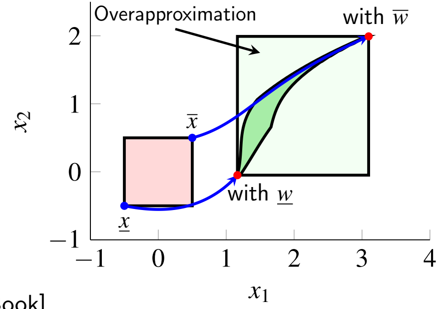
Example:

$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} x_2^3 - x_1 + w \\ x_1 \end{bmatrix}$$

$$\mathcal{W} = [2.2\ ,\ 2.3] \quad \mathcal{X}_0 = \left[\begin{bmatrix} -0.5 \\ -0.5 \end{bmatrix}, \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix}\right]$$



[4] MW Hirsch, H Smith. Monotone dynamical systems, 2006 [Book]

Theorem (classical)[4]

For a monotone system with $\mathcal{W} = [\underline{w}, \overline{w}]$

$$\mathcal{R}_f(t, [\underline{x}_0, \overline{x}_0], [\underline{w}, \overline{w}]) \subseteq [x_{\underline{w}}(t), x_{\overline{w}}(t)]$$

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Proof: $x_{\underline{w}}(0) = \underline{x}_0 \leq x(0) \leq \overline{x}_0 = x_{\overline{w}}(0)$. By monotonicity of the system

$$x_{\underline{w}}(t) \leq x(t) \leq x_{\overline{w}}(t), \text{ for all } t \geq 0$$

$$\implies \mathcal{R}_f(t, [\underline{x}_0, \overline{x}_0], [\underline{w}, \overline{w}]) \subseteq [x_{\underline{w}}(t), x_{\overline{w}}(t)]$$

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does not hold for non-monotone systems

Example:

$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} x_2^3 - x_2 + w \\ x_1 \end{bmatrix}$$

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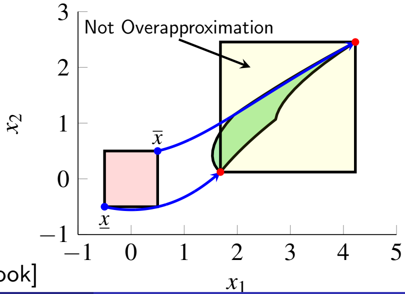

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- **Key idea:** embed the dynamical system on $\mathbb{R}^n$ into a dynamical system on $\mathbb{R}^{2n}$
- Assume $\mathcal{W} = [\underline{w}, \overline{w}]$ and $\mathcal{X}_0 = [\underline{x}_0, \overline{x}_0]$

Original system

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

Embedding system

$$\dot{\underline{x}} = \underline{d}(\underline{x}, \overline{x}, \underline{w}, \overline{w}),$$
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J-L. Gouze and L. P. Hadeler. Monotone flows and order intervals. Nonlinear World, 1994

G. Enciso, H. Smith, and E. Sontag. Nonmonotone systems decomposable into monotone systems with negative feedback . Journal of Differential Equations, 2006.

H. Smith. Global stability for mixed monotone systems. Journal of Difference Equations and Applications, 2008

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Computing decomposition function

- close connection with **inclusion function** in Numerical Analysis[5]
- mean-value inequality and interval arithmetic[6]

[e] L. Jaulin, et al. Applied Interval Analysis, 2001 [Book]

[f] A. Harapanahalli, **SJ**, S. Coogan, A toolbox for fast interval arithmetic in numpy, 2023

Mixed Monotone Theory

Embedding into higher dimensional systems

- **Key idea:** embed the dynamical system on $\mathbb{R}^n$ into a dynamical system on $\mathbb{R}^{2n}$
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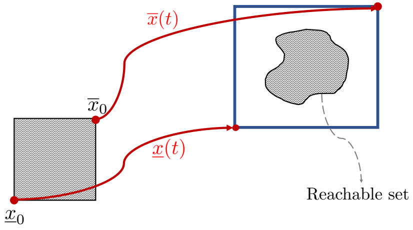
In this talk: we use mixed monotone theory for reachability analysis

Theorem[7]

Assume $\mathcal{W} = [\underline{w}, \overline{w}]$ and $\mathcal{X}_0 = [\underline{x}_0, \overline{x}_0]$ and

$$\begin{aligned} \dot{\underline{x}} &= \underline{d}(\underline{x}, \overline{x}, \underline{w}, \overline{w}), & \underline{x}(0) &= \underline{x}_0 \\ \dot{\overline{x}} &= \overline{d}(\overline{x}, \underline{x}, \overline{w}, \underline{w}), & \overline{x}(0) &= \overline{x}_0 \end{aligned}$$

Then $\mathcal{R}_f(t, \mathcal{X}_0, \mathcal{W}) \subseteq [\underline{x}(t), \overline{x}(t)]$



[7] **SJ**, et al. Efficient interaction-aware interval analysis of neural network feedback loops, 2024.

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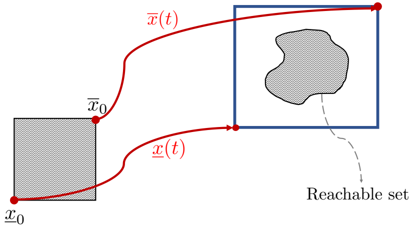

a single trajectory of embedding system provides **lower bound** ($\underline{x}$) and **upper bound** ($\overline{x}$) for the trajectories of the original system.

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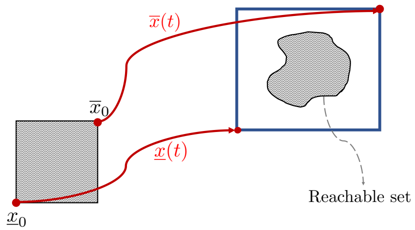


a single trajectory of embedding system provides **lower bound** ($\underline{x}$) and **upper bound** ($\overline{x}$) for the trajectories of the original system.

(Computational efficient): solve for one trajectory of embedding system

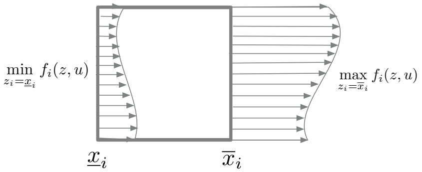
(Scalable): embedding system is $2n$-dimensional

[7] **SJ**, et al. Efficient interaction-aware interval analysis of neural network feedback loops, 2024.

The tight decomposition function is given by

$$\underline{F}_i(\underline{x}, \overline{x}, \underline{w}, \overline{w}) = \min_{\substack{z \in [\underline{x}, \overline{x}], z_i = \underline{x}_i \\ u \in [\underline{w}, \overline{w}]}} f_i(z, u),$$

$$\overline{F}_i(\underline{x}, \overline{x}, \underline{w}, \overline{w}) = \max_{\substack{z \in [\underline{x}, \overline{x}], z_i = \overline{x}_i \\ u \in [\underline{w}, \overline{w}]}} f_i(z, u)$$



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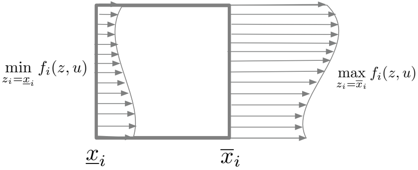

The embedding system from tight decomposition is a monotone system on $\mathbb{R}^{2n}$ with respect to the **southeast** partial order $\leq_{\mathrm{SE}}$:

$$\begin{bmatrix} x \\ \widehat{x} \end{bmatrix} \leq_{\mathrm{SE}} \begin{bmatrix} y \\ \widehat{y} \end{bmatrix} \iff x \leq y \quad \text{and} \quad \widehat{y} \leq \widehat{x}$$

In terms of cones, $\leq_{\mathrm{SE}}$ is induced by the cone $\mathbb{R}^n_{\geq 0} \times -\mathbb{R}^n_{\geq 0}$.

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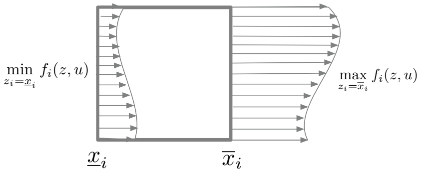

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By monotone reachability theorem: $\begin{bmatrix} x(t) \\ x(t) \end{bmatrix} \leq_{\mathrm{SE}} \begin{bmatrix} \overline{x}(t) \\ \underline{x}(t) \end{bmatrix}$

For every other decomposition function $\underline{d}, \overline{d}$,

$$\text{(tight decomposition)} \quad \underline{F}(\underline{x}, \overline{x}, \underline{w}, \overline{w}) \geq \underline{d}(\underline{x}, \overline{x}, \underline{w}, \overline{w})$$
$$\text{(tight decomposition)} \quad \overline{F}(\underline{x}, \overline{x}, \underline{w}, \overline{w}) \leq \overline{d}(\underline{x}, \overline{x}, \underline{w}, \overline{w})$$

Compare two dynamical systems using **classical monotone comparison results**[8]

$$\frac{d}{dt}\begin{bmatrix}\underline{x}\\ \overline{x}\end{bmatrix} = \begin{bmatrix}\underline{F}(\underline{x}, \overline{x}, \underline{w}, \overline{w})\\ \overline{F}(\underline{x}, \overline{x}, \underline{w}, \overline{w})\end{bmatrix}, \qquad \frac{d}{dt}\begin{bmatrix}\underline{y}\\ \overline{y}\end{bmatrix} = \begin{bmatrix}\underline{d}(\underline{y}, \overline{y}, \underline{w}, \overline{w})\\ \overline{d}(\underline{y}, \overline{y}, \underline{w}, \overline{w})\end{bmatrix}$$

This leads to

$$\begin{bmatrix}\overline{x}(t)\\ \underline{x}(t)\end{bmatrix} \leq_{\mathrm{SE}} \begin{bmatrix}\overline{y}(t)\\ \underline{y}(t)\end{bmatrix} x(t) \in [\underline{x}(t), \overline{x}(t)] \subseteq [\underline{y}(t), \overline{y}(t)].$$

[8] A. N. Michel, et al. Stability of dynamical systems: Continuous, discontinuous, and discrete systems, 2008

Outline of this talk

- Reachability Analysis
- Mixed Monotonicity Reachability
- **Safety of Learning-enabled Systems**
- Future Research Directions

Extremely fragile wrt input perturbations

Adversarial Perturbations[9]

Small changes in the input

$\downarrow$

Large changes in the output

[11] C. Szegedy, et al. Intriguing properties of neural networks, 2014

Extremely fragile wrt input perturbations

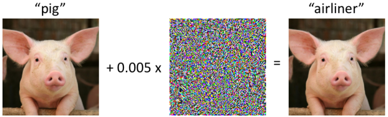

Image credit: MIT CSAIL

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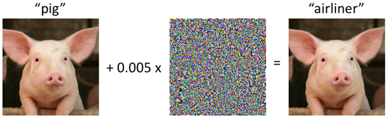
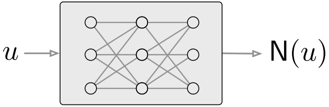


Image credit: MIT CSAIL

Safety of learning-based systems

Input perturbation set $\mathcal{U}$ and unsafe output domain $\mathcal{S}$:

$$\mathsf{N}(\mathcal{U}) \cap \mathcal{S} = \emptyset.$$



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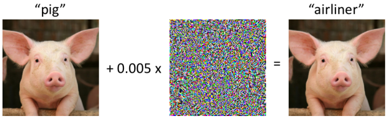

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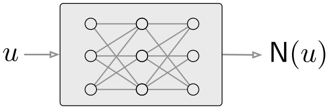
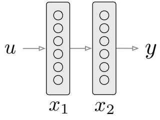


- large # of parameters with nonlinearity

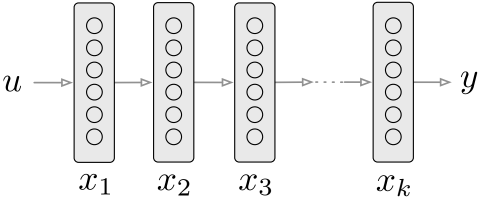


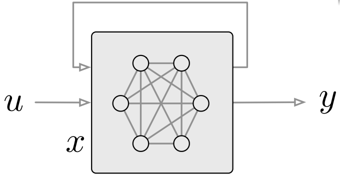
computationally efficient methods to over-approximate $\mathsf{N}(\mathcal{U})$.

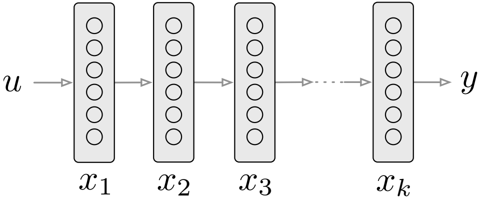
[11] C. Szegedy, et al. Intriguing properties of neural networks, 2014

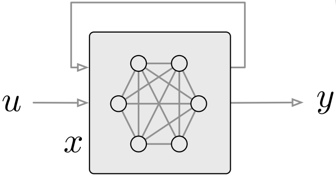
Generalized Neural Networks

Definition via fixed-point equations









- Feedforward neural networks:

$$x^{i+1} = \Phi(A_i x^i + b_i), \quad x^0 = u$$
$$y = A_k x^k + b_k$$

- Generalized neural networks:

$$x = \Phi(Ax + Bu + b)$$
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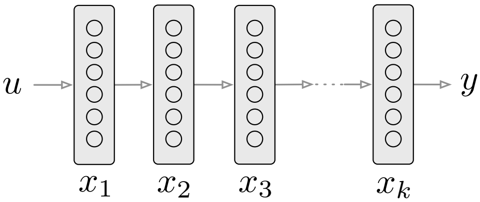

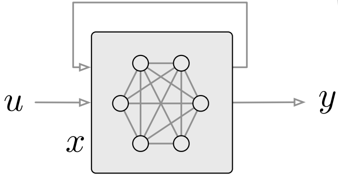

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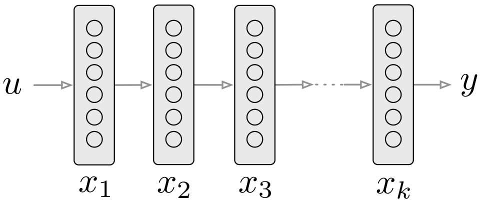
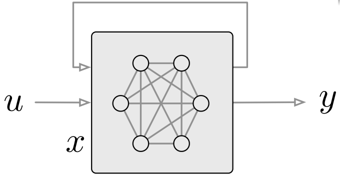
- activation functions are slope-restricted in $[0, 1]$, i.e., $0 \leq \frac{\phi_i(x) - \phi_i(y)}{x - y} \leq 1$ for all $x, y \in \mathbb{R}$





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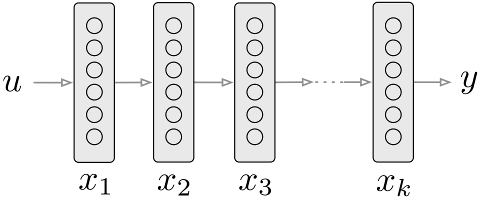
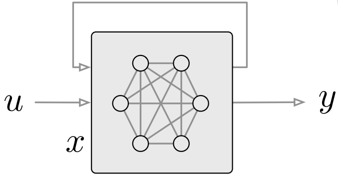
Notion of Layer: output is defined **implicitly** as a function of input

e.g., fixed-point equation, differential equations, optimization problem





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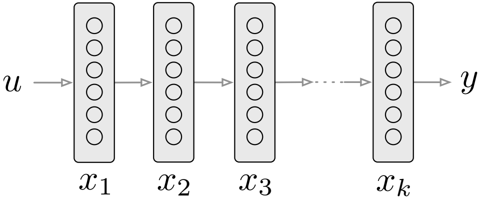
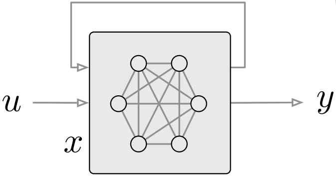
- $\Phi(y_1, \dots, y_n) = (\phi_1(y_1), \dots, \phi_n(y_n))^\top$ is a diagonal activation function
- activation functions are slope-restricted in $[0, 1]$, i.e., $0 \leq \frac{\phi_i(x) - \phi_i(y)}{x - y} \leq 1$ for all $x, y \in \mathbb{R}$

1. S. Bai, J. Z. Kolter, and V. Koltun. Deep equilibrium models, NeurIPS, 2019
2. L. El Ghaoui, F. Gu, B. Travacca, A. Askari, and A. Y. Tsai. Implicit deep learning. SIMODS, 2019





- Feedforward neural networks:

$$x^{i+1} = \Phi(A_i x^i + b_i), \quad x^0 = u$$
$$y = A_k x^k + b_k$$

- Generalized neural networks:

$$x = \Phi(Ax + Bu + b)$$
$$y = Cx + c$$

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Advantages: Representation, Performance, Memory

Main Questions

$$x = \Phi(Ax + Bu + b)$$
$$u = Cx + c$$

1. Existence and computation of solutions?
2. How to estimate the input-output $x \mapsto u$ robustness?

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Key insight

Fixed-point equation	$\Longleftrightarrow$	Dynamical system
$x = \Phi(Ax + Bu + b)$		$\dot{x} = -x + \Phi(Ax + Bu + b)$
fixed-points	$\Longleftrightarrow$	**equilibrium points**
robustness	$\Longleftrightarrow$	**reachability** $(t = \infty)$

- We can use tools from dynamical systems to study generalized neural networks

- **Metzler/non-Metzler** decomposition: $A = \lceil A \rceil^{\mathrm{Mzl}} + \lfloor A \rfloor^{\mathrm{Mzl}}$
- Example: $A = \begin{bmatrix} 2 & -1 \\ 1 & -3 \end{bmatrix} \implies \lceil A \rceil^{\mathrm{Mzl}} = \begin{bmatrix} 2 & 0 \\ 1 & -3 \end{bmatrix} \quad \lfloor A \rfloor^{\mathrm{Mzl}} = \begin{bmatrix} 0 & -1 \\ 0 & 0 \end{bmatrix}$

[12] **SJ**, et al. Robust implicit networks via non-Euclidean contractions, 2022

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Dynamical system perspective

Original system $u \in [\underline{u}, \overline{u}]$

$$\dot{x} = -x + \Phi(Ax + Bu + b) \implies$$

Tight embedding system

$$\begin{bmatrix} \dot{\underline{x}} \\ \dot{\overline{x}} \end{bmatrix} = - \begin{bmatrix} \underline{x} \\ \overline{x} \end{bmatrix} + \begin{bmatrix} \Phi(\lceil A \rceil^{\mathrm{Mzl}} \underline{x} + \lfloor A \rfloor^{\mathrm{Mzl}} \overline{x} + [B]^{+} \underline{u} + [B]^{-} \overline{u} + b) \\ \Phi(\lceil A \rceil^{\mathrm{Mzl}} \overline{x} + \lfloor A \rfloor^{\mathrm{Mzl}} \underline{x} + [B]^{+} \overline{u} + [B]^{-} \underline{u} + b) \end{bmatrix}$$

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Theorem[10]

If $\max_i \{a_{ii} + \sum_{i \neq j} |a_{ij}|\} < 1$ and $u \in [\underline{u}, \overline{u}]$

1. tight embedding system has a unique equilibrium point $\begin{bmatrix} \underline{x}^* \\ \overline{x}^* \end{bmatrix}$
2. $\left([C]^{+} \ [C]^{-}\right) \begin{bmatrix} \underline{x}^* \\ \overline{x}^* \end{bmatrix} + c \leq y \leq \left([C]^{-} \ [C]^{+}\right) \begin{bmatrix} \underline{x}^* \\ \overline{x}^* \end{bmatrix} + c$

[12] **SJ**, et al. Robust implicit networks via non-Euclidean contractions, 2022

- MNIST dataset: 28×28 pixel handwritten digits between $0 - 9$.
- Generalized NN with $n = 100$.

- $\epsilon =$ size of perturbation, $\mathcal{U} = [u - \epsilon \mathbb{1}_{784}, u + \epsilon \mathbb{1}_{784}]$.

Numerical Experiments

MNIST dataset classification

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Lipschitz Approach

$$\mathsf{N}(\mathcal{U}) \subset [y - L_{\infty}\epsilon, y + L_{\infty}\epsilon]$$

Mixed Monotone Approach

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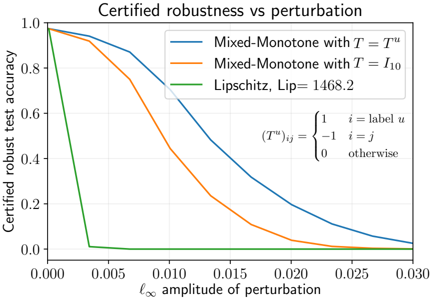

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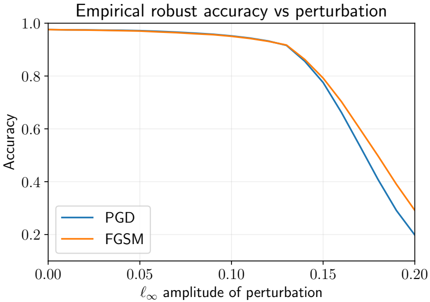

Outline of this talk

- Reachability Analysis
- Mixed Monotonicity Reachability
- Safety of Learning-enabled Systems
- **Future Research Directions**

Future Research Directions

Reachability of stochastic dynamical systems

Mixed monotone reachability: uncertainty $w \in \mathcal{W} = [\underline{w}, \overline{w}]$ are treated as worst-case using $\underline{w}$ and $\overline{w}$

[10] **SJ**, Z. Liu, and Y. Chen, "Probabilistic Reachability of Stochastic Systems", submitted to TAC 2024

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$$dX = f(X, w)dt + dV \quad \text{where } V \sim \mathcal{D}$$

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Separation Strategy: a suitable Lyapunov function to separate the stochastic noise and deterministic disturbance

[10] **SJ**, Z. Liu, and Y. Chen, "Probabilistic Reachability of Stochastic Systems", submitted to TAC 2024

Reachability of large-scale interconnected hybrid systems
Example: power grids

[11] **SJ**, P. Cisneros, F. Bullo, Contraction Theory for Dynamical Systems on Hilbert Spaces, 2022

Reachability of large-scale interconnected hybrid systems
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- Mixed monotone reachability for hybrid and switched systems
- Pattern of interconnection structure in embedding system

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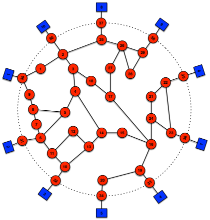
Coupled oscillator model of power grids

$$\dot{\theta}_i = \omega_i$$
$$M_i \dot{\omega}_i = p_i - D_i \omega_i + \sum_{j=1}^{n} a_{ij} \sin(\theta_j - \theta_i)$$

where $a_{ij} = |Y_{ij}| V_i V_j$ is the active power capacity of line (i, j)



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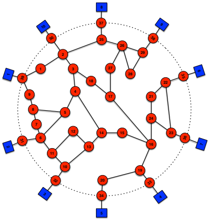

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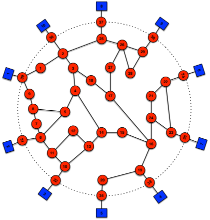

- **Question:** how to choose a suitable cone K for Mixed monotone reachability?
- **Question:** how to extend Mixed monotone reachability to infinite dimensional spaces?[11]

[11]**SJ**, P. Cisneros, F. Bullo, Contraction Theory for Dynamical Systems on Hilbert Spaces, 2022

Future Research Directions

Safety beyond reachability

Safety using Barrier and Lyapunov functions for **monotone systems**

Safety using Barrier and Lyapunov functions for monotone systems

- Barrier function $B : \mathbb{R}^n \to \mathbb{R}$ for dynamical system $\dot{x} = f(x, w)$:

$$B(x) \leq 0 \quad \text{for all } x \in \mathcal{X}_0$$

$$B(x) > 0 \quad \text{for all } x \in \mathcal{U}$$

$$\frac{\partial B}{\partial x}(x) f(x, w) \leq 0 \quad \text{for all } w \in [\underline{w}, \overline{w}] \text{ and } x \text{ s.t. } B(x) = 0$$

Then system is always safe (never enters the unsafe region)

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Barrier introduce a functional perspective toward safety analysis

- Numerous efficient methods for finding B in the literature
- **Question:** Does monotonicity of $\dot{x} = f(x, w)$ impose any structure on B?

Teaching Interests

Plans and vision for teaching

- 1550: Differential and Integral Calculus
- 2030 Discrete Dynamical Systems
- 2065 Elementary Differential Equations
- 2070 Mathematical Methods in Engineering
- 2090 Elementary Differential Equations and Linear Algebra
- 4025 Optimization Theory and Applications
- 4027 Differential Equations
- 7320 Ordinary Differential Equations

1. **Contraction theory for dynamical systems and optimization algorithms**
   topics: monotone operator theory, normed spaces, dynamical systems
2. **Dynamical systems on networks**
   topics: Nonlinear dynamical systems, algebraic graph theory, matrix theory

Thank you for your attention!

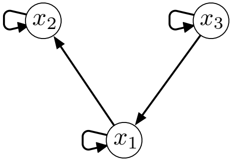
Back up Slides

A system $\dot{x} = f(x, w)$ satisfies Kamke– Müller condition if, for every $x \leq y$, every $u \leq w$, and every $i \in \{1, \ldots, n\}$,

$$x_i = y_i \implies f_i(x, u) \leq f_i(y, w)$$

- **Metzler/non-Metzler** decomposition: $A = \lceil A \rceil^{\mathrm{Mzl}} + \lfloor A \rfloor^{\mathrm{Mzl}}$
- Example: $A = \begin{bmatrix} 2 & 0 & -1 \\ 1 & -3 & 0 \\ 0 & 0 & 1 \end{bmatrix} \implies \lceil A \rceil^{\mathrm{Mzl}} = \begin{bmatrix} 2 & 0 & 0 \\ 1 & -3 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \lfloor A \rfloor^{\mathrm{Mzl}} = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$

Linear systems



Original system

$$\dot{x} = Ax + Bw$$

Embedding system

$$\dot{\underline{x}} = \lceil A \rceil^{\mathrm{Mzl}} \underline{x} + \lfloor A \rfloor^{\mathrm{Mzl}} \overline{x} + B^{+} \underline{w} + B^{-} \overline{w}$$
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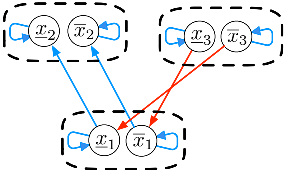

How to compute a decomposition function for a system?

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- Assume $f : \mathbb{R} \to \mathbb{R}$ is scalar:

Mean-value Inequality

$$f(\underline{x}) + \left[\min_{z\in[\underline{x},\overline{x}]} \frac{\partial f}{\partial x}\right] (\overline{x} - \underline{x}) \leq f(x) \leq f(\underline{x}) + \left[\max_{z\in[\underline{x},\overline{x}]} \frac{\partial f}{\partial x}\right] (\overline{x} - \underline{x})$$

where $[A]^+ = \max\{A, 0\}$ and $[A]^- = \min\{A, 0\}$.

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The effect of $\overline{x}$ on $\underline{d}(\underline{x}, \overline{x})$ is competitive.

The effect of $\overline{x}$ on $\overline{d}(\underline{x}, \overline{x})$ is cooperative.

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Punchline

sign pattern of $\frac{\partial f}{\partial x}$ separates cooperative and competitive effect of states.

How to compute a decomposition function for a system?

Theorem[12]

Jacobian-based: $\dot{x} = f(x,u)$ such that $\frac{\partial f}{\partial x} \in [\underline{J}_{[\underline{x},\overline{x}]}, \overline{J}_{[\underline{x},\overline{x}]}]$ and $\frac{\partial f}{\partial u} \in [\underline{J}_{[\underline{u},\overline{u}]}, \overline{J}_{[\underline{u},\overline{u}]}]$, then

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$\underline{x} \mapsto R_1 \mapsto R_2 \mapsto \ldots \mapsto R_n \mapsto \overline{x}$, then the i-th column of $\underline{M}$ is $\min_{z \in R_i, w \in [\underline{u},\overline{u}]} \frac{\partial f_i}{\partial x}(z,w)$

[4] **SJ** and A. Harapanahalli and S. Coogan, IEEE TAC, 2023

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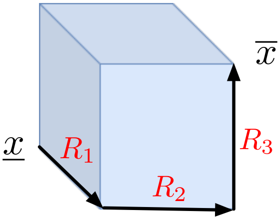
- Interval analysis for computing Jacobian bounds.
- Use tools and techniques from interval analysis.



[4] **SJ** and A. Harapanahalli and S. Coogan, IEEE TAC, 2023

Differential condition

Logarithmic norm

Given a matrix $A \in \mathbb{R}^{n\times n}$ and a norm $\|\cdot\|$:

$$\mu_{\|\cdot\|}(A) := \lim_{h\to 0^+} \frac{\|I_n + hA\| - 1}{h}$$

- Directional derivative of norm $\|\cdot\|$ in direction of A,

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[1] A. Davydov, **SJ**, F. Bullo, Non-Euclidean contraction theory for robust nonlinear stability, 2022

Differential condition

Logarithmic norm

Given a matrix $A \in \mathbb{R}^{n\times n}$ and a norm $\|\cdot\|$:

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Integral condition

Weak pairing[13]

Given a norm $\|\cdot\|$, the associated weak pairing is $[\![\cdot,\cdot]\!] : \mathbb{R}^n \times \mathbb{R}^n \to \mathbb{R}$:

- Subadditive and weakly homogeneity
- Positive definite
- Cauchy-Schwarz inequality
- $[\![x, x]\!] = \|x\|^2$

$$[\![x, y]\!]_2 = y^\top x$$
$$[\![x, y]\!]_1 = \mathrm{sign}(y)^\top x$$
$$[\![x, y]\!]_\infty = \max_{i\in I_\infty(x)} x_i y_i$$

$$I_\infty(x) = \{i \mid |x_i| = \|x\|_\infty\}$$

[1] A. Davydov, **SJ**, F. Bullo, Non-Euclidean contraction theory for robust nonlinear stability, 2022

Theorem[14]

$\dot{x} = f(x,u)$ is contracting wrt $\|\cdot\|$ with rate c iff

Differential: $\mu_{\|\cdot\|}(D_x f(x,u)) \leq -c,$ for all x, u

Integral: $[\![f(x,u) - f(y,u), x - y]\!] \leq -c\|x-y\|^2,$ for all x, y, u

[2] A. Davydov, S. Jafarpour, F. Bullo, TAC 2022

Theorem

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- Connection between **contraction theory** and **monotone operator theory**

f is a contracting vector field wrt to $\|\cdot\|_2$
iff
$-f$ is a strongly monotone operator wrt to the inner product $\langle \cdot, \cdot \rangle$.

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- Connection between **contraction theory** and **monotone operator theory**

f is a contracting vector field wrt to $\|\cdot\|$
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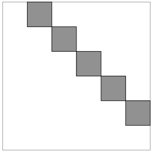
Generalized neural networks

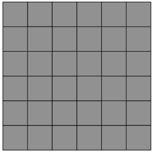
Origin and motivations

- Origins:

- Generalizing feedforward neural networks to fully-connected synaptic matrices

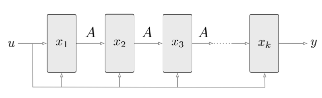
Intuition: $z^{i+1} = \phi_i(A_i z^i + b_i) \quad \Longleftrightarrow \quad z = \Phi(Ax + Bu + b)$, where A has upper diagonal structure.

$A_{\text{upper-diagonal}} =$ 

$A_{\text{complete}} =$ 

- comparable accuracy to traditional neural networks with significant memory reduction

Intuition: generalized neural network = weight-tied infinite-layer network



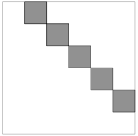
$z^{i+1} = \phi_i(Az^i + B_i x + b_i) \implies \lim_{i\to\infty} z^i = x^*$ solution to the generalized neural network

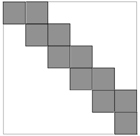
- suitable for learning constrained optimization problems

Intuition: casting KKT condition as an implicit layer

- vanishing and exploding gradient

Intuition: the notion of "autapse" (time-delayed self-feedback) from neuroscience

$A_{\text{upper-diagonal}} =$ 

$A_{\text{Autapse}} =$ 

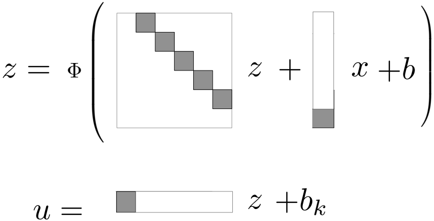
- suitable for learning stiff problems or problems with discontinuity

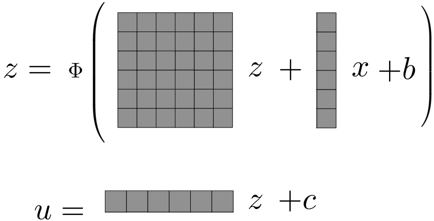
- Feedforward neural networks:

$$z^{(\ell+1)} = \Phi(A_\ell z^{(\ell)} + b_\ell), \quad z^{(0)} = x$$
$$u = A_k z^{(k)} + b_k$$

- Generalized neural networks:

$$z = \Phi(Az + Bx + b)$$
$$u = Cz + c$$





1. loss function $\mathcal{L}$ and training data $(\widehat{x}_i, \widehat{u}_i)_{i=1}^N$
2. $\epsilon =$ size of ℓ_∞-perturbation in input: $\mathcal{X} = [\underbrace{x - \epsilon \mathbb{1}_r}_{\underline{x}}, \underbrace{x + \epsilon \mathbb{1}_r}_{\overline{x}}]$

Training generalized neural networks

$$\min_{A,B,b,c} \sum_{i=1}^{N} \mathcal{L}(\widehat{u}_i, Cz_i + c)$$
$$z_i = \Phi(Az_i + B\widehat{u}_i + b),$$
$$a_{ii} + \sum_{j=1} |a_{ij}| \leq \gamma \qquad \text{well-posedness}$$

Training FFNNs

$$\min_{A,B,b,c} \sum_{i=1}^{N} \mathcal{L}(\widehat{u}_i, Cz_i^{(k)} + c)$$
$$z_i^{(\ell+1)} = \Phi(A_\ell z_i^{(\ell)} + b_\ell), \quad \ell \in \{1, \dots, k-1\}$$

Training generalized neural networks

Promoting robustness via regularization

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2. $\epsilon =$ size of ℓ_∞-perturbation in input: $\mathcal{X} = [\underbrace{x - \epsilon \mathbb{1}_r}_{\underline{x}}, \underbrace{x + \epsilon \mathbb{1}_r}_{\overline{x}}]$

output $u \in [\underline{u}(\epsilon), \overline{u}(\epsilon)]$

Training generalized neural networks

$$\min_{A,B,b,c} \sum_{i=1}^N \mathcal{L}(\widehat{u}_i, Cz_i + c) + \kappa \underbrace{\mathcal{R}(\underline{u}_i(\epsilon), \overline{u}_i(\epsilon))}_{\text{robustness}}$$

$$z_i = \Phi(Az_i + B\widehat{u}_i + b),$$

$$a_{ii} + \sum_{j=1} |a_{ij}| \leq \gamma < 1 \qquad \text{well-posedness}$$

Training FFNNs (S. Gowal, et. al., 2018)

$$\min_{A,B,b,c} \sum_{i=1}^N \mathcal{L}(\widehat{u}_i, Cz_i^{(k)} + c) + \kappa \underbrace{\mathcal{R}(\underline{u}_i(\epsilon), \overline{u}_i(\epsilon))}_{\text{robustness}}$$

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- $\mathcal{R}(\underline{u}(\epsilon), \overline{u}(\epsilon))$ uses $\underline{y}(\epsilon)$ and $\overline{u}(\epsilon)$ to estimate robustness margin
- κ, ϵ, γ are hyperparameters

Accuracy of Mixed Monotone Reachability

How accurate are hyper-rectangular over-approximations?

Monotone reachability is tight

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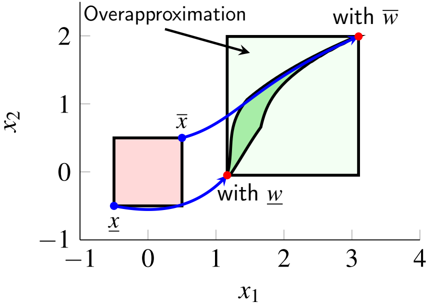
$$\frac{d}{dt}\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} x_2^3 - x_1 + w \\ x_1 \end{bmatrix}$$

$$\mathcal{W} = [2.2\ ,\ 2.3] \quad \mathcal{X}_0 = \left[\begin{bmatrix} -0.5 \\ -0.5 \end{bmatrix}, \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix}\right]$$



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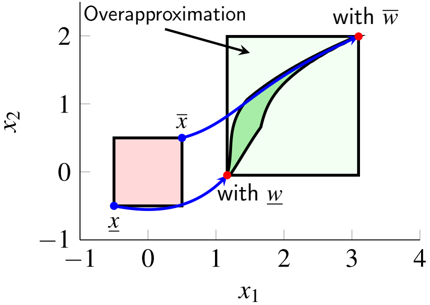

Question: how accurate is mixed monotone reachability?

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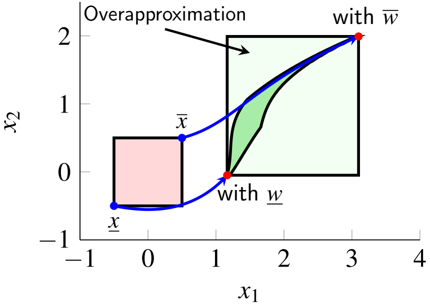

Question: how accurate is mixed monotone reachability?

Accuracy = the distance between trajectories of **embedding system**

$\begin{bmatrix} x^*(t) \\ x^*(t) \end{bmatrix}$ and $\begin{bmatrix} \underline{x}(t) \\ \overline{x}(t) \end{bmatrix}$ traj of embedding system $\implies$ provide bounds on $\|x^*(t) - \underline{x}(t)\|$ and $\|x^*(t) - \overline{x}(t)\|$

Definition: Contracting systems

$\dot{x} = f(x, w)$ is contracting wrt $\|\cdot\|$ with rate c if

$$\|x_w(t) - y_w(t)\| \leq e^{ct}\|x_w(0) - y_w(0)\|, \text{ for all } w \in \mathcal{W}, \quad t \geq 0.$$

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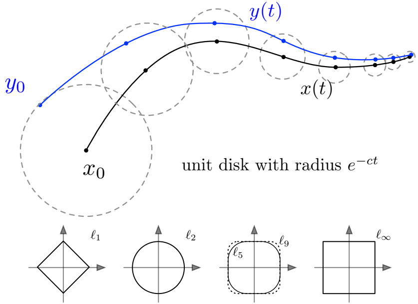
Highly regular properties

- existence of a globally stable equilibrium point
- efficient equilibrium point computation
- input-output robustness
- entrainment to periodic orbits



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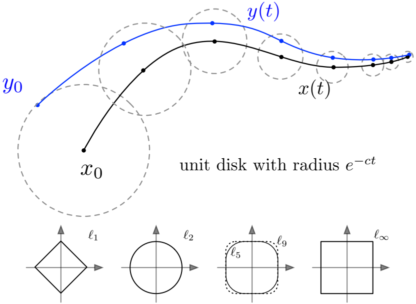

How to characterize contractivity using vector fields?

Definition: Matrix measure

Given a matrix $A \in \mathbb{R}^{n \times n}$ and a norm $\|\cdot\|$:

$$\mu_{\|\cdot\|}(A) := \lim_{h \to 0^+} \frac{\|I_n + hA\| - 1}{h}$$

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[9] W. Lohmiller and J. Slotine, On Contraction Analysis for Nonlinear Systems, 1998

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Theorem (Classical result)[15]

$\dot{x} = f(x, w)$ is contracting wrt $\|\cdot\|$ with rate c iff

$$\mu_{\|\cdot\|}\left(\tfrac{\partial f}{\partial x}(x, w)\right) \leq c, \qquad \text{for all } x, w$$

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Embedding Systems

Contraction rate wrt ℓ_∞-norm

Theorem[16]

Let $\frac{d}{dt}\begin{bmatrix}\underline{x}\\ \overline{x}\end{bmatrix} = \begin{bmatrix}\underline{F}(\underline{x},\overline{x},\underline{w},\overline{w})\\ \overline{F}(\underline{x},\overline{x},\underline{w},\overline{w})\end{bmatrix} := e(\underline{x},\overline{x},\underline{w},\overline{w})$ be the embedding system from the tight decomposition function for $\dot{x} = f(x,w)$. For $x \in [\underline{x},\overline{x}]$, $w \in [\underline{w},\overline{w}]$

$$\mu_\infty\left(\frac{\partial f}{\partial x}(x,w)\right) \leq c \quad \Longleftrightarrow \quad \mu_\infty\left(\frac{\partial e}{\partial\left[\begin{smallmatrix}\underline{x}\\ \overline{x}\end{smallmatrix}\right]}(\underline{x},\overline{x},\underline{w},\overline{w})\right) \leq c$$

[10]**SJ** and S. Coogan, Monotoncity and contraction on polyhedral cones, 2024

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hyper-rectangles evolve with ℓ_∞ contraction rate of original system

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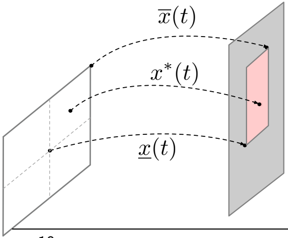

Gray = contraction tube
Red = Mixed Monotone hyper-rectangle

$$\left\|\begin{bmatrix}x^*(t)\\ x^*(t)\end{bmatrix} - \begin{bmatrix}\underline{x}(t)\\ \overline{x}(t)\end{bmatrix}\right\|_\infty \leq e^{ct}\left\|\begin{bmatrix}x^*(0)\\ x^*(0)\end{bmatrix} - \begin{bmatrix}\underline{x}(0)\\ \overline{x}(0)\end{bmatrix}\right\|_\infty$$

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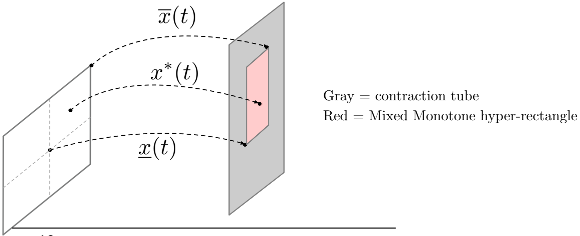

$$\|x^*(t) - \underline{x}(t)\|_\infty \leq e^{ct}L$$
$$\|x^*(t) - \overline{x}(t)\|_\infty \leq e^{ct}L$$

$$L = \max\{\|x^*(0) - \underline{x}(0)\|_\infty, \|x^*(0) - \overline{x}(0)\|_\infty\}$$

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Idea of proof

connecting the **order structure** and **metric structure** of system

Definition: Gauge norm

Given a pointed proper cone K, $\|v\|_K = \inf\{\lambda \geq 0 \mid -\lambda\mathbb{1}_n \preceq_K v \preceq_K \lambda\mathbb{1}_n\}$

ℓ_∞-norm is the gauge norm for the proper pointed cone $\mathbb{R}^n_{\geq 0}$.

[10]**SJ** and S. Coogan, Monotoncity and contraction on polyhedral cones, 2024