Interaction-aware Reachability of Neural Network Controlled Systems:

A Mixed Monotone Approach

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SJ and A. Harapanahalli and S. Coogan. Efficient Interaction-Aware Interval Analysis of Neural Network Feedback Loops. arXiv, 2023.

A. Harapanahalli an **SJ** and S. Coogan. A Toolbox for Fast Interval Arithmetic in numpy with an Application to Formal Verification of Neural Network Controlled Systems. 2nd ICML workshop on Formal Verification of Machine Learning, 2023

A. Harapanahalli and **SJ** and S. Coogan. Forward Invariance in Neural Network Controlled Systems. arXiv, 2023.

Neural Network Controllers

• Neural Networks as controllers in safety-critical applications (examples: autonomous vehicles and mobile robots)



Issues with neural network controllers:

- large # of parameters with nonlinearity
- sensitive wrt to input perturbations
- limited closed-loop safety guarantees



Challenges

Rigorous verification and computational efficiency vs. accuracy.

Safety Verification via Reachability Analysis Problem Statement

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



• reachable sets characterize evolution of the system

 $\mathcal{R}^f(t, \mathcal{X}_0) = \{x_w(t) \mid x_w(\cdot) \text{ is a traj of the system for some } w \text{ with } x_0 \in \mathcal{X}_0\}$

- over-approximation of reachable sets for safety and verification
- reachability of dynamical system is an old problem with several classical approaches

Classical approaches are not scalable to large-scale nonlinear systems

Monotone Dynamical Systems

Definition and Characterization

A dynamical system $\dot{x} = f(x, w)$ is monotone¹(with respect to cones K, C) if

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

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



¹D. Angeli and E. Sontag, "Monotone control systems", IEEE TAC, 2003

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In this talk: monotone system theory for reachability analysis

¹D. Angeli and E. Sontag, "Monotone control systems", IEEE TAC, 2003

Reachability of Monotone Dynamical Systems

Hyper-rectangular over-approximations

Theorem (classical result)

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

$$\mathcal{R}^{f}(t, [\underline{x}_{0}, \overline{x}_{0}]) \subseteq [x_{\underline{w}}(t), x_{\overline{w}}(t)]$$

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

Example:

$$\frac{d}{dt} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} x_2^3 - x_1 + w \\ x_1 \end{bmatrix}$$
$$\mathcal{W} = \begin{bmatrix} 2.2 , 2.3 \end{bmatrix} \quad \mathcal{X}_0 = \begin{bmatrix} \begin{bmatrix} -0.5 \\ -0.5 \end{bmatrix}, \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} \end{bmatrix}$$



• For non-monotone dynamical systems the extreme trajectories do not provide any over-approximation of reachable sets

Example:

$$\frac{d}{dt} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} x_2^3 - x_2 + w \\ x_1 \end{bmatrix}$$
$$\mathcal{W} = \begin{bmatrix} 2.2 \\ , \end{bmatrix} \\ \mathcal{X}_0 = \begin{bmatrix} \begin{bmatrix} -0.5 \\ -0.5 \end{bmatrix}, \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} \end{bmatrix}$$



Mixed Monotone Theory

Embedding into a larger system

- 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 $\mathcal{X}_0 = [\underline{x}_0, \overline{x}_0]$



 $\underline{d}, \overline{d} \text{ are decomposition functions s.t.}$ $f(x, w) = \underline{d}(x, x, w, w) \text{ for every } x, w$ $cooperative: (\underline{x}, \underline{w}) \mapsto \underline{d}(\underline{x}, \overline{x}, \underline{w}, \overline{w})$ $competitive: (\overline{x}, \overline{w}) \mapsto \underline{d}(\underline{x}, \overline{x}, \underline{w}, \overline{w})$

④ the same properties for \overline{d}

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

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

In terms of cones, $\leq_{\rm SE}$ is induced by the cone $\mathbb{R}^n_{>0} imes - \mathbb{R}^n_{>0}$.

Mixed Monotone Theory

Versatility and History

• f locally Lipschitz \implies a decomposition function exists

The best (tightest) decomposition function is given by

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

A short (and incomplete) history:

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

Reachability using Embedding Systems

Hyper-rectangular over-approximations

Theorem ²	
Assume $\mathcal{W} = [\underline{w}, \overline{w}]$ and $\mathcal{X}_0 =$	$[\underline{x}_0,\overline{x}_0]$ and
$ \underline{\dot{x}} = \underline{d}(\underline{x}, \overline{x}, \underline{w}, \overline{w}), \\ \underline{\dot{x}} = \overline{d}(\overline{x}, x, \overline{w}, w), $	$\underline{x}(0) = \underline{x}_0$ $\overline{x}(0) = \overline{x}_0$
Then $\mathcal{R}^f(t, \mathcal{X}_0) \subseteq [x(t), \overline{x}(t)]$	() 0



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

²Coogan and Arcak, "Efficient finite abstraction of mixed monotone systems", HSCC, 2015.

Reachability using Embedding Systems

Example

Original System:

$$\frac{d}{dt} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} x_2^3 - x_2 + w \\ x_1 \end{bmatrix}$$
$$\mathcal{W} = \begin{bmatrix} 2.2 , 2.3 \end{bmatrix} \quad \mathcal{X}_0 = \begin{bmatrix} \begin{bmatrix} -0.5 \\ -0.5 \end{bmatrix}, \begin{bmatrix} 0.5 \\ 0.5 \end{bmatrix} \end{bmatrix}$$

red = cooperative, blue = competitive

Embedding System:







Systems with NN Controllers

A Mixed Monotone Approach

Given the open-loop nonlinear system with a neural network controller

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

study reachability of the closed-loop system

 $\dot{x} = f(x, N(x), w) := f^c(x, w)$



Challenge: find a decomposition function for closed-loop system

Key observation: Interval bounds for neural networks combines nicely with mixed monotone theory for the open-loop system!

• Interval bounds for NN using verification algorithms (CROWN, LipSDP, IBP, etc)

Question: How to capture the interaction between NN and the system

Decomposition Functions for Systems

A Jacobian-based Approach

$$\begin{aligned} \mathbf{Jacobian-based:} \ \dot{x} &= f(x,w) \text{ such that } \frac{\partial f}{\partial x} \in [\underline{J}_{[\underline{x},\overline{x}]}, \overline{J}_{[\underline{x},\overline{x}]}] \text{ and } \frac{\partial f}{\partial w} \in [\underline{J}_{[\underline{w},\overline{w}]}, \overline{J}_{[\underline{w},\overline{w}]}], \text{ then} \\ \\ \left[\frac{d(\underline{x},\overline{x},\underline{w},\overline{w},\overline{w})}{\overline{d}(\underline{x},\overline{x},\underline{w},\overline{w})} \right] &= \begin{bmatrix} -[\underline{J}_{[\underline{x},\overline{x}]}]^{-} & [\underline{J}_{[\underline{x},\overline{x}]}]^{-} \\ -[\overline{J}_{[\underline{x},\overline{x}]}]^{+} & [\overline{J}_{[\underline{x},\overline{x}]}]^{+} \end{bmatrix} \begin{bmatrix} \underline{x} \\ \overline{x} \end{bmatrix} + \begin{bmatrix} -[\underline{J}_{[\underline{w},\overline{w}]}]^{-} & [\underline{J}_{[\underline{w},\overline{w}]}]^{-} \\ -[\overline{J}_{[\underline{w},\overline{w}]}]^{+} & [\overline{J}_{[\underline{w},\overline{w}]}]^{+} \end{bmatrix} \begin{bmatrix} \underline{w} \\ \overline{w} \end{bmatrix} + \begin{bmatrix} f(\underline{x},\underline{w}) \\ f(\underline{x},\underline{w}) \end{bmatrix} \end{aligned}$$

- Interval arithmetic allows computing Jacobian bounds efficiently using *inclusion functions*.
- npinterval³: Toolbox that implements intervals as native data-type in numpy.



³Harapanahalli, Jafarpour, Coogan. "A Toolbox for Fast Interval Arithmetic in numpy with an Application to Formal Verification of Neural Network Controlled Systems", 2nd WFVML, ICML, 2023

Interval Bounds for Neural Networks

Input-output Bounds vs. Functional Bounds

Input-output bounds: Given a neural network controller u = N(x)

 $\underline{u}_{[\underline{x},\overline{x}]} \leq N(x) \leq \overline{u}_{[\underline{x},\overline{x}]}, \quad \text{ for all } x \in [\underline{x},\overline{x}]$

Functional bounds: Given a neural network controller u = N(x) $\underline{N}_{[x,\overline{x}]}(x) \le N(x) \le \overline{N}_{[x,\overline{x}]}(x), \text{ for all } x \in [\underline{x},\overline{x}]$

• Example: CROWN⁴can provide both input-output and functional bounds.

 $\begin{array}{ll} \text{CROWN functional bounds:} \\ \underline{N}_{[\underline{x},\overline{x}]}(x) = \underline{A}_{[\underline{x},\overline{x}]}x + \underline{b}_{[\underline{x},\overline{x}]}, \\ \overline{N}_{[\underline{x},\overline{x}]}(x) = \overline{A}_{[\underline{x},\overline{x}]}x + \overline{b}_{[\underline{x},\overline{x}]} \end{array} \end{array} \xrightarrow{} \begin{array}{l} \text{CROWN input-output bounds:} \\ \underline{u}_{[\underline{x},\overline{x}]} = \underline{A}^+_{[\underline{x},\overline{x}]}\overline{x} + \overline{A}^-_{[\underline{x},\overline{x}]}\underline{x} + \underline{b}_{[\underline{x},\overline{x}]}, \\ \overline{u}_{[\underline{x},\overline{x}]} = \overline{A}^+_{[\underline{x},\overline{x}]}\overline{x} + \underline{A}^-_{[\underline{x},\overline{x}]}\underline{x} + \overline{b}_{[\underline{x},\overline{x}]}, \\ \end{array}$

⁴Zhang, Weng, Chen, Hsieh, Daniel. "Efficient neural network robustness certification with general activation functions." NeurIPS, 2018.

Approach #1: Interconnection-based Approach

A pictorial explanation

Original system:



Embedding system:



How does the interconnection-based approach work?

- closed-loop embedding system = interconnection of NN interval bounds + open-loop embedding system
- NN bounds are evaluated on each edge instead of the whole box, i.e., we use <u>u[x_{i:x}, x]</u> and <u>u[x_{i:x}, x]</u> instead of <u>u[x, x]</u> and <u>u[x, x]</u>.



Systems with NN Controllers

Interconnection-based Approach

Theorem⁵

1 Decomposition function $\underline{d}, \overline{d}$ for the open-loop system $\dot{x} = f(x, u, w)$

② Interval input-output bounds $\underline{u}_{[\underline{x},\overline{x}]}, \overline{u}_{[\underline{x},\overline{x}]}$ for the neural network controller u = N(x), Then

$$\frac{\underline{d}_{i}^{c}(\underline{x},\overline{x},\underline{w},\overline{w})}{\overline{d}_{i}^{c}(\underline{x},\overline{x},\underline{w},\overline{w},\overline{w})} = \underline{d}_{i}(\underline{x},\overline{x},\underline{\eta}^{i},\overline{\eta}^{i},\underline{w},\overline{w})$$
$$\overline{d}_{i}^{c}(\underline{x},\overline{x},\underline{w},\overline{w},\overline{w}) = \overline{d}_{i}(\underline{x},\overline{x},\underline{\nu}^{i},\overline{\nu}^{i},\underline{w},\overline{w})$$

where

$$\underline{\eta}^{i} = \underline{u}_{[\underline{x},\overline{x}_{i:\underline{x}}]} \quad \overline{\eta}^{i} = \overline{u}_{[\underline{x},\overline{x}_{i:\underline{x}}]}, \qquad \underline{\nu}^{i} = \underline{u}_{[\underline{x}_{i:\overline{x}},\overline{x}]} \quad \overline{\nu}^{i} = \overline{u}_{[\underline{x}_{i:\overline{x}},\overline{x}]},$$

is a **decomposition function for the closed-loop system** where $v_{i:w}$ is the vector v with ith component replaced with ith component of w.

⁵Jafarpour, Harapanahalli, Coogan. "Efficient Interaction-aware Interval Reachability of Neural Network Feedback Loops", arXiv, 2003

Approach #2: Interaction-based Approach

A pictorial explanation

Original system:

$$\longrightarrow \left[\dot{x} = f(x, \mathbf{N}(x), w) \right] \longrightarrow$$

closed-loop system

Embedding system:

$$\longrightarrow \left[\frac{\dot{x}}{\dot{x}}\right] = \begin{bmatrix} [\underline{H}]^+ - \underline{J}_{[\underline{x},\overline{x}]} & [\underline{H}]^- \\ [\overline{H}]^+ - \overline{J}_{[\underline{x},\overline{x}]} & [\overline{H}]^- \end{bmatrix} \begin{bmatrix} \underline{x} \\ \overline{x} \end{bmatrix} + \begin{bmatrix} -[\underline{J}_{[\underline{w},\overline{w}]}]^- & [\underline{J}_{[\underline{w},\overline{w}]}]^+ \\ [-[\overline{J}_{[\underline{w},\overline{w}]}]^- & [\overline{J}_{[\underline{w},\overline{w}]}]^+ \end{bmatrix} \begin{bmatrix} \underline{w} \\ \overline{w} \end{bmatrix} + Q \end{bmatrix} \longrightarrow \left[\begin{bmatrix} \underline{w} \\ \underline{w} \end{bmatrix} + \begin{bmatrix} \underline{w} \\ \underline{w} \end{bmatrix} + Q \end{bmatrix} \right]$$

closed-loop embedding system

How does the interaction-based approach work?

- Closed-loop decomposition function = Jacobian based for f(x, N(x), w).
- Neural Network affine functional bounds $\frac{N_{[\underline{x},\overline{x}]}}{\overline{N}_{[\underline{x},\overline{x}]}} = \underline{A}_{[\underline{x},\overline{x}]}x + \underline{b}_{[\underline{x},\overline{x}]},$ $\overline{N}_{[\underline{x},\overline{x}]} = \overline{A}_{[\underline{x},\overline{x}]}x + \overline{b}_{[\underline{x},\overline{x}]}$ are used to compute the interactions.

$$\begin{split} & \underline{H} = \underline{J}_{[\underline{x},\overline{x}]} + [\underline{J}_{[\underline{u},\overline{u}]}]^+ \underline{A}_{[\underline{x},\overline{x}]} + [\underline{J}_{[\underline{u},\overline{u}]}]^- \overline{A}_{[\underline{x},\overline{x}]} \\ & \overline{H} = \overline{J}_{[\underline{x},\overline{x}]} + [\underline{J}_{[\underline{u},\overline{u}]}]^+ \overline{A}_{[\underline{x},\overline{x}]} + [\underline{J}_{[\underline{u},\overline{u}]}]^- \underline{A}_{[\underline{x},\overline{x}]} \end{split}$$

Interaction-based Approach

Theorem⁶

Let
$$\frac{\partial f}{\partial x} \in [\underline{J}_{[\underline{x},\overline{x}]}, \overline{J}_{[\underline{x},\overline{x}]}], \ \frac{\partial f}{\partial u} \in [\underline{J}_{[\underline{u},\overline{u}]}, \overline{J}_{[\underline{u},\overline{u}]}], \text{ and } \ \frac{\partial f}{\partial w} \in [\underline{J}_{[\underline{w},\overline{w}]}, \overline{J}_{[\underline{w},\overline{w}]}].$$
 Then

$$\begin{bmatrix} \underline{d}_i^c(\underline{x}, \overline{x}, \underline{w}, \overline{w}) \\ \overline{d}_i^c(\underline{x}, \overline{x}, \underline{w}, \overline{w}) \end{bmatrix} = \begin{bmatrix} [\underline{H}]^+ - \underline{J}_{[\underline{x},\overline{x}]} & [\underline{H}]^- \\ [\overline{H}]^+ - \overline{J}_{[\underline{x},\overline{x}]} & [\overline{H}]^- \end{bmatrix} \begin{bmatrix} \underline{x} \\ \overline{x} \end{bmatrix} + \begin{bmatrix} -[\underline{J}_{[\underline{w},\overline{w}]}]^- & [\underline{J}_{[\underline{w},\overline{w}]}]^+ \\ -[\overline{J}_{[\underline{w},\overline{w}]}]^+ \end{bmatrix} \begin{bmatrix} \underline{w} \\ \overline{w} \end{bmatrix} + Q$$

where

$$\begin{split} \underline{\underline{H}} &= \underline{J}_{[\underline{x},\overline{x}]} + [\underline{J}_{[\underline{u},\overline{u}]}]^+ \underline{\underline{A}}_{[\underline{x},\overline{x}]} + [\underline{J}_{[\underline{u},\overline{u}]}]^- \overline{\underline{A}}_{[\underline{x},\overline{x}]} \\ \overline{\underline{H}} &= \overline{J}_{[\underline{x},\overline{x}]} + [\underline{J}_{[\underline{u},\overline{u}]}]^+ \overline{\underline{A}}_{[\underline{x},\overline{x}]} + [\underline{J}_{[\underline{u},\overline{u}]}]^- \underline{\underline{A}}_{[\underline{x},\overline{x}]} \end{split}$$

is a decomposition function for the closed-loop system.

S. Jafarpour (CU Boulder)

⁶Jafarpour, Harapanahalli, Coogan. "Efficient Interaction-aware Interval Reachability of Neural Network Feedback Loops", arXiv, 2003

Case Study: Bicycle Model

Design of the neural network



Goal: steer the bicycle to the origin avoiding the obstacles

- offline controller: MPC with hard constraint to avoid the obstacles
- run MPC for 65000 randomly chosen initial condition (20 sample per trajectory)
- train a feedforward neural network $4 \mapsto 100 \mapsto 100 \mapsto 2$ with this data

Case Study: Bicycle Model

Numerical Experiments



S. Jafarpour (CU Boulder)

- reachability using mixed monotone theory
- mixed monotone theory for reachability of NN controlled systems
- two methods for capturing the interaction between system and NN controller
 - interconnection-based approach
 - interaction-based approach

Future directions:

- forward invariance of systems with NN controllers
- design of suitable correction actions
- ensuring safety in the training of NN

Embedding System for Linear Dynamical System

A structure preserving decomposition

• Metzler/non-Metzler decomposition: $A = [A]^{Mzl} + |A|^{Mzl}$

• Example:
$$A = \begin{bmatrix} 2 & 0 & -1 \\ 1 & -3 & 0 \\ 0 & 0 & 1 \end{bmatrix} \implies \lceil A \rceil^{Mzl} = \begin{bmatrix} 2 & 0 & 0 \\ 1 & -3 & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad \lfloor A \rfloor^{Mzl} = \begin{bmatrix} 0 & 0 & -1 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$

Linear systems

Original system

 $\dot{x} = Ax + Bw$

Embedding system

$$\underline{\dot{x}} = \begin{bmatrix} A \end{bmatrix}^{\mathrm{Mzl}} \underline{x} + \begin{bmatrix} A \end{bmatrix}^{\mathrm{Mzl}} \overline{x} + B^{+} \underline{w} + B^{-} \overline{w}$$
$$\underline{\dot{x}} = \begin{bmatrix} A \end{bmatrix}^{\mathrm{Mzl}} \overline{x} + \begin{bmatrix} A \end{bmatrix}^{\mathrm{Mzl}} \underline{x} + B^{+} \overline{w} + B^{-} \underline{w}$$



