Contraction-guided reachability analysis of neural network controlled systems

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Acknowledgements

- S. Jafarpour, A. Harapanahalli, S. Coogan, "Interval Reachability of Nonlinear Dynamical Systems with Neural Network Controllers", L4DC, 2023, arXiv:2301.07912
- A. Harapanahalli, S. Jafarpour, S. Coogan, "Contraction-Guided Adaptive Partitioning for Reachability Analysis of Neural Network Controlled Systems", in submission to IEEE CDC, arXiv:2304.03671
- S. Jafarpour and S. Coogan, "Monotonicity and Contraction on Polyhedral Cones", in submission to IEEE TAC, arXiv:2210.11576





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



- Reachable sets characterize possible system evolution
- Overapproximations of reachable sets are appropriate for verification and safety

Neural network feedback controllers: The reachability problem



Goal: compute reachable sets of closed-loop system

Challenges: soundness, efficiency-vs-conservatism tradeoff

In this talk:

- Interval-based reachability using monotone systems theory
- Contraction-based adaptive partitioning
- Contraction with alternate partial orders for improved fidelity

A starting point: Reachability estimates from contraction theory

For $\dot{x} = f(x, w)$, $x \in \mathbb{R}^n$ and $w \in \mathcal{W} \subseteq \mathbb{R}^m$, define reachable set as

$$\mathcal{R}^{f}(t;X_{0}) = \{x(t): x(\cdot) \text{ is sol'n for some } w(\cdot) \text{ with } x_{0} \in X_{0}\}.$$

Suppose

$$\mu\left(\frac{\partial f}{\partial x}(x,w)\right) \leq c \quad \text{and} \quad \left\|\frac{\partial f}{\partial w}(x,w)\right\|_{w\to x} \leq \ell.$$



If $X_0 = B(r_1, x_0^*)$ and $\mathcal{W} = B(r_2, w^*)$ where $B(\cdot, \cdot)$ is ball with radius and center, then $\mathcal{R}^f(t; X_0) \subseteq B\left(e^{ct}r_1 + \frac{\ell}{c}(e^{ct} - 1)r_2, x^*(t)\right)$ where $\dot{x}^*(\tau) = f(x^*(\tau), w^*)$ for all τ .

(Pf. Rewriting of Grönwall Comparison Lemma, [Bullo, Corollary 3.17, p. 81].)

The system $\dot{x} = f(x, w)$, $x \in \mathbb{R}^n$, $w \in \mathbb{R}^m$ is monotone¹ if

 $x_0 \preceq_{K_x} x_0'$ implies that $x(t) \preceq_{K_x} x'(t)$ for all time,

for any $w(\cdot)$ and $w'(\cdot)$ such that $w(t) \preceq_{K_w} w'(t)$ for all t, where \preceq_K is some partial order induced by cone K ($K_x \subset \mathbb{R}^n$ or $K_w \subset \mathbb{R}^m$).

Test for monotonicity (standard order
$$\leq$$
):
 $\frac{\partial f}{\partial x}(x,w)$ is Metzler (≥ 0 off-diag. entries)
 $\frac{\partial f}{\partial w}(x,w) \geq 0$



¹D. Angeli and E. Sontag, "Monotone Control Systems", *IEEE TAC*, 2003 S. Coogan

Reachability estimates for monotone systems

Reachability Analysis for Monotone Systems. For a monotone system,

Reachable set \subseteq [lower trajectory, upper trajectory].



Reachability estimates from monotonicity are tight.

Theorem. A monotone system $\dot{x} = f(x)$ (wrt. \leq) contracts at rate c any box with sidelengths a multiple of $\eta \in \mathbb{R}^n_{>0}$ if (equivalently, contracts w.r.t. $\|\cdot\|_{\infty,[\eta]^{-1}}$):

i)
$$\left(\frac{\partial f}{\partial x}(x)\right)\eta \le c\eta$$
 for all x or, equivalently,
ii) $f(y)-f(x) \le c(y-x)$ for all x and $y = x + \beta\eta$ for some $\beta > 0$

Proof for i): Follows from the fact that $\frac{\partial f}{\partial x}(x)$ is Metzler and that $\mu_{\infty}(A) = \max_{i} A_{ii} + \sum_{j \neq i} |A_{ij}|.$ Proof sketch for ii):



²[Bullo, Ch. 4.5, Lemma 4.17, p. 117]

 3 S. Coogan, "A contractive approach to separable Lyapunov functions for monotone systems", s. Coogan dutomatica, 2019.

Example

 $\rightarrow (x_3) \leftarrow$ (x_5)

Consensus on line graph with anchored Distribute "excess negativity" from first column by choosing

$$\dot{x} = \underbrace{\begin{bmatrix} -2 & 1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \ddots & \vdots & \vdots \\ 0 & \cdots & 0 & 1 & -2 & 1 \\ 0 & \cdots & 0 & 0 & 1 & -1 \end{bmatrix}}_{A} x$$

► A1 ≤ 0, so hypersquares are nonexpansive

$$\eta = \begin{bmatrix} 1\\ 1+\varepsilon_1\\ 1+\varepsilon_1+\varepsilon_2\\ \vdots\\ 1+\varepsilon_1+\ldots+\varepsilon_{n-1} \end{bmatrix}$$
 with $1 > \varepsilon_1 > \varepsilon_2 > \ldots > \varepsilon_{n-1} > 0$, then $A\eta < 0$.

Reachability for nonmonotone systems

Generally, cannot bound the reachable set between two extreme trajectories for nonmonotone systems





Mixed monotonicity embeds nonmonotone systems in a monotone system

• Given $\dot{x} = f(x, w)$, disturbance input $w \in \mathcal{W} = [\underline{w}, \overline{w}] = \{w : \underline{w} \le w \le \overline{w}\}$

Mixed monotone approach: find decomposition functions \underline{d} , \overline{d} such that: **1** $\underline{d}(x,x,w,w) = \overline{d}(x,x,w,w)$ for all x, w and

2 the 2n dimensional embedding system^{4,5}

$$\begin{bmatrix} \underline{\dot{x}} \\ \overline{\dot{x}} \end{bmatrix} = \begin{bmatrix} \underline{d}(\underline{x}, \overline{x}, \underline{w}, \overline{w}) \\ \overline{d}(\underline{x}, \overline{x}, \underline{w}, \overline{w}) \end{bmatrix}$$

is monotone w.r.t the *southeast order* \leq_{SE} on \mathbb{R}^{2n} defined as:

 $(x, \hat{x}) \leq_{\mathsf{SE}} (y, \hat{y})$ if and only if $x \leq y$ and $\hat{y} \leq \hat{x}$.

⁴G. Enciso, H. Smith, E. Sontag, "Non-monotone systems decomposable into monotone systems with negative feedback", *Journal of Diff. Eq.*, 2006

⁵H. Smith, "Global stability for mixed monotone systems", *Journal of Difference Equations and Applications*, 2008

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Reachable set from embedding trajectory:
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\mathcal{R}^{f}(T; [\underline{x}_{0}, \overline{x}_{0}]) \subseteq [\underline{x}(T), \overline{x}(T)]
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where $\underline{x}(t),\overline{x}(t)$ is embedding system solution with initial condition $(\underline{x}_0,\overline{x}_0)$



- MM is fast: A single trajectory of the deterministic embedding bounds reachable sets of the original system
- ▶ MM is scalable: If $(\underline{x}_{eq}, \overline{x}_{eq})$ is an equilibrium for embedding system, then hyperrectangle $[\underline{x}_{eq}, \overline{x}_{eq}]$ is robustly forward invariant⁶

⁶S. Coogan, "Mixed monotonicity for reachability and safety in dynamical systems", IEEE CDC, 2020 (tutorial paper)

Example

Mixed Monotone System:

$$\begin{bmatrix} \dot{x}_1\\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} x_2^2 + 2\\ x_1 \end{bmatrix}$$
$$[\underline{x}_0, \overline{x}_0] = [(-0.5, -0.5), (0.5, 0.5)]$$
$$T = 1$$

Decomposition Function:

$$\underline{d}_{1}(x,\hat{x}) = \begin{cases} x_{2}^{2} + 2 & \text{if } x_{2} \ge 0 \text{ and } x_{2} \ge -\hat{x}_{2}, \\ \widehat{x}_{2}^{2} + 2 & \text{if } \widehat{x}_{2} \le 0 \text{ and } x_{2} < -\widehat{x}_{2}, \\ 2 & \text{if } x_{2} < 0 \text{ and } \widehat{x}_{2} > 0. \end{cases}$$
$$\underline{d}_{2}(x,\hat{x}) = x_{1}, \qquad \overline{d}(x,\hat{x}) = \underline{d}(\widehat{x}, x)$$



Stability in the embedding space implies robust invariance

Mixed Monotone System:

 $\begin{bmatrix} \dot{x}_1 \\ \dot{x}_2 \end{bmatrix} = \begin{bmatrix} -x_1^3 - x_2 - w \\ x_1^2 - x_2 + w^3 \end{bmatrix}$

W = [-1, 1]

Decomposition Function:

$$d_1(x, w, \widehat{x}, \widehat{w}) = -x_1^3 - \widehat{x}_2 - \widehat{w}$$

$$d_2(x, w, \widehat{x}, \widehat{w}) = \begin{cases} x_1^2 - x_2 + w^3 & \text{if } x_1 \ge 0 \text{ and } x_1 \ge -\widehat{x}_1, \\ \widehat{x}_1^2 - x_2 + w^3 & \text{if } \widehat{x}_1 \le 0 \text{ and } x_1 < -\widehat{x}_1, \\ -x_2 + w^3 & \text{if } x_1 < 0 \text{ and } \widehat{x}_1 > 0. \end{cases}$$



Theorem⁷. Any system has best (i.e, tightest) decomposition functions satisfying $\underline{d}_i(x, \hat{x}, w, \hat{w}) = \min_{y \in [x, \hat{x}], y_i = x_i, z \in [w, \hat{w}]} f_i(y, z)$ $\overline{d}_i(x, \hat{x}, w, \hat{w}) = \max_{y \in [x, \hat{x}], y_i = \hat{x}_i, z \in [w, \hat{w}]} f_i(y, z)$

Closed form sometimes possible, otherwise, several automated approaches for





 $^{8}\mbox{A}.$ Harapanahalli, S. Jafarpour, S. Coogan, Python-based toolbox, forthcoming.

Theorem. Let
$$\begin{bmatrix} \dot{x} \\ \dot{\bar{x}} \end{bmatrix} = \begin{bmatrix} \underline{d}(\underline{x}, \overline{x}, \underline{w}, \overline{w}) \\ \overline{d}(\underline{x}, \overline{x}, \underline{w}, \overline{w}) \end{bmatrix} =: e(\underline{x}, \overline{x})$$
 be the embedding system construction from tight decomposition functions. For any $\eta \in \mathbb{R}^n$,
 $\mu_{\infty, [\eta]^{-1}} \left(\frac{\partial f}{\partial x}(x, w) \right) \leq c \quad \text{for all } x$
if and only if
 $\mu_{\infty, [(\eta, \eta)]^{-1}} \left(\frac{\partial e}{\partial (x, \overline{x})}(\underline{x}, \overline{x}) \right) \leq c \quad \text{for all } \underline{x}, \overline{x}.$

Reachable sets computed from a trajectory of the tight embedding system are at least as good as using contraction alone on the original system



- ▶ Fixing # of partitions, adaptive is faster and can be more accurate
- Fixing computation time, adaptive allows for more partitions



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- Fixing # of partitions, adaptive is faster and can be more accurate
- Fixing computation time, adaptive allows for more partitions

Algorithm overview

Given

 $\dot{x} = f^{ol}(x, u, w)$ (open-loop system) u = N(x) (NN controller),

obtain decomposition function for closed-loop system

$$\dot{x} = f^{cl}(x, w) = f^{ol}(x, N(x), w)$$

from

- ▶ Open-loop decomposition function for f^{ol} and
- Bounding functions for open-loop controller N(x) (next slides)
- 2 Efficiently evolve embedding system to obtain overapproximation set
- 3 Adaptively (in space and time) partition to avoid compounding conservatism



Neural network bounding functions

Given NN N(x) and bounds $[\underline{z}, \overline{z}]$, $\underline{N}_{(\underline{z}, \overline{z})}(\underline{x}, \overline{x})$ and $\overline{N}_{(\underline{z}, \overline{z})}(\underline{x}, \overline{x})$ are bounding functions for N(x) valid on $[\underline{z}, \overline{z}]$ if

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

Example: CROWN⁹ is a NN verifier that produces affine bounds:

$$\underline{A}_{(\underline{z},\overline{z})}x + \underline{b}_{(\underline{z},\overline{z})} \le N(x) \le \overline{A}_{(\underline{z},\overline{z})}x + \overline{b}_{(\underline{z},\overline{z})}$$

Lemma. Given CROWN bounds $\underline{A}_{(\underline{z},\overline{z})}x + \underline{b}_{(\underline{z},\overline{z})} \leq N(x) \leq \overline{A}_{(\underline{z},\overline{z})}x + \overline{b}_{(\underline{z},\overline{z})}$, then

$$\begin{split} \underline{N}_{(\underline{z},\overline{z})}(\underline{x},\overline{x}) &= [\underline{A}_{(\underline{z},\overline{z})}]^+ \underline{x} + [\underline{A}_{(\underline{z},\overline{z})}]^- \overline{x} + \underline{b}_{(\underline{z},\overline{z})}, \\ \overline{N}_{(\underline{z},\overline{z})}(\underline{x},\overline{x}) &= [\overline{A}_{(\underline{z},\overline{z})}]^+ \overline{x} + [\overline{A}_{(\underline{z},\overline{z})}]^- \underline{x} + \overline{b}_{(\underline{z},\overline{z})} \end{split}$$

are bounding functions for N(x) valid on $[\underline{z}, \overline{z}]$.

⁹Zhang, Weng, Chen, Hsieh,Daniel, "Efficient neural network robustness certification with general activation functions." *Advances in neural information processing systems*, 2018. S. Coogan Assume we have:

- **①** Open-loop decomposition function d^{ol} for $f^{ol}(x, u, w)$
- 2 Ability to construct NN bounding functions $\underline{N}_{(z,\overline{z})}$, $\overline{N}_{(z,\overline{z})}$
 - Construction is expensive while queries are cheap (e.g., CROWN vs matrix multiply)

For reachability of $f^{cl}(x,w) = f^{ol}(x,N(x),w)$, we propose an algorithm that features:

- 1 Separation of bounding function construction from queries
- Spatially and temporally adaptive partitioning for accuracy

Theorem.¹⁰ Let $\underline{N}_{(\underline{z},\overline{z})}$, $\overline{N}_{(\underline{z},\overline{z})}$ be bounding functions for N(x) valid on some $[\underline{z},\overline{z}]$, and let d^{ol} be a decomposition function for f^{ol} . Then d_i defined by

$$\begin{split} \underline{d}_i(\underline{x}, \overline{x}, \underline{w}, \overline{w}) &= d_i^{ol}(\underline{x}, \overline{x}, \underline{\eta}, \overline{\eta}, \underline{w}, \overline{w}), \\ \overline{d}_i(\underline{x}, \overline{x}, \underline{w}, \overline{w}) &= d_i^{ol}(\overline{x}, \underline{x}, \overline{v}, \underline{v}, \overline{w}, \underline{w}), \end{split}$$

where

$$\begin{split} \underline{\eta} &= \underline{N}_{(\underline{z},\overline{z})}(\underline{x},\overline{x}_{[i:\underline{x}]}) \quad \overline{\eta} &= \overline{N}_{(\underline{z},\overline{z})}(\underline{x},\overline{x}_{[i:\underline{x}]}), \\ \underline{\nu} &= \underline{N}_{(\underline{z},\overline{z})}(\overline{x},\underline{x}_{[i:\overline{x}]}), \quad \overline{\nu} &= \overline{N}_{(\underline{z},\overline{z})}(\overline{x},\underline{x}_{[i:\overline{x}]}), \end{split}$$

is a decomposition function for f^{cl} for any $(\underline{x}, \overline{x})$ such that $[\underline{x}, \overline{x}] \subseteq [\underline{z}, \overline{z}]$, where $v_{[i:v']}$ is the vector v with its *i*-th component replaced with that of v'.

¹⁰S. Jafarpour, A. Harapanahalli, S. Coogan, "Interval Reachability of Nonlinear Dynamical Systems with Neural Network Controllers", *L4DC*, 2023

Spatially and temporally adaptive partitioning for accuracy

- Evolving tree structure tracks partitionings, leaves are current partitions
- Along an evolution step (e.g., control update step) if partition expansion exceeds threshold, add a partition and reevolve
- S NN bounding construction performed at some nodes, used for all descendent leaves



Case study: kinematic bicycle



 Obstacle-avoiding go-to-origin NN controller (4×100×100×2 ReLU) trained from nonlinear MPC data



	D_p	D_{N}	Runtime (s)	Volume
non-adaptive	2	1	1.851 ± 0.010	1.988
adaptive	2	1	1.583 ± 0.010	1.689
non-adaptive	2	2	4.274 ± 0.023	0.803
adaptive	2	2	3.332 ± 0.012	0.787

Benchmark: Double integrator

$$x_{t+1} = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix} x_t + \begin{bmatrix} 0.5 \\ 1 \end{bmatrix} u_t$$

► $2 \times 10 \times 5 \times 1$ ReLU NN controller from literature





Benchmark: Double integrator



Generalizing rectangular compatibility of monotonicity and contraction

Given a partial order \leq_K induced by a cone K, for any $\eta \in int(K)$, the corresponding gauge norm (or seminorm) is defined as

$$\|v\|_{\eta,K} = \inf\{\lambda \in \mathbb{R}_{\geq 0} \mid -\eta \preceq_{K} v \preceq_{K} \eta\}.$$

► For the standard order ≤, gauge norms are weighted ℓ_∞ norms and intervals





Monotonicity w.r.t. polyhedral cones

A polyhedral cone has the form $K = \{x \in \mathbb{R}^n \mid Hx \ge \mathbb{O}_m\} = \{Vx \in \mathbb{R}^n \mid x \ge \mathbb{O}_m\}$ Halfspace rep Vertex rep **Theorem.**¹¹ The system $\dot{x} = f(x)$ is monotone w.r.t. \leq_K , K a polyhedral cone, if anv of the following equivalent conditions hold: **①** There exists $\alpha(x, u)$ such that $H\left(\frac{\partial f}{\partial x}(x) + \alpha(x,u)I_n\right)V \ge \mathbb{O}_{m imes m} \quad \text{for all } x,u,$ There exists Metzler P(x, u) such that 2 $H\frac{\partial f}{\partial x}(x) = P(x,u)H$ for all x, u, There exists Metzler Q(x, u) such that 3 $\frac{\partial f}{\partial x}(x)V = VQ(x,u)$ for all x, u. ¹¹S. Jafarpour and S. Coogan, "Monotonicity and Contraction on Polyhedral Cones", in submission to IEEE TAC.

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Theorem.¹² Let $\dot{x} = f(x)$ be monotone w.r.t. \leq_K , K polyhedral. Let $\eta \in int(K)$, $c \in \mathbb{R}$. The following are equivalent: **1** $\frac{\partial f}{\partial x}(x)\eta \leq_K c\eta$, **2** $H\frac{\partial f}{\partial x}(x) \leq cH\eta$, **3** $\|y(t) - x(t)\|_{\eta,K} \leq e^{ct} \|y(0) - x(0)\|_{\eta,K}$ for any two trajectories x(t), y(t)

¹²S. Jafarpour and S. Coogan, "Monotonicity and Contraction on Polyhedral Cones", in submission to *IEEE TAC*.

Example: Inverted pendulum

Inverted pendulum:

 $\dot{x}_1 = x_2$ $\dot{x}_2 = \sin(x_1) + u$

► Choose u = -k₁x₁ - k₂x₂, to stabilize origin, then

$$\frac{\partial f}{\partial x}(x) = \begin{bmatrix} 0 & 1\\ \cos(x_1) - k_1 & -k_2 \end{bmatrix}$$

 No controller contracts a rectangle around the origin



- Alternative cone
 - $K = \left\{ x \mid \begin{bmatrix} 1 & 0 \\ 1 & \gamma \end{bmatrix} x \ge \mathbb{O}_m \right\}$

Example: Network flow

► Nodal flows:

$$\dot{x} = -\underbrace{B_{\nu}B_{\nu}^{T}}_{L}x, \quad B_{\nu} = \begin{bmatrix} 1 & 0 & 1 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & -1 & -1 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

• Edge flows: $z = B_v^T x$.

▶ Non-pointed
$$K = \{x \in \mathbb{R}^n : B_v^T x \ge \mathbb{O}_4\}$$
:

$$-B_{\nu}L = \underbrace{\begin{bmatrix} -3 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & -1 & -1 & 1 \\ 0 & 0 & 0 & 1 \end{bmatrix}}_{\text{Metzler}} B_{\nu}^{T},$$

so edge flow dynamic are monotone: $B_{\nu}^{T}x(0) \leq B_{\nu}^{T}y(0) \implies B_{\nu}^{T}x(t) \leq B_{\nu}^{T}y(t) \forall t$



In this talk:

- Contraction (and [mixed] monotonicity) for computing reachable sets, applications to learning-based controllers
- ② Gauge norms induced by partial orders are natural for computing with intervals
- Opportunities for "computational contraction theory"

coogan.ece.gatech.edu for papers and code

Thank you

Bounding accuracy

Theorem (informal).

$$\begin{aligned} \mathsf{partition}(t) \|_{\infty} &\leq e^{ct} \|\mathsf{partition}(0)\|_{\infty} + \frac{L^{\mathrm{ol}}_{w}(e^{ct}-1)}{c} \|\overline{w}-\underline{w}\|_{\infty} \\ &+ \frac{L^{\mathrm{ol}}_{u}(e^{ct}-1)}{c} \sup_{z} \max\{\|\underline{N}(z,z)-N(z)\|_{\infty}, \|\overline{N}(z,z)-N(z)\|_{\infty}\} \end{aligned}$$

where

 $c = {\rm local}$ contraction rate of closed-loop embedding system $L_u^{\rm ol} = {\rm local} \ {\rm Lipschitz} \ {\rm constant} \ {\rm of} \ {\rm open-loop} \ {\rm embedding} \ {\rm system} \ {\rm w.r.t.} \ u$ $L_w^{\rm ol} = {\rm local} \ {\rm Lipschitz} \ {\rm constant} \ {\rm of} \ {\rm open-loop} \ {\rm embedding} \ {\rm system} \ {\rm w.r.t.} \ w$

• Separation \implies improve term 1 independent of term 3

• Spatial awareness \implies improved local Lipschitz constant L_w^{ol} , L_u^{ol}

• Temporal awareness \implies controlled $e^{ct} \| partition(0) \|_{\infty}$

Theorem (informal). Contraction rate c of closed loop system satisfies $c \leq c^{\text{ol}} + L_u^{\text{ol}} \sup_{(\underline{x},\overline{x})} \max \left\{ \left\| \frac{\partial \underline{N}}{\partial(\underline{x},\overline{x})}(\underline{x},\overline{x}) \right\|_{\infty}, \left\| \frac{\partial \overline{N}}{\partial(\underline{x},\overline{x})}(\underline{x},\overline{x}) \right\|_{\infty} \right\}$ where c^{ol} is contraction rate of the open-loop embedding system.

Moreover, when the open-loop decomposition function is tight, $c^{\rm ol}$ matches the contraction rate of the open-loop system.