Bridging Neural ODE and ResNet: A Formal Error Bound for Safety Verification

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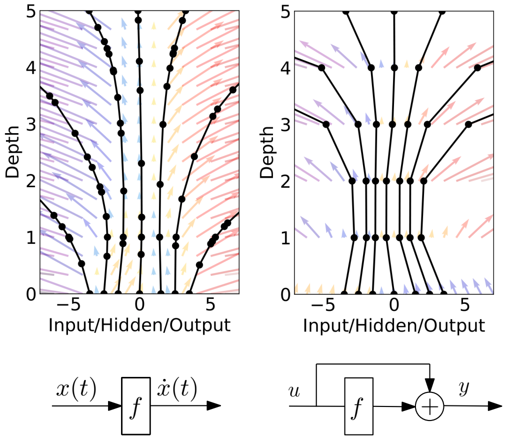
Motivations

Relations

- Continuous-depth generalization of ResNet
- Euler-discretization of neural ODE



$$\dot{x}(t) = f(x(t))$$

$$y = u + f(u)$$

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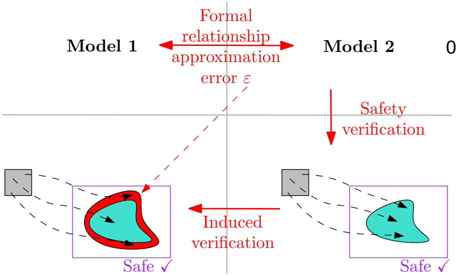
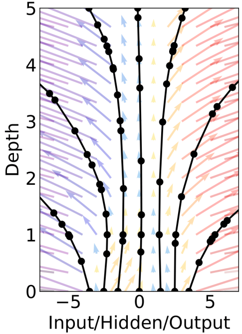
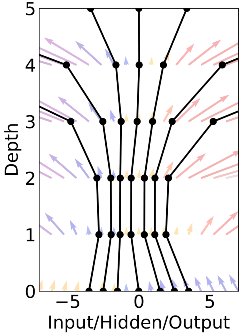
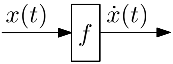
Proposed Framework









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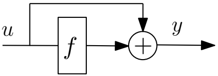

$$y = u + f(u)$$

Problem Definition

- $\mathcal{X}_{in}$: input set
- neural ODE reachable set:

$$\mathcal{R}_{\text{neural ODE}}(\mathcal{X}_{in}) = \{y \in \mathbb{R}^n \mid y = \Phi(1, u) \;\; u \in \mathcal{X}_{in}\}$$

- ResNet reachable set:

$$\mathcal{R}_{\text{ResNet}}(\mathcal{X}_{in}) = \{y \in \mathbb{R}^n \mid y = u + f(u) \;\; u \in \mathcal{X}_{in}\}$$

- *Problem 1* (*Error Bounding*):

$$\mathcal{R}_{\varepsilon}(\mathcal{X}_{in}) = \{\Phi(1, u) - (u + f(u)) \mid u \in \mathcal{X}_{in}\}$$

Proposed Approach

- Lagrange remainder:

$$x(t) = x(0) + t\frac{dx(0)}{dt} + \frac{t^2}{2!}\frac{d^2x(t^*)}{dt^2}, \text{ for unkown } t^* \in [0, t]$$

Proposed Approach

- Lagrange remainder:

$$x(1) = x(0) + \frac{dx(0)}{dt} + \frac{1}{2}\frac{d^2x(t^*)}{dt^2}, \text{ for unkown } t^* \in [0,1]$$

- neural ODE based on ResNet:

$$\Phi(1,u) = (u + f(u)) + \varepsilon(u)$$

- Where ε:

$$\varepsilon(u) = \frac{1}{2} f'(x(t^*)) f(x(t^*))$$

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- ResNet based on neural ODE:

$$u + f(u) = \Phi(1,u) - \varepsilon(u)$$

Numerical Example

Fixed-Point Attractor System

- 5 dimensional neural ODE
- $\dot{x} = f(x) = \tau x + W\text{tanh}(x)$,
  where:
  - → $\tau = -10^{-6}$
  - → W is a 5×5 matrix
  - → $tanh$: hyperbolic tangent AF

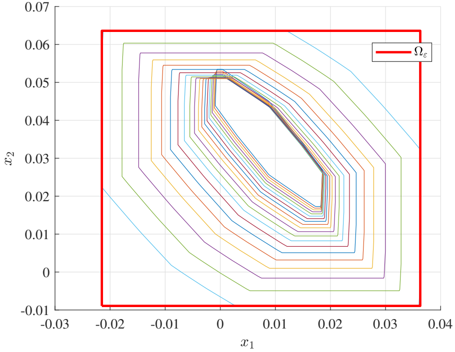
Bounding Ω_ε

- neural ODE reachable tube:

$$\mathcal{R}^{\text{tube}}_{\text{neural ODE}}(\mathcal{X}_{in}) = \{\Phi(t,u) \in \mathbb{R}^n \mid t \in [0,1],\ u \in \mathcal{X}_{in}\}$$

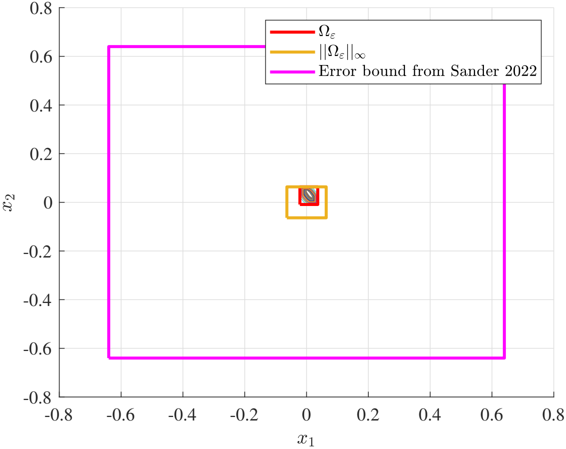
- Bound the error term:

$$\varepsilon(u) = \frac{1}{2} f'(\Phi(t^*,u)) f(\Phi(t^*,u))$$



Error Bound Comparison

- $\Omega_\varepsilon < 16$ million times $\times$ Sander 2022



Verification Proxy

- $\mathcal{X}_s$: safe set
- *Problem 2 (Safety Specification)*:

$$\mathcal{R}(\mathcal{X}_{in}) \subseteq \mathcal{X}_s$$

- neural ODE based on ResNet:

$$\mathcal{R}_{\text{neural ODE}}(\mathcal{X}_{in}) \subseteq \Omega_{\text{ResNet}}(\mathcal{X}_{in}) + \Omega_{\varepsilon}(\mathcal{X}_{in})$$

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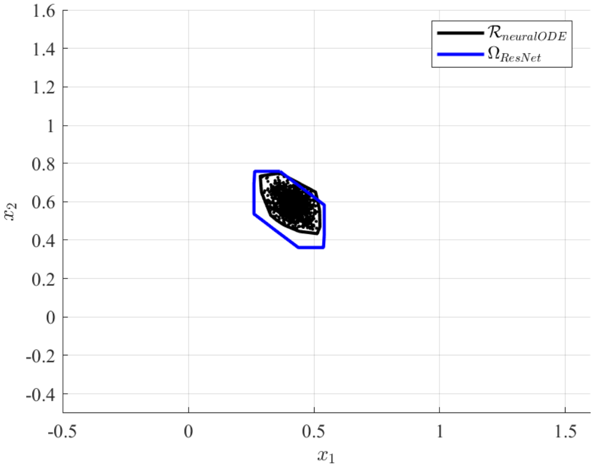
- ResNet based on neural ODE:

$$\mathcal{R}_{\text{ResNet}}(\mathcal{X}_{in}) \subseteq \Omega_{\text{neural ODE}}(\mathcal{X}_{in}) + \Omega_{-\varepsilon}(\mathcal{X}_{in})$$

Verification of neural ODE based on ResNet

- $\mathcal{X}_s \supseteq \Omega_{\text{ResNet}}(\mathcal{X}_{in}) + \Omega_{\varepsilon}(\mathcal{X}_{in}) \supseteq \mathcal{R}_{\text{neural ODE}}$



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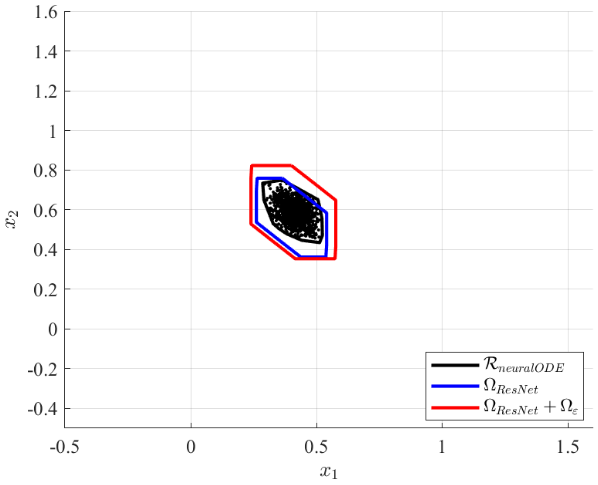

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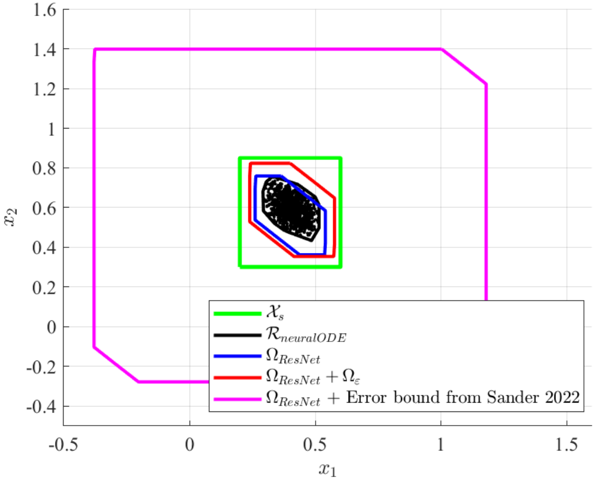

Verification of ResNet based on neural ODE

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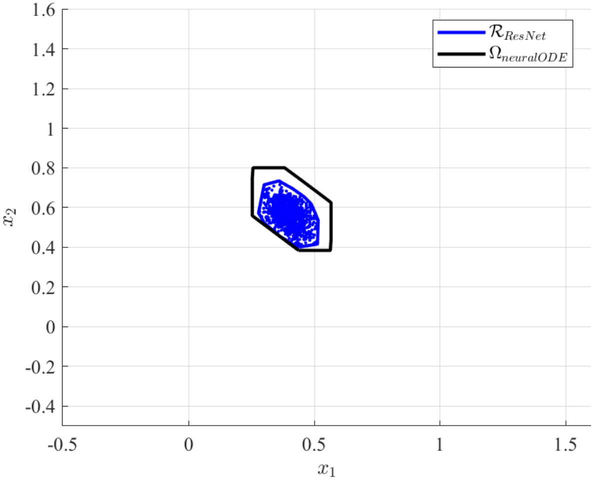

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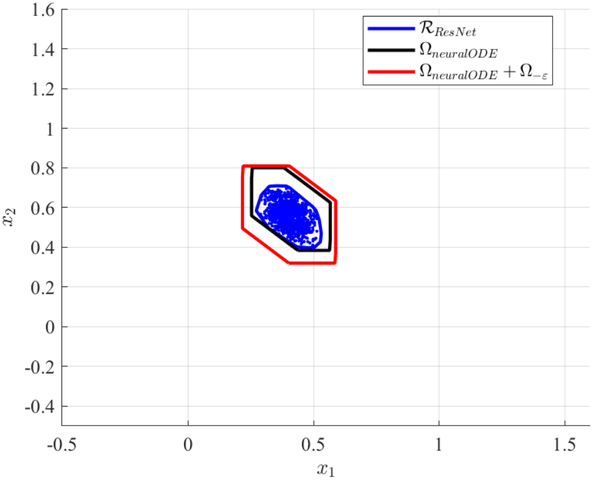

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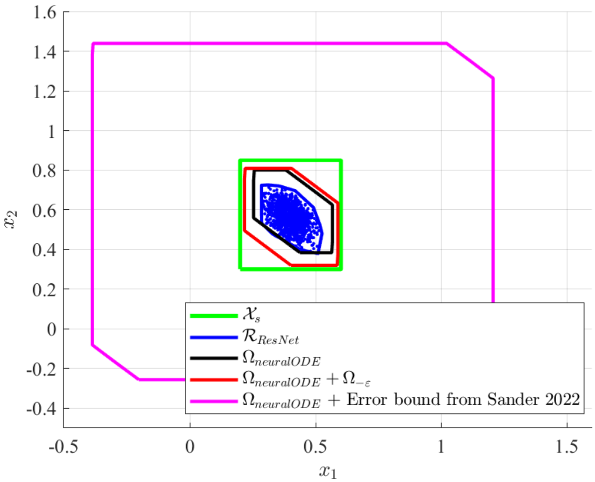

Conclusions

Set-based method bounding neural ODE and ResNet approximation

- Tighter over-approximation than SOTA
- Use reachability/verification tools on one model to verify the other

Future Work

- Explore additional complexity sources
  - Handle non-smooth activation functions (e.g., ReLU)
- Study versatility of verification proxy approach
  - Apply to complex nonlinear dynamical systems
  - Extend to other neural network architectures (e.g., RNN or CNN)

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