Certifying Differential Invariants of Neural Networks using Abstract Duals

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The Setup

Safety Property

Given a neural network classifier $f : \mathbb{R}^n \to \mathbb{R}^k$, an input x_0, and a perturbation radius ϵ. Verify that classification of x_0 is invariant within an ϵ-ball i.e.,

$$\forall x \in \mathbb{B}_\infty(x_0, \epsilon) : \quad \text{argmax}(f(x)) = \text{argmax}(f(x_0))$$

Original Image

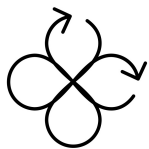
Original Image $+ \epsilon = 0.25$

Original Image $+ \epsilon = 0.1$

The Problem

Neural Networks are highly non-linear and vulnerable to *adversarial attacks*.

Original Image + tiny perturbations



Continuous input spaces

Safety-Critical Domains

Possible solution

Try computing an over-approximation of the reachable output set $\mathcal{R}_f(X_0)$ to prove safety

Why is it Interesting?

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The power of global bounds with simplicity of gradient analysis

1. **Simplicity beats complexity**
   - → DeepPoly[1] is strictly better than our method
   - → However, *suprising results found!*
2. **Gradient Instability**
   - → Found 100% correlation between instability and failure at high ϵ
   - → Our method detects when the *local linearity assumption collapses*

[1] Singh, G. et. al. (2019). An abstract domain for certifying neural networks. 3(POPL), pp.1–30.

The Conceptual Shift

Mathematical Bridge: Mean Value Theorem

$$|f(x) - f(x_0)| \leq \underbrace{\sup_{z \in X} ||\nabla f(z)||}_{\text{Abstract Duals}} \cdot ||x - x_0||$$

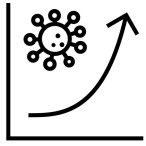
Key Difference

→ **DeepPoly:** Tracks affine constraints layer-by-layer ($x_j \geq \sum w_i x_i$). Precise but accumulates error ($O(L)$)

→ **Ours:** Approximates the derivative $\nabla f(x)$. Coarser, but "jumps" by bypassing intermediate wrapping errors

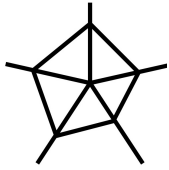
Contributions

Formalization:
Affine Arithmetic



Gradient Anomaly:
Depth < 3; Sigmoid

Instability Metric:
Identifies failures



Evaluation:
Tiny/Small/Std. ϵ

Statement

"Global gradient bounds provide a simpler verification domain for shallow, smooth networks, while relational domains are essential for deep, non-smooth architectures"

Contribution Idea

Lift standard dual numbers $\mathbb{D} = \{a + b\eta\}$ to Affine Forms to compute global gradient bounds.

→ **Value Component**: $\hat{x} = \alpha_0 + \sum_{i=1}^{n} \alpha_i \epsilon_i$ (Abstract Input Region)

→ Propogate the interval through the network:

$$\hat{y} = f(\hat{x}) = \underbrace{\left(y_0 + \sum y_i \epsilon_i\right)}_{\text{Value Interval}} + \underbrace{\left(d_0 + \sum d_i \epsilon_i\right)}_{\text{Gradient } \nabla f} \eta$$

→ *Global Lipschitz bound is the supremum*:

$$K = \sup_{x \in X_0} ||\nabla f(x)||_1 = \sum_j \left(|\beta_{0,j}| + \sum_i |\beta_{i,j}| \right)$$

Contribution Idea

A neuron n is **gradient-unstable** if its gradient interval $[\underline{g}, \overline{g}]$ contains 0

$$\exists x_1, x_2 \in X_0 \text{ s.t. } \text{sign}\left(\frac{\partial f}{\partial n}(x_1)\right) \neq \text{sign}\left(\frac{\partial f}{\partial n}(x_2)\right)$$

Implication

→ **Geometric Interpretation**: The function is non-monotonic with respect to neuron n within the input region.

→ Linear approximations (DeepPoly) become loose when curvature is high

Experimental Results I

Counter-Intuitive Finding

In **16.1%** of Tiny Net cases ($\epsilon = 0.01$), the simpler Gradient method certified robustness where DeepPoly failed.

Network	ϵ	**Count**	**%**
Tiny Net	0.01	5	16.1%
Tiny Net	0.02	3	9.7%
Tiny Net	0.03	2	6.5%
Small/Std	All	0	0.0%

Table: Gradient method outperforms DeepPoly in shallow, smooth networks; {Tiny: 2×10, Small: 5×20, Standard: 10×20}

Experimental Results II

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1. Gradient Instability Analysis

→ **Hypothesis:** Does instability (zero-crossing gradient) predict failure?

→ **Result:** 100% Correlation at high perturbation ($\epsilon = 0.12$)

2. ReLU vs. Sigmoid

→ **Hypothesis:** Does activation smoothness affect performance?

→ **Result:** DeepPoly dominates (100% win rate) on ReLU networks, whereas, smooth derivatives of Sigmoid allow tight global bounds.

Leveraged ocaml-nn[2] library to run on MNIST classifiers with perturbation $\epsilon \in \{0.01 \dots 0.12\}$.

[2] https://github.com/ck090/ocaml-nn/tree/main

Thank You!

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→ **Shallow + Smooth** → Use **Gradient (Abstract Duals)**

→ **Deep + Non-smooth** → Use **Relational (DeepPoly)**

Final Takeaway

"Domain complexity does not dictate robustness, however, alignment with function smoothness does. Expanding to Physics-Informed Neural Networks is an exciting future direction"