



Probably Approximately Global Robustness Certification Peter Blohm, Patrick Indri, Thomas Gärtner, Sagar Malhotra, RuML @ TU Wien December 19, 2024



Problem Setting: Certification of Neural Network Robustness

Goodfellow et al (2015)







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 $oldsymbol{x}$

"panda" 57.7% confidence

$$\operatorname{sign}(\nabla_{\boldsymbol{x}} J(\boldsymbol{\theta}, \boldsymbol{x}, y))$$

"nematode" 8.2% confidence

Image Source: Goodfellow et al (2015)

 $\begin{array}{c} \boldsymbol{x} + \\ \epsilon \text{sign}(\nabla_{\boldsymbol{x}} J(\boldsymbol{\theta}, \boldsymbol{x}, y)) \\ \text{"gibbon"} \\ 99.3 \% \text{ confidence} \end{array}$

Athalye et al (2018)



Image Source: Youtube Video

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Adversarial examples are a security risk

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Definition (Robust Classifier)

We call a classifier $f : \mathcal{X} \to \mathbb{R}^n$ robust around a point $\mathbf{x} \in \mathcal{X}$ iff $\forall \mathbf{x}' \in \mathcal{N}(\mathbf{x}) : \text{class}(f(\mathbf{x}')) = \text{class}(f(\mathbf{x}))$



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We focus on certification of robustness



Adversarial Robustness: Projected Gradient Descent (PGD) Madry et al (2018)

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$$\mathbf{x}^{(t+1)} = \Pi_{\mathcal{N}(\mathbf{x})}(\mathbf{x}^{(t)} + \alpha \operatorname{sgn}(\nabla_{\mathbf{x}} L(\mathbf{x}, y)))$$
(1)

Where $\Pi(.)$ projects its argument back into $\mathcal{N}(x)$



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Where $\Pi(.)$ projects its argument back into $\mathcal{N}(x)$ Good at finding adversaries...but not exhaustive! (Finding adversarial examples is hard Garini and Wagner (2017))



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| Method | Architecture | PGD10 | AutoAttack | Remark |
|--------|--------------|-------|------------|-----------|
| AT | ResNet18 | 52.73 | 48.67 | |
| MART | ResNet18 | 54.73 | 47.51 | |
| TRADES | ResNet18 | 53.47 | 49.45 | |
| AT | ResNet18 | 55.52 | 50.80 | |
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Image Source: MAIR Framework Github

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- Results depend attack parameters
- Information gain about f is limited

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$$\forall \mathbf{x} \in \mathcal{X} : \forall \mathbf{x}' \in \mathcal{N}(\mathbf{x}) : \mathsf{class}(f(\mathbf{x})) = \mathsf{class}(f(\mathbf{x}'))$$
(3)

Is too strict!



(Leino et al (2021); Athavale et al (2024))

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 $conf_f(x)$ can be e.g. the *Softmax confidence Very* expensive, infeasible above 100s of neurons



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Global Robustness: Adversarial vs. Formal

Adversarial Robustness Techniques

- sample based
- fast
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- expensive locally
- intractable globally
- Proof or Counterexample
- Model needs to be encoded
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Global Robustness: Adversarial vs. Formal

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Our Objective:

- give sample based guarantees about global robustness
- Stay model-agnostic
- Give specific robustness bounds for each prediction

Formal Verification

- expensive locally
- intractable globally
- Proof or Counterexample
- Model needs to be encoded
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Background: Probabilistic Coverage Guarantees with Epsilon-nets



For a classifier $f : \mathcal{X} \to \mathbb{R}^n$, we want to define a notion of *coverage* of a space under a data distribution \mathcal{D}



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Definition (Range-Space)

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ϵ-Nets

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Definition (ϵ -Nets)

Given a range space (\mathcal{X}, \mathcal{R}) and a probability distribution \mathcal{D} , a finite set $N \subset \mathcal{X}$ is called an ϵ -net, iff N intersects each ϵ -probable $R \in \mathcal{R}$, i.e.,

$$\forall \mathsf{R} \in \mathcal{R} : \Pr(\mathsf{R}) \ge \epsilon \Rightarrow \mathsf{N} \cap \mathsf{R} \neq \emptyset \quad \Leftrightarrow \tag{5}$$

$$\forall \mathsf{R} \in \mathcal{R} : \mathsf{N} \cap \mathsf{R} = \emptyset \Rightarrow \mathsf{Pr}(\mathsf{R}) < \epsilon \tag{6}$$

e-Nets: Example

We consider the range space (\mathbb{R}^2 , \mathcal{B}), with \mathcal{B} is some set of circles



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An ϵ -net intersects all likely enough circles



Definition (VC-Dimension (Vapnik and Chervonenkis (2015)))

Let $(\mathcal{X}, \mathcal{R})$ be a range space. The Vapnik-Chervonenkis (VC) dimension d of $(\mathcal{X}, \mathcal{R})$ is the size of the largest set $S \subseteq \mathcal{X}$, such that

$$\forall S' \subseteq S : \exists R \in \mathcal{R} : R \cap S = S' \tag{7}$$

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Well studied for common hypothesis spaces

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ϵ -Nets from iid Samples

Theorem (ϵ -nets from iid samples (Mitzenmacher and Upfal (2017)))

Let $(\mathcal{X}, \mathcal{R})$ be a range-space with VC-dimension d and \mathcal{D} be a probability distribution. For any $0 < \delta, \epsilon \leq \frac{1}{2}$, an iid sample N will be an ϵ -net with probability at least $1 - \delta$ iff

$$|N| = \mathcal{O}\left(\frac{d}{\epsilon}\ln\frac{d}{\epsilon} + \frac{1}{\epsilon}\ln\frac{1}{\delta}\right)$$
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We are interested in obtaining minimal samples of sufficient size, so we find |N| = s with

$$s(\epsilon, \delta, d) = \min_{s \in \mathbb{N}} \left\{ s : s \ge \frac{2}{\epsilon} \left(\log \left(\frac{2}{\delta} \right) + d \log(2s) \right) \right\}$$
(9)

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Distillation with probably approximately global coverage



We have formal tools that can prove global robustness for only very small NNs





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Where we will use $y = class(f_T(\mathbf{x}))$

Gradient-Aligned Distillation Share

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 f_{S}

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Y

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 $\mathcal{L}_{CF}(f_{s}(\mathbf{x}), \mathbf{v}) + \mathcal{L}_{KI}(f_{s}(\mathbf{x}), f_{t}(\mathbf{x})) +$

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Where we will use $y = class(f_T(\mathbf{x}))$ Under *perfect conditions*, f_S is as robust as f_T Assumes both functions are linear in a metric ball $B_r(\mathbf{x})$!

 $\|\nabla_{\mathbf{x}} \mathcal{L}_{CF}(f_t(\mathbf{x}), \mathbf{y}) - \nabla_{\mathbf{x}} \mathcal{L}_{CF}(f_s(\mathbf{x}), \mathbf{y})\|$

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Distill on an ϵ -net *N* over metric balls! Informally:

- 1. We will intersect all ϵ -likely metric balls under \mathcal{D}
- 2. For $\mathbf{x} \in N$, f_S and f_T have same robustness around \mathbf{x} in $B_r(\mathbf{x})$
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We sample sufficiently *N* iid from some dataset with additive noise

Does It Work? Experimental Results

We constructed f_T with known robustness properties and checked if robustness transferred through distillation



Image Source: Indri et al (2024)

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 - How can we detect ϵ -likely balls?

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- Robustness around x transfers if f_S,f_T are linear around x This trivializes checking robustness! Why not use tangent planes directly?
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But what does this mean?

- How can we detect ϵ -likely balls?
- If we consider balls of any size: we require local linearity at arbitrary scale
- If we consider only small balls: maybe none are ϵ -likely (high dimensional data)



Property-Based Robustness Guarantees

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For a classifier $f : \mathcal{X} \to \mathbb{R}^n$, a *robustness oracle* is defined as

$$\operatorname{rob}_{f}(\mathbf{x}) = \min_{\mathbf{x}' \in \mathcal{N}(\mathbf{x})} \{ \|\mathbf{x} - \mathbf{x}'\| : \operatorname{class}(\mathbf{x}) \neq \operatorname{class}(\mathbf{x}') \}$$
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We can also use (non-exact) oracles that find a counterexample with attacks (e.g. PGD)

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$$\mathsf{R}(\rho,\kappa) = \{(\rho',\kappa') \in \mathbb{R}^2 : \rho' < \rho, \kappa' \ge \kappa\}$$
(14)



Confidence

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Answer: We can sample ϵ -nets in Q!

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$$q(\mathbf{x}) = R(\rho, \kappa)$$

10

(17)

Confidence

 $|N| = s(\epsilon, \delta, d)$ depends only on the VC-dimension d of \mathcal{R} , not on \mathcal{X}

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We choose (ρ_1,κ_1) and N tells us f is (ρ_1,κ_1) robust with probability at least $1 - \epsilon$ Now we use f and obtain 100 points with confidence exactly κ_1

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$$\Pr(\mathbf{rob}_{f}(\mathbf{x}) < \rho \mid \mathbf{conf}_{f}(\mathbf{x}) \geq \kappa) \Pr(\mathbf{conf}_{f}(\mathbf{x}) \geq \kappa) < \epsilon$$
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$$\Pr(\mathsf{rob}_f(\mathbf{x}) < \rho \mid \mathsf{conf}_f(\mathbf{x}) \ge \kappa) < \frac{\epsilon}{\Pr(\mathsf{conf}_f(\mathbf{x}) \ge \kappa)}$$

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(21)
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If we can give a conditional statement $\forall (\rho, \kappa)$ we can obtain a robustness radius from the confidence:

$$M(\kappa) = \max_{\rho \in \mathbb{R}} : \Pr(\mathbf{rob}_{f}(\mathbf{x}) < \rho \mid \mathbf{conf}_{f}(\mathbf{x}) \ge \kappa) < \epsilon$$
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We can use conditional guarantees to give "*customized*" robustness lower bounds for each prediction!

With $\epsilon\text{-nets}$ we can only get the bound

$$\mathsf{Pr}(\mathsf{rob}_f(\mathsf{x}) <
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For the case $Pr(conf_f(\mathbf{x}) \ge \kappa) > 1 - p_{max}$

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We use *rank statistics* to estimate a bound from the sample!

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Given a sample *N*, for which κ : Pr(conf_f(**x**) < κ) $\leq p_{max}$? We estimate *the rank* of the p_{max} -quantile κ_{max} of κ ... Let $N_{(i)}$ be the element in *N* with *i*th-biggest confidence

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... and use Chernoff bounds

$$\Pr(\kappa_{\mathsf{max}} < \mathsf{N}_{(i)}) < \delta ext{ s.t.}$$

(25)
$$i < c(|N|, p_{\max}, \delta) = \left[|N|p_{\max} - \sqrt{2|N|p_{\max} \ln\left(\frac{1}{\delta}\right)} \right]$$
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less confident elements in N

Theorem (PAG Robustness)

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Given a classifier $f : \mathcal{X} \to \mathbb{R}^n$, a robustness oracle \mathbf{rob}_f and a data distribution \mathcal{D} over \mathcal{X} For parameters $\epsilon, \delta, p_{max}$

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$$\forall \rho \forall \kappa \leq \kappa_{\max} : \{q(\mathbf{x}) : \mathbf{x} \in \mathsf{N}\} \cap \mathsf{R}(\rho, \kappa) = \emptyset \Rightarrow \Pr\left(\mathsf{rob}_{f}(\mathsf{X}) < \rho | \mathsf{conf}_{f}(\mathsf{X}) \geq \kappa\right) < \frac{\epsilon}{1 - p_{\max}}$$
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If we have no counterexample in N, f is probably approximately globally (ho,κ)-robust

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$$\Pr(\mathbf{rob}_{f}(\mathbf{x}) < \mathcal{M}(\kappa) \mid \mathbf{conf}_{f}(\mathbf{x}) \geq \kappa) < 0.01$$
(28)

Experimental Results



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This method also generalizes to learning other rules in black-box ML
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