Theoretic Fundamentals of Machine and Deep Learning

Certified Robustness I: Randomized Smoothing

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Winter-Spring, 2023

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Content

1. Certified robustness definitions
2. Certified robustness via Lipschitzness
3. Randomized Smoothing and its variants

Robustness in Machine Learning

Robustness [informally]

Ability for a machine learning algorithm a to provide similar outputs on the similar data (i.e. having the same class or other invariant features)

Two types of **Robustness** in ML:

Generalization

Dataset issue: algorithm needs to be robust if the dataset to evaluate it differs (sometimes significantly: we can treat it is a distribution shift) from the training dataset

Adversarial Robustness

Noise issue: algorithm needs to provide the similar output w.r.t. both clean and noisy images (where the model of noise is the topic to consider itself)

For now we'll consider the **Adversarial Robustness**.

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Adversarial Robustness topics

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Certified Robustness: for classification

- Let us NN function $f(x)$ is the classifier to K classes: $f : \mathbb{R}^d \to Y, Y = \{1, \dots, K\}$
- Usually we have NN $h(x) : \mathbb{R}^d \to \mathbb{R}^K$, and $f(x) = \arg\max_{i \in Y} h(x)_i$

Deterministic approach

Need to find the class of input perturbation $S(x, f)$ so as the classifier's output doesn't not change, or more formally:

$$f(x + \delta) = f(x) \quad \forall \delta \in S(x, f)$$

Probabilistic approach

Need to find the class of input perturbation $S(x, f, P)$ w.r.t. robustness probability P s.t.:

$$Prob_{\delta \in S(x,f,P)}(f(x + \delta) = f(x)) = P$$

Remark: Probabilistic approach coincides with Deterministic one when $P = 1$.

Certified Robustness: for regression

- Let us NN function $f(x)$ NN f(x) is the regressor: $f:\mathbb{R}^d \to \mathbb{R}$

Deterministic approach

Need to find the class of input perturbation $S(x, f, f_{low}, f_{up})$ w.r.t. the upper and lower bounds on the output perturbation f_{low}, f_{up} s.t.:

$$f(x) - f_{low} \leq f(x+\delta) \leq f(x) + f_{up} \quad \forall \delta \in S(x, f, f_{low}, f_{up})$$

Probabilistic approach

Need to find the class of input perturbation $S(x, f, f_{low}, f_{up}, P)$ w.r.t. robustness probability P and the upper / lower bounds on the output perturbation f_{low}, f_{up} s.t.:

$$Prob_{\delta \in S(x, f, f_{low}, f_{up}, P)}(f(x) - f_{low} \leq f(x+\delta) \leq f(x) + f_{up}) = P$$

Certified Robustness: inverse tasks for classification

- Suppose that we know the input perturbation class S
- For classification we have only probabilistic formulation

Classification

Need to measure the probability P of retaining the classifier's output under some class of input perturbations S:

$$Prob_{\delta \in S}(f(x+\delta) = f(x)) = P$$

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Certified Robustness: inverse tasks for regression

- Suppose that we know the input perturbation class S
- For regression we have both deterministic and probabilistic formulations

Regression (deterministic formulation)

Need to find the upper and lower bounds $f_{low}(f, x, S)$, $f_{up}(f, x, S)$ of the output perturbation under some class of input perturbations S:

$$f(x) - f_{low}(f, x, S) \leq f(x + \delta) \leq f(x) + f_{up}(f, x, S)$$

Regression (probabilistic formulation)

Need to measure the probability P of keeping the classifier's output inside the lower / upper bounds f_{low}, f_{up} under some class of input perturbations S:

$$Prob_{\delta \in S}(f(x) - f_{low} \leq f(x + \delta) \leq f(x) + f_{up}) = P$$

Certified Robustness via Lipschitzness (1)

- NN classifier to K classes is $f(x)$: $f : \mathbb{R}^d \to Y, Y = \{1, \ldots, K\}$
- NN itself is $h(x) : \mathbb{R}^d \to \mathbb{R}^K$, and $f(x) = \arg\max_{i \in Y} h(x)_i$
- Consider binary case (other cases are treated similarly) $K = 2$ and probabilistic (SoftMax) output: $h(x)_1 + h(x)_2 = 1, \quad h(x)_i \geq 0 \quad \forall i$

Definition of Lipschitz function

Lipschitz function g: $g : \mathbb{R}^d \to \mathbb{R}$ with a Lipschitz constant L so as $\forall x_1, x_2$ it holds $|g(x_1) - g(x_2)| \leq L \|x_1 - x_2\|$

Definition of Local Lipschitz function

Local Lipschitz function g: $g : \mathbb{R}^d \to \mathbb{R}$ with a Lipschitz constant $L(x_0)$ so as $\forall x \in S(x_0)$ it holds $|g(x_0) - g(x)| \leq L(x_0) \|x_0 - x\|$

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Certified Robustness via Lipschitzness (2)

- Let $j = \arg\max_{i \in Y} h(x_0)_i$, and $h(x_0)_j - h(x_0)_{i \neq j} \geq \epsilon$
- Let $h(x_0)_j$ — local Lipschitz function with a Lipschitz constant $L(x_0)$
- Then if $S(x_0) = \{x : \|x_0 - x\| \leq \frac{\epsilon}{2L(x_0)}\}$ we have $|h(x_0)_j - h(x)_j| \leq L(x_0)\frac{\epsilon}{2L(x_0)} = \frac{\epsilon}{2}$
- Therefore $j = \arg\max_{i \in Y} h(x)_i$ and $f(x) = f(x_0) = j$ in the vicinity $S(x_0) = \{x : \|x_0 - x\| \leq \frac{\epsilon}{2L(x_0)}\}$
- $\Rightarrow$ Certified Robustness!

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Certified Robustness via Lipschitzness (3)

But:

Problems

- The certified radius can be much bigger than the local Lipschitz vicinity $S(x_0)$
- It is hard to provide the adequate (not tending to ∞) Lipschitz constant for any industrial Deep Neural Network

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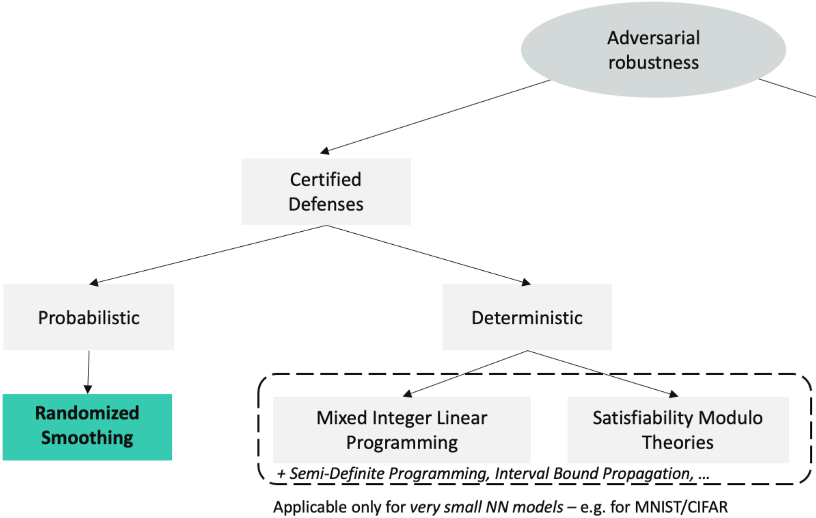
Adversarial Robustness: overview



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Adversarial Robustness: empirical vs certified

Empirical robustness

Bound

The upper bound on the true robust accuracy

Cons

Only valid *until* the *new* – and stronger – *attack* appears

Certified robustness

Bound

The lower bound on the true robust accuracy

Pros

It is what has been *theoretically proven*, and no one attack can beat it

Empirical Robustness: Adversarial Training

- Let us have the training dataset $D = \{(x_i, y_i)_{i=1}^{M}\}$
- Parameters of the neural net f are denoted as θ
- Loss function is $L(f_\theta(x), y) \Rightarrow$ the training process is

$$\min_\theta \mathbf{E}_{(x,y)\in D} L(f_\theta(x), y)$$

Adversarial Training (AT)

Idea: train on the **hardest examples** using some class of perturbations $S(x)$ around training examples $\Rightarrow$ AT is

$$\min_\theta \mathbf{E}_{(x,y)\in D}[\max_{x+\delta\in S(x)} L(f_\theta(x+\delta), y)]$$

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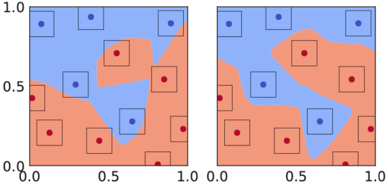
Adversarial Training: pros and cons

AT pros

Very simple methodological principle of training

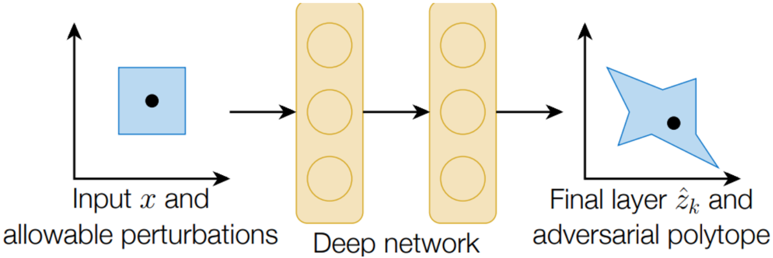


AT cons

- Quite *inefficient training* (longer than usual because need to find hard perturbation for **every training example** for **every iteration**)
- The *accuracy on clean samples is lower* than for usual training

The problem with l_p-balls

- Usually the robustness is studied under the l_p-balls perturbations of input ($S = \{\delta : \|\delta\|_p \leq \epsilon\}$)
- The problem is while the *input* l_p-ball is *convex*, for the output it could be of *any form and convexity*[1]. That's why it is hard to prove anything.



[1] Image source: `https://arxiv.org/pdf/1711.00851.pdf`

Convex relaxation

- Main idea: let's make our regions convex by relaxation!
- E.g., we need to *convexify* the non-linearity ReLU
- Then it can be proved[2] that if some relaxed objective $J_\epsilon(x, g_\theta) \geq 0$ for the dual problem, then there is no an adversarial example $\tilde{x}$ such that $\|\tilde{x} - x\|_\infty \leq \epsilon$ and $f_\theta(\tilde{x}) \neq y_{gt}$
  - g_θ is the neural net constructed from initial f_θ by relaxing ReLU
- This is the example of using *MILP* and, unfortunately, *cannot be generalized* to ImageNet

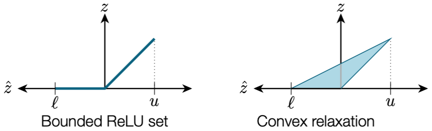
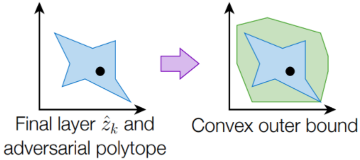


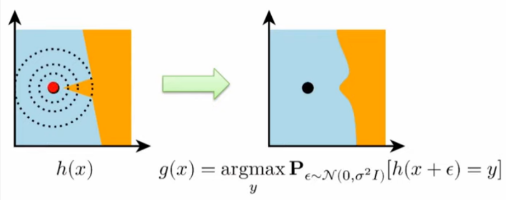
Figure 2. **Illustration of the convex ReLU relaxation over the bounded set $[\ell, u]$.**



[2]Wong, Eric, and Zico Kolter. "Provable defenses against adversarial examples via the convex outer adversarial polytope." 2017

Adversarial Examples: boundary curvature

- Very **curved boundary** leads to *adversarial examples* looking very similar to ones near the classification boundary
- So let's **diminish** this curvature **spike** influence!
- Different approaches exist e.g. by *Lecuyer et al.*[3] and *Li et al.*[4], but the most famous one is by *Cohen et al.*[5]



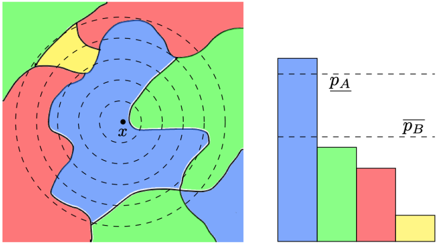
[3] Lecuyer, Mathias, et al. "Certified robustness to adversarial examples with differential privacy." 2018
[4] Li, Bai, et al. "Certified adversarial robustness with additive noise." 2018
[5] Cohen, Jeremy, et al. "Certified adversarial robustness via randomized smoothing." 2019

Randomized Smoothing

Idea of Randomized Smoothing (RS)

- Let's use the **T**est **T**ime **A**ugmentation (**TTA**) in order to mitigate the boundary effect
- The new classifier $g(x)$ is defined as:

$$g(x) = \underset{c \in Y}{\arg\max}\, P(f(x+\epsilon) = c), \epsilon \sim N(0, \sigma^2)$$



RS main result

- If the initial classifier $f(x)$ is robust under Gaussian noise,
- Then the new classifier $g(x)$ is robust under **ANY** noise

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Randomized Smoothing: Theory overview

Theorem: Certification Radius

Suppose $c_A \in Y$ and $\underline{p_A}, \overline{p_B} \in [0,1]$ satisfy
$\mathbb{P}(f(x+\epsilon) = c_A) \geq \underline{p_A} \geq \overline{p_B} \geq \max_{c_B \neq c_A} \mathbb{P}(f(x+\epsilon) = c_B)$. Then
$g(x+\delta) = c_A \quad \forall \|\delta\|_2 < R$, where

$$R = \frac{\sigma}{2}(\Phi^{-1}(\underline{p_A}) - \Phi^{-1}(\overline{p_B}))$$

Tightness of Radius R

Assume $\underline{p_A} + \overline{p_B} \leq 1$. Then for any perturbation $\delta, \|\delta\|_2 > R$ there exist a base classifier f s.t. $\mathbb{P}(f(x+\epsilon) = c_A) \geq \underline{p_A} \geq \overline{p_B} \geq \max_{c_B \neq c_A} \mathbb{P}(f(x+\epsilon) = c_B)$ so as $g(x+\delta) \neq c_A$

Remark. Φ^{-1} is the inverse of the standard Gaussian CDF: $\Phi(x) = \frac{1}{2\pi}\int_{-\infty}^{x} e^{-\frac{t^2}{2}} dt$.

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Randomized Smoothing: Theory insights

Why $\underline{p_A}$ and $\overline{p_B}$ instead of p_A and p_B?

Because in most cases we cannot get exact probabilities for $P(f(x+\epsilon)=c), \epsilon \sim N(0,\sigma^2)$, and we need to estimate.

How to get the R?

Use so called Neyman-Pearson Lemma[6].

[6] Neyman, Jerzy, and Egon Sharpe Pearson. "On the problem of the most efficient tests of statistical hypotheses." 1933

Randomized Smoothing: Interesting cases

Let us consider the linear binary classifier $f(x) = \text{sign}(w^T x + b)$

It is a smoothed version of itself

If g is a smoothed version of f with any σ, then $f(x) = g(x)$.

Certified radius just a distance to the boundary

If g is a smoothed version of f with any σ, then using the previous Theorem for certification radius R with $\underline{p_A} = p_A$ and $\underline{p_B} = p_B$ will yield $R = \frac{|w^T x + b|}{\|w\|}$.

But sometimes the certification radius can be really big (for non-linear binary classifier):

Certified radius can be of any value

For any $\tau > 0$, there exists a base classifier f and an input x_0 for which the corresponding g is robust around x_0 at radius ∞, whereas the previous Theorem for certification radius R only certifies a radius $R = \tau$ around x_0.

Randomized Smoothing: Training

- To certify the classifiers, authors **trained the base models with Gaussian noise** from $N(0, \sigma^2 I)$ — actually, to make the classifier $f(x)$ to be more robust to Gaussian noise
- So no any other training-specific tricks aside from simple **augmentation**

Randomized Smoothing: Inference

- Trained models are compared using "**approximate certified accuracy**":
  - $\forall$ test radius $\delta = r$ the fraction of examples is returned so as the procedure CERTIFY:
    - Provides the answer
    - Returns the correct class
    - Returns a radius R so as $r \leq R$

Procedure CERTIFY

- Can return ABSTAIN if confidence bounds are too loose (done by **Clopper-Pearson** confidence intervals for the Binomial distribution[7])
- If not ABSTAIN, then return the majority class $\hat{c}_A$ and certification radius $R = \sigma\Phi^{-1}(\underline{p_A})$

Remark1. Quantile of Gaussian distribution corresponding to the error rate is denoted as α (larger α, tighter the **c**onfidence **i**nterval (CI), but less reliable).

Remark2. Class estimation and CI of g are done by Monte Carlo sampling n times.

[7] Clopper, Charles J., and Egon S. Pearson. "The use of confidence or fiducial limits illustrated in the case of the binomial." 1934

Randomized Smoothing: Results on ImageNet

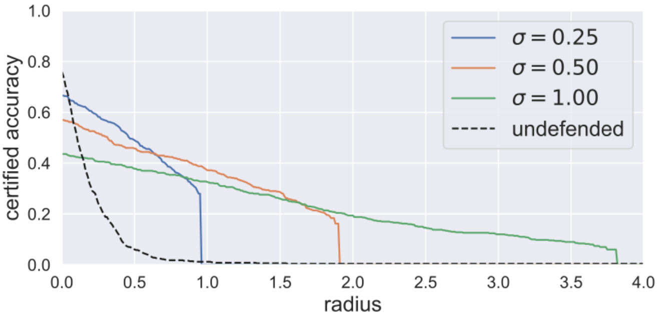

Table 1. Approximate certified accuracy on ImageNet. Each row shows a radius r, the best hyperparameter σ for that radius, the approximate certified accuracy at radius r of the corresponding smoothed classifier, and the standard accuracy of the corresponding smoothed classifier. To give a sense of scale, a perturbation with ℓ_2 radius 1.0 could change one pixel by 255, ten pixels by 80, 100 pixels by 25, or 1000 pixels by 8. Random guessing on ImageNet would attain 0.1% accuracy.

ℓ_2 RADIUS	BEST σ	CERT. ACC (%)	STD. ACC(%)
0.5	0.25	49	67
1.0	0.50	37	57
2.0	0.50	19	57
3.0	1.00	12	44

Remark1. Waterfall just because the trained model is robust usually under some $r \leq R$.
Remark2. "Certified accuracy" = approximate certified accuracy.
Remark3. The difference between "clean" and "certified" accuracy is not order of magnitude (it works! and can be useful).

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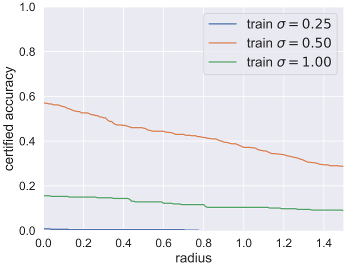
Randomized Smoothing: Influence of training noise parameter σ

- Main outcomes:
  - Best results are when the inference σ_I and training σ_T parameters of noise σ are exactly the same: $\sigma_T = \sigma_I = \sigma$
  - If not the same, better results are when the training noise is more severe than the inference one: $\sigma_T > \sigma_I$

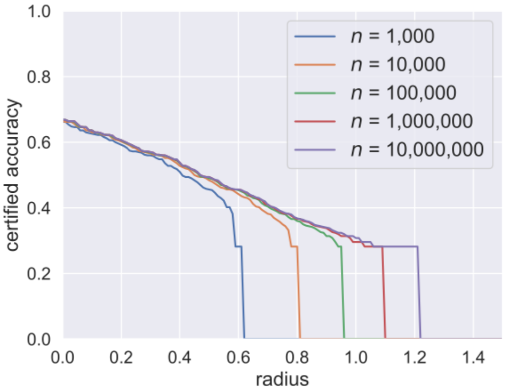


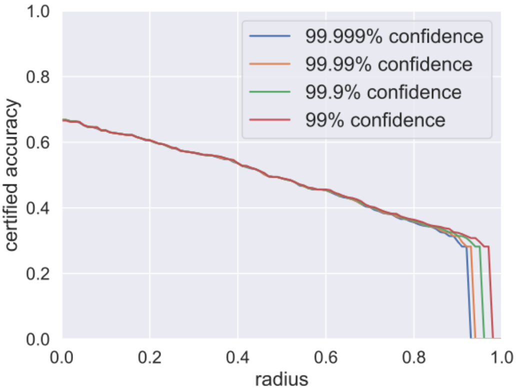
(b) ImageNet

Remark. Here the inference noise level is $\sigma_I = 0.5$.

Randomized Smoothing: Influence of Inference parameters n and α

- Main outcomes:
  - Larger number of Monte Carlo samples n, the larger the certified radius R (significantly; but veeery slow)
  - Larger confidence in results $(1-\alpha)$, the smaller the certified radius R (but not much)



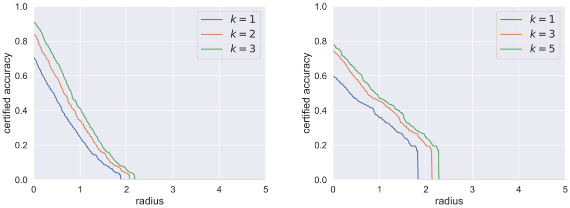


Randomized Smoothing: Robustness radius in practice

- Actually, with NN classifier $f(x)$ we can have **larger real robustness radius** than R from Theorem
- Authors just tried to find the real adversaries under $r > R$ and measure the success of the attack (cf. the **inverse formulation** of Certified Robustness)
- (The lower the success rate the more robust the model):
  - $r = 1.5 \cdot R \Rightarrow 17\%$ of success rate
  - $r = 2 \cdot R$: $\Rightarrow 53\%$ of success rate

Improvement: Certified Robustness for Top-k Predictions[8]

- Sometimes we need to concentrate not on the biggest in probability prediction ("top-1") but on the whole set of "top-k" predictions with largest probabilities
- It turned out that the very similar results can be transferred to the top-k setting
  - Certification guarantees that the correct answer still be presented among top-k answers of the smoothed classifier
  - **Results**: Certified top-1 / top-3 / top-5 accuracy = 46.6% / 57.8% / 62.8% when perturbation radius $\|\delta\|_2 = 0.5$



(a) CIFAR10 (b) ImageNet

[8] Jia, Jinyuan, et al. "Certified robustness for top-k predictions against adversarial perturbations via randomized smoothing." 2019

Certification: intermediate takeaway

- Randomized Smoothing = Smoothing distribution + norm l_p of perturbation
- Randomized Smoothing requires multiple inferences :(
- Certified robustness is better than empirical adversarial training in certification, but worse than clean performance (and too much time to train)

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Thank you!