CC-Cert: A Probabilistic Approach to Certify General Robustness of Neural Networks

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Abstract

In safety-critical machine learning applications, it is crucial to defend models against adversarial attacks — small modifications of the input that change the predictions. Besides rigorously studied $\ell_p$-bounded additive perturbations, semantic perturbations (e.g., rotation, translation) raise a serious concern on deploying ML systems in real-world. Therefore, it is important to provide provable guarantees for deep learning models against semantically meaningful input transformations. In this paper, we propose a new universal probabilistic certification approach based on Chernoff-Cramer bounds that can be used in general attack settings. We estimate the probability of a model to fail if the attack is sampled from a certain distribution. Our theoretical findings are supported by experimental results on different datasets.

Introduction

Deep neural network (DNN) models have achieved tremendous success in many tasks. On the other hand, it is well known that they are intriguingly susceptible to adversarial attacks of different kinds (Szegedy et al. 2013), thus there is a pressing lack of models that are robust to such attacks. Several mechanisms are proposed as empirical defenses to various known adversarial perturbations. However, these defenses have been later circumvented by new more aggressive attacks (Carlini and Wagner 2017b,a; Athalye, Carlini, and Wagner 2018; Tramer et al. 2020).

Therefore, a natural question arises: given a DNN model $f$, can we provide any provable guarantee on its prediction under a certain threat model, i.e. $f(x) = f(x_T)$, where $x_T$ is a transformed input? This is precisely the topic of a growing field of certified robustness. A part of the existing research relies on the analysis of the Lipschitz properties of a classifier: its output’s Lipschitz-continuity leads to a robustness certificate for additive attacks (Anil, Lucas, and Grosse 2019; Li et al. 2019; Serrurier et al. 2021). Another excellent tool for such a task is smoothing: the inference of the model is replaced by averaging of predictions over the set of transformed inputs. First, this approach was developed for small-norm attacks (Cohen, Rosenfeld, and Kolter 2019; Levine and Feizi 2020), but then it was successfully generalized to a much more general class of transforms such as translations or rotations (Balunović et al. 2019; Fischer, Baader, and Vechev 2020). A recent work (Li et al. 2021) and its follow-up (Alfarra et al. 2021) study a general smoothing framework that is able to provide useful certificates for the most common synthetic image modifications and their compositions.

However, a drawback of smoothing methods is that they can only certify a smoothed model which is significantly slower than the original one due to a large number of samples to approximate the expectation. Thus, we need a method that a) can certify any given black-box model, and b) is general and not tailored to a specific threat model (such as small-norm perturbations). Providing an exact rigorous certification in this setting is a very challenging task.

Instead, in this paper, we propose and investigate a probabilistic approach that produces robustness guarantees of a black-box model against different threat models. In this approach, we estimate the probability of misclassification, if the attack is sampled randomly from the admissible set of attacks. We bound this quantity by the probability of the large deviation of a certain random variable $Z$, which is derived from the distance between the probability vectors (see Lemma 1). To estimate the probability of the large deviation, we propose to use the empirical version of the Chernoff-Cramer bound and show that under the additional assumption on $Z$ this bound holds with high probability (see Theorem 1).

Our contributions are summarized as follows:

• We propose a new framework called Chernoff-Cramer Certification (CC-Cert) for probabilistic robustness bounds and theoretically justify them based on the empirical version of Chernoff-Cramer inequality;

• We test those bounds and demonstrate their efficacy for several models trained in different ways for single semantic parametric transformations and some of their compositions.

Preliminaries

We consider the classification task with fixed set of data samples $S = \{(x_1, y_1), \ldots, (x_m, y_m)\}$ where $x_i \in \mathbb{R}^D$ is
Robustness and Large Deviations

Probabilistic Certification of Robustness

Our proposal is to certify the robustness of the classifier $f$ by estimating the probability of large deviations of its output probability vectors. The following lemma shows how the discrepancy $f(x) - f(x_T)$ between the output vectors $f(x)$ and $f(x_T)$ assigned by $f$ to the original sample $x$ and its transformed version $x_T$ is connected to their predicted class labels.

**Lemma 1.** Let $f : \mathbb{R}^D \rightarrow [0, 1]^C$ be the classifier with a known inference procedure and $x$ be an input sample. Let $x_T$ be a transformation of $x$ after transform $T \in T$ where $T$ is a given class of transforms. Assume that $p = f(x)$ and $p_T = f(x_T)$ are the probability vectors of the original sample $x$ and its transformed version $x_T$, respectively. Let $c = \arg\max p$ and $\hat{c} = \arg\max p_T$ be the classes assigned by $f$ to $x$ and $x_T$, respectively and let $d = \frac{m-n}{2}$ be the half of the difference between two largest components of $p$.

Then, if $\|p - p_T\|_\infty < d$ holds, $\hat{c} = c$.

**Proof.** Suppose that $c \neq \hat{c}$, then, $p_{T\hat{c}} > p_{Tc}$ and $p_c > p_{\hat{c}}$. On the other hand, since the difference norm $\|p - p_T\|_\infty = \max(|p_1 - p_{T1}|, \ldots, |p_C - p_{TC}|) < d$,
we have $p_c - d < p_{Tc}$ and $p_{Tc} - d < p_{c}$, which leads to $p_{Tc} - p_{Tc} > (p_c - d) - (p_c + d) = p_c - p_{c} - 2d$.

Since $2d = p_1 - p_2 = p_c - p_2$,

$$p_c - p_c - 2d = p_2 - p_{c} \geq 0,$$

yielding a contradiction. Thus, $c = c$.

Intuitively, the lemma states that whenever the maximum change in the output $p_T$ does not exceed half the distance $d$ between the two largest components in $p$, the argument of the maximum in $p_T$ does not change in comparison to the one in $p$.

We suggest to estimate the right tail of the probability distribution of $Z = Z_{x,T} = \|p - p_T\|_{\infty}$. Namely, we want to bound from above the probability $P(Z \geq d)$ to provide guarantees that transformations from class $T$ applied to $x$ do not lead to a change of class label assigned by $f$.

**Deriving the Bound: Estimates of the Tail of the Distribution**

In this section, we describe our method to estimate the tail of probability distribution. Namely, we refer to the Chernoff-Cramer approach and propose a technique that allows us to use a sample mean instead of the population mean in the right-hand side of the bound.

**Lemma 2** (Markov’s inequality). Let $Z$ be a non-negative scalar random variable with finite expectation and $t \in \mathbb{R}, t > 0$, then

$$P(Z \geq t) \leq \frac{\mathbb{E}(Z)}{t}.$$  

**Lemma 3** (Chernoff-Cramer method, (Boucheron, Lugosi, and Bousquet 2003)). Let $Z$ be a scalar random variable, $t \in \mathbb{R}, t > 0$ and $d \in \mathbb{R}$. Then

$$P(Z \geq d) = P(e^{Zt} \geq e^{dt}) \leq \frac{\mathbb{E}(e^{Zt})}{e^{dt}}$$  

by a Markov’s inequality.

The right-hand side of Eq. 2 is the upper-bound for $\epsilon$ in Eq. 1. Note that depending on the value of $t$, Eq. 2 produces a lot of bounds, so it is natural to choose $t$ that minimizes its right-hand side.

**Sample Mean Instead of True Expectation**. Overall, we want to use Eq. (2) to bound the probability that the deviation between $p$ and $p_T$ is greater than half the difference between the two largest components of $p$, i.e. $d$. Unfortunately, it is impractical to compute its right hand side directly, because the population mean of $e^{Zt}$ is unknown in general. Instead, the task is to estimate the density of

$$Y = \exp(-dt) \frac{1}{n} \sum_{i=1}^{n} \exp(Z_it),$$

where $\forall i \in \{1, \ldots, n\}$ $Z_i = \|p - p_{Tc}\|_{\infty}$ is the norm of the difference in the probability vectors of original and transformed samples. There is a certain challenge in such an approach: when the population mean is replaced by the sample mean, it is possible to underestimate the true expectation, and thus, provide an incorrect bound which is less than the right-hand side of Eq. (2). It implies that the inequality

$$P(Z \geq d) \leq Y,$$  

which is the modification of (2) by the replacement of the true expectation by a sample mean, holds with some probability: it is guaranteed to hold only in case $Y \geq e^{-dt}\mathbb{E}(e^{Zt})$.

Thus, the probability of the sample mean to underestimate the population mean,

$$P(Y \leq \frac{\mathbb{E}(e^{Zt})}{e^{dt}}),$$

needs to be small as it regulates the correctness of computation of the bound in the form of Eq. (3). Our proposal is to bound from above the probability in Eq. (5) by sampling $k$ i.i.d. sample means $\{Y_1, \ldots, Y_k\}$ in the form of (3) and exploit the statistics of the random variable max($\{Y_1, \ldots, Y_k\}$).

The pseudo-code in Algorithm (1) summarizes the bound computation for a single input $x$.

**Several Sample Means Instead of One**. In this section, we show that, under certain assumptions, bound provided by the Algorithm (1) may be used instead of the right-hand side of Eq. (2).

**Lemma 4** (Paley-Zygmund, (Paley and Zygmund 1930)). Suppose a random variable $X$ is positive and have finite variance, $\sigma_X^2 < \infty$. Then, $\forall \delta \in (0, 1)$,

$$P(X < \delta \mathbb{E}(X)) \leq \frac{\sigma_X^2}{\sigma_X^2 + (1 - \delta)^2(\mathbb{E}(X))^2}.$$  

**Theorem 1** (Worst-out-of-k-bounds). Suppose that random variable $X$ takes values from $[0, 1]$, probability density function of random variable $\xi = e^{Xt}$ is positively skewed and has coefficient of variation $C_\xi = \frac{\sigma_\xi}{\mathbb{E}(\xi)} \sim 1$. Then, given $b$ as the bound produced by the Algorithm 1,

$$P\left(\frac{b}{\mathbb{E}(\xi)} < \left(\frac{1}{1 + \frac{n(1-\delta)^2}{C_\xi^2}}\right)^k\right).$$  

Proof. As one of the steps of the Algorithm 1, sample means $Y_j = \xi_j e^{-dt} = \left\{\frac{\sum_{i=1}^{n} X_{ij}}{n} \right\}_j$ are computed. Note that the expectation and variance of $\xi$ and $\xi$ are related as $\mathbb{E}(\xi) = \mathbb{E}(\xi) = \mu_\xi$ and $\sigma_\xi^2 = \frac{\sigma_\xi^2}{n}$, respectively.

Then, according to (6),

$$P(\xi < \delta \mathbb{E}(\xi)) = P(\xi < \delta \mu_\xi) \leq \frac{\sigma_\xi^2}{\sigma_\xi^2 + (1 - \delta)^2(\mu_\xi)^2}$$

$$= \frac{\sigma_\xi^2}{\sigma_\xi^2 + n(1-\delta)^2 \mu_\xi^2} = \frac{1}{1 + \frac{n(1-\delta)^2}{C_\xi^2}} = p(n, C_\xi).$$

\[1\]In our repository the code is parallelized for batches.
Algorithm 1: Chernoff-Cramer bound calculation algorithm.

1: function BOUND(f, x, y, t, transform, n, k, δ)
2: p ← f(x) ▶ compute model output on original x
3: d = \frac{P[0]−p[1]}{2} ▶ Compute the difference between top 2 classes
4: y = \max(p) ▶ compute predicted class
5: hit ← y == y ▶ boolean variable indicating correctness of prediction for initial input
6: x_n = repeat(x, n) ▶ repeat original input n times
7: p_n = repeat(p, n) ▶ repeat p n times
8: bounds ← \{0, \ldots, 0\} ▶ initialize placeholder for bounds with k zeros
9: for i=0, i<k, i++ do
10: x_T = transform(x_n) ▶ apply random transforms to input x_n
11: p_T ← f(x_T) ▶ compute model output on transformed x_T
12: Z = \|p_n−p_T\|_\infty ▶ compute the change in output vector in terms of max norm
13: Zd_T = outer(Z, t) ▶ multiply every diff by vector of temperatures t
14: \mathbb{E}(e^{Zd_T}) = \text{mean}(\exp(Zd_T)) ▶ compute sample mean over n random transforms
15: e^{dt} = \exp(dt)
16: b = \mathbb{E}(e^{Zd_T})/e^{dt} ▶ get the bounds vector over temperatures
17: b_{\text{min}} = \min(b) ▶ compute the smallest bound over temperatures
18: bounds[k] ← b_{\text{min}}
19: bound = \frac{1}{k}\max(bounds) ▶ compute the largest of obtained bounds and normalize by δ
20: return min(1.0, bound), hit

Since sample means $\xi_j = Y_j e^{dt}$, $j \in [1, \ldots, k]$, in Algorithm (1) are i.i.d.,

$$\mathbb{P}\left(\max(\xi_1, \ldots, \xi_k) < \delta \mu_\xi\right) = \prod_{j=1}^{k} \mathbb{P}(\xi_j < \delta \mu_\xi) \leq \prod_{j=1}^{k} p(n, C_v) = p(n, C_v)^k.$$ 

Thus, since the left-hand side of the above inequality is the one from (7), namely

$$\mathbb{P}\left(\max(\xi_1, \ldots, \xi_k) < \delta \mu_\xi\right) = \mathbb{P}\left(\frac{1}{\delta} \max(\xi_1, \ldots, \xi_k) < \mu_\xi\right) = \mathbb{P}\left(\hat{b} < \frac{\mathbb{E}(\xi)}{e^{dt}}\right),$$

inequality (7) holds. \qed

**Remark.** When the number of samples in the Algorithm 1 is enough, namely, $n > n_\delta = (1−\delta)^{-2}C_v^2$, the right hand side of inequality (7) is less than $\left(\frac{1}{2}\right)^k$. In other words, there exists a number $n_\delta$ such that for all $n > n_\delta$ the probability can be made small for not very large $k$. In Figure 2, we present an example of positively skewed probability density.

![Positively skewed probability density](image)

**Figure 2:** Example of positively skewed probability density function.

### Types of Model Training and Computation Cost of Inference

It should be mentioned that our method can be applied for certification of any model $f(x)$, i.e. it does not require changing the inference procedure as it is done in smoothing methods. However, if the model training is done in the standard way, the overall robust accuracy is expected to be significantly lower than the plain accuracy of the model. A straightforward way to improve the robustness of the model is to modify the training procedure. We can adapt the training procedure used in smoothing methods such as (Li et al. 2021). Such procedure can be implemented through data augmentation: the model is trained on transformed samples, thus we expect it will have higher robust accuracy. During the inference stage, the smoothed model has to be evaluated many times (Horváth et al. 2021), thus increasing the complexity. In our approach, we can apply the certification directly to the original model trained in an augmented way. Our numerical experiments confirm that such models typically have better accuracy, however, there are notable exceptions. This means that more research is needed in training more robust plain models and/or mixed approaches such as smoothing with a small number of samples.

### Experiments

In order to evaluate our method, we assess the proposed bounds on the public datasets, namely, MNIST and CIFAR-10.

All the models, training and testing procedures are implemented in PyTorch (Paszke et al. 2019), and the transformations considered are implemented with use of Kornia framework (Riba et al. 2020). We use architectures, training parameters and procedures from (Li et al. 2021) and evaluate our approach on 500 random test samples for each experiment, following (Cohen, Rosenfeld, and Kolter 2019).
As a result of the experiments, we provide probabilistically certified accuracy, \( \text{PCA} \), in dependence on probability threshold \( \varepsilon \) and show how it is connected to empirical robust accuracy, \( \text{ERA} \), under corresponding adaptive attack. Namely, given the classifier \( h(\cdot) \), set of images \( S = \{(x_1, y_1), \ldots, (x_m, y_m)\} \) and threshold \( \varepsilon \), probabilistically certified accuracy is computed as

\[
\text{PCA}(S, \varepsilon) = \frac{|(x, y) \in S : \text{BOUND}(x) < \varepsilon \text{ and } h(x) = y|}{m}.
\]

At the same time, given the discretization \( \Theta = \{\theta_1, \ldots, \theta_r\} \) of space of parameters of the transform \( T \), empirical robust accuracy is computed as a fraction of objects from \( S \) that are correctly classified under all the transformations \( T_{\theta_i}, i \in [1, \ldots, r] \):

\[
\text{ERA}(S) = \frac{|(x, y) \in S : h(T_{\theta_i}(x)) = y \forall i \in [1, \ldots, r]|}{m}.
\]

**Bound Computation Parameters and Cost**

In all our experiments, we use the following parameters for the Algorithm 1: number of samples \( n = 200 \), number of bounds \( k = 30 \), parameter \( \delta = 0.9 \) for Lemma (4), temperature vector \( t \) consists of 500 evenly spaced numbers from interval \([10^{-4}, 10^4] \). We use \( r = 20 \) as discretization parameter for space of parameters for each transform. Execution of the Algorithm 1 on single GPU Tesla V100-SXM2-16GB takes 30 – 1000 seconds on MNIST and 60 – 2000 seconds on CIFAR-10 depending on the transform complexity.

**Considered Transformations**

Here we present the set of transformations studied in this work and provide the set of corresponding parameters used in the experiments with single transformations.

**Image Rotation.** The transformation of rotation is parameterized by the rotation angle \( \phi \) and is assumed to be followed by the bilinear interpolation with zero-padding of rotated images. In case of CIFAR-10 dataset, we use \( \Theta = \{\phi \in [-10^\circ, 10^\circ]\} \), and \( \Theta = \{\phi \in [-50^\circ, 50^\circ]\} \) for MNIST.

**Image Translation.** The transformation of image translation is parameterized by a translation vector and is also assumed to be followed by bilinear interpolation. We use zero-padding and are not restricted to discrete translations. In case of CIFAR-10, we use \( \Theta = \{v \in \mathbb{R}^2 : |v| \leq 0.2 \times w\} \), and for MNIST \( \Theta = \{v \in \mathbb{R}^2 : |v| \leq 0.3 \times w\} \), with \( w \) equal to the width/height of the image, i.e. translation by no more than 20\% of image for CIFAR-10 and no more than 30\% of image for MNIST, respectively.

**Brightness Adjustment.** The transformation of brightness adjustment is just an element-wise addition of a brightness factor to an image. We change the brightness by no more than 40\% for CIFAR-10 and by no more than 50\% for MNIST.

**Gaussian Blurring.** The transformation of Gaussian blurring (Li et al. 2021) convolves an image with the Gaussian function

\[
G_\sigma(k) = \frac{1}{\sqrt{2\pi}\sigma} e^{-k^2/2\sigma^2},
\]

where a squared kernel radius \( \sigma \) is a parameter. In our experiments, \( \Theta = \{\sigma \in (0, 9]\} \) for both CIFAR-10 and MNIST.

**Contrast Adjustment.** The transformation of contrast adjustment is just an element-wise multiplication of image by a contrast factor. We change contrast by no more than 40\% for CIFAR-10 and by no more than 50\% for MNIST.

**Image Scaling.** The transform of image scaling is resize of one by two factors corresponding to spatial dimensions. In our work, we zero-pad downscaled images and use \( \Theta = \{s \in \mathbb{R}^2 : ||s||_2 \in [0.7, 1.3]\} \) for CIFAR-10 and \( \Theta = \{s \in \mathbb{R}^2 : ||s||_2 \in [0.5, 1.5]\} \) for MNIST. In other words, we adjust no more than 30\% of image size on CIFAR-10 and no more than 50\% of image size on MNIST.

**Quantitative Results of Experiments.** We present considered transformations, corresponding parameters, and quantitative results in Table 1 and visualize our results in the Technical Appendix. In almost all cases, PCA bounds are smaller than ERA, and the difference is small. This confirms that our bounds are sufficiently tight for a wide class of transformations.

**Evaluation Protocol Illustration**

Figure 3 illustrates the certification of the model to brightness adjustment on CIFAR-10. Following Theorem 1, it is
at least $1 - \left(\frac{1}{2}\right)^{30}$ chance that almost 60% of considered samples will be correctly classified by a considered model trained with smoothing after no more than 40% brightness adjustment with probability $1 - \varepsilon \geq 1 - 10^{-7}$.

**Comparison with the Clopper-Pearson Confidence Intervals**

It is natural to compare upper bound for probability of a model to fail obtained via proposed method with the upper limit of corresponding Clopper-Pearson confidence interval (Clopper and Pearson 1934) for an unknown binomial probability $p$. Namely, we randomly sample $n$ transforms and count the number $k$ of the ones that mislead a classifier. If it is zero, we can upper bound the probability $p \leq \frac{C(\alpha)}{n}$ given confidence level $\alpha$. Thus, in order to get bound of $10^{-4}$ we need at least 10000 transformed version of a sample. Analogously to **probabilistically certified accuracy**, Clopper-Pearson certified accuracy (CPCA) is computed as

$$CPCA(S, \varepsilon) = \frac{|\{x, y\} \in S : CP(x) < \varepsilon \& h(x) = y\}}{m},$$

where $CP(x) = CP(x, n, k, \alpha)$ is the upper limit of the classical Clopper-Pearson bound for sample $x$ given $n$, $k$, $\alpha$ from above.

In Figures 4, 5, we compare Clopper-Pearson certified accuracy for different number of trials $n$ and probabilistically certified accuracy for the same experiment, respectively.

It can be seen that the method proposed in this paper allows to get a better bound with smaller number of samples. The reason is that we use additional information – the distribution of the random variable $Z$, unlike the CP approach which relies solely on the fact of misclassification.

**Related Work**

**Adversarial Vulnerability.** Adversarial examples (Szegedy et al. 2013; Goodfellow, Shlens, and Szegedy 2014) have
attracted significant attention due to vulnerability of neural networks in safety-critical scenarios. Although initially found as \( \ell_p \)-bounded attacks (Goodfellow, Shlens, and Szegedy 2014; Moosavi-Dezfooli, Fawzi, and Frossard 2016), several beyond \( \ell_p \) adversaries have been proposed that degrade performance of deep models. They include semantic perturbations, such as rotation and translation (Kanbak, Moosavi-Dezfooli, and Frossard 2018; Xiao et al. 2018), color manipulation (Hosseini and Poovendran 2018), renderer-based lightness and geometry transformation (Liu et al. 2018), parametric attribute manipulation (Joshi et al. 2019), 3d scene parameters such as camera pose, sun position, global translation, rotation (Li et al. 2018b). These threats present a serious obstacle for model deployment in safety-critical real-world applications.

**Certified Defenses Against Additive Perturbations.** To overcome the adversarial vulnerability of deep models, several empirical defenses have been presented, however, they were found to fail against new adaptive attacks (Tramer et al. 2020). This forced researchers to provide certified defenses that guarantee stable performance. A number of works have been tackling this problem for small additive perturbations from different perspectives. This includes semi-definite programming (Raghunathan, Steinhardt, and Liang 2018), interval bound propagation (Gowal et al. 2018), convex relaxation (Wong and Kolter 2018), duality perspective (Dvijotham et al. 2018), Satisfiability Modulo Theory (Bunel et al. 2017; Katz et al. 2017; Ehlers 2017). Although these methods consider small networks, randomized smoothing (Cohen, Rosenfeld, and Kolter 2019; Li et al. 2018a; Lecuyer et al. 2019) and its improvements (Salman et al. 2019; Zhai et al. 2020) have been proposed as a certified defense for any network that can be applied to large-scale datasets.

**Certified Defenses Against Image Transformations.** Following certificates for \( \ell_p \)-bounded perturbations, several methods proposed certified robustness against semantic perturbations. Generating linear relaxation and propagating through a neural network was used in (Singh et al. 2019; Balunović et al. 2019; Mohapatra et al. 2020b). Extensions of MCMC-based randomized smoothing (Cohen, Rosenfeld, and Kolter 2019) to the space of semantic transformations were presented in (Fischer, Baader, and Vechev 2020; Li et al. 2021; Alfarra et al. 2021). Our work presents a probabilistic approach for certifying neural networks against different semantic perturbations. Perhaps, the closest to our approach are PROVEN (Weng et al. 2019), where authors present a framework to probabilistically certify neural networks against \( \ell_p \) perturbations and work of (Mangal, Nori, and Orso 2019), where authors certify a neural network in a probabilistic way by overapproximation of input regions that violate model’s robustness. However, these works do not consider probabilistic certifications under semantic transformations.

**Conclusion and Future Work**

We proposed a new framework CC-Cert for probabilistic certification of the robustness of DNN models to synthetic transformations and provide theoretical bounds on its robustness guarantees. Our experiments show the applicability of our approach for certification of model’s robustness to a random transformation of input. An important question that is not considered in our work is the worst-case analysis of robustness to synthetic transformations. Future work includes analysis of the discrepancy between worst-case transformations of general type and corresponding random transformations. A possible gap between certification with probability and certification in worst-case should be carefully analyzed and narrowed.

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