Consistency Regularization for Certified Robustness of Smoothed Classifiers

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Abstract
A recent technique of randomized smoothing has shown that the worst-case (adversarial) $\ell_2$-robustness can be transformed into the average-case Gaussian-robustness by “smoothing” a classifier, i.e., by considering the averaged prediction over Gaussian noise. In this paradigm, one should rethink the notion of adversarial robustness in terms of generalization ability of a classifier under noisy observations. We found that the trade-off between accuracy and certified robustness of smoothed classifiers can be greatly controlled by simply regularizing the prediction consistency over noise. This relationship allows us to design a robust training objective without approximating a non-existing smoothed classifier, e.g., via soft smoothing. Our experiments under various deep neural network architectures and datasets demonstrate that the “certified” $\ell_2$-robustness can be dramatically improved with the proposed regularization, even achieving better or comparable results to the state-of-the-art approaches with significantly less training costs and hyperparameters.

1 Introduction

Despite achieving even super-human level performance on i.i.d. datasets [He et al., 2016; Silver et al., 2017; Devlin et al., 2019], deep neural network (DNN) classifiers usually make substantially fragile predictions than humans on the samples not from the data-generating distribution. The broad existence of adversarial examples [Szegedy et al., 2014; Goodfellow et al., 2015] are arguably the most crucial instance of this phenomenon: a small, adversarially-crafted perturbation on input can easily change the prediction of a classifier, even when the perturbation does not affect the semantic information perceived by humans at all.

This intriguing weakness of DNNs has encouraged many researchers to develop robust neural networks, along with a parallel attempt to break them with stronger attacks [Carlini and Wagner, 2017a; Uesato et al., 2018; Athalye et al., 2018]. Currently, the community has agreed that adversarial training [Goodfellow et al., 2015; Madry et al., 2018; Zhang et al., 2019], i.e., augmenting the training dataset with adversarial examples, is an effective defense method, but the “scalability” of the method is often questionable in several aspects: (a) it is generally hard to guarantee that an adversarially-trained classifier is indeed robust, (b) generalizing the robustness beyond the training threat model is still challenging [Tramèr and Boneh, 2019; Kang et al., 2019], and (c) the network capacity required for robust representation seems to be much larger than practice, e.g., a recent observation shows empirical robustness does not saturate even at ResNet-638 on ImageNet dataset [Xie and Yuille, 2020].

Alternatively, a growing body of the research has developed methods that can provide certified robustness [Sinha et al., 2018; Wong and Kolter, 2018; Zhang et al., 2020]. Randomized smoothing [Lecuyer et al., 2019; Cohen et al., 2019] is a recent idea in this direction, which shows that any classifier (e.g., a neural network) that performs well under Gaussian noise can be “smoothed” into a certifiably robust classifier. This opens a new, scalable notion of adversarial robustness: a neural network may not have to be perfectly smooth, as a proxy of another classifier.
However, it has been relatively under-explored that how to train a good base classifier to maximize the certified robustness of the smoothed counterpart, e.g., Cohen et al. [2019] only explored the standard training with Gaussian augmentation. A few recent works [Salman et al., 2019; Zhai et al., 2020] have shown that a more sophisticated training algorithm can indeed improve the certified robustness, but the common downside is that they require a sensitive choice of many hyperparameters to optimally trade-off between accuracy and robustness, often imposing a significant amount of additional training costs.

**Contribution.** In this paper, we show that a simple consistency regularization term added on a standard training scheme surprisingly improves the certified robustness of smoothed classifiers. Maintaining the prediction consistency over a certain noise, e.g., Gaussian, can be regarded as a natural and desirable property for a classifier under noisy observations. Indeed, for example, forcing such consistency is now considered as one of the most popular techniques in the semi-supervised learning literature [Sajjadi et al., 2016; Miyato et al., 2018; Oliver et al., 2018; Berthelot et al., 2019]. We examine this regularization, motivated by the observation that perfect consistency is a sufficient condition for minimizing the robust 0-1 loss of smoothed classifiers. This observation connects certified robustness of smoothed classifiers to the general corruption robustness [Hendrycks and Dietterich, 2019; Gilmer et al., 2019], supporting a great potential of smoothed inference as a scalable alternative of adversarially-trained, deterministic classifiers.

We verify the effectiveness of our proposed regularization based on extensive evaluation covering MNIST [LeCun et al., 1998], CIFAR-10 [Krizhevsky, 2009], and ImageNet [Russakovsky et al., 2015] classification datasets. We show that our simple technique upon a naive training achieves a very comparable, or even better, certified $\ell_2$-robustness to other recent, robust training methods [Li et al., 2019; Salman et al., 2019; Zhai et al., 2020]. For example, one of our models for CIFAR-10 shows a better robustness than those trained by other tested methods with 2.7× faster training due to its simplicity. Furthermore, we also demonstrate that applying our method upon a more sophisticated training even further improves the certified robustness, e.g., our method applied upon state-of-the-art training could further improve the average certified $\ell_2$-radius $0.785 \rightarrow 0.799$ on CIFAR-10.

Despite its effectiveness, our proposed regularization is easy-to-use with only a single additional hyperparameter, and could run significantly faster than existing approaches without additional backward computation as in adversarial training. We observe that our method does not introduce instability in training for a wide range of the hyperparameter, offering a new, stable trade-off between accuracy and certified robustness of smoothed classifiers. Finally, our concept of regularizing prediction consistency can be extended to other families of noise other than Gaussian, which are often corresponded to different types of adversary, e.g., Laplace noise for $\ell_1$-robustness [Lecuyer et al., 2019; Dvijotham et al., 2020].

## 2 Preliminaries

### 2.1 Adversarial robustness

We consider a classification task with $K$ classes from a dataset $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n$, where $x \in \mathbb{R}^d$ and $y \in \mathcal{Y} := \{1, \ldots, K\}$ denote an input and the corresponding class label, respectively. Usually, $\mathcal{D}$ is assumed to be i.i.d. samples from a data-generating distribution $P$. Let $f : \mathbb{R}^d \rightarrow \mathcal{Y}$ be a classifier. In many cases, e.g., neural networks, this mapping is modeled by $f(x) := \arg\max_{k \in \mathcal{Y}} F(x) \big|_k$ with a differentiable mapping $F : \mathbb{R}^d \rightarrow \Delta^{K-1}$ for a gradient-based optimization, where $\Delta^{K-1}$ denotes the probability simplex in $\mathbb{R}^K$.

In the literature of general robustness research [Dodge and Karam, 2017; Biggio and Roli, 2018; Hendrycks and Dietterich, 2019], $f$ is required to perform well not only on $P$, but also on a certain extension of it without changing the semantics, say $\hat{P}$. In particular, the notion of adversarial robustness considers the worst-case distribution near $P$ under a certain distance metric. More concretely, a common way to define the adversarial robustness is to consider the average minimum-distance of adversarial perturbation [Moosavi-Dezfooli et al., 2016; Carlini and Wagner, 2017b; Carlini et al., 2019], namely:

$$R(f; P) := \mathbb{E}_{(x,y) \sim P} \left[ \min_{\|f(x') - f(y')\| \neq 0} \|x' - x\|_2 \right].$$


Therefore, our goal is to train \( f \) that (a) performs well on \( P \), while (b) maximizing \( R(f; P) \) as well.

### 2.2 Randomized smoothing

In practice, the inner minimization objective in (1) is usually not easy to optimize exactly, and mostly results in near-zero value on standard neural network classifiers. The key idea of randomized smoothing [Cohen et al., 2019] is rather to consider the robustness of a “smoothed” transformation of the base classifier \( f \) over Gaussian noise, namely \( \hat{f} \):

\[
\hat{f}(x) := \arg \max_{k \in \mathcal{Y}} \mathbb{E}_{\delta \sim N(0, \sigma^2 I)} \left[ 1_{f(x+\delta)=k} \right],
\]

(2)

where \( \sigma^2 \) is a hyperparameter that controls the level of smoothing. For a given input \( x \), Cohen et al. [2019] guarantees a certified radius in \( \ell_2 \) distance, the current state-of-the-art lower bound of the minimum-distance of adversarial perturbation around \( \hat{f}(x) \): suppose \( f(x + \delta) \) returns a class \( \hat{f}(x) \in \mathcal{Y} \) with probability \( p^{(1)} \) and the “runner-up” (i.e., the second best) class with probability \( p^{(2)} := \max_{c \neq \hat{f}(x)} \Pr(f(x + \delta) = c) \). Then, the lower bound can be given as follows:

\[
R(\hat{f}; x, y) := \min_{f(x') \neq y} ||x' - x||_2 \geq \frac{\sigma}{2} \left( \Phi^{-1}(p^{(1)}) - \Phi^{-1}(p^{(2)}) \right)
\]

(3)

provided that \( \hat{f}(x) = y \), otherwise \( R(\hat{f}; x, y) := 0 \). Here, \( \Phi \) denotes the standard Gaussian CDF. Since the inequality holds for any upper bound of \( p^{(2)} \), say \( \tilde{p}^{(2)} \), one could also obtain a bit loose, but simpler bound of certified radius by letting \( \tilde{p}^{(2)} = 1 - p^{(1)} \geq p^{(2)} \):

\[
R(\hat{f}; x, y) \geq \sigma \cdot \Phi^{-1}(p^{(1)}) := R(\hat{f}, x, y).
\]

(4)

### 3 Consistency regularization for smoothed classifiers

Our intuition on the proposed consistency regularization is based on minimizing the 0-1 robust classification loss, in a similar manner to the recent attempts of decomposing the training objective with respect to the accuracy and robustness [Zhang et al., 2019; Zhai et al., 2020]. Specifically, we attempt minimize the following:

\[
\mathbb{E}_{(x,y) \in \mathcal{D}} \left[ 1 - \mathbb{I}(\hat{f}(x,y) \geq \epsilon) \right] = \mathbb{E} \left[ 1_{f(x) \neq y} \right] + \mathbb{E} \left[ 1_{f(x)=y, \ R(\hat{f}, x, y) < \epsilon} \right],
\]

(5)

where \( \mathbb{R} \) is the certified lower bound of \( R \) as defined in (4), and \( \epsilon > 0 \) is a pre-defined constant. Assuming that the natural error term can be optimized via a standard surrogate loss, e.g., cross-entropy, we rather focus on how to minimize the robust error term. Here, the key difficulties to consider a gradient-based optimization is that (a) computing \( \hat{f} \) exactly is intractable, and more importantly, (b) \( \hat{f} \) is practically a non-differentiable object when estimated via Monte Carlo sampling (see (2)), so that even a proper surrogate loss function would not make the optimization differentiable.

To bypass these issues, we instead concentrate on a sufficient condition to minimize the given robust 0-1 loss. Recall that we assume \( f(x) = \arg \max_{k \in \mathcal{Y}} F(x) \) for a differentiable function \( F : \mathbb{R}^d \to A^{K-1} \). Intuitively, we notice that the robust loss would anyway become zero if \( F(x + \delta) \) returns a “constant” output over \( \delta \) for a given \( x \). More concretely, the condition implies \( \Pr_{\epsilon}(f(x + \delta) = f(x)) \) to become 1 regardless of what \( \hat{f} \) is, and minimizes an upper bound of the robust loss in (5) due to the following:

\[
\mathbb{E} \left[ 1_{f(x)=y, \ R(\hat{f}, x, y) < \epsilon} \right] = \mathbb{E} \left[ 1_{\hat{f}(x)=y, \ R(f, x, \hat{f}(x)) < \epsilon} \right] \leq \mathbb{E} \left[ 1_{\mathbb{R}(f, x, \hat{f}(x)) < \epsilon} \right] = \mathbb{E} \left[ 1_{\Pr_{\epsilon}(f(x+\delta)=f(x)) < \Phi(\epsilon)} \right],
\]

(6)
Figure 1: Comparison of log-probability gap distributions under Gaussian noise sampled at a fixed test point of MNIST. For each histogram, we used 10,000 samples of noise. The left, shaded area indicates where a classifier makes a misclassification.

where the last equality is from the definition of $R$ in (4). Therefore, we attempt to optimize the robust training objective on $\hat{f}$ via regularizing $F(x + \delta)$ to be consistent across $\delta$. Specifically, we propose the following consistency regularization upon any standard training objective:

$$L^{\text{con}} := E_\delta [L(F(x + \delta), \hat{F}(x))],$$

(7)

where $\hat{F}(x) := E[F(x + \delta)]$ is the mean prediction of $F(x + \delta)$, and $L$ indicates the cross-entropy loss. In other words, this regularization enforces $F$, correspondingly $f$ as well, to reduce the variance of predictions under Gaussian noise for a given sample $x$.

3.1 Comparison to prior works

There have been a few prior approaches in attempts to improve the robustness of smoothed classifiers with a more sophisticated training method beyond that of Cohen et al. [2019]. Salman et al. [2019] proposed SmoothAdv, which shows that adversarial training directly on smoothed classifiers improve the certified robustness. More recently, Zhai et al. [2020] proposed a faster training method called MACER, via maximizing a soft approximation of the certified radius given in (3).\footnote{For the interested readers, we present a more detailed overview of Salman et al. [2019] and Zhai et al. [2020] in Appendix C.} The essential difference of our regularization to the previous works is at how the non-differentiable $\hat{f}$ is handled, namely, prior works commonly approximate $\hat{f}$ directly by the inner soft-classifier $F$:

$$E_\delta[1_{f(x+\delta) = k}] \approx E_\delta[F_k(x + \delta)],$$

(8)

for each class $k \in \mathcal{Y}$. A key caveat here is that, however, optimizing $\hat{f}$ with this approximation would implicitly count out much optimal solutions of $F$. More specifically, we remark that an optimal soft classifier $F$ does not require to have confidence near to 1 for maximizing the certified radius (3), which is a usual solution found by minimizing the cross-entropy based on (8). Our approach rather considers an “indirect” regularizer of $\hat{f}$ without assuming such an approximation, thereby allows a more flexible optimization.

On the other hand, Li et al. [2019] proposed stability training, as a parallel attempt to the Gaussian training of randomized smoothing [Cohen et al., 2019] to obtain a robust smoothed classifier: namely, in order to perform well on Gaussian noise, stability training trains $F$ with the following loss:

$$\min_F \mathcal{L}(F(x), y) + \lambda \cdot \mathcal{L}(F(x), F(x + \delta)), \tag{9}$$

where $\mathcal{L}$ is the cross-entropy loss. The regularization term used in (9) has a seemingly similar formula to ours (7), but there is a fundamental difference: our method (7) does not require $F$ to jointly minimize $\mathcal{L}(F(x), y)$ and $\mathcal{L}(F(x + \delta), y)$ to perform well on $(x + \delta, y)$. Consequently, our method again allows a more flexible solution compared to (9). In Section 4.3, we empirically show that our form of regularization (7) attains a significantly better robustness than (9). We also show in Table 9 that, due to such flexibility, our method is more robust on the choice of $\lambda$.\footnote{For the interested readers, we present a more detailed overview of Salman et al. [2019] and Zhai et al. [2020] in Appendix C.}
In Figure 1, we illustrate how the optimal classifier found by our method differs from others, by comparing the distribution of logits under Gaussian noise. Specifically, we compare the log-probability gap for a given noisy sample \((x + \delta, y)\): \(\log F_y(x + \delta) - \max_{\tau \neq y} \log F_\tau(x + \delta)\). We notice that our method learns relatively lower, yet more consistent, confidences than others. We also found that MACER [Zhai et al., 2020] tends to vary on much larger values in logits (see Figure 1(b)): MACER essentially maximizes the gap between the first- and second-best logits of \(E[F(x + \delta)]\), which leads \(F\) to have an arbitrary large value when optimized. Finally, Figure 1(c) supports that our method is fundamentally different to the stability training [Li et al., 2019]: one can observe that stability training does not give a particular consistency that our method shows.

### 3.2 Training with consistency regularization

**Overall training objective.** Combining our regularization \(L_{\text{con}}\) to a natural surrogate loss \(L_{\text{nat}}\) leads to a full objective to minimize. Any form of \(L_{\text{nat}}\) is possible to use, as long as it minimizes the natural error of \(\hat{f}\) in (5), e.g., the standard cross-entropy loss on \(f\) may not be proper for \(L_{\text{nat}}\). As a plain example, we use the loss proposed by Cohen et al. [2019], which simply performs Gaussian augmentation during training: for a given sample \((x, y) \sim D\), the authors suggest to minimize:

\[
L_{\text{nat}} := E_{\delta \sim \mathcal{N}(0, \sigma^2)} [L(F(x + \delta), y)].
\] (10)

The overall objective with consistency regularization is then:

\[
L := L_{\text{nat}} + \lambda \cdot L_{\text{con}} = E_{\delta} \left[ L(F(x + \delta), y) + \lambda \cdot L(F(x + \delta), \tilde{F}(x)) \right]
\approx \frac{1}{m} \sum_i \left( L(F(x + \delta_i), y) + \lambda \cdot L(F(x + \delta_i), \hat{F}(x)) \right),
\] (11)

where \(\lambda > 0\) is a hyperparameter that controls the relative strength compared to \(L_{\text{nat}}\), and (12) shows a concrete training procedure with respect to (11) via Monte Carlo sampling over \(\delta\). Nevertheless, our regularization scheme is not limited to a specific choice of \(L_{\text{nat}}\), and one can also apply others in a similar way. In our experiments, for example, we show that using SmoothAdv [Salman et al., 2019] as \(L_{\text{nat}}\) could further improve the certified robustness, although it is significantly more expensive to optimize compared to (10).

**Computational overhead.** We use \(m\) independent samples of Gaussian noise in (12) to estimate (11), and this is the only source of extra training costs compared to the original [Cohen et al., 2019]. Nevertheless, we empirically observe that the minimal choice of \(m = 2\) is fairly enough for our method, as demonstrated in Figure 4(b). Considering that other existing methods also use this inner-sampling procedure, often requiring an additional outer-loop of backward computations for adversarial training [Salman et al., 2019], or a large number of \(m\) for a stable training [Zhai et al., 2020], our method offers a significantly less training cost with less hyperparameters, as further discussed in Section 4.5.

**Other design choices.** We also remark that one can adopt other forms of consistency regularization instead of the cross-entropy loss \(L\) in (7) as well, as long as the regularization leads (6) to be zero. For example, in the literature of semi-supervised learning, the mean-squared-error [Sajjadi et al., 2016] or KL-divergence [Miyato et al., 2018] are commonly-used forms to enforce prediction consistency. In our experiments, we examine both as well, and it turns out indeed they are also effective to improve the certified robustness. Nevertheless, we empirically observe that our cross-entropy form (7) shows a particular robustness compared to them (see Section 4.6 for more details).

### 4 Experiments

We validate the effectiveness of our proposed consistency regularization for a wide range of image classification datasets: MNIST [LeCun et al., 1998], CIFAR-10 [Krizhevsky, 2009], and ImageNet [Russakovsky et al., 2015].

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2 Code is available at https://github.com/jh-jeong/smoothing-consistency.
Figure 2: Comparison of approximate certified accuracy via randomized smoothing for various training methods on MNIST. A sharp drop of certified accuracy in the plots exists since there is a hard upper bound that CERTIFY can output for a given σ and n = 100,000.

...to the other baseline training methods greatly boosts the certified ℓ2-robustness via randomized smoothing. Remarkably, we show that our method even further improves the previous state-of-the-art results of SmoothAdv [Salman et al., 2019]. We also perform an ablation study to further investigate the detailed components proposed in our method.

4.1 Setups

**Evaluation metrics.** To evaluate certified robustness for a given classifier \( f \), we aim to compute the certified test accuracy at radius \( r \), which is defined by the fraction of the test dataset that \( f \) can certify the robustness of radius \( r \) with respect to the certifiable lower bound in (3). Due to the intractability of this metric, however, we instead measure the approximate certified test accuracy [Cohen et al., 2019]. More concretely, Cohen et al. [2019] proposed a practical Monte Carlo based certification procedure, namely CERTIFY, which returns the prediction of \( f \) and a “safe” lower bound of certified radius over the randomness of \( n \) samples with probability at least \( 1 - \alpha \), or abstains the certification. The approximate certified test accuracy is then defined by the fraction of the test dataset which CERTIFY classifies correctly with radius larger than \( r \) without abstaining.

In our experiments, we use the official implementation\(^3\) of CERTIFY for evaluation, with \( n = 100,000 \), \( n_0 = 100 \) and \( \alpha = 0.001 \), following the prior work [Cohen et al., 2019; Salman et al., 2019]. We mainly report the approximate certified test accuracy at various radii, but also report the average certified radius (ACR) considered by Zhai et al. [2020], i.e., the averaged value of certified radii returned by CERTIFY, as another metric for better comparison of robustness between two models under the trade-offs between accuracy and robustness [Tsipras et al., 2019; Zhang et al., 2019]: namely, \( \text{ACR} := \frac{1}{|D_{\text{test}}|} \sum_{(x, y) \in D_{\text{test}}} \text{CR}(f, \sigma, x) \cdot \mathbf{1}_{f(x) = y'} \) where \( D_{\text{test}} \) is the test dataset, and \( \text{CR} \) denotes the certified radius returned from \( \text{CERTIFY}(f, \sigma, x) \).

**Training details.** We use the same base classifier used in the prior work [Cohen et al., 2019; Salman et al., 2019; Zhai et al., 2020]: namely, we use LeNet [LeCun et al., 1998] for MNIST, ResNet-110 [He et al., 2016] for CIFAR-10, and ResNet-50 [He et al., 2016] for ImageNet. For a fair comparison, we follow the same training details used in Cohen et al. [2019] and Salman et al. [2019]. For each model configuration, we consider three different models as varying the noise level \( \sigma \in \{0.25, 0.5, 1.0\} \). During inference, we apply randomized smoothing with the same \( \sigma \) used in the training. When our regularization is used, we use \( m = 2 \) unless otherwise specified. More training details are specified in Appendix A.

**Baseline methods.** We evaluate how consistency regularization would affect the certified robustness when applied to a baseline training method. In our experiments, we consider two baseline methods proposed for training smoothed classifiers to apply our regularization scheme: (a) Gaussian [Cohen et al., 2019]: training with Gaussian augmentation over \( \mathcal{N}(0, \sigma^2 I) \); (b) SmoothAdv [Salman et al., 2019]: adversarial training on a soft approximation of the smoothed classifier. We also consider stability training [Li et al., 2019] in (9) and MACER [Zhai et al., 2020] to compare, as other regularization-based approaches.

\(^3\)https://github.com/locuslab/smoothing
Table 1: Comparison of approximate certified test accuracy on MNIST dataset. For each model, training and certification are done with the same smoothing factor specified in $\sigma$. Each of the values indicates the fraction of test samples those have $\ell_2$ certified radius larger than the threshold specified at the top row. We set our result bold-faced whenever the value improves the baseline. For ACR, we underlined the best-performing model per each $\sigma$.

| $\sigma$ | Models (MNIST) | ACR | 0.00 | 0.25 | 0.50 | 0.75 | 1.00 | 1.25 | 1.50 | 1.75 | 2.00 | 2.25 | 2.50 |
|----------|----------------|-----|------|------|------|------|------|------|------|------|------|------|------|
| 0.25     | Gaussian [Cohen et al., 2019] | 0.911 | 99.2 | 98.5 | 96.7 | 93.3 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |
|          | + Consistency ($\lambda = 20$) | 0.930 | 99.5 | 99.0 | 98.0 | 96.4 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |
|          | SmoothAdv [Salman et al., 2019] | 0.933 | 99.4 | 99.0 | 98.2 | 96.9 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |
|          | + Consistency ($\lambda = 5$) | 0.932 | 99.2 | 98.8 | 98.0 | 96.8 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |
|          | Stability training [Li et al., 2019] | 0.915 | 99.3 | 98.6 | 97.1 | 93.8 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |
|          | MACER [Zhai et al., 2020] | 0.920 | 99.3 | 98.7 | 97.5 | 94.8 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |
| 0.50     | Gaussian [Cohen et al., 2019] | 1.553 | 99.2 | 98.3 | 96.8 | 94.3 | 89.7 | 81.9 | 67.3 | 43.6 | 0.0  | 0.0  | 0.0  |
|          | + Consistency ($\lambda = 20$) | 1.665 | 98.9 | 98.3 | 97.4 | 95.6 | 93.0 | 88.1 | 79.5 | 62.9 | 0.0  | 0.0  | 0.0  |
|          | SmoothAdv [Salman et al., 2019] | 1.687 | 99.0 | 98.3 | 97.3 | 95.8 | 93.2 | 88.5 | 81.1 | 67.5 | 0.0  | 0.0  | 0.0  |
|          | + Consistency ($\lambda = 5$) | 1.690 | 98.2 | 97.5 | 96.5 | 94.7 | 91.7 | 87.7 | 81.5 | 71.2 | 0.0  | 0.0  | 0.0  |
|          | Stability training [Li et al., 2019] | 1.570 | 99.2 | 98.5 | 97.1 | 94.8 | 90.7 | 83.2 | 69.2 | 45.4 | 0.0  | 0.0  | 0.0  |
|          | MACER [Zhai et al., 2020] | 1.594 | 98.5 | 97.5 | 96.2 | 93.7 | 90.0 | 83.7 | 72.2 | 54.0 | 0.0  | 0.0  | 0.0  |
| 1.00     | Gaussian [Cohen et al., 2019] | 1.620 | 96.4 | 94.4 | 91.4 | 87.0 | 79.9 | 71.0 | 59.6 | 46.2 | 32.6 | 19.7 | 10.8 |
|          | + Consistency ($\lambda = 20$) | 1.750 | 92.5 | 89.8 | 86.5 | 81.7 | 76.3 | 69.6 | 61.4 | 52.9 | 44.2 | 35.9 | 26.8 |
|          | SmoothAdv [Salman et al., 2019] | 1.780 | 95.7 | 93.8 | 90.8 | 86.6 | 80.9 | 73.6 | 64.6 | 54.0 | 43.5 | 33.0 | 22.4 |
|          | + Consistency ($\lambda = 5$) | 1.804 | 92.8 | 90.3 | 86.8 | 82.2 | 76.9 | 69.8 | 62.3 | 53.4 | 45.1 | 37.4 | 29.4 |
|          | Stability training [Li et al., 2019] | 1.634 | 96.5 | 94.6 | 91.7 | 87.4 | 80.6 | 72.0 | 60.5 | 46.8 | 33.1 | 20.0 | 11.2 |
|          | MACER [Zhai et al., 2020] | 1.570 | 92.0 | 88.5 | 84.0 | 78.1 | 71.5 | 63.8 | 55.3 | 46.3 | 36.5 | 26.2 | 16.3 |

4.2 Results on MNIST

We train every MNIST model for 90 epochs. We consider a fixed configuration of hyperparameters when SmoothAdv is used in MNIST: specifically, we perform a 10-step projected gradient descent (PGD) attack constrained in $\ell_2$ ball of radius $\epsilon = 1.0$ for each input, while the objective is approximated with $m = 4$ noise samples. For the MACER models, on the other hand, we generally follow the hyperparameters specified in the original paper [Zhai et al., 2020]: we set $m = 16$, $\lambda = 16.0$, $\gamma = 8.0$ and $\beta = 16.0$. In $\sigma = 1.0$, however, we had to reduce $\lambda$ to 6 for a successful training. Nevertheless, we have verified that the ACRs computed from the reproduced models are comparable to those reported in the original paper. We use $\lambda = 2$ when stability training [Li et al., 2019] is applied in this section.

We report the results in Table 1. We also plot full curves of certified accuracy over the full range of radii per each $\sigma$ in Figure 2. Overall, we observe that our consistency regularization stably improve Gaussian and SmoothAdv baselines in ACR, except when applied to SmoothAdv on $\sigma = 0.25$. This corner-case is possibly due to that the model is already achieve to the best capacity via SmoothAdv, regarding that MNIST on $\sigma = 0.25$ is relatively a trivial task. For the rest non-trivial cases, nevertheless, our regularization shows a remarkable effectiveness in two aspects: (a) applying our consistency regularization on Gaussian, the simplest baseline, dramatically improves the certified test accuracy and ACR even outperforming the recently proposed MACER by a large margin, and (b) when applied to SmoothAdv, our method could further improve ACR. In particular, one could observe that our regularization significantly improves the certified accuracy especially at large radii, where a classifier should attain a high value of $p^{(1)}(3)$, i.e., a consistent prediction is required.

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4We refer the readers to Zhai et al. [2020] for the details on each hyperparemeter.
Figure 3: Comparison of approximate certified accuracy via randomized smoothing for various training methods on CIFAR-10. A sharp drop of certified accuracy in the plots exists since there is a hard upper bound that CERTIFY can output for a given \( \sigma \) and \( n = 100,000 \).

### 4.3 Results on CIFAR-10

We train CIFAR-10 models for 150 epochs following the training details of SmoothAdv [Salman et al., 2019]. Whenever possible, we use the pre-trained models officially released by the authors for our evaluation to reproduce the baseline results.\(^5\) For the SmoothAdv models, we report the results for two different configurations: (a) for a fixed, pre-defined configuration across \( \sigma \), and (b) for the “best” configuration per each \( \sigma \), which is heavily examined by Salman et al. [2019] over hundreds of models. In case of \( \sigma = 0.25 \), however, we only report (b) as they show nearly identical results. For (a), we consider a 10-step PGD attack constrained in \( \ell_2 \) ball of radius \( \varepsilon = 1.0 \), using \( m = 8 \) noise samples.\(^6\) In case of stability training [Li et al., 2019], we report the best models in terms of ACR across varying \( \lambda \) tested: namely, we consider \( \lambda \in \{1, 2, 5, 10, 20\} \) for each \( \sigma \), and report \( \lambda = 2 \) for \( \sigma = 0.25, 0.5 \) and \( \lambda = 1 \) for \( \sigma = 1.0 \). The full results can be found in Table 9.

The results are presented in Table 2 and Figure 3. Our results in CIFAR-10 is even more significant than MNIST, in terms of consistent improvement both in certified test accuracy and ACR. Specifically, when \( \sigma = 0.50 \), we found our regularization with \( \lambda = 20 \) applied on the naïve Gaussian baseline could surpass the best-performing SmoothAdv model reported in “SmoothAdv + Hyperparameter search”, in terms of ACR. Furthermore, in case of \( \sigma = 1.00 \), consistency regularization upon the best SmoothAdv model even further improve the current state-of-the-art baseline by a significant margin, which verifies an orthogonal contribution of our method compared to the prior work. These observations suggest our method works better on more complex tasks, where forcing “confident” prediction (as done in the prior works) might be difficult. We also notice that, despite its similarity with our method, the stability training [Li et al., 2019] itself does not improve ACRs even compared to the Gaussian baselines. This is because this training (9) would require \( f \) to perform well both in \( x \) and \( x + \delta \), which is harder to force compared to that of (11) in the context of randomized smoothing.

### 4.4 Results on ImageNet

We also evaluate our regularization scheme on ImageNet classification dataset, to show that our method is scalable on large-scale datasets. We train each model on \( \sigma \in \{0.5, 1.0\} \) for 90 epochs. We perform our evaluation on a subsampled test dataset of 500 samples as done by Cohen et al. [2019]. As presented in Table 3, we observe that consistency regularization still effectively improves the certified robustness, both in terms of ACR and certified test accuracy, despite its simple and efficient nature of our method. Compared to

\(^5\)https://github.com/Hadisalman/smoothing-adversarial

\(^6\)https://github.com/RuntianZ/macer

\(^7\)In case of the pre-trained MACER models, we observe a slight discrepancy between our evaluation and those reported in Zhai et al. [2020]. We have verified that this is due to a sampling bias: we found [Zhai et al., 2020] used 500 contiguous subsamples by default in the official code, while our evaluation uses the full CIFAR-10 test set.

\(^8\)The detailed configurations for (b), the best models, are specified in Appendix A.3.
Table 2: Comparison of approximate certified test accuracy (%) on CIFAR-10 dataset. For each model, training and certification are done with the same smoothing factor specified in $\sigma$. Each of the values indicates the fraction of test samples those have $\ell_2$ certified radius larger than the threshold specified at the top row. We set our result bold-faced whenever the value improves the baseline. For ACR, we underlined the best-performing model per each $\sigma$. For the results in “+ Hyperparameter search”, we evaluate the best model among those released by Salman et al. [2019] trained for a given $\sigma$.

| $\sigma$ | Models (CIFAR-10) | ACR | 0.00 | 0.25 | 0.50 | 0.75 | 1.00 | 1.25 | 1.50 | 1.75 | 2.00 | 2.25 |
|----------|-------------------|-----|------|------|------|------|------|------|------|------|------|------|
| 0.25     | Gaussian [Cohen et al., 2019] | 0.424 | 76.6 | 61.2 | 42.2 | 25.1 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |
|          | + Consistency ($\lambda = 20$) | 0.551 | 75.9 | 67.5 | 57.6 | 46.9 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |
|          | SmoothAdv [Salman et al., 2019] | 0.544 | 73.4 | 65.6 | 57.0 | 47.5 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |
|          | + Consistency ($\lambda = 5$) | 0.555 | 73.3 | 66.3 | 57.7 | 49.3 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |
|          | Stability training [Li et al., 2019] | 0.421 | 72.3 | 58.0 | 43.3 | 27.3 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |
|          | MACER [Zhai et al., 2020] | 0.531 | 79.5 | 69.0 | 55.8 | 40.6 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |
| 0.50     | Gaussian [Cohen et al., 2019] | 0.525 | 65.7 | 54.9 | 42.8 | 32.5 | 22.0 | 14.1 | 8.3  | 3.9  | 0.0  | 0.0  |
|          | + Consistency ($\lambda = 10$) | 0.725 | 64.8 | 58.2 | 50.9 | 43.8 | 36.4 | 29.4 | 22.8 | 16.1 | 0.0  | 0.0  |
|          | + Consistency ($\lambda = 20$) | 0.737 | 59.0 | 53.9 | 48.7 | 43.4 | 37.8 | 32.7 | 27.0 | 21.0 | 0.0  | 0.0  |
|          | SmoothAdv [Salman et al., 2019] | 0.689 | 64.4 | 57.2 | 49.0 | 40.6 | 33.6 | 27.4 | 21.8 | 14.0 | 0.0  | 0.0  |
|          | + Hyperparameter search | 0.717 | 53.1 | 49.2 | 44.9 | 41.0 | 37.2 | 33.2 | 29.1 | 24.0 | 0.0  | 0.0  |
|          | + Consistency ($\lambda = 5$) | 0.716 | 52.7 | 48.8 | 44.6 | 41.1 | 37.5 | 33.3 | 28.8 | 24.3 | 0.0  | 0.0  |
|          | Stability training [Li et al., 2019] | 0.521 | 60.6 | 51.5 | 41.4 | 32.5 | 23.9 | 15.3 | 9.6  | 5.0  | 0.0  | 0.0  |
|          | MACER [Zhai et al., 2020] | 0.691 | 64.2 | 57.5 | 49.9 | 42.3 | 34.8 | 27.6 | 20.2 | 15.8 | 10.0 | 0.0  |
| 1.00     | Gaussian [Cohen et al., 2019] | 0.542 | 47.2 | 39.2 | 34.0 | 27.8 | 21.6 | 17.4 | 14.0 | 11.8 | 10.0 | 7.6  |
|          | + Consistency ($\lambda = 10$) | 0.727 | 47.1 | 42.7 | 38.1 | 33.5 | 29.2 | 25.3 | 21.9 | 18.4 | 15.6 | 12.4 |
|          | + Consistency ($\lambda = 20$) | 0.742 | 43.8 | 40.1 | 36.0 | 32.3 | 28.4 | 25.0 | 21.7 | 18.9 | 16.3 | 13.8 |
|          | SmoothAdv [Salman et al., 2019] | 0.682 | 50.2 | 44.0 | 37.6 | 33.8 | 28.8 | 24.0 | 20.2 | 15.8 | 13.2 | 10.2 |
|          | + Hyperparameter search | 0.785 | 45.6 | 41.9 | 38.0 | 34.2 | 30.9 | 27.4 | 24.1 | 20.7 | 17.7 | 14.9 |
|          | + Consistency ($\lambda = 2$) | 0.799 | 45.2 | 41.9 | 38.1 | 34.6 | 31.1 | 27.9 | 24.3 | 21.1 | 18.4 | 15.5 |
|          | Stability training [Li et al., 2019] | 0.526 | 43.5 | 38.9 | 32.8 | 27.0 | 23.1 | 19.1 | 15.4 | 11.3 | 7.8  | 5.7  |
|          | MACER [Zhai et al., 2020] | 0.744 | 41.4 | 38.5 | 35.2 | 32.3 | 29.3 | 26.4 | 23.4 | 20.2 | 17.4 | 14.5 |

Table 4: Comparison of training time statistics on CIFAR-10 with $\sigma = 0.50$. All the baselines are trained on their official implementations separately.

| Models (CIFAR-10) | # HP | ACR | Mem. | Time (h) |
|-------------------|------|-----|------|----------|
| Gaussian [Cohen et al., 2019] | 0.525 | 75.9 | 67.5 | 57.6 | 46.9 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |
| + Consistency ($\lambda = 20$) | 0.551 | 75.9 | 67.5 | 57.6 | 46.9 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |
| SmoothAdv [Salman et al., 2019] | 0.544 | 73.4 | 65.6 | 57.0 | 47.5 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |
| + Consistency ($\lambda = 5$) | 0.555 | 73.3 | 66.3 | 57.7 | 49.3 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |
| Stability training [Li et al., 2019] | 0.421 | 72.3 | 58.0 | 43.3 | 27.3 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |
| MACER [Zhai et al., 2020] | 0.531 | 79.5 | 69.0 | 55.8 | 40.6 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |

the best results of SmoothAdv [Salman et al., 2019], our results achieve a comparable robustness, despite using a single fixed configuration of hyperparameter, namely $\lambda = 10$.

4.5 Runtime analysis

With much effectiveness on the certified robustness, consistency regularization also offers a great efficiency in terms of training costs compared to other competitive methods. We compare our method with the baselines in several training statistics, including the number of hyper-parameter (# HP), ACR, memory usage in GPU on peak computation (Mem.), and the total training time (Time). In this experiment, every model is trained on CIFAR-10 using one GPU of NVIDIA TITAN X (Pascal). We use $\sigma = 0.5$ with hyperparameters specified in Section 4.3. In case of SmoothAdv, we choose the best-performing configuration for training. Our method to compare runs upon the Gaussian baseline with $m = 2$ and $\lambda = 20$. The results summarized in the Table 4 show that our regularization indeed costs about twice the Gaussian baseline due to additional sampling procedure, but one can immediately notice that this overhead is far less...
Table 3: Comparison of approximate certified test accuracy (%) on ImageNet dataset. For each model, training and certification are done with the same smoothing factor specified in \( \sigma \). Each of the values indicates the fraction of test samples those have \( \ell_2 \) certified radius larger than the threshold specified at the top row. We set our result bold-faced whenever the value improves the baseline.

| \( \sigma \) | Models (ImageNet) | ACR 0.0 | ACR 0.5 | ACR 1.0 | ACR 1.5 | ACR 2.0 | ACR 2.5 | ACR 3.0 | ACR 3.5 |
|---|---|---|---|---|---|---|---|---|---|
| 0.50 | Gaussian [Cohen et al., 2019] + Consistency (\( \lambda = 10 \)) | 0.733 | 57 | 46 | 37 | 29 | 0 | 0 | 0 | 0 |
| 0.50 | SmoothAdv [Salman et al., 2019] | 0.825 | 54 | 49 | 43 | 37 | 0 | 0 | 0 | 0 |
| 1.00 | Gaussian [Cohen et al., 2019] + Consistency (\( \lambda = 10 \)) | 0.875 | 44 | 38 | 33 | 26 | 19 | 15 | 12 | 9 |
| 1.00 | SmoothAdv [Salman et al., 2019] | 1.040 | 40 | 37 | 34 | 30 | 27 | 25 | 20 | 15 |

![Figure 4: Comparison of approximate certified accuracy via randomized smoothing across various types of ablation models. A sharp drop of certified accuracy in the plots exists since there is a hard upper bound that CERTIFY can output for a given \( \sigma \) and \( n = 100,000 \).](image)

than other baselines, e.g., compared to adversarial training. Furthermore, our method even achieves better ACR than other methods, which verifies a clear efficiency of consistency regularization compared to the prior work.

4.6 Ablation study

We conduct an ablation study for a detailed analysis on the proposed method. All the experiments in this section are performed on MNIST. When consistency regularization is used, we assume it is applied upon Gaussian training. We report all the detailed results in Appendix B.

**Design choices on loss.** In order to enforce the prediction consistency, our regularization uses cross-entropy loss between individual prediction and their mean (7). Here, we examine two other popular designs for consistency regularization, namely, mean-squared-error [Sajjadi et al., 2016] and KL-divergence [Miyato et al., 2018] by considering the following alternative forms:

\[
L_{\text{MSE}} := \| F(x + \delta_1) - F(x + \delta_2) \|^2_2 \quad \text{and} \quad L_{\text{KL}} := \text{KL}(\hat{F}(x) \| F(x + \delta)),
\]

where \( \delta_1, \delta_2 \sim \mathcal{N}(0, \sigma^2 I) \). We evaluate certified test accuracy on \( \sigma = 1.00 \) for these regularization with varying \( \lambda \in \{20, 50, 100\} \), and compare the results with \( L_{\text{con}} \) with \( \lambda = 20 \). The results are presented in Figure 4(a). In general, we observe that both regularizers, namely \( L_{\text{MSE}} \) and \( L_{\text{KL}} \), are also capable to improve the certified robustness, but they could not achieve a better ACR than \( L_{\text{con}} \) even with a moderately large \( \lambda \). This observation indicates the importance of regularizing the entropy of the mean prediction, once noticing that \( L_{\text{con}} = L_{\text{KL}} + H(\hat{F}(x)) \) where \( H \) denotes the entropy. Indeed, we empirically observe that both \( L_{\text{MSE}} \) and \( L_{\text{KL}} \) often lead the predictions to be too close to the uniform when \( \lambda \) is large, which may harm the discriminative performance of the base classifier.
Effect of $m$. As mentioned in Section 3, the computational costs for our regularization scheme highly depends on the number of noise samples used, namely $m > 1$. Nevertheless, we observe that our regularization is fairly robust on the choice of $m$, so that $m = 2$ usually leads to good enough performance. In Figure 4(b), we compare the certified robustness of models trained with our regularization with varying $m \in \{2, 4, 8\}$. For each $m$, we present three different models under various $\sigma \in \{0.25, 0.5, 1.0\}$. The results show that models using $m = 2$ perform nearly identically to others, while one could observe a slight improvement at $\sigma = 1.0$ for larger $m$. In practice, this observation reduces much of the hyperparameter complexity in our method: by simply letting $m$ to be small, e.g., $m = 2$, $\lambda$ becomes the only crucial hyperparameter.

Effect of $\lambda$. We also investigate the effect of having different $\lambda$ in Figure 4(c). As expected, we observe a clear trade-off between accuracy and robustness of the corresponding smoothed classifier by controlling $\lambda$. Furthermore, for a sufficiently large $\lambda$, e.g., $\lambda = 40$ in Figure 4(c), a classifier is often trained to return maximal certifiable radius for any input when smoothed, even the accuracy falls into chance-level. Nevertheless, this would be a desirable property for a trade-off term between accuracy and robustness, which has not been explored much for smoothed classifiers.

5 Conclusion

In this paper, we show consistency regularization can play a key role in certifiable robustness of smoothed classifiers. We think our work would emphasize the importance of noise-consistent inference in deep neural networks, one of under-explored topics despite its desirable property. We also expect our work can be a useful guideline when other researchers will study the noise-consistency in other problems in the future. Many questions are related: how can we design a “noise-invariant” neural network, or for which family of noise this would be allowed, just to name a few.

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## A Details on experimental setups

### A.1 Training details

We train every model via stochastic gradient descent (SGD) with Nesterov momentum of weight 0.9 without dampening. We set a weight decay of $10^{-4}$ for all the models. We use different training schedules for each dataset: (a) MNIST: The initial learning rate is set to 0.01; We train a model for 90 epochs with mini-batch size 256, and the learning rate is decayed by 0.1 at 30-th and 60-th epoch, (b) CIFAR-10: The initial learning rate is set to 0.1; We train a model for 150 epochs with mini-batch size 256, and the learning rate is decayed by 0.1 at 50-th and 100-th epoch, and (c) ImageNet: The initial learning rate is set to 0.1; We train a model for 90 epochs with mini-batch size 200, and the learning rate is decayed by 0.1 at 30-th and 60-th epoch. When SmoothAdv is used, we adopt the warm-up strategy on attack radius $\epsilon$ [Salman et al., 2019], i.e., $\epsilon$ is initially set to zero, and linearly increased during the first 10 epochs to a pre-defined hyperparameter.

### A.2 Datasets

**MNIST** dataset [LeCun et al., 1998] consists 70,000 gray-scale hand-written digit images of size $28 \times 28$, 60,000 for training and 10,000 for testing. Each of the images is labeled from 0 to 9, i.e., there are 10 classes. When training on MNIST, we do not perform any pre-processing except for normalizing the range of each pixel from 0-255 to 0-1. The full dataset can be downloaded at [http://yann.lecun.com/exdb/mnist/](http://yann.lecun.com/exdb/mnist/).

**CIFAR-10** dataset [Krizhevsky, 2009] consist of 60,000 RGB images of size $32 \times 32$ pixels, 50,000 for training and 10,000 for testing. Each of the images is labeled to one of 10 classes, and the number of data per class is set evenly, i.e., 6,000 images per each class. We follow the same data-augmentation scheme used in Cohen et al. [2019]; Salman et al. [2019] for a fair comparison, namely, we use random horizontal flip and random translation up to 4 pixels. We also normalize the images in pixel-wise by the mean and the standard deviation calculated from the training set. Here, an important practical point is that this normalization is done after a noise is added to input when regarding randomized smoothing, following Cohen et al. [2019]. This is to ensure that noise is given to the original image coordinates. In practical implementations, this can be done by placing the normalization as the first layer of base classifiers, instead of as a pre-processing step. The full dataset can be downloaded at [https://www.cs.toronto.edu/~kriz/cifar.html](https://www.cs.toronto.edu/~kriz/cifar.html).

**ImageNet** classification dataset [Russakovsky et al., 2015] consists of 1.2 million training images and 50,000 validation images, which are labeled by one of 1,000 classes. For data-augmentation, we perform $224 \times 224$ random cropping with random resizing and horizontal flipping to the training images. At test time, on the other hand, $224 \times 224$ center cropping is performed after re-scaling the images into $256 \times 256$. This pre-processing scheme is also used in Cohen et al. [2019]; Salman et al. [2019] as well. Similar to CIFAR-10, all the images are normalized after adding a noise in pixel-wise by the pre-computed mean and standard deviation. A link for downloading the full dataset can be found in [http://image-net.org/download](http://image-net.org/download).
Table 5: Detailed specification of hyperparameters used in the best-performing SmoothAdv models.

| Dataset    | $\sigma$ | Method | # steps | $\varepsilon$ | $m$ |
|------------|----------|--------|---------|--------------|-----|
| CIFAR-10   | 0.25     | PGD    | 10      | 255          | 4   |
|            | 0.50     | PGD    | 10      | 512          | 2   |
|            | 1.00     | PGD    | 10      | 512          | 2   |
| ImageNet   | 0.50     | PGD    | 1       | 255          | 1   |
|            | 1.00     | PGD    | 1       | 512          | 1   |

A.3 Detailed configurations of SmoothAdv models

In Table 5, we specify the exact configurations used in our evaluation for the best-performing SmoothAdv models. These configurations have originally explored by Salman et al. [2019] via a grid search over 4 hyperparameters: namely, (a) attack method (Method): PGD [Madry et al., 2018] or DDN [Rony et al., 2019], (b) the number of steps (# steps), (c) the maximum allowed $\ell_2$ perturbation on the input ($\varepsilon$), and (d) the number of noise samples ($m$). We choose one pre-trained model per $\sigma$ for CIFAR-10 and ImageNet, among those officially released and classified as the best-performing models by Salman et al. [2019]. The link to download all the pre-trained models can be found in https://github.com/Hadisalman/smoothing-adversarial.

B Detailed results in ablation study

We report the detailed results for the experiments performed in ablation study (see Section 4.6). Table 6, 7, and 8 are corresponded to Figure 4(a), 4(b), and 4(c), respectively.

Table 6: Comparison of approximate certified test accuracy (%) on MNIST, for varying loss functions and $\lambda$. We set our result bold-faced whenever the value improves the baseline. For ACR, we underlined the best-performing model.

| Model        | $\lambda$ | ACR | 0.00 | 0.25 | 0.50 | 0.75 | 1.00 | 1.25 | 1.50 | 1.75 | 2.00 | 2.25 | 2.50 |
|--------------|-----------|-----|------|------|------|------|------|------|------|------|------|------|------|
| Gaussian     | 0         | 1.620 | 96.4 | 94.4 | 91.4 | 87.0 | 79.9 | 71.0 | 59.6 | 46.2 | 32.6 | 19.7 | 10.8 |
| MSE          | 20        | 1.677 | 93.6 | 91.0 | 87.5 | 83.0 | 77.1 | 69.9 | 60.8 | 50.3 | 39.5 | 28.6 | 18.4 |
|             | 50        | 1.603 | 92.5 | 90.0 | 86.1 | 81.3 | 75.5 | 67.7 | 58.6 | 47.4 | 35.7 | 24.1 | 14.5 |
|             | 100       | 1.570 | 91.5 | 88.8 | 84.7 | 80.0 | 73.8 | 65.9 | 57.0 | 46.5 | 34.6 | 23.5 | 14.3 |
| KL-divergence| 20        | 1.713 | 94.0 | 91.7 | 88.2 | 83.5 | 77.7 | 70.5 | 61.5 | 51.4 | 41.2 | 31.1 | 21.4 |
|             | 50        | 1.707 | 93.4 | 90.7 | 87.1 | 82.3 | 76.8 | 69.4 | 60.6 | 50.9 | 41.3 | 31.8 | 22.6 |
|             | 100       | 1.683 | 92.7 | 89.9 | 85.9 | 81.3 | 75.4 | 68.0 | 59.5 | 49.9 | 40.4 | 31.2 | 22.6 |
| Cross-entropy| 20        | 1.750 | 92.5 | 89.8 | 86.5 | 81.7 | 76.3 | 69.6 | 61.4 | 52.9 | 44.2 | 35.9 | 26.8 |
Table 7: Comparison of approximate certified test accuracy on MNIST for varying $m \in \{2, 4, 8\}$. For each model, training and certification are done with the same smoothing factor specified in $\sigma$.

| $\sigma$ | 0.00 | 0.25 | 0.50 | 0.75 | 1.00 | 1.25 | 1.50 | 1.75 | 2.00 | 2.25 | 2.50 |
|----------|------|------|------|------|------|------|------|------|------|------|------|
| 0.25     | 0.930| 99.5 | 99.0 | 98.0 | 96.4 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |
| 0.50     | 1.665| 98.9 | 98.3 | 97.4 | 95.6 | 93.0 | 88.1 | 79.5 | 62.9 | 0.0  | 0.0  |
| 1.00     | 1.750| 92.5 | 89.8 | 86.5 | 81.7 | 76.3 | 69.6 | 61.4 | 52.9 | 44.2 | 35.9 | 26.8 |

Table 8: Comparison of approximate certified test accuracy on MNIST for varying $\lambda$. We set our result bold-faced whenever the value improves the baseline ($\lambda = 0.0$). For ACR, we underlined the best-performing model.

| $\lambda$ | ACR 0.00 | 0.25 | 0.50 | 0.75 | 1.00 | 1.25 | 1.50 | 1.75 | 2.00 | 2.25 | 2.50 |
|-----------|----------|------|------|------|------|------|------|------|------|------|------|
| 0.0       | 1.620    | 96.4 | 94.4 | 91.4 | 87.0 | 79.9 | 71.0 | 59.6 | 46.2 | 32.6 | 19.7 |
| 1.0       | 1.707    | 96.0 | 94.1 | 91.3 | 86.9 | 81.0 | 73.0 | 63.1 | 51.2 | 38.7 | 26.8 |
| 5.0       | 1.741    | 95.0 | 92.9 | 89.8 | 85.4 | 79.5 | 72.6 | 63.3 | 52.8 | 41.8 | 31.0 |
| 10.0      | 1.743    | 94.2 | 92.0 | 88.8 | 84.3 | 78.7 | 71.7 | 62.9 | 52.8 | 42.7 | 32.3 |
| 15.0      | 1.749    | 93.7 | 91.2 | 87.8 | 83.2 | 77.6 | 70.6 | 62.2 | 52.8 | 43.7 | 34.1 |
| 20.0      | 1.750    | 92.5 | 89.8 | 86.5 | 81.7 | 76.3 | 69.6 | 61.4 | 52.9 | 44.2 | 35.9 |
| 25.0      | 1.737    | 90.5 | 88.0 | 84.3 | 79.7 | 74.4 | 67.6 | 60.6 | 52.6 | 44.8 | 37.3 |
| 30.0      | 1.713    | 87.4 | 84.6 | 81.0 | 76.5 | 71.4 | 65.5 | 59.1 | 52.4 | 45.6 | 38.3 |
| 35.0      | 1.654    | 81.6 | 78.8 | 75.7 | 71.3 | 66.7 | 62.0 | 56.6 | 51.4 | 45.3 | 39.0 |
| 40.0      | 0.432    | 11.3 | 11.3 | 11.3 | 11.3 | 11.3 | 11.3 | 11.3 | 11.3 | 11.3 | 11.3 |

Table 9: Comparison of our method to stability training [Li et al., 2019] on CIFAR-10 dataset. Each of the values indicates the fraction of test samples those have $\ell_2$ certified radius larger than the threshold specified at the top row. We set our result bold-faced whenever the value improves the baseline.

| $\sigma$ | Models (CIFAR-10) | ACR 0.00 | 0.25 | 0.50 | 0.75 | 1.00 | 1.25 | 1.50 | 1.75 | 2.00 | 2.25 |
|----------|-------------------|----------|------|------|------|------|------|------|------|------|------|
| 0.25     | Gaussian [Cohen et al., 2019] | 0.424    | 76.6 | 61.2 | 42.2 | 25.1 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |
|          | + Consistency ($\lambda = 20$) | 0.551    | 75.9 | 67.5 | 57.6 | 46.9 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |
|          | Stability [Li et al., 2019] ($\lambda = 1$) | 0.408    | 71.6 | 57.8 | 40.7 | 27.0 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |
|          | Stability [Li et al., 2019] ($\lambda = 2$) | 0.421    | 72.3 | 58.0 | 43.3 | 27.3 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |
|          | Stability [Li et al., 2019] ($\lambda = 5, 10, 20$) | 0.102    | 10.7 | 10.7 | 10.7 | 10.7 | 0.0  | 0.0  | 0.0  | 0.0  | 0.0  |
| 0.50     | Gaussian [Cohen et al., 2019] | 0.525    | 65.7 | 54.9 | 42.8 | 32.5 | 22.0 | 14.1 | 8.3  | 3.9  | 0.0  |
|          | + Consistency ($\lambda = 20$) | 0.737    | 59.0 | 53.9 | 48.7 | 43.4 | 37.8 | 32.7 | 27.0 | 21.0 | 0.0  |
|          | Stability [Li et al., 2019] ($\lambda = 1$) | 0.496    | 61.1 | 51.5 | 40.9 | 29.8 | 21.1 | 14.0 | 8.3  | 3.6  | 0.0  |
|          | Stability [Li et al., 2019] ($\lambda = 2$) | 0.521    | 60.6 | 51.5 | 41.4 | 32.5 | 23.9 | 15.3 | 9.6  | 5.0  | 0.0  |
|          | Stability [Li et al., 2019] ($\lambda = 5, 10, 20$) | 0.206    | 10.8 | 10.8 | 10.8 | 10.8 | 10.8 | 10.8 | 10.8 | 10.8 | 0.0  |
| 1.00     | Gaussian [Cohen et al., 2019] | 0.542    | 47.2 | 39.2 | 34.0 | 27.8 | 21.6 | 17.4 | 14.0 | 11.8 | 10.0 |
|          | + Consistency ($\lambda = 20$) | 0.742    | 43.8 | 40.1 | 36.0 | 32.3 | 28.4 | 25.0 | 21.7 | 18.9 | 16.3 |
|          | Stability [Li et al., 2019] ($\lambda = 1$) | 0.526    | 43.5 | 38.9 | 32.8 | 27.0 | 23.1 | 19.1 | 15.4 | 11.3 | 7.8  |
|          | Stability [Li et al., 2019] ($\lambda = 2$) | 0.414    | 17.0 | 16.3 | 15.4 | 14.6 | 13.7 | 12.6 | 12.1 | 11.2 | 10.3 |
|          | Stability [Li et al., 2019] ($\lambda = 5, 10, 20$) | 0.381    | 10.0 | 10.0 | 10.0 | 10.0 | 10.0 | 10.0 | 10.0 | 10.0 | 10.0 |
C Overview on prior works

For completeness, we present a brief introduction to the prior works mainly considered in our experiments. We use the notations defined in Section 2 throughout this appendix.

C.1 SmoothAdv

Recall (2) that a smoothed classifier \( \hat{f} \) is defined from a hard classifier \( f : \mathbb{R}^d \to \mathcal{Y} \). Here, SmoothAdv [Salman et al., 2019] attempts to perform adversarial training [Madry et al., 2018] directly on \( \hat{f} \):

\[
\min_{\hat{f}} \max_{||x' - x||_2 \leq \varepsilon} \mathcal{L}(\hat{f}; x', y), \tag{14}
\]

where \( \mathcal{L} \) denotes the standard cross-entropy loss. As mentioned in Section 3, however, \( \hat{f} \) is practically a non-differentiable object when (2) is approximated via Monte Carlo sampling, making it difficult to optimize the inner maximization of (14). To bypass this, Salman et al. [2019] propose to attack the soft-smoothed classifier \( \tilde{F} := \mathbb{E}_\delta[F_y(x + \delta)] \) instead of \( \hat{f} \), as \( \tilde{F} : \mathbb{R}^d \to \Delta^{k-1} \) is rather differentiable. Namely, SmoothAdv finds an adversarial example via solving the following:

\[
\hat{x} = \arg \max_{||x' - x||_2 \leq \varepsilon} \mathcal{L}(\tilde{F}; x', y) = \arg \max_{||x' - x||_2 \leq \varepsilon} \left( -\log \mathbb{E}_\delta \left[ F_y(x' + \delta) \right] \right). \tag{15}
\]

In practice, the expectation in this objective (15) is approximated via Monte Carlo integration with \( m \) samples of \( \delta \), namely \( \delta_1, \ldots, \delta_m \sim N(0, \sigma^2I) \):

\[
\hat{x} = \arg \max_{||x' - x||_2 \leq \varepsilon} \left( -\log \left( \frac{1}{m} \sum_{i} F_y(x' + \delta_i) \right) \right). \tag{16}
\]

To optimize the outer minimization objective in (14), on the other hand, SmoothAdv simply minimize the averaged loss over \( (\hat{x} + \delta_1, y), \ldots, (\hat{x} + \delta_m, y) \), i.e., \( \min_{\hat{F}} \frac{1}{m} \sum_{i} \mathcal{L}(\hat{F}; \hat{x} + \delta_i, y) \). Notice that the noise samples \( \delta_1, \ldots, \delta_m \) are re-used for the outer minimization as well.

C.2 MACER

On the other hand, MACER [Zhai et al., 2020] attempts to improve robustness of \( \hat{F} \) via directly maximizing the certified lower bound (3) on \( \ell_2 \)-adversarial perturbations [Cohen et al., 2019] for \( (x, y) \in \mathcal{D} \). Again, directly maximizing (3) is difficult due to the non-differentiability of \( \hat{f} \), thereby MACER instead maximizes the certified radius of \( \hat{F} \), in a similar manner to SmoothAdv [Salman et al., 2019]:

\[
\text{CR}(\hat{F}; x, y) := \sigma \left( \Phi^{-1}(\mathbb{E}_\delta[F_y(x + \delta)]) - \Phi^{-1}(\max_{c \neq y} \mathbb{E}_\delta[F_c(x + \delta)]) \right). \tag{17}
\]

Motivated from the 0-1 robust classification loss (18) in the following, Zhai et al. [2020] propose a robust training objective for maximizing \( \text{CR}(\hat{F}; x, y) \) along with the standard cross-entropy loss \( \mathcal{L} \) on \( \hat{F} \) as a surrogate loss for the natural error term:

\[
\mathcal{L}_d(f) := \mathbb{E}_{(x, y) \in \mathcal{D}} \left[ 1 - \mathbb{1}_{\text{CR}(\hat{f}; x, y) \geq \varepsilon} \right] = \mathbb{E} \left[ \mathbb{1}_{\hat{f}(x) \neq y} \right] + \mathbb{E} \left[ \mathbb{1}_{\hat{f}(x) = y, \text{CR}(\hat{f}; x, y) < \varepsilon} \right] \tag{18}
\]

\[
\mathcal{L}_{\text{MACER}}(F; x, y) := \mathcal{L}(f(x), y) + \frac{\gamma}{2} \max_{c \neq y} \{ \gamma - \text{CR}(\hat{F}; x, y) \} \cdot \mathbb{1}_{\hat{f}(x) = y} \tag{19}
\]

where \( \gamma, \lambda \) are hyperparameters. Here, notice that (19) uses the hinge loss to maximize \( \text{CR}(\hat{F}; x, y) \), only for the samples that \( \hat{F}(x) \) is correctly classified to \( y \). In addition, MACER uses an inverse temperature \( \beta > 1 \) to calibrate \( \hat{F} \) as another hyperparameter, mainly for reducing the practical gap between \( \hat{F} \) and \( \hat{f} \).