SmoothMix: Training Confidence-calibrated Smoothed Classifiers for Certified Robustness

Anonymous Author(s)
Affiliation
Address
email

Abstract

Randomized smoothing is currently a state-of-the-art method to construct a *certifiably robust* classifier from neural networks against ℓ_2-adversarial perturbations. Under the paradigm, the robustness of a classifier is aligned with the *prediction confidence*, *i.e.*, the higher confidence from a smoothed classifier implies the better robustness. This motivates us to rethink the fundamental trade-off between accuracy and robustness in terms of *calibrating* confidences of smoothed classifier. In this paper, we propose a simple training scheme, coined *SmoothMix*, to control the robustness of smoothed classifiers via *self-mixup*: it trains convex combinations of samples along the direction of adversarial perturbation for each input. The proposed procedure effectively identifies over-confident, near off-class samples as a cause of limited robustness in case of smoothed classifiers, and offers an intuitive way to adaptively set a new decision boundary between these samples for better robustness. Our experimental results demonstrate that the proposed method can significantly improve the certified ℓ_2-robustness of smoothed classifiers compared to existing state-of-the-art robust training methods.

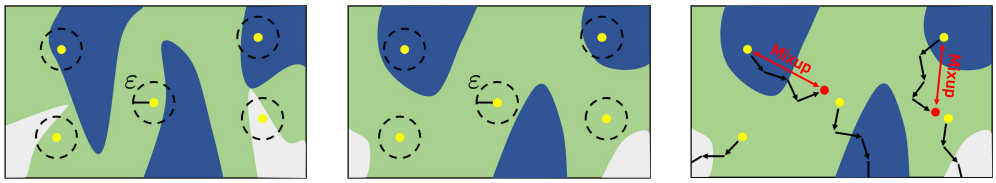
1 Introduction

Adversarial examples [53, 17] in deep neural networks clearly highlight that neural networks often generalize differently from humans, at least without an additional prior of *local smoothness* of predictions with respect to the input space: an adversarially-crafted, yet imperceptible input perturbation can drastically change the prediction of a neural network based classifier. Due to the intrinsic complexity of neural networks, however, the community has noticed that it is extremely hard to directly encode this smoothness prior into neural networks [6, 3, 55], especially without relying on *adversarial training* [40, 66], *i.e.*, augmenting training data with its adversarial examples. Even with adversarial training, (a) the non-convex, minimax nature of the training introduces many optimization difficulties, often resulting in a harsh over-fitting [51, 47], and (b) it is generally hard to provably guarantee that the learned classifier is indeed smooth.

Randomized smoothing [33, 11] is relatively a recent idea that aims to *indirectly* encode the smoothness prior: Cohen et al. [11] have shown that any classifier, regardless of whether it is smooth or not, can be transformed into a *certifiably robust* classifier via averaging its predictions over Gaussian noise, where the (certified) robustness of the classifier depends on how well the base classifier performs with the noise. Compared to adversarial training, this notion of "indirect" smoothness can be favorable in a sense that (a) it is easier to optimize, and (b) offers a provable guarantee on the robustness. Currently, randomized smoothing is considered as the state-of-the-art approach in the context of building a neural network based classifier that is certifiably robust on ℓ_2-perturbations [39].

In this respect, a growing body of research has focused on improving the robustness guarantee that randomized smoothing can give, *e.g.*, via different smoothing measures [34, 62] or improved

Submitted to 35th Conference on Neural Information Processing Systems (NeurIPS 2021). Do not distribute.



(a) Adversarial training [40] (b) SmoothAdv [49] (c) SmoothMix (Ours)

Figure 1: Illustrations of how each training method obtains adversarial robustness: adversarial training [40] considers an ε-ball around each sample and corrects adversarial examples found in these balls; SmoothAdv [49] directly employs adversarial training on smoothed classifiers; SmoothMix (ours) can be differentiated from SmoothAdv as it (*i*) does not assume an explicit norm restriction on adversarial examples, and (*ii*) applies the *mixup* [67] instead of correcting the adversarial examples.

certification procedures [14, 43]. One of important directions on this line of research is to investigate *which training* of the base classifier could maximize the certified robustness of smoothed classifiers [49, 65, 23]. In particular, Salman et al. [49] have proposed *SmoothAdv*, showing that employing adversarial training [40] for smoothed classifiers could further improve the robustness, akin to the standard neural networks. This motivates us to develop a new form of adversarial training, more specialized for smoothed classifiers.

Contribution. In this paper, we propose *SmoothMix*, a novel adversarial training method designed for improving the certified robustness of smoothed classifiers. One of the key features that smoothed classifiers offer is a direct correspondence from *prediction confidence* to adversarial robustness: achieving a higher confidence in a smoothed classifier implies that the classifier can give a better certified robustness. Inspired by this, we found that the certified robustness of a given data sample can be significantly decreased by nearby *off-class* but *over-confident* [45] inputs: such "harmful" inputs would occupy an unnecessarily large robust radius near the sample of our interest, especially when they do not contain much information to be discriminated by the classifier.

Under the finding, we aim to calibrate the confidence of these off-class inputs to improve the certified robustness at the original input. More specifically, we first observe that such over-confident examples can be efficiently found along the direction of *adversarial* perturbations for a given input. Then, we suggest to regularize the over-confident predictions along the adversarial direction toward the *uniform* prediction through a *mixup* loss [67] (see Figure 1 for an overview). This new approach of incorporating adversarial examples effectively permits more distant examples in training, even when they goes off-class, based on the local-smoothness of smoothed classifiers. It also suggests an intuitive way of defining confidence beyond the given data samples to smoothed classifiers.

We evaluate our proposed SmoothMix against with various state-of-the-art robust training methods for smoothed classifiers on a wide range of image classification benchmarks, including MNIST [32], CIFAR-10 [29], and ImageNet [48] datasets. Overall, the results consistently show that our new adversarial training scheme for smoothed classifiers significantly improves the certified robustness compared to existing methods, *e.g.*, one of our CIFAR-10 model could largely outperform an existing state-of-the-art result on the average certified robustness in ℓ_2-radius $0.720 \to 0.737$. Through an extensive ablation study, we also verify that our method is (a) robust to the choice of hyperparameters, and (b) can effectively trade-off between the accuracy and robustness [66] of smoothed classifiers.

Overall, our work suggests that the robustness of a classifier should be set individually per sample considering its nearby inputs: we approach this problem by leveraging the relationship between the prediction confidence and robustness of smoothed classifiers. Recently, there have been also some initial attempts to incorporate a *sample-wise* treatment for robustness by allowing input-dependent noise scales in randomized smoothing [1, 58, 10]. However, our theoretical analysis shows that such an approach would eventually suffer from the curse of dimensionality (Theorem 1 in Appendix H), highlighting our approach of focusing on a "better calibration" as a promising alternative.

2 Preliminaries

We assume an *i.i.d.* dataset $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^n \sim P$, where $x_i \in \mathbb{R}^d$ and $y_i \in \mathcal{Y} := \{1, \cdots, C\}$, and focus on the problem of correctly classifying a given input x into one of C classes. Let $f : \mathbb{R}^d \to \mathcal{Y}$

be a classifier modeled by $f(x) := \arg\max_{c \in \mathcal{Y}} F_c(x)$ with $F : \mathbb{R}^d \to \Delta^{C-1}$, where Δ^{C-1} denotes the probability simplex in $\mathbb{R}^C$. For example, F can be a neural network followed by a softmax layer.

In the context of *adversarial robustness*, we require f not only to correctly classify $(x, y) \sim P$, but also to be *locally-constant* around x, *i.e.*, f should not contain any adversarial examples around x. In this respect, one can measure and attempt to maximize the adversarial robustness of a classifier f by considering the *minimum-distance* of adversarial perturbation [44, 7, 8], namely:

$$R(f; x, y) := \min_{f(x') \neq y} \|x' - x\|_2. \tag{1}$$

Randomized smoothing. In cases when f is too complex to control its predictions in practice, *e.g.*, if f is a neural network on high-dimensional data, directly solving and maximizing (1) can be hard. *Randomized smoothing* [11] instead construct a new classifier $\hat{f}$ from f that is easier to obtain robustness by transforming the base classifier f with a certain *smoothing measure*, where in this paper we focus on the case of Gaussian distributions $\mathcal{N}(0, \sigma^2 I)$:

$$\hat{f}(x) := \arg\max_{c \in \mathcal{Y}} \mathbb{P}_{\delta \sim \mathcal{N}(0, \sigma^2 I)} \left(f(x + \delta) = c \right). \tag{2}$$

For a given (x, y), Cohen et al. [11] have shown that $R(\hat{f}; x, y)$ can be lower-bounded by the *certified radius* $\underline{R}(\hat{f}, x, y)$, which can be derived from the *confidence* of $\hat{f}$ at x, namely we denote it by $p_f(x)$:

$$R(\hat{f}; x, y) \geq \sigma \cdot \Phi^{-1}(p_f(x)) =: \underline{R}(\hat{f}, x, y) \text{ where } p_f(x) := \mathbb{P}_{\delta \sim \mathcal{N}(0, \sigma^2 I)}(f(x + \delta) = \hat{f}(x)), \tag{3}$$

provided that $\hat{f}(x) = y$, and otherwise $R(\hat{f}; x, y) := 0$.[1] This lower bound is known as tight for the ℓ_2-minimum distance, *e.g.*, the bound is optimal for linear classifiers [11].

Although randomized smoothing can be applied for any classifier $f : \mathbb{R}^d \to \mathcal{Y}$, the robustness of smoothed classifiers can vary depending on p_f as in (3), *i.e.*, how f performs on a given input under the presence of Gaussian noise. In this sense, to obtain a robust $\hat{f}$, Cohen et al. [11] simply propose to train f using Gaussian augmentation by default:

$$\min_F \mathbb{E}_{\substack{(x,y) \sim P \\ \delta \sim \mathcal{N}(0, \sigma^2 I)}} \left[\mathcal{L}(F(x + \delta), y) \right], \tag{4}$$

where $\mathcal{L}$ denotes the standard cross-entropy loss.

Adversarial training for smoothed classifiers. To obtain f that gives a more robust classifier when smoothed into $\hat{f}$, Salman et al. [49] propose *SmoothAdv* that employs adversarial training [40] on $\hat{f}$:

$$\min_{\hat{f}} \max_{\|x' - x\|_2 \leq \epsilon} \mathcal{L}(\hat{f}; x', y). \tag{5}$$

Due to the intractability of $\hat{f}$, however, it is hard to directly optimize the inner maximization of (5) via gradient methods. To bypass this, SmoothAdv attacks the *soft-smoothed* classifier $\hat{F} := \mathbb{E}_\delta[F_y(x+\delta)]$ instead. Specifically, SmoothAdv finds an adversarial example via solving the following:

$$\hat{x} = \arg\max_{\|x' - x\|_2 \leq \epsilon} \mathcal{L}(\hat{F}; x', y) \approx \arg\max_{\|x' - x\|_2 \leq \epsilon} \left(-\log \left(\frac{1}{m} \sum_i F_y(x' + \delta_i) \right) \right), \tag{6}$$

using Monte Carlo integration with m samples of δ, namely $\delta_1, \cdots, \delta_m \sim \mathcal{N}(0, \sigma^2 I)$.

3 Method

Our goal in this paper is to develop a more suitable form of adversarial training (AT) for smoothed classifiers, taking into account their unique characteristics on adversarial robustness over standard neural networks. Figure 1 illustrates a motivating example: as shown in Figure 1(a), AT typically assumes a fixed-sized ball of radius ε that each adversarial perturbation must be in, as the goal of the training is to defend the classifier against adversaries under a specific threat model. However, in a case when AT is applied to a smoothed classifier, *e.g.*, as done by SmoothAdv, this assumption may

[1] Here, Φ denotes the cumulative distribution function of the standard normal distribution.

be too restrictive, particularly for inputs where the classifier already certifies robustness of radii larger than ε (*e.g.*, Figure 1(b)). This demands for a new form of AT specially for smoothed classifiers, *e.g.*, that allows more distant adversarial examples, despite its fundamental difficulty in the context of standard neural networks [25, 69].

In this regard, our proposed training method of *SmoothMix* takes a completely different approach to incorporate adversarial examples during training. More specifically, for a given sample $(x, y) \sim P$, our method finds an adversarial example of x *without* an explicit norm constraint, *i.e.*, "unrestrictively." This is because our focus is not to find an input for correcting its label to y (as in the standard AT), but to find an input that is *over-confident* and *semantically off-class*, *i.e.*, it is not beneficial to the classifier to label this input to y. Once we have such an example, SmoothMix then labels it as the *uniform confidence*, and considers a *mixup* training [67] with the original x: by linearly interpolating with the uniform confidence, SmoothMix effectively calibrates the over-confident inputs in between, re-balancing the certified radius at the original sample of x at the end.

3.1 Exploring over-confident adversarial examples in smoothed classifiers

Recall that we have a (base) classifier f of the form $f(x) = \arg\max_{c \in \mathcal{Y}} F_c(x)$, $\hat{f}$ is its smoothed counterpart, and we aim to improve the robustness of $\hat{f}$ by incorporating adversarial examples in training. In this paper, we are particularly interested in adversarial examples of $\hat{f}$ that is found *without* a hard restriction in its perturbation size. More concretely, for a given training sample $(x, y) \sim P$, we find adversarial examples by solving the following optimization:

$$\tilde{x} := \arg\max_{x'} \left(\mathcal{L}(\hat{f}; x', y) - \beta \cdot \|x' - x\|_2^2 \right), \tag{7}$$

where $\mathcal{L}$ is the cross-entropy loss, and $\beta > 0$ is to ensure that (7) cannot be arbitrarily far from x.

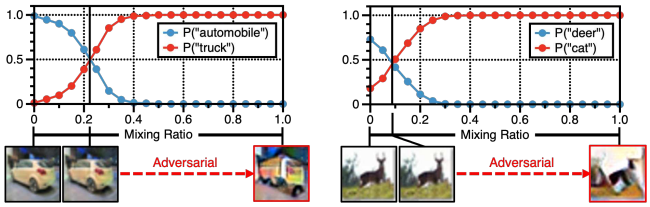
As proposed by Salman et al. [49] (see Section 2), one can optimize (7) by approximating the intractable $\hat{f}$ with the soft-smoothed classifier $\hat{F} := \mathbb{E}_\delta[F(x + \delta)]$, in a similar manner to (6). Based on this approximation, we simply perform a T-step gradient ascent from $\tilde{x}^{(0)} := x$ with step size $\alpha > 0$ to solve (7) using m samples of δ, namely $\delta_1, \cdots, \delta_m \sim \mathcal{N}(0, \sigma^2 I)$:[2]

$$\tilde{x}^{(t+1)} := \tilde{x}^{(t)} + \alpha \cdot \frac{\nabla_x J(\tilde{x}^{(t)})}{\|\nabla_x J(\tilde{x}^{(t)})\|_2}, \text{ where } J(x) := -\log \left(\frac{1}{m} \sum_i F_y(x + \delta_i) \right). \tag{8}$$

Figure 2 demonstrates two particular instances of these "unrestricted" adversarial examples found from (8) on x, and plots how the confidence of inputs changes as they are linearly interpolated from the clean input to its adversarial counterpart. From this illustration, we make several remarks those would lead to a more direct motivation to our method:

- We observe that adversarial perturbations found via (8), *i.e.*, from a smoothed classifier, could contain enough amount of semantic changes even in a perceptual sense, in either ways of translating the input to another class (Figure 2(a)), or simply removing some relevant information for the current class (Figure 2(b)). At least for these cases, therefore, it is reasonable for the classifier to keep their low confidence to the original class. Such a "perceptually-aligned" representation is not a unique property of smoothed classifiers, but have been generally observed on adversarially-robust classifiers [50, 15, 26]: in other words, we leverage the provable robustness of smoothed classifiers during training to reasonably obtain a semantically off-class samples those to be labeled as the uniform confidence.
- A major problem we rather highlight here is the tendency of *over-confidence* [45] toward the direction of adversarial perturbation: Figure 2 also presents how the confidence of the given smoothed classifier changes as we linearly interpolate the input from x to $\tilde{x}$. Overall, the adversarially-crafted samples $\tilde{x}$ usually attain significantly higher confidence compared to those of x, consequently their *certified radius* (3) would be much larger as well. Therefore, considering that $\tilde{x}$ are still nearby x, such the over-confidence at $\tilde{x}$ would negatively affect

[2] Here, we note that the β-term in (7) are omitted in (8). In practice, we do not use nor tune β in our method mainly for simplicity, as the role of β can be replaced by assuming a finite $\alpha \cdot T$, *i.e.*, by the *Lagrangian duality*: an unconstrained optimization with ℓ_2-regularization implicitly defines a hard constraint in its ℓ_2-norm.



(a) In-class translation (b) Out-of-class translation

Figure 2: Illustration of adversarial examples unrestrictively found in CIFAR-10 with a smoothed ResNet-110 ($\sigma = 0.25$). The plot demonstrates the change of confidence between two classes as the input is linearly interpolated.

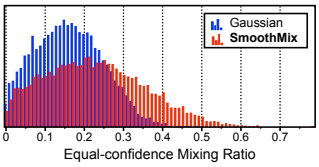


Figure 3: *Equal-confidence mixing ratios* on CIFAR-10, *i.e.*, the minimal mixing ratios for changing the correct prediction when each input is linearly interpolated to its adversarial example.

the certified radius of x, especially when $\tilde{x}$ does not contain much semantically meaningful information as observed in Figure 2(b). We nevertheless remark that such $\tilde{x}$ is still sufficiently far from x compared to the case of SmoothAdv, that has a hard ℓ_2-norm restriction.

3.2 SmoothMix for confidence-calibrated training of smoothed classifiers

Based on the observations from Section 3.1, we hypothesize that the *miscalibration* of confidences between x and its unrestricted adversarial example $\tilde{x}$ is an important factor that degrades the certified robustness of smoothed classifiers, and propose to penalize the over-confidence by mixing the *uniform* confidence to them. More concretely, we consider the *mixup* [67] training between x and $\tilde{x}$, *i.e.*, by augmenting the given training data with the following pairs:

$$x^{\texttt{mix}} := (1-\lambda)\cdot x + \lambda \cdot \tilde{x}^{(T)}, y^{\texttt{mix}} := (1-\lambda)\cdot \hat{F}(x) + \lambda \cdot \tfrac{\mathbb{1}}{C}, \text{ where } \lambda \sim \mathcal{U}\left(\left[0, \tfrac{1}{2}\right]\right) \quad (9)$$

where $\hat{F}(x) \in \Delta^{C-1}$ is the soft-smoothed prediction of x, $\mathcal{U}$ denotes the uniform distribution, λ is a random variable that represents the mixing ratio between $(x, \hat{F}(x))$ and $(\tilde{x}^{(T)}, \mathcal{U}(\mathcal{Y}))$, and $\mathbb{1}$ denotes the C-dimensional vector of ones. Here, we notice that λ is sampled only from $[0, \frac{1}{2}]$, unlike the standard choice [67] of $\mathcal{U}([0,1])$: recall from Figure 2(a) that $\tilde{x}$ can be often semantically in-class, so that a direct supervision of the uniform confidence on it could harm the classifier. By simply taking only the half part of the mixed samples closer to x, we could reasonably avoid these cases while maintaining its effect to prevent the over-confidence issue. The actual loss to minimize for these new data simply follows the cross-entropy loss with Gaussian augmentation, similarly to (4):

$$L^{\texttt{mix}} := \mathbb{E}_{\delta \sim \mathcal{N}(0, \sigma^2 I)} \left[\mathcal{L}(F(x^{\texttt{mix}} + \delta), y^{\texttt{mix}}) \right]. \quad (10)$$

Recall the over-confidence issue observed in Figure 2 as we follow from x to $\tilde{x}^{(T)}$. Minimizing $L^{\texttt{mix}}$ (10) directly corresponds to calibrating the high confidence at $\tilde{x}^{(T)}$ and the samples in-between, while keeping the original prediction of $\hat{F}(x)$ at x.

Incorporating SmoothAdv for free. As our method focuses on adversarial examples that are moderately far from the original inputs assuming that the classifier is already locally-smooth, one may still enjoy the effectiveness of SmoothAdv if it could further enforce the local smoothness. We indeed observe that the joint training can be helpful for the robustness of smoothed classifiers, but a naïve combination of them could incur too much costs for finding separate adversarial examples for each method. Instead, we found that simply taking $x \leftarrow \tilde{x}^{(1)}$ without modifying our current training, *i.e.*, using the *single-step adversarial example* found during (8) instead of the clean sample, can reasonably bring a similar effect. In this respect, we allow SmoothMix to use $(\tilde{x}^{(1)}, y)$ instead of (x, y) depending on demand of more robustness at expense of decreased clean accuracy.

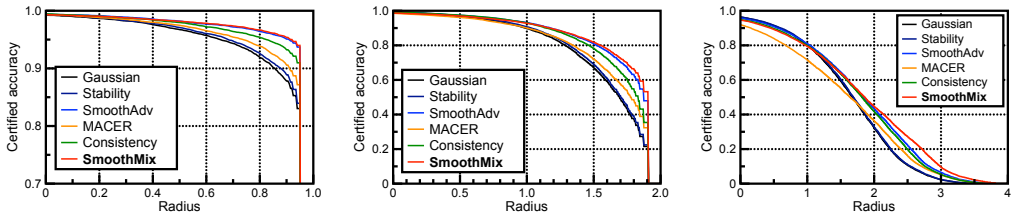
Overall training. Combining the proposed loss with the standard Gaussian training (4) gives the full objective to minimize for our training method. For a given sample $(x, y) \sim P$, and by letting $L^{\texttt{nat}} := \mathbb{E}_{\delta}\left[\mathcal{L}(F(x+\delta), y)\right]$, the final loss of SmoothMix is given by:

$$L := L^{\texttt{nat}} + \eta \cdot L^{\texttt{mix}} \quad (11)$$

where $\eta > 0$ is a hyperparameter to control the trade-off between accuracy and robustness. Algorithm 1 in Appendix A demonstrates a concrete training procedure of SmoothMix using m samples of δ for the Monte Carlo approximation.

Table 1: Comparison of approximate certified test accuracy (%) and ACR on MNIST. All the models are trained and evaluated with the same smoothing factor specified by σ. Each value except ACR indicates the fraction of test samples those have ℓ_2 certified radius larger than the threshold specified at the top row. We set our results bold-faced whenever the value improves the Gaussian baseline, and underlined whenever the value improves the best among the considered baselines.

σ	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	2.75
0.25	Gaussian [11]	0.911	99.2	98.5	96.7	93.3	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	Stability training [38]	0.915	99.3	98.6	97.1	93.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	SmoothAdv [49]	0.932	99.4	99.0	98.2	96.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	MACER [65]	0.920	99.3	98.7	97.5	94.8	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	Consistency [23]	0.928	99.5	98.9	98.0	96.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	SmoothMix ($\eta = 1.0$)	**0.931**	**99.5**	**98.9**	**98.2**	**96.4**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	+ One-step adversary	**0.933**	**99.4**	**99.0**	**98.2**	**96.9**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	SmoothMix ($\eta = 5.0$)	**0.932**	**99.4**	**99.0**	**98.2**	**96.7**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
	+ One-step adversary	**0.933**	**99.3**	**99.0**	**98.2**	**97.0**	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
0.50	Gaussian [11]	1.553	99.2	98.3	96.8	94.3	89.7	81.9	67.3	43.6	0.0	0.0	0.0	0.0
	Stability training [38]	1.570	99.2	98.5	97.1	94.8	90.7	83.2	69.2	45.4	0.0	0.0	0.0	0.0
	SmoothAdv [49]	1.687	99.0	98.3	97.3	95.8	93.2	88.5	81.1	67.5	0.0	0.0	0.0	0.0
	MACER [65]	1.594	98.5	97.5	96.2	93.7	90.0	83.7	72.2	54.0	0.0	0.0	0.0	0.0
	Consistency [23]	1.657	99.2	98.6	97.6	95.9	93.0	87.8	78.5	60.5	0.0	0.0	0.0	0.0
	SmoothMix ($\eta = 1.0$)	**1.678**	99.0	**98.4**	**97.4**	**95.7**	**93.0**	**88.1**	**80.0**	**65.6**	0.0	0.0	0.0	0.0
	+ One-step adversary	**1.694**	98.8	98.1	**97.1**	**95.3**	**92.7**	**88.3**	**81.7**	**69.5**	0.0	0.0	0.0	0.0
	SmoothMix ($\eta = 5.0$)	**1.694**	98.7	98.0	**97.0**	**95.3**	**92.7**	**88.5**	**81.8**	**70.0**	0.0	0.0	0.0	0.0
	+ One-step adversary	**1.685**	98.2	97.5	96.3	**94.5**	**91.3**	**87.4**	**81.0**	**70.7**	0.0	0.0	0.0	0.0
1.00	Gaussian [11]	1.620	96.3	94.4	91.4	86.8	79.8	70.9	59.4	46.2	32.5	19.7	10.9	5.8
	Stability training [38]	1.634	96.5	94.6	91.6	87.2	80.7	71.7	60.5	47.0	33.4	20.6	11.2	5.9
	SmoothAdv [49]	1.779	95.8	93.9	90.6	86.5	80.8	73.7	64.6	53.9	43.3	32.8	22.2	12.1
	MACER [65]	1.598	91.6	88.1	83.5	77.7	71.1	63.7	55.7	46.8	38.4	29.2	20.0	11.5
	Consistency [23]	1.740	95.0	93.0	89.7	85.4	79.7	72.7	63.6	53.0	41.7	30.8	20.3	10.7
	SmoothMix ($\eta = 1.0$)	**1.788**	95.5	93.5	90.5	86.2	**80.6**	**73.4**	**64.3**	**53.7**	**43.2**	**33.5**	**23.9**	**14.1**
	+ One-step adversary	**1.816**	94.7	92.4	89.2	84.6	79.4	**72.5**	**64.0**	**54.5**	**44.8**	**36.2**	**27.4**	**18.7**
	SmoothMix ($\eta = 5.0$)	**1.820**	93.7	91.6	88.1	83.5	77.9	70.9	**62.7**	**53.8**	**44.8**	**36.6**	**28.9**	**21.5**
	+ One-step adversary	**1.823**	93.3	90.9	87.5	83.0	77.5	70.6	**62.7**	**53.4**	**44.9**	**37.1**	**29.3**	**22.4**



(a) $\sigma = 0.25$ (b) $\sigma = 0.50$ (c) $\sigma = 1.00$

Figure 4: Comparison of approximate certified accuracy for various training methods on MNIST. The sharp drop of certified accuracy in each plots is due to that there is a strict upper bound in radius that CERTIFY can output for a given σ and $n = 100,000$.

4 Experiments

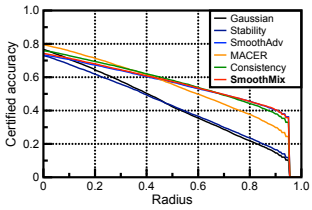
We evaluate the effectiveness of our method extensively on MNIST [32], CIFAR-10 [29], and ImageNet [48][3] classification datasets. Overall, the results consistently highlight that our newly proposed training can significantly improve the certified robustness of smoothed classifiers compared to existing robust training methods. We point out the improvements are especially remarkable on the certified accuracy at larger perturbations, at which SmoothMix mainly focus compared to prior arts. We also conduct an ablation study on the proposed method to convey a detailed analysis on the individual components. The detailed experimental setups, *e.g.*, trainig details, datasets, and hyperparameters for the baseline methods, are specified in Appendix B.

Baseline methods. We compare our method with a variety of existing techniques proposed for a robust training of smoothed classifiers, as listed in what follows: (a) Gaussian [11]: standard training with Gaussian augmentation; (b) Stability training [38]: a cross-entropy regularization between $F(x)$ and $F(x+\delta)$; (c) SmoothAdv [49]: adversarial training on smoothed classifier; (d) MACER

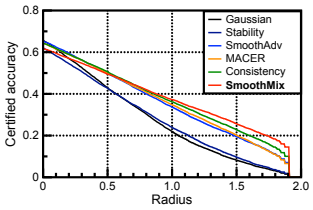
[3]Results on the ImageNet dataset can be found in Appendix E.

Table 2: Comparison of approximate certified test accuracy (%) and ACR on CIFAR-10. We set our results bold-faced whenever the value improves the Gaussian baseline, and underlined whenever the value improves the best among the considered baselines. * indicates that the results are evaluated from the official pre-trained models released by authors.

σ	Models (CIFAR-10)	ACR	0.00	0.25	0.50	0.75	1.00	1.25	1.50	1.75
0.25	Gaussian [11]	0.424	76.6	61.2	42.2	25.1	0.0	0.0	0.0	0.0
	Stability training [38]	0.421	72.3	58.0	43.3	27.3	0.0	0.0	0.0	0.0
	SmoothAdv* [49]	0.544	73.4	65.6	57.0	47.5	0.0	0.0	0.0	0.0
	MACER* [65]	0.531	79.5	69.0	55.8	40.6	0.0	0.0	0.0	0.0
	Consistency [23]	0.552	75.8	67.6	58.1	46.7	0.0	0.0	0.0	0.0
	SmoothMix (Ours)	**<u>0.553</u>**	**77.1**	**67.9**	**57.9**	**46.7**	0.0	0.0	0.0	0.0
	+ One-step adversary	**0.548**	74.2	**66.1**	**57.4**	**<u>47.7</u>**	0.0	0.0	0.0	0.0
0.50	Gaussian [11]	0.525	65.7	54.9	42.8	32.5	22.0	14.1	8.3	3.9
	Stability training [38]	0.521	60.6	51.5	41.4	32.5	23.9	15.3	9.6	5.0
	SmoothAdv* [49]	0.684	65.3	57.8	49.9	41.7	33.7	26.0	19.5	12.9
	MACER* [65]	0.691	64.2	57.5	49.9	42.3	34.8	27.6	20.2	12.6
	Consistency [23]	0.720	64.3	57.5	50.6	43.2	36.2	29.5	22.8	16.1
	SmoothMix (Ours)	**0.715**	65.0	**56.7**	**49.2**	**41.2**	**34.5**	**<u>29.6</u>**	**<u>23.5</u>**	**<u>18.1</u>**
	+ One-step adversary	**<u>0.737</u>**	61.8	**55.9**	**49.5**	**<u>43.3</u>**	**<u>37.2</u>**	**<u>31.7</u>**	**<u>25.7</u>**	**<u>19.8</u>**



(a) $\sigma = 0.25$



(b) $\sigma = 0.50$

Figure 5: Comparison of approximate certified accuracy for various training methods on CIFAR-10. The sharp drop of certified accuracy in each plots is due to that there is a strict upper bound in radius that CERTIFY can output for a given σ and $n = 100,000$.

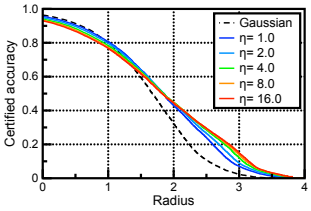


Figure 6: Comparison of approximate certified test accuracy of SmoothMix for varying η. "Gaussian" indicates the baseline training with Gaussian augmentation.

[65]: a regularization that maximizes an approximative form of the certified radius (3); and (e) Consistency [23]: a KL-divergence based regularization that minimizes the variance of $F(x+\delta)$ across δ. Whenever possible, we use the pre-trained models released by authors for our evaluation to reproduce the baselines. The more detailed training configurations are specified in Appendix B.2.

Evaluation metrics. Our evaluation of the robustness for a given smoothed classifier $\hat{f}$ is largely based on the protocol proposed by Cohen et al. [11], similarly to prior works [49, 65, 23]: more concretely, Cohen et al. [11] proposed a practical Monte Carlo based certification procedure, namely CERTIFY, that returns the prediction of $\hat{f}$ and a "safe" lower bound of certified radius over the randomness of n samples with probability at least $1-\alpha$, or abstains the certification.

From CERTIFY, we consider two evaluation metrics: (a) the *approximate certified test accuracy* at various radii: the fraction of the test dataset which CERTIFY classifies correctly with radius larger than r without abstaining, and (b) the *average certified radius* (ACR) [65]: the average of certified radii returned by CERTIFY on the test dataset counting only the correctly classified samples, namely $\mathrm{ACR} := \frac{1}{|\mathcal{D}_{\texttt{test}}|}\sum_{(x,y)\in\mathcal{D}_{\texttt{test}}} \mathrm{CR}(f,\sigma,x)\cdot \mathbf{1}_{\hat{f}(x)=y}$, where $\mathcal{D}_{\texttt{test}}$ is the test dataset, and CR denotes the certified radius from $\mathrm{CERTIFY}(f,\sigma,x)$. Here, the latter metric, ACR, is for a better comparison of robustness under trade-off between accuracy and robustness [56, 66]. We use the official PyTorch implementation[4] of CERTIFY, with $n = 100,000$, $n_0 = 100$ and $\alpha = 0.001$, following [11, 49, 23].

4.1 Results on MNIST

For MNIST [32] experiments, we report the approximate certified accuracy and ACR of smoothed classifiers obtained from LeNet [32] with different training methods, including SmoothMix, using the full MNIST test dataset. 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 σ used in the

[4] https://github.com/locuslab/smoothing

training. When SmoothMix is used, we consider a fixed hyperparameter value for $\alpha = 1.0$ and $m = 4$, the step size and the number of noise samples. We empirically observe that it is beneficial to set $\alpha \cdot T$ to be proportional to σ, the noise level, as there exist different upper bounds on the certified radius statistical achievable in practice depending on σ: in this respect, we set $T = 2, 4, 8$ for the models with $\sigma = 0.25, 0.5, 1.0$, respectively. We apply the same $m = 4$ for SmoothAdv, *i.e.*, for adversarial training, as well, and $T = 10$ with an ℓ_2-constraint of radius $\varepsilon = 1.0$.

The results are presented in Table 1 and Figure 4. Overall, we observe that our proposed SmoothMix loss (10) added to the Gaussian training dramatically improve the certified test accuracy from "Gaussian". By considering the one-step adversary (Section 3.2) in training, we could further improve the robust accuracy, significantly improving ACRs compared to the previous state-of-the-art training methods: *e.g.*, our method could improve ACRs with $\sigma = 1.0$ from $1.779 \to 1.823$. This shows that improvements from SmoothMix can be orthogonal to those from SmoothAdv. It is also remarkable that even without the one-step adversarial example, one could further improve the certified robustness by simply increasing the relative strength η of the SmoothMix loss, *e.g.*, by $1.0 \to 5.0$ as presented in Table 1: *e.g.*, "SmoothMix" with $\eta = 5.0$ still outperforms "SmoothAdv" by $1.779 \to 1.820$ at $\sigma = 1.0$. Finally, we note that our models could substantially improve the robustness at larger perturbations with less degradation in the clean accuracy, *e.g.*, compared to "MACER" or "Consistency": considering that they are also regularization based approaches those allow to control the robustness via controlling their regularization strength, the results show that our form of loss could better compensate the trade-off between accuracy and robustness.

4.2 Results on CIFAR-10

For CIFAR-10 [29] experiments, we report the approximate certified accuracy and ACR of smoothed classifiers from ResNet-110 [20] using the full CIFAR-10 test dataset. Again, we consider three different models as varying the noise level $\sigma \in \{0.25, 0.5, 1.0\}$,[5] and apply the same σ for inference as well. When SmoothMix is used, we consider a fixed hyperparameter value for $T = 4$ and $m = 2$, the number of steps and the number of noise samples, respectively. We also fix $\eta = 5.0$ throughout the experiments, as also used for MNIST (see Table 1). Again, we make sure that $\alpha \cdot T$ to be proportional to σ, so that we set $\alpha = 0.5, 1.0, 2.0$ for the models with $\sigma = 0.25, 0.5, 1.0$, respectively. For SmoothAdv, we report the performance evaluated from the pre-trained models released by the authors[6] for a fixed configuration of $T = 10, \varepsilon = 1.0$, and $m = 8$.

The results are summarized in Table 2 and Figure 5. Again, we still observe that our method generally exhibits better trade-offs between accuracy and certified robustness compared to other baselines: *e.g.*, at $\sigma = 0.5$, "SmoothMix" could improve the previous best result from "Consistency" by a significant margin of $0.720 \to 0.737$. Without the single-step adversary, "SmoothMix" can effectively preserve the clean accuracy while also improving ACR, *e.g.*, at $\sigma = 0.25$, "SmoothMix" could even improve the clean accuracy of "Gaussian": although "MACER" could improve the clean accuray as well, one could see that their improvements in robust accuracy are relatively limited.

4.3 Ablation study

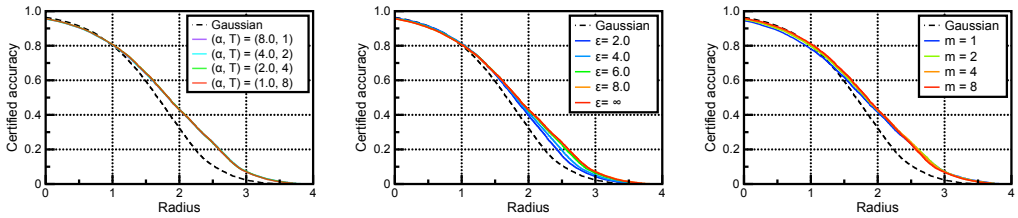
We also conduct an ablation study to investigate the individual effects of the hyperparameters in our method. Unless otherwise noted, we perform experiments on MNIST with $\sigma = 1.0$. All the detailed results from this study and additional study, *e.g.*, the effect of m, are reported in Appendix G.

Effect of η. By design, SmoothMix controls the trade-off between accuracy and robustness by adjusting η, the relative strength of $L^{\texttt{mix}}$ over $L^{\texttt{nat}}$ (11). Here, we further examine the effect of η by comparing the certified robustness on varying $\eta \in \{1, 2, 4, 8, 16\}$: the results in Figure 6 show that increasing η consistently improves the certified robustness of the classifier, which confirms $L^{\texttt{mix}}$, the mixup loss, as an effective term to trade-off the robustness against $L^{\texttt{nat}}$ for accuracy.

Trade-off between α and T. In practice, SmoothMix can trade-off between the step size α and the number of steps T to compensate between a more accurate optimization of (7) and its computational cost, while maintaining the effective range of the perturbation by $\alpha \cdot T$. Figure 7(a) explores this trade-off, by comparing models trained with different combinations of (α, T) under control of $\alpha \cdot T = 8.0$.

[5] Due to the space limitation, we defer the CIFAR-10 results with $\sigma = 1.0$ to Appendix D, considering that the scenario can be less practical compared to the others: *e.g.*, the clean accuracy in this setup is $< 50\%$ in most cases, even for the Gaussian baseline [11].

[6] https://github.com/Hadisalman/smoothing-adversarial



(a) Effect of α and T (b) Hard restriction of ε on attacks (c) Effect of m

Figure 7: Comparison of approximate certified test accuracy of SmoothMix and its ablations. "Gaussian" indicates the baseline training with Gaussian augmentation.

Interestingly, the results indicate that the choice of α and T does not significantly affect the final performance as long as $\alpha \cdot T$ is constant: all the considered combinations achieve similar robustness, with only a slight degradation in ACR even at $(\alpha, T) = (8.0, 1)$ (see Table 7 in Appendix G). This suggests that (a) finding adversarial examples in a smoothed classifier can be simpler than one might expect, and (b) one can effectively reduce the training cost of SmoothMix using small T in practice.

Hard restriction on adversarial attacks. One of key features of SmoothMix is at its *unrestricted* search of adversarial examples. Here, we examine the case when there is a hard restriction on each search, namely in ℓ_2-radius of $\varepsilon \in \{2, 4, 6, 8\}$. The results presented in Figure 7(b) along with the Gaussian baseline ("Gaussian") and the original unrestricted setup ("$\varepsilon = \infty$") show that SmoothMix indeed works best when there is no such restrictions, although these ablations still reasonably improve the Gaussian baseline, *i.e.*, calibrating with adversarial examples outside the ε-ball can indeed help to improve the certified robustness in our training scheme.

Equal-confidence mixing ratios. Recall from Figure 2 that we are motivated by the problem of *miscalibration* in smoothed classifiers between clean and its adversarial example. To see how much the proposed SmoothMix could alleviate this issue, we compare the distributions of the minimal mixing ratios that changes its prediction of a given classifier on the test dataset, namely the *equal-confidence mixing ratios*, before and after training with SmoothMix. For this comparison, we use ResNet-110 on CIFAR-10 assuming $\sigma = 0.25$. Figure 3 shows the result, and it indeed confirms SmoothMix has an effect of improving calibration between clean and adversarial examples.

5 Discussion and conclusion

We observe that adversarial training with an *unrestricted* adversary can be feasible and even more promising (compared to the *restricted* ones) when it comes with smoothed classifiers, by showing their effectiveness to improve the certified adversarial robustness with a novel mixup-based training. We address the brittleness of deep neural networks through the lens of smoothed classifiers, which could give us a simpler view on them. We believe our research could be a useful step toward understanding what essentially constitutes adversarial examples in deep neural networks.

Broader impact. Adversarial robustness in deep learning is arguably an essential requirement for *AI safety* [2], with much impact on various security-concerned systems: *e.g.*, medical diagnosis [9], speech recognition [46] and autonomous driving [64]. Thanks to their certifiable guarantees, we believe a practical success of systems based on *randomized smoothing* would be fatal for those who maliciously attempt to break down the system via adversarial attacks. Nevertheless, one should also recognize that current techniques for robustness in deep learning, including randomized smoothing as well, indeed have a clear gap to be practically used in real-world, *e.g.*, defending against challenging unrestricted attacks [60, 5], which should be further investigated in the future research. Consequently, it is particularly important for the defense techniques not to be misused in practical systems, as a failure of such systems may lead practitioners to have a biased, false sense of security.

Limitation. While our ultimate goal is to find optimal smoothed classifiers in terms of the accuracy and robustness trade-off, SmoothMix should not be considered as the final solution for the problem; our method is a promising proof-of-concept showing the close relationship between randomized smoothing and *confidence-calibrated* classifiers [19, 36]. Although our focus in this paper is currently limited only to the over-confidence issue, we believe there are still many rooms to be explored in future for another such connection, *e.g.*, could the recent developments in the literature of uncertainty estimation of deep neural networks [22, 54] help to improve the robustness of smoothed classifiers.

References

[1] Motasem Alfarra, Adel Bibi, Philip H. S. Torr, and Bernard Ghanem. Data dependent randomized smoothing, 2020.

[2] Dario Amodei, Chris Olah, Jacob Steinhardt, Paul Christiano, John Schulman, and Dan Mané. Concrete problems in AI safety. *arXiv preprint arXiv:1606.06565*, 2016.

[3] Anish Athalye, Nicholas Carlini, and David Wagner. Obfuscated gradients give a false sense of security: Circumventing defenses to adversarial examples. In *Proceedings of the 35th International Conference on Machine Learning*, volume 80 of *Proceedings of Machine Learning Research*, pages 274–283, Stockholmsmässan, Stockholm Sweden, 10–15 Jul 2018. PMLR. URL http://proceedings.mlr.press/v80/athalye18a.html.

[4] Mislav Balunovic and Martin Vechev. Adversarial training and provable defenses: Bridging the gap. In *International Conference on Learning Representations*, 2020. URL https://openreview.net/forum?id=SJxSDxrKDr.

[5] Anand Bhattad, Min Jin Chong, Kaizhao Liang, Bo Li, and D. A. Forsyth. Unrestricted adversarial examples via semantic manipulation. In *International Conference on Learning Representations*, 2020. URL https://openreview.net/forum?id=Sye_OgHFwH.

[6] Nicholas Carlini and David Wagner. Adversarial examples are not easily detected: Bypassing ten detection methods. In *Proceedings of the 10th ACM Workshop on Artificial Intelligence and Security*, pages 3–14, 2017.

[7] Nicholas Carlini and David Wagner. Towards evaluating the robustness of neural networks. In *IEEE Symposium on Security and Privacy*, pages 39–57. IEEE, 2017.

[8] Nicholas Carlini, Anish Athalye, Nicolas Papernot, Wieland Brendel, Jonas Rauber, Dimitris Tsipras, Ian Goodfellow, and Aleksander Madry. On evaluating adversarial robustness. *arXiv preprint arXiv:1902.06705*, 2019.

[9] Rich Caruana, Yin Lou, Johannes Gehrke, Paul Koch, Marc Sturm, and Noemie Elhadad. Intelligible models for healthcare: Predicting pneumonia risk and hospital 30-day readmission. In *Proceedings of the 21th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, pages 1721–1730, 2015.

[10] Chen Chen, Kezhi Kong, Peihong Yu, Juan Luque, Tom Goldstein, and Furong Huang. Insta-RS: Instance-wise randomized smoothing for improved robustness and accuracy, 2021.

[11] Jeremy Cohen, Elan Rosenfeld, and Zico Kolter. Certified adversarial robustness via randomized smoothing. In Kamalika Chaudhuri and Ruslan Salakhutdinov, editors, *Proceedings of the 36th International Conference on Machine Learning*, volume 97 of *Proceedings of Machine Learning Research*, pages 1310–1320, Long Beach, California, USA, 09–15 Jun 2019. PMLR. URL http://proceedings.mlr.press/v97/cohen19c.html.

[12] Francesco Croce and Matthias Hein. Provable robustness against all adversarial l_p-perturbations for $p \geq 1$. In *International Conference on Learning Representations*, 2020. URL https://openreview.net/forum?id=rklk_ySYPB.

[13] Francesco Croce, Maksym Andriushchenko, and Matthias Hein. Provable robustness of ReLU networks via maximization of linear regions. In Kamalika Chaudhuri and Masashi Sugiyama, editors, *Proceedings of Machine Learning Research*, volume 89 of *Proceedings of Machine Learning Research*, pages 2057–2066. PMLR, 16–18 Apr 2019. URL http://proceedings.mlr.press/v89/croce19a.html.

[14] Krishnamurthy (Dj) Dvijotham, Jamie Hayes, Borja Balle, Zico Kolter, Chongli Qin, Andras Gyorgy, Kai Xiao, Sven Gowal, and Pushmeet Kohli. A framework for robustness certification of smoothed classifiers using f-divergences. In *International Conference on Learning Representations*, 2020. URL https://openreview.net/forum?id=SJlKrkSFPH.

[15] Logan Engstrom, Andrew Ilyas, Shibani Santurkar, Dimitris Tsipras, Brandon Tran, and Aleksander Madry. Adversarial robustness as a prior for learned representations. *arXiv preprint arXiv:1906.00945*, 2019.

[16] Timon Gehr, Matthew Mirman, Dana Drachsler-Cohen, Petar Tsankov, Swarat Chaudhuri, and Martin Vechev. Ai2: Safety and robustness certification of neural networks with abstract interpretation. In *2018 IEEE Symposium on Security and Privacy*, pages 3–18. IEEE, 2018.

[17] Ian J Goodfellow, Jonathon Shlens, and Christian Szegedy. Explaining and harnessing adversarial examples. In *International Conference on Learning Representations*, 2015.

[18] Sven Gowal, Krishnamurthy Dj Dvijotham, Robert Stanforth, Rudy Bunel, Chongli Qin, Jonathan Uesato, Relja Arandjelovic, Timothy Mann, and Pushmeet Kohli. Scalable verified training for provably robust image classification. In *Proceedings of the IEEE/CVF International Conference on Computer Vision*, pages 4842–4851, 2019.

[19] Chuan Guo, Geoff Pleiss, Yu Sun, and Kilian Q. Weinberger. On calibration of modern neural networks. In Doina Precup and Yee Whye Teh, editors, *Proceedings of the 34th International Conference on Machine Learning*, volume 70 of *Proceedings of Machine Learning Research*, pages 1321–1330, International Convention Centre, Sydney, Australia, 06–11 Aug 2017. PMLR. URL http://proceedings.mlr.press/v70/guo17a.html.

[20] Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Deep residual learning for image recognition. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pages 770–778, 2016.

[21] Dan Hendrycks and Kevin Gimpel. A baseline for detecting misclassified and out-of-distribution examples in neural networks. In *International Conference on Learning Representations*, 2017. URL https://openreview.net/forum?id=Hkg4TI9xl.

[22] Dan Hendrycks, Mantas Mazeika, Saurav Kadavath, and Dawn Song. Using self-supervised learning can improve model robustness and uncertainty. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d'Alché-Buc, E. Fox, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 32. Curran Associates, Inc., 2019. URL https://proceedings.neurips.cc/paper/2019/file/a2b15837edac15df90721968986f7f8e-Paper.pdf.

[23] Jongheon Jeong and Jinwoo Shin. Consistency regularization for certified robustness of smoothed classifiers. In *Advances in Neural Information Processing Systems*, 2020.

[24] Heinrich Jiang, Been Kim, Melody Guan, and Maya Gupta. To trust or not to trust a classifier. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 31, pages 5541–5552. Curran Associates, Inc., 2018. URL https://proceedings.neurips.cc/paper/2018/file/7180cffd6a8e829dacfc2a31b3f72ece-Paper.pdf.

[25] Daniel Kang, Yi Sun, Dan Hendrycks, Tom Brown, and Jacob Steinhardt. Testing robustness against unforeseen adversaries, 2020.

[26] Simran Kaur, Jeremy Cohen, and Zachary C Lipton. Are perceptually-aligned gradients a general property of robust classifiers? *arXiv preprint arXiv:1910.08640*, 2019.

[27] Jang-Hyun Kim, Wonho Choo, and Hyun Oh Song. Puzzle Mix: Exploiting saliency and local statistics for optimal mixup. In Hal Daumé III and Aarti Singh, editors, *Proceedings of the 37th International Conference on Machine Learning*, volume 119 of *Proceedings of Machine Learning Research*, pages 5275–5285. PMLR, 13–18 Jul 2020. URL http://proceedings.mlr.press/v119/kim20b.html.

[28] JangHyun Kim, Wonho Choo, Hosan Jeong, and Hyun Oh Song. Co-Mixup: Saliency guided joint mixup with supermodular diversity. In *International Conference on Learning Representations*, 2021. URL https://openreview.net/forum?id=gvxJzw8kW4b.

[29] Alex Krizhevsky. Learning multiple layers of features from tiny images. Technical report, Department of Computer Science, University of Toronto, 2009.

[30] Ananya Kumar, Percy S Liang, and Tengyu Ma. Verified uncertainty calibration. In *Advances in Neural Information Processing Systems*, volume 32, pages 3792–3803. Curran Associates, Inc., 2019. URL https://proceedings.neurips.cc/paper/2019/file/f8c0c968632845cd133308b1a494967f-Paper.pdf.

[31] Alex Lamb, Vikas Verma, Juho Kannala, and Yoshua Bengio. Interpolated adversarial training: Achieving robust neural networks without sacrificing too much accuracy. In *Proceedings of the 12th ACM Workshop on Artificial Intelligence and Security*, pages 95–103, 2019.

[32] Y. LeCun, L. Bottou, Y. Bengio, and P. Haffner. Gradient-based learning applied to document recognition. *Proceedings of the IEEE*, 86(11):2278–2324, Nov 1998. ISSN 1558-2256. doi: 10.1109/5.726791.

[33] Mathias Lecuyer, Vaggelis Atlidakis, Roxana Geambasu, Daniel Hsu, and Suman Jana. Certified robustness to adversarial examples with differential privacy. In *2019 IEEE Symposium on Security and Privacy (SP)*, pages 656–672. IEEE, 2019.

[34] Guang-He Lee, Yang Yuan, Shiyu Chang, and Tommi Jaakkola. Tight certificates of adversarial robustness for randomly smoothed classifiers. In *Advances in Neural Information Processing Systems*, volume 32, pages 4910–4921. Curran Associates, Inc., 2019.

[35] Kimin Lee, Changho Hwang, KyoungSoo Park, and Jinwoo Shin. Confident multiple choice learning. In Doina Precup and Yee Whye Teh, editors, *Proceedings of the 34th International Conference on Machine Learning*, volume 70 of *Proceedings of Machine Learning Research*, pages 2014–2023, International Convention Centre, Sydney, Australia, 06–11 Aug 2017. PMLR. URL http://proceedings.mlr.press/v70/lee17b.html.

[36] Kimin Lee, Honglak Lee, Kibok Lee, and Jinwoo Shin. Training confidence-calibrated classifiers for detecting out-of-distribution samples. In *International Conference on Learning Representations*, 2018. URL https://openreview.net/forum?id=ryiAv2xAZ.

[37] Saehyung Lee, Hyungyu Lee, and Sungroh Yoon. Adversarial vertex mixup: Toward better adversarially robust generalization. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 272–281, 2020.

[38] Bai Li, Changyou Chen, Wenlin Wang, and Lawrence Carin. Certified adversarial robustness with additive noise. In *Advances in Neural Information Processing Systems 32*, pages 9464–9474. Curran Associates, Inc., 2019.

[39] Linyi Li, Xiangyu Qi, Tao Xie, and Bo Li. SoK: Certified robustness for deep neural networks. *arXiv preprint arXiv:2009.04131*, 2020.

[40] Aleksander Madry, Aleksandar Makelov, Ludwig Schmidt, Dimitris Tsipras, and Adrian Vladu. Towards deep learning models resistant to adversarial attacks. In *International Conference on Learning Representations*, 2018. URL https://openreview.net/forum?id=rJzIBfZAb.

[41] Alexander Meinke and Matthias Hein. Towards neural networks that provably know when they don't know. In *International Conference on Learning Representations*, 2020. URL https://openreview.net/forum?id=ByxGkySKwH.

[42] Matthew Mirman, Timon Gehr, and Martin Vechev. Differentiable abstract interpretation for provably robust neural networks. In Jennifer Dy and Andreas Krause, editors, *Proceedings of the 35th International Conference on Machine Learning*, volume 80 of *Proceedings of Machine Learning Research*, pages 3578–3586, Stockholmsmässan, Stockholm Sweden, 10–15 Jul 2018. PMLR. URL http://proceedings.mlr.press/v80/mirman18b.html.

[43] Jeet Mohapatra, Ching-Yun Ko, Tsui-Wei Weng, Pin-Yu Chen, Sijia Liu, and Luca Daniel. Higher-order certification for randomized smoothing. In *Advances in Neural Information Processing Systems*, 2020.

[44] Seyed-Mohsen Moosavi-Dezfooli, Alhussein Fawzi, and Pascal Frossard. DeepFool: a simple and accurate method to fool deep neural networks. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, pages 2574–2582, 2016.

[45] Gabriel Pereyra, George Tucker, Jan Chorowski, Łukasz Kaiser, and Geoffrey Hinton. Regularizing neural networks by penalizing confident output distributions. *arXiv preprint arXiv:1701.06548*, 2017.

[46] Yao Qin, Nicholas Carlini, Garrison Cottrell, Ian Goodfellow, and Colin Raffel. Imperceptible, robust, and targeted adversarial examples for automatic speech recognition. In *Proceedings of the 36th International Conference on Machine Learning*, volume 97 of *Proceedings of Machine Learning Research*, pages 5231–5240, Long Beach, California, USA, 09–15 Jun 2019. PMLR. URL http://proceedings.mlr.press/v97/qin19a.html.

[47] Leslie Rice, Eric Wong, and Zico Kolter. Overfitting in adversarially robust deep learning. In Hal Daumé III and Aarti Singh, editors, *Proceedings of the 37th International Conference on Machine Learning*, volume 119 of *Proceedings of Machine Learning Research*, pages 8093–8104. PMLR, 13–18 Jul 2020. URL http://proceedings.mlr.press/v119/rice20a.html.

[48] Olga Russakovsky, Jia Deng, Hao Su, Jonathan Krause, Sanjeev Satheesh, Sean Ma, Zhiheng Huang, Andrej Karpathy, Aditya Khosla, Michael Bernstein, Alexander C. Berg, and Li Fei-Fei. ImageNet Large Scale Visual Recognition Challenge. *International Journal of Computer Vision*, 115(3):211–252, 2015. doi: 10.1007/s11263-015-0816-y.

[49] Hadi Salman, Jerry Li, Ilya Razenshteyn, Pengchuan Zhang, Huan Zhang, Sebastien Bubeck, and Greg Yang. Provably robust deep learning via adversarially trained smoothed classifiers. In *Advances in Neural Information Processing Systems 32*, pages 11289–11300. Curran Associates, Inc., 2019.

[50] Shibani Santurkar, Andrew Ilyas, Dimitris Tsipras, Logan Engstrom, Brandon Tran, and Aleksander Madry. Image synthesis with a single (robust) classifier. In *Advances in Neural Information Processing Systems*, volume 32, pages 1262–1273. Curran Associates, Inc., 2019. URL https://proceedings.neurips.cc/paper/2019/file/6f2268bd1d3d3ebaabb04d6b5d099425-Paper.pdf.

[51] Ludwig Schmidt, Shibani Santurkar, Dimitris Tsipras, Kunal Talwar, and Aleksander Madry. Adversarially robust generalization requires more data. In *Advances in Neural Information Processing Systems*, 2018.

[52] David Stutz, Matthias Hein, and Bernt Schiele. Confidence-calibrated adversarial training: Generalizing to unseen attacks. In Hal Daumé III and Aarti Singh, editors, *Proceedings of the 37th International Conference on Machine Learning*, volume 119 of *Proceedings of Machine Learning Research*, pages 9155–9166. PMLR, 13–18 Jul 2020. URL http://proceedings.mlr.press/v119/stutz20a.html.

[53] Christian Szegedy, Wojciech Zaremba, Ilya Sutskever, Joan Bruna, Dumitru Erhan, Ian Goodfellow, and Rob Fergus. Intriguing properties of neural networks. In *International Conference on Learning Representations*, 2014.

[54] Jihoon Tack, Sangwoo Mo, Jongheon Jeong, and Jinwoo Shin. CSI: Novelty detection via contrastive learning on distributionally shifted instances. In H. Larochelle, M. Ranzato, R. Hadsell, M. F. Balcan, and H. Lin, editors, *Advances in Neural Information Processing Systems*, volume 33, pages 11839–11852. Curran Associates, Inc., 2020. URL https://proceedings.neurips.cc/paper/2020/file/8965f76632d7672e7d3cf29c87ecaa0c-Paper.pdf.

[55] Florian Tramer, Nicholas Carlini, Wieland Brendel, and Aleksander Madry. On adaptive attacks to adversarial example defenses. In *Advances in Neural Information Processing Systems*, volume 33, 2020.

[56] Dimitris Tsipras, Shibani Santurkar, Logan Engstrom, Alexander Turner, and Aleksander Madry. Robustness may be at odds with accuracy. In *International Conference on Learning Representations*, 2019. URL https://openreview.net/forum?id=SyxAb30cY7.

[57] Vikas Verma, Alex Lamb, Christopher Beckham, Amir Najafi, Ioannis Mitliagkas, David Lopez-Paz, and Yoshua Bengio. Manifold mixup: Better representations by interpolating hidden states. In Kamalika Chaudhuri and Ruslan Salakhutdinov, editors, *Proceedings of the*

36th International Conference on Machine Learning, volume 97 of *Proceedings of Machine Learning Research*, pages 6438–6447. PMLR, 09–15 Jun 2019. URL http://proceedings.mlr.press/v97/verma19a.html.

[58] Lei Wang, Runtian Zhai, Di He, Liwei Wang, and Li Jian. Pretrain-to-finetune adversarial training via sample-wise randomized smoothing, 2021. URL https://openreview.net/forum?id=Te1aZ2myPIu.

[59] Eric Wong and Zico Kolter. Provable defenses against adversarial examples via the convex outer adversarial polytope. In Jennifer Dy and Andreas Krause, editors, *Proceedings of the 35th International Conference on Machine Learning*, volume 80 of *Proceedings of Machine Learning Research*, pages 5286–5295, Stockholmsmässan, Stockholm Sweden, 10–15 Jul 2018. PMLR. URL http://proceedings.mlr.press/v80/wong18a.html.

[60] Chaowei Xiao, Jun-Yan Zhu, Bo Li, Warren He, Mingyan Liu, and Dawn Song. Spatially transformed adversarial examples. In *International Conference on Learning Representations*, 2018. URL https://openreview.net/forum?id=HyydRMZC-.

[61] Kai Y. Xiao, Vincent Tjeng, Nur Muhammad (Mahi) Shafiullah, and Aleksander Madry. Training for faster adversarial robustness verification via inducing ReLU stability. In *International Conference on Learning Representations*, 2019. URL https://openreview.net/forum?id=BJfIVjAcKm.

[62] Greg Yang, Tony Duan, J. Edward Hu, Hadi Salman, Ilya Razenshteyn, and Jerry Li. Randomized smoothing of all shapes and sizes. In Hal Daumé III and Aarti Singh, editors, *Proceedings of the 37th International Conference on Machine Learning*, volume 119 of *Proceedings of Machine Learning Research*, pages 10693–10705. PMLR, 13–18 Jul 2020. URL http://proceedings.mlr.press/v119/yang20c.html.

[63] Sangdoo Yun, Dongyoon Han, Seong Joon Oh, Sanghyuk Chun, Junsuk Choe, and Youngjoon Yoo. CutMix: Regularization strategy to train strong classifiers with localizable features. In *Proceedings of the IEEE/CVF International Conference on Computer Vision*, pages 6023–6032, 2019.

[64] Ekim Yurtsever, Jacob Lambert, Alexander Carballo, and Kazuya Takeda. A survey of autonomous driving: Common practices and emerging technologies. *IEEE Access*, 8:58443–58469, 2020.

[65] Runtian Zhai, Chen Dan, Di He, Huan Zhang, Boqing Gong, Pradeep Ravikumar, Cho-Jui Hsieh, and Liwei Wang. MACER: Attack-free and scalable robust training via maximizing certified radius. In *International Conference on Learning Representations*, 2020. URL https://openreview.net/forum?id=rJx1Na4Fwr.

[66] Hongyang Zhang, Yaodong Yu, Jiantao Jiao, Eric Xing, Laurent El Ghaoui, and Michael Jordan. Theoretically principled trade-off between robustness and accuracy. In *Proceedings of the 36th International Conference on Machine Learning*, volume 97 of *Proceedings of Machine Learning Research*, pages 7472–7482, Long Beach, California, USA, 09–15 Jun 2019. PMLR. URL http://proceedings.mlr.press/v97/zhang19p.html.

[67] Hongyi Zhang, Moustapha Cisse, Yann N. Dauphin, and David Lopez-Paz. mixup: Beyond empirical risk minimization. In *International Conference on Learning Representations*, 2018. URL https://openreview.net/forum?id=r1Ddp1-Rb.

[68] Huan Zhang, Hongge Chen, Chaowei Xiao, Sven Gowal, Robert Stanforth, Bo Li, Duane Boning, and Cho-Jui Hsieh. Towards stable and efficient training of verifiably robust neural networks. In *International Conference on Learning Representations*, 2020. URL https://openreview.net/forum?id=Skxuk1rFwB.

[69] Jingfeng Zhang, Xilie Xu, Bo Han, Gang Niu, Lizhen Cui, Masashi Sugiyama, and Mohan Kankanhalli. Attacks which do not kill training make adversarial learning stronger. In *Proceedings of the 37th International Conference on Machine Learning*, volume 119 of *Proceedings of Machine Learning Research*, pages 11278–11287. PMLR, 13–18 Jul 2020. URL http://proceedings.mlr.press/v119/zhang20z.html.

[70] Linjun Zhang, Zhun Deng, Kenji Kawaguchi, Amirata Ghorbani, and James Zou. How does mixup help with robustness and generalization? In *International Conference on Learning Representations*, 2021. URL https://openreview.net/forum?id=8yKEo06dKNo.

Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes] See Section 5.
   (c) Did you discuss any potential negative societal impacts of your work? [Yes] See Section 5.
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [Yes] See Appendix H.
   (b) Did you include complete proofs of all theoretical results? [Yes] See Appendix H.
3. If you ran experiments...
   (a) Did you include the code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL)? [Yes]
   (b) Did you specify all the training details (e.g., data splits, hyperparameters, how they were chosen)? [Yes] See Section 4 and Appendix B.
   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes] See Appendix F.
   (d) Did you include the total amount of compute and the type of resources used (e.g., type of GPUs, internal cluster, or cloud provider)? [Yes] See Appendix B.
4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets...
   (a) If your work uses existing assets, did you cite the creators? [Yes]
   (b) Did you mention the license of the assets? [N/A]
   (c) Did you include any new assets either in the supplemental material or as a URL? [N/A]
   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [N/A]
   (e) Did you discuss whether the data you are using/curating contains personally identifiable information or offensive content? [N/A]
5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
   (b) Did you describe any potential participant risks, with links to Institutional Review Board (IRB) approvals, if applicable? [N/A]
   (c) Did you include the estimated hourly wage paid to participants and the total amount spent on participant compensation? [N/A]