Towards Bridging the gap between Empirical and Certified Robustness against Adversarial Examples

Abstract

The current state-of-the-art defense methods against adversarial examples typically focus on improving either empirical or certified robustness. Among them, adversarially trained (AT) models produce empirical state-of-the-art defense against adversarial examples without providing any robustness guarantees for large classifiers or higher-dimensional inputs. In contrast, existing randomized smoothing based models achieve state-of-the-art certified robustness while significantly degrading the empirical robustness against adversarial examples. In this paper, we propose a novel method, called *Certification through Adaptation*, that transforms an AT model into a randomized smoothing classifier during inference to provide certified robustness for ℓ_2 norm without affecting their empirical robustness against adversarial attacks. We also propose *Auto-Noise* technique that efficiently approximates the appropriate noise levels to flexibly certify the test examples using randomized smoothing technique. Our proposed *Certification through Adaptation* with *Auto-Noise* technique achieves an *average certified radius (ACR) scores* up to 1.102 and 1.148 respectively for CIFAR-10 and ImageNet datasets using AT models without affecting their empirical robustness or benign accuracy. Therefore, our paper is a step towards bridging the gap between the empirical and certified robustness against adversarial examples by achieving both using the same classifier.

1 Introduction

Deep neural network (DNN) based models are found to be brittle to minor, adversarially-chosen perturbations for their inputs that remain undetectable to human eyes. A DNN classifier that correctly classifies a clean image x, can be easily fooled by choosing such *adversarial attacks* to misclassify $x + \delta$ (Szegedy et al., 2014; Goodfellow et al., 2015; Madry et al., 2018). Here, δ is a minor *adversarial perturbation* such that the change between x and $x + \delta$ remains imperceptible.

Among the existing successful defense models, *adversarial training* (AT) produces the best empirical robustness against the known adversarial attacks, however, without providing any guarantee Madry et al. (2018); Tramèr & Boneh (2019); Zhang et al. (2019); Rice et al. (2020); Gowal et al. (2020). It trains a DNN classifier using strong adversaries from a specific class of perturbation (e.g., a small ℓ_p-norm) to provide robustness for the same perturbation types. Several certification techniques are proposed that can be applied to adversarially trained models to certifiably verify if the prediction of a test example, x remains constant within its neighborhood Wong & Kolter (2018); Wang et al. (2018); Salman et al. (2019b); Dvijotham et al. (2018); Gehr et al. (2018); Sheikholeslami et al. (2021). However, these certification techniques typically do not scale for larger networks (e.g., ResNet50) and datasets (e.g., ImageNet). Hence, we cannot guarantee for large networks or data-sets that a powerful, not yet known attack would not break these defenses. In fact, several recently proposed empirical defense models are later broken by stronger *adaptive* adversarial attacks, indicating the importance of investigating certified defenses with suitable robustness guarantees Carlini & Wagner (2017); Athalye et al. (2018). In contrast to these models, the *randomized smoothing* based models can provide scalable ℓ_2-certification framework for any classification model, which is robust against large isotropic Gaussian noise (Cohen et al., 2019; Salman et al., 2019a). However, the existing randomized smoothing-based models significantly degrade the empirical robustness compared to the

CIFAR-10 models with the best hyper-parameters for ℓ_2 certifications													
ℓ_2 Radius	0.0	0.25	0.5	0.75	1.0	1.25	1.5	1.75	2.0	2.25	2.5	2.75	3.0	ACR
Baseline	10.49	6.96	2.04	0.09	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.035
Baseline + Auto-Noise	33.57	18.56	10.25	4.44	0.83	0.07	0.01	0.0	0.0	0.0	0.0	0.0	0.0	0.124
Baseline + Adaptation + Auto-Noise	59.64	21.66	7.81	3.97	1.28	0.36	0.07	0.0	0.0	0.0	0.0	0.0	0.0	0.154
$\text{Rand}_{\sigma=0.5}$ (Cohen et al., 2019)	62.13	51.68	40.38	30.25	20.81	13.36	7.71	3.38	0.0	0.0	0.0	0.0	0.0	0.494
$\text{Rand}_{\sigma=0.5}$ + Auto-Noise	**79.48**	71.75	**60.23**	48.72	35.97	25.16	15.09	10.13	6.98	5.58	4.18	2.94	1.76	0.821
$\text{Rand}_{\sigma=0.5}$ + Adaptation + Auto-Noise	78.27	69.51	57.16	44.73	31.19	19.27	10.4	4.25	1.65	0.57	0.14	0.01	0.0	0.695
$\text{SmoothAdv}_{\sigma=0.5}$ (Salman et al., 2019a)	57.59	52.82	47.67	42.68	37.55	32.64	27.52	22.42	0.0	0.0	0.0	0.0	0.0	0.733
$\text{SmoothAdv}_{\sigma=0.5}$ + Auto-Noise	61.27	57.27	52.52	48.17	**43.49**	38.02	33.15	27.47	21.86	15.81	9.5	4.97	2.01	0.965
$\text{SmoothAdv}_{\sigma=0.5}$ + Adaptation + Auto-Noise	61.23	56.9	51.33	46.44	41.05	35.65	30.11	24.35	18.48	12.8	7.76	4.27	2.3	0.908
Adv_∞ (Rice et al., 2020)	13.82	12.22	10.48	9.12	7.69	6.32	5.1	3.79	0.0	0.0	0.0	0.0	0.0	0.154
Adv_∞ + Auto-Noise	69.46	63.12	35.73	30.63	17.54	14.78	10.27	9.16	8.01	7.2	6.21	5.31	3.78	0.649
Adv_∞ + Adaptation + Auto-Noise	70.75	64.54	50.63	43.38	32.5	24.43	18.05	12.2	8.31	5.37	3.36	1.96	1.23	0.76
Adv_2 (Rice et al., 2020)	30.37	26.98	23.98	21.35	18.4	15.94	13.52	10.63	0.0	0.0	0.0	0.0	0.0	0.367
Adv_2 + Auto-Noise	64.45	60.57	45.73	41.06	28.48	22.92	15.1	10.77	7.23	4.8	2.77	1.67	1.1	0.702
Adv_2 + Adaptation + Auto-Noise	61.96	58.58	53.64	**49.67**	42.76	**38.69**	**34.54**	**30.36**	**24.65**	**20.77**	**17.09**	**13.66**	**9.18**	**1.102**
$\text{Marcer}_{\sigma=0.5}$ (Zhai et al., 2020)	64.2	57.5	49.9	42.3	34.8	27.6	20.2	12.6	0.0	0.0	0.0	0.0	0.0	0.691
$\text{Consistency}_{\sigma=0.5}$ (Jeong & Shin, 2020)	52.3	48.9	45.1	41.3	37.8	33.9	29.9	25.2	0.0	0.0	0.0	0.0	0.0	0.726
$\text{Boosting}_{\sigma=0.5}$ (Horváth et al., 2022)	65.0	59.0	49.4	44.8	38.6	32.0	26.2	19.8	0.0	0.0	0.0	0.0	0.0	0.756

Table 1: CIFAR-10: Certified accuracy at different ℓ_2 radii and ACR scores using the best hyper-parameters. Existing randomized-smoothing based models are trained and certified using noise-level, $\sigma = 0.5$. We also present the best reported results for Marcer and Consistency at (Jeong & Shin, 2020) and for Boosting at (Horváth et al., 2022) for our comparisons. For detailed results and hyper-parameters for both ImageNet and CIFAR-10 datasets, please refer to Table 3 and 4 respectively in Appendix.

state-of-the-art AT models. In summary, a high empirical robustness along with certification guarantees are necessary to improve the reliability of a DNN model for sensitive real-world applications. However, to the best of our knowledge, none of the existing techniques provide both high performance for both empirical robustness with such certified guarantees using the same DNN classifier. Towards this, we aim to bridge this gap by providing robustness certification for AT models without degrading their state-of-the-art empirical robustness against adversarial examples.

In this paper, we propose a novel *certification through adaptation* framework that transforms an AT model into a randomized smoothing framework during inference to provide non-trivial ℓ_2 certification without any additional training or architecture modifications. Our proposed certification technique consists of two steps: We first adapt the AT model using popular batch normalization adaptation technique using appropriate levels of Gaussian noises separately for each test example (Cariucci et al., 2017; Li et al., 2016). This process significantly boosts the performance of the AT models against the random isotropic Gaussian noises. Hence, we can now directly apply the *randomized smoothing* based certification technique to provide ℓ_2 certification in the next step. However, choosing the Gaussian noise for each test example is a challenging task. The existing randomized smoothing based models that use Gaussian noises for training, use the same noise levels to certify each test example, significantly compromising their certification performance. Towards this, we also propose an *Auto-Noise* technique to efficiently approximate the appropriate Gaussian noise levels for correctly certifying each test example during inference.

In the following, we summarize the list of contributions for our paper:

1. We propose a novel *certification through adaptation* framework that adapts an AT model using Gaussian noises to provide non-trivial robustness certifications at large ℓ_2 radii. Our proposed technique only requires a set of *clean images*, obtained from training/validation or test set to adapt the AT models using popular BN-adaptation technique (Cariucci et al., 2017; Li et al., 2016).

2. We also propose *Auto-Noise technique* to efficiently approximate the appropriate Gaussian noise levels for certifying each test example during inference. Auto-Noise is applicable even for existing randomized smoothing based models and often significantly improves the certification performance. Our *Certification through Adaptation* together with *Auto-Noise* technique produces *average certified radius (ACR) scores* upto 1.102 and 1.148 for CIFAR-10 and ImageNet for AT models, achieving the state-of-the-art performance for CIFAR-10. Notably, our proposed method is applied during inference, without affecting the empirical robustness or benign accuracy of AT models to produce these non-trivial ℓ_2 certification results.

3. Our results also suggests a stronger correlation between empirical and certified robustness that empirically stronger AT models also produce better ℓ_2 certification performance.

2 Related Work

2.1 Adversarial Robustness for DNN models

Empirical Defenses and Adversarial Training. Defense models against adversarial examples can be broadly categorized as: *empirical* and *certified* defenses. Empirical defenses demonstrate empirical robustness against adversarial attacks, typically without out providing any certification guarantees (Schott et al., 2019; Moosavi Dezfooli et al., 2019; Nandy et al., 2020; Mao et al., 2021). *Adversarial training* achieves the state-of-the-art empirical defense (Madry et al., 2018). It optimizes the following loss function for a DNN classifier, f, to provide robustness within an ϵ-bounded *threat model* for an ℓ_p norm, where the perturbations, $\delta \in \Delta$ are constrained as $\Delta = \{\delta : ||\delta||_p \leq \epsilon\}$:

$$\min_{\theta} \mathbb{E}_{(x,y)}[\max_{\delta \in \Delta} \mathcal{L}(f_\theta(x + \delta), y)] \tag{1}$$

where, θ denotes the model parameters. $\mathcal{L}$ is the classification loss.

The *inner maximization* in Eq. 1 is solved by producing adversarial examples using strong iterative adversaries, e.g., *projected gradient descent (PGD)* attack (Kurakin et al., 2016; Madry et al., 2018). Wong et al. (2020) found that even a single-step *fast gradient sign method (FGSM)* attack-based AT models also achieves high empirical robustness (Goodfellow et al., 2015). Zhang et al. (2020) proposed to use the least adversaries for training. Recently TRADES (Zhang et al., 2019), Adv-LLR (Qin et al., 2019) introduced additional regularizers to achieve higher empirical robustness by smoothing the loss surface. Rice et al. (2020) showed that even the standard PGD based AT model with early-stopping criteria provides one of the best empirical defenses for a given perturbation type. Recent works also explored the importance of different hyper-parameters for adversarial training (Gowal et al., 2020; Pang et al., 2021) as well as incorporating additional data in a semi-supervised fashion (Carmon et al., 2019; Uesato et al., 2019) to further improve their empirical robustness against adversarial attacks. Recently, Kireev et al. (2021) also demonstrated that adversarial training with smaller perturbation can also improve the performance against random corruptions.

Certified Defenses. Empirical defenses demonstrate robustness only against the *known* adversaries without providing any guarantees. In fact, most empirical defenses proposed in the literature were later *broken* by stronger adversaries, highlighting the importance of certified defenses to provide robustness guarantees (Athalye et al., 2018; Uesato et al., 2018; Jalal et al., 2019).

Several recent works proposed to train neural network models with provable robustness guarantees. These works include methods based on semidefinite relaxations (Raghunathan et al., 2018), linear relaxations and duality (Wong & Kolter, 2018; Wong et al., 2018), abstract interpretation (Mirman et al., 2018), and interval bound propagation (Gowal et al., 2018). Parallel to training a certified defense, several works also focus on certifying the already trained models (Tjeng et al., 2017; Gehr et al., 2018; Weng et al., 2018; Wang et al., 2018; Bunel et al., 2018). Recently Mueller et al. (2021) combined a *small* certification network with a *large*, empirically robust AT model using some selection criteria to boost overall benign accuracy along with empirical robustness for the certified framework. However, most of these techniques do not scale well for large DNN classifiers (e.g., ResNet50) or higher-dimensional datasets (e.g., ImageNet).

Randomized Smoothing is a promising certification technique that can be scaled to larger networks and higher-dimensional datasets. It was initially proposed as a heuristic defense (Cao & Gong, 2017; Liu et al., 2018) and later shown to be certifiable (Lecuyer et al., 2019; Li et al., 2019). Recently, Cohen et al. (2019) and Salman et al. (2019a) separately provided strong robustness guarantees for ℓ_2-norm. A randomized smoothing based certification model requires their base-classifier to be robust against large Gaussian perturbations to produce non-trivial results. Cohen et al. (2019) proposed to train their base-classifier by incorporating random Gaussian noises. Several recent works focused on improving the base classifiers to achieve better certification performance by adversarially choosing the noise (Salman et al., 2019a), incorporating additional regularizers (Zhai et al., 2020; Jeong & Shin, 2020), by ensembling multiple base-models (Horváth et al.,

2022) etc. Several works also investigated on improving certification guarantees using different smoothing measures (Li et al., 2019; Lee et al., 2019; Yang et al., 2020) or divergences (Dvijotham et al., 2020). Salman et al. (2020) also demonstrated that we can achieve non-trivial certified robustness even for a standard DNN classifier by incorporating an additional denoising module as a pre-processing unit. Notably, randomized smoothing is the only scalable certification framework and also provides superior performance for different perturbation types (Dvijotham et al., 2020).

However, while achieving the state-of-the-art certification performance, randomized smoothing significantly degrades the empirical robustness against adversarial attacks compared to the state-of-the-art AT models (Lecuyer et al., 2019; Salman et al., 2019a; Cohen et al., 2019). Towards this, our proposed technique transforms an AT model into a randomized smoothing classifier without requiring additional training or architectural modification. Since AT models already provide the state-of-the-art empirical defense, we achieve both empirical and certified robustness against adversarial examples using the same classifier.

Batch-normalization and Robustness. Several recent papers investigate the effects of batch-normalization layers for different aspects of robustness. Many of these works focused on improving robustness against random corruptions by adapting batch-normalization using a sufficiently large set of test images from the same covariate shift (Schneider et al., 2020; Nado et al., 2020; Benz et al., 2021a). By hypothesizing that clean and adversarial examples belongs to different domains, several recent works proposed to apply different branches of BN to separately capture their distributions (Xie et al., 2020a; Xie & Yuille, 2020; Jiang et al., 2020; Wang et al., 2020b; 2021). Benz et al. (2021b) presents empirical evidence to argue that BN shifts a model towards being more dependent on non-robust features (NRFs). Unlike these previous works, we proposed to adapt BN layers using appropriate Gaussian noise levels to provide ℓ_2 certified robustness for AT models.

2.2 Test-time Adaptation & applications

Test-time adaptation techniques have been widely explored before in the field of domain adaptation (Sun et al., 2017; Roy et al., 2019; Huang et al., 2018; Li et al., 2016) and covariate-shift adaptation (Sun et al., 2020; French et al., 2017; Xie et al., 2020b; Wang et al., 2020a; Schneider et al., 2020; Nado et al., 2020; Benz et al., 2021a). However, to the best of our knowledge, such techniques are never applied for adversarial robustness and certification. Our paper mainly focuses on one of the most popular and effective mechanisms, called *adaptive batch-normalization*.

A batch-normalization (BN) layer computes the mean and variance of the hidden activation maps across the channels to normalize these activations to $\mathcal{N}(0,1)$ before feeding into the next hidden layer (Ioffe & Szegedy, 2015). This process reduces the dependencies among different hidden layers, improving the training efficiency for deep architectures. However, the distributional shifts in the test examples lead to different activation statistics compared to the training examples. Hence, the statistics estimated during training fail to correctly normalize the activation tensors to $\mathcal{N}(0,1)$. Consequently, it breaks the crucial assumption for the subsequent hidden layers to work. Adaptive BN technique computes the BN statistics from the feature activations, μ_t, s_t^2, of the test batch. We can adapt them with the existing *training* statistics, μ_T, s_T^2, learned using the training batches as (Cariucci et al., 2017; Li et al., 2016; Schneider et al., 2020):

$$\overline{\mu} = \rho \cdot \mu_t + (1-\rho) \cdot \mu_T \quad \overline{s} = \rho \cdot s_t + (1-\rho) \cdot s_T \tag{2}$$

where, $\rho \in [0,1]$ is the momentum. The choice of $\rho = 0$ is equivalent to the standard inference setup with a deterministic DNN classifier in the IID settings. We should choose $\rho = 1$ when receiving larger test batches as it can provide a better estimation of the test distributions.

Assumptions and Limitations. The existing BN-adaptation techniques typically require a *large set of test images* from the same "unknown" test distributions. However, this assumption may not hold for several real-world applications, e.g., stateless web APIs. Also, these test images should be *semantically diverse*, preferably over multiple classes, to effectively estimate the test distributions. Hence, it further limits the practical usability of these frameworks for real-world applications, e.g., autonomous cars.

Unlike these models for domain adaptation and corruption robustness, our proposed certification framework does not make any such assumptions. As we shall see that we can appropriately approximate the required Gaussian noise level for adaptation to certify a test image. Therefore, we can pre-select a diverse set of clean images, $\mathbf{X}_{clean}$ and inject the random Gaussian noises to appropriately adapt the models as required, addressing both of these limitations.

3 Proposed Methodology

In this section, we first present the background of the randomized smoothing technique and explain why it is not directly applicable to AT models. Next, we present our proposed *certification through adaptation* framework that adapts a DNN model during inference to provide certified robustness without additional training or architectural modifications.

3.1 Background on Randomized Smoothing

Consider a classification model, f, that maps inputs in $\mathbb{R}^d$ to $\mathcal{Y}$ classes. The randomized smoothing framework transforms the original base classifier, f into a new, smoothed classifier g Cohen et al. (2019). In particular, for an input $x \in \mathbb{R}^d$, the smoothed classifier g returns the most probable class to be predicted by the base classifier f under isotropic Gaussian noises of x. That is,

$$g(x) = arg \max_{y \in \mathcal{Y}} \mathbb{P}(f(x + \delta) == y) \quad \text{s.t.} \quad \delta \sim \mathcal{N}(0, \sigma^2 I). \tag{3}$$

where, $\sigma^2 I$ is the covariance matrix and σ denotes the noise level for certifying x. σ controls the trade-off between robustness at different ℓ_2 radii: Increasing σ improves the robustness of g at higher ℓ_2 radii. However, it degrades the robustness at smaller ℓ_2 radii.

Cohen et al. (2019) presented a tight robustness guarantee using Neyman-Pearson lemma for the smoothed classifier, g and provided an efficient algorithm using Monte Carlo sampling for certification. We can also obtain the same guarantee by explicitly computing the Lipschitz constant of the smoothed classifier as shown in (Salman et al., 2019a; Yang et al., 2020). The certification procedure is as follows: Suppose a base classifier f classifies $\mathcal{N}(x, \sigma^2 I)$ to return the *"most probable"* class, c_A with probability $p_A = \mathbb{P}(f(x + \delta) == c_A)$ and the *"runner-up"* class c_B with probability $p_B = \max_{y \neq c_A} \mathbb{P}(f(x + \delta) == y)$. Then, the smooth classifier, g is certifiably robust around x within an ℓ_2 radius of R, as follows:

$$R = \frac{\sigma}{2} \Big(\Phi^{-1}(p_A) - \Phi^{-1}(p_B) \Big) \tag{4}$$

where, Φ^{-1} denotes the inverse of the standard Gaussian CDF.

However, computing the exact values for p_A and p_B is impossible in practice when f is a DNN. Cohen et al. (2019) addressed this problem using Monte Carlo sampling to estimate $\underline{p_A}$ and $\overline{p_B}$ such that $\underline{p_A} \leq p_A$ and $\overline{p_B} \geq p_B$ with arbitrarily high probability. The certified radius for input x is then computed by replacing p_A and p_B with $\underline{p_A}$ and $\overline{p_B}$ respectively in Eq. 4.

As we can see in Equation 3 that the base classifier, f needs to be robust against large Gaussian noises to produce non-trivial robustness certification results. Otherwise, it leads to lower p_A and hence a lower certification of R for the test examples. Existing randomized smoothing-based models applies custom-trained using explicit Gaussian noises to learn their original base classifier (Lecuyer et al., 2019; Cohen et al., 2019; Salman et al., 2019a; Zhai et al., 2020; Jeong & Shin, 2020). However, these models produce significantly lower empirical robustness compared to the AT models (Madry et al., 2018; Zhang et al., 2019; Rice et al., 2020; Gowal et al., 2020). In contrast, AT models are not robust against large Gaussian noises in the standard inference settings (Gilmer et al., 2019). In our paper, we bridge this gap between these two research directions by certifying the AT models through adaptation, as described in the following.

Algorithm 1: CERTIFICATION-THROUGH-ADAPTATION

Input: f: classifier, x_{test}: test example, σ: desired noise-level, $\mathbf{X}_{clean}$: batch of clean images sampled from train/validation data or test stream, N: No. of noisy samples for Monte-Carlo estimation (Eq. 4)

Output: Certifiably robust ℓ_2 radius of R for x_{test}.

/* Step 1: Adapt BN parameters using $\mathbf{X}_{clean}$ with $\rho = 1$ (Eqn 2). */

1 $\tilde{\mathbf{X}}_{clean} = [x + \mathcal{N}(0, \sigma I) \ \forall \ x \ \in \ \mathbf{X}_{clean}]$ // perturb $\mathbf{X}_{clean}$ with random noise.

2 $f_{adapt} = \text{CLONE}(f.train())$ // clone f with *train-mode*.

3 $f_{adapt}(\tilde{\mathbf{X}}_{clean})$ // forward pass for BN parameter adaptation.

4 $f_{adapt}.eval()$ // fix the parameters.

/* Step 2: Certify x_{test} using Randomized Smoothing framework. */

5 $g = \text{GETRANDOMIZEDMODEL}(f_{adapt})$ // Convert f_{adapt} to randomized-smoothing classifier g (Eqn 3).

6 $R = \text{CERTIFY}(g, x_{test}; \sigma, N)$ // Execute 4 for ℓ_2 certification.

7 return R // Return ℓ_2 certification for x_{test}.

3.2 Proposed Certification through Adaptation

Our proposed *certification through adaptation* framework consists of two steps: Given a test image x_{test}, we first adapt the original classification model, f using adaptive BN technique with an appropriate/ pre-selected level of Gaussian noise, σ to obtain the base classifier, f_{adapt} for certification using randomized smoothing. Next, we freeze the model parameters and use the fixed adapted model, f_{adapt}, as our base classifier to certify the test example, x_{test} using randomized smoothing technique (Equation 4). The proposed *certification through adaptation* method is presented in Algorithm 1.

Training versus Test images for model adaptation. Recall that adaptive BN requires a large set of diverse test images to correctly re-estimate the BN layer statistics. However, to provide certification for ℓ_2-norm, we only need to adapt our model against Gaussian perturbations. Hence, unlike existing test-time adaptation-based models for covariate shift or domain adaptation problems, we can pre-select a sufficiently large and diverse set of clean images, $\mathbf{X}_{clean}$. We apply the selected level of Gaussian noise, σ to obtain the base classifier, f_{adapt} for certifying test examples, x_{test}. Notably, we can sample $\mathbf{X}_{clean}$ from training/validation or test sets. Since the underlying distribution of these clean images remains the same, it does not affect the certification performance. In Figure 1, we compare the performance as we randomly sample $\mathbf{X}_{clean}$ from training vs. test sets for CIFAR-10. We can see that the certification performance of AT models remains almost the same in both cases. The slight differences in their performances typically arise due to the underlying randomization of the set, $\mathbf{X}_{clean}$ and added Gaussian noise to estimate the BN parameters.

Figure 1: Certification performance on CIFAR-10 as we apply training data vs test data for adaptation in Algorithm 1. $\text{Adv}_\infty[8/255]$ and $\text{Adv}_2[1.0]$ respectively denote AT models, trained at $\ell_\infty \leq 8/255$ and $\ell_2 \leq 1.0$ threat-boundaries.

Effect on empirical robustness and benign (clean) accuracy. The main advantage of our proposed framework is that we can provide certification for AT models without affecting their state-of-the-art empirical robustness and benign accuracy. Given a test example, we first obtain the predicted class label from the original classifier, f (i.e., without making any change). Next, we adapt the model to f_{adapt} using appropriate σ to certify the classification prediction using proposed Algorithm 1. Hence, we maintain the same empirical robustness and benign accuracy as reported in the existing papers (Rice et al., 2020; Madry et al., 2018).

Applicability. Our proposed "certification through adaptation" technique can be applied to any classification model, f with batch-normalization layers. However, achieving high accuracy against large random Gaussian perturbations is a necessary condition: a randomized smoothing classifier, g needs to *consistently* predict the correct class to provide higher certification guarantees at larger radii. Hence for standard non-robust DNN classifiers, we can only achieve higher ℓ_2 certification guarantees at very small ℓ_2 radii (see in Table 3 and Table 4). Further,we also observe that adapting the existing randomized smoothing models does not necessarily improve the overall certification performance (see Table 1 and Figure 6 in Section 4.3) In contrast, AT models with our proposed "offline" adaptation significantly improve their performance against large Gaussian perturbations, providing non-trivial certification robustness.

3.3 Proposed Auto-Noise: Appropriate Noise level for Certification

Robustness of a classification model can significantly vary at different input spaces. Hence, choosing appropriate noise-level for certifying is an important but challenging task for randomized smoothing based certification techniques. While choosing a lower noise level produces significantly lower-estimates of certified radii, over-estimation of noise may fail to provide any certification robustness for a test example. A brute-force approach to address this problem would be to evaluate the certification results on multiple noise levels and report the maximum certified ℓ_2 radii. However, certification using randomized smoothing is an extremely time-consuming process: it requires to evaluate a large number of noisy samples (of cardinality $N = 100,000$) to estimate $\underline{p_A}$ and $\overline{p_B}$ using Monte-Carlo sampling (Eq. 4). For example, it can take upto 110 seconds to certify an ImageNet test example with ResNet-50 models on NVIDIA RTX 2080 Ti (Cohen et al., 2019). Notably, as we choose a smaller set of noisy samples to estimate $\underline{p_A}$ and $\overline{p_B}$, it provides significantly lower ℓ_2 certified radii. Hence, existing randomized smoothing based models typically use the same Gaussian noise level as applied to train their base classifiers (Cohen et al., 2019; Salman et al., 2019a; Zhai et al., 2020; Jeong & Shin, 2020). However, we demonstrate that it significantly underestimates the certification performance of the randomized smoothing framework. Here, we present a simple but effective Auto-Noise technique to choose appropriate σ for a given test example, x_{test}.

Auto-Noise technique aims to approximate the appropriate noise-level from a given set, $\boldsymbol{\sigma} = \{\sigma_1, \sigma_2, \cdots\}$. The key idea of our proposed Auto-Noise method is as follows: *Although a small set of noisy examples underestimates the ℓ_2 certified noise levels, it can provide a fair comparison of different noise levels for certifying x_{test}.* We propose to use a small set of N_{auto} noisy examples, N_{auto} to approximately obtain the ℓ_2 certification radii for different noise levels, $\sigma \in \boldsymbol{\sigma}$. We select the noise level σ_{auto} that produces the maximum ℓ_2 radius using N_{auto} noisy examples, i.e.:

$$\sigma_{auto} = arg \max_{\sigma \in \boldsymbol{\sigma}} \quad \text{CERTIFY}(g, x_{test}; \sigma, N_{auto}) \tag{5}$$

where, g denotes the randomized-smoothing classifier obtained using the base classifier, f (Eq. 3). For AT models, we should adapt the models, f_{adapt} with noise level σ as the base classifier.

Finally, we use σ_{auto} for certifying x_{test} with a large number of noisy samples, $N = 100,000$.

Computational Overhead. In practice, the ideal choices of noise levels as $\boldsymbol{\sigma}$ remains reasonably small. For example, in our experiments, we select $\boldsymbol{\sigma} = \{0.12, 0.25, 0.37, 0.50, 0.67, 0.75, 0.87, 1.0\}$, i.e. of cardinality=8 and set $N_{auto} = 1,000$. Hence, we require an additional $8,000$ iterations to obtain the appropriate σ for each test-examples, along with $100,000$ iterations to get the final certification. In other words, with very little computational overhead, we can approximate the appropriate noise levels for each test example.

Note that our Auto-Noise algorithm using a small set, $N_{auto} = 1,000$ may not provide reliable estimation of the most appropriate noise-level, σ. However, as shown in Table 1, it significantly improves the certification performance for both AT models and the existing randomized smoothing based models, compared to the fixed choices of σ (Cohen et al., 2019; Li et al., 2019). Furthermore, by using certification through adaptation along with Auto-Noise method, we can produce state-of-the-art certification performance for AT models, trained using ℓ_2 bounded adversarial examples.

4 Experimental Results

Setup.   We use CIFAR-10 (Krizhevsky et al., 2009) and ImageNet (Deng et al., 2009) datasets for our experiments. For CIFAR-10, we use pre-activation ResNet18 and for ImageNet, we use ResNet50 (He et al., 2016a;b). For our experiments, we train the AT models using the *early stopping* criteria (Rice et al., 2020). For ImageNet, we use two AT models, $\mathrm{Adv}_\infty[4/255]$ and $\mathrm{Adv}_2[3]$, learned at ℓ_∞ and ℓ_2 threat models with threat boundaries of 4/255 and 3 respectively. For CIFAR-10, we train multiple AT models with different threat boundaries. We denote them by incorporating their corresponding threat boundaries, applied for training. For example, we denote an AT model, trained with threat boundary of 8/255 as $\mathrm{Adv}_\infty[8/255]$.

For our comparisons, we use the standard DNN Baseline and $\mathrm{Rand}_{\sigma=0.5}$ models. Baseline models are trained using clean images. $\mathrm{Rand}_{\sigma=0.5}$ models are trained by augmenting random noise, sampled from $\mathcal{N}(0, \sigma^2 I)$ with $\sigma = 0.5$ Cohen et al. (2019). We also compare with the current state-of-the-art certification models, SmoothAdv for CIFAR-10 (Salman et al., 2019a). Please refer to Appendix A.2 for additional details [1].

(a) ImageNet						(b) CIFAR-10				
Model	$\sigma = 0$	$\sigma = 0.25$	$\sigma = 0.5$	$\sigma = 0.75$		Model	$\sigma = 0$	$\sigma = 0.25$	$\sigma = 0.5$	$\sigma = 0.75$
Baseline	$\mathbf{75.2}_{\pm 0.0}$	$11.8_{\pm 0.22}$	$0.3_{\pm 0.01}$	$0.1_{\pm 0.0}$		Baseline	$\mathbf{95.2}_{\pm 0.0}$	$10.9_{\pm 0.88}$	$10.6_{\pm 0.76}$	$10.5_{\pm 1.19}$
+ adaptive BN	$74.4_{\pm 0.04}$	$\mathbf{31.0}_{\pm 0.27}$	$\mathbf{7.7}_{\pm 0.24}$	$\mathbf{2.4}_{\pm 0.01}$		+ adaptive BN	$95.0_{\pm 0.57}$	$\mathbf{40.1}_{\pm 0.97}$	$\mathbf{22.0}_{\pm 0.83}$	$\mathbf{17.2}_{\pm 0.66}$
$\mathrm{Adv}_\infty[4/255]$	$\mathbf{62.8}_{\pm 0.0}$	$3.9_{\pm 0.03}$	$0.4_{\pm 0.01}$	$0.2_{\pm 0.01}$		$\mathrm{Adv}_\infty[8/255]$	$\mathbf{82.1}_{\pm 0.0}$	$40.2_{\pm 4.56}$	$16.1_{\pm 7.85}$	$12.2_{\pm 5.23}$
+ adaptive BN	$60.8_{\pm 0.16}$	$\mathbf{53.4}_{\pm 0.15}$	$\mathbf{44.9}_{\pm 0.08}$	$\mathbf{33.7}_{\pm 0.28}$		+ adaptive BN	$81.6_{\pm 0.96}$	$\mathbf{74.2}_{\pm 0.95}$	$\mathbf{62.4}_{\pm 0.64}$	$\mathbf{51.0}_{\pm 1.03}$
$\mathrm{Adv}_2[3]$	$\mathbf{59.8}_{\pm 0.0}$	$9.8_{\pm 0.08}$	$0.9_{\pm 0.01}$	$0.3_{\pm 0.0}$		$\mathrm{Adv}_2[1]$	$\mathbf{81.6}_{\pm 0.0}$	$47.5_{\pm 5.1}$	$21.5_{\pm 7.79}$	$14.3_{\pm 5.63}$
+ adaptive BN	$58.3_{\pm 0.08}$	$\mathbf{53.7}_{\pm 0.14}$	$\mathbf{47.3}_{\pm 0.14}$	$\mathbf{39.8}_{\pm 0.18}$		+ adaptive BN	$81.8_{\pm 0.7}$	$\mathbf{75.8}_{\pm 0.43}$	$\mathbf{64.9}_{\pm 0.73}$	$\mathbf{53.5}_{\pm 1.71}$

Table 2: Top-1 accuracy of AT models significantly improve using adaptive BN under different levels of Gaussian noises (when $\sigma > 0$). We randomly sample the noises and report ($mean \pm 2 \times sd$) for five different runs.

4.1 Performance under Gaussian Noise.

We first investigate the performance of AT models as we significantly increase the Gaussian noises. As we note in Section 3.1, it is a necessary condition to provide non-trivial robustness certification at larger ℓ_2 radii. In Table 2, we present a comparative performance for Baseline, Adv_∞, and Adv_2 models for both ImageNet and CIFAR-10 datasets. We can see that the classification performance of all these models sharply degrades under large Gaussian noises in standard inference settings. However, we can improve these performances by adapting them under the same level of Gaussian noises using adaptive BN techniques. In particular, we observe that AT models achieve significantly higher performance gain using adaptive BN than the non-robust, Baseline models under Gaussian noise levels. For example, at $\sigma = 0.5$, Baseline, $\mathrm{Adv}_2[3]$ and $\mathrm{Adv}_\infty[4/255]$ respectively achieve top-1 accuracy of 0.3%, 0.4%, and 0.9% for ImageNet without using BN adaptation (Table 2 (a)). However, adaptive BN for $\mathrm{Adv}_2[3]$ and $\mathrm{Adv}_\infty[4/255]$ significantly improves the top-1 accuracy to 47.3% and 44.9% respectively. In contrast, the baseline model only achieves 7.7% accuracy. We also observe similar results for CIFAR-10 in Table 2 (b).

Adaptive BN for AT models correctly extracts robust features under Gaussian noises.   In Figure 2, we further investigate the performance of AT models by visualizing the *loss gradients* of individual pixels of an image as we increase the noise level , σ. *Loss-gradients* reflect the most relevant input pixels for classification predictions. Here, we scale, translate and clip the loss-gradient values without using any sophisticated techniques (as in Tsipras et al. (2019)). At $\sigma = 0$ (i.e., for clean images), the loss-gradients from AT models align properly with perceptually relevant features (as observed previously (Tsipras et al., 2019; Etmann et al., 2019)). However, as we choose higher noise using $\sigma=0.5$ and $\sigma=0.75$, the overall loss gradients become noisier. Specifically, we can see that AT models without BN adaptation produce larger gradient values (i.e., greater importance) even for background pixels. In contrast, AT models with BN adaptation using Gaussian noises allows to correctly extract perceptually relevant features from the object of interest, suppressing the gradients for background (refer to Figure 2(c) and Figure 2(d)). In other words,

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[1]For ImageNet, we obtain Adv_∞ and Adv_2 from https://github.com/locuslab/robust_overfitting and Baseline and $\mathrm{Rand}_{\sigma=0.5}$ models from https://github.com/locuslab/smoothing.

(a) $\sigma = 0$ (Clean)   (b) $\sigma = 0.25$ (c) $\sigma = 0.5$ (d) $\sigma = 0.75$

Figure 2: Visualizing loss-gradients produced by AT models as we apply different levels of Gaussian noises.

it allows us to extract the required semantic information for correct classifications. Also, it is interesting to note that Adv_2 produces significantly more human-aligned loss gradients compared to Adv_∞. This behavior is also reflected in their classification performance in Table 2 and certification robustness in Table 1. We can see that Adv_2 overall produces better performance compared to Adv_∞. These results indicate that we can achieve non-trivial certification results by appropriately adapting the AT models, as demonstrated in the following sections.

4.2 Certified Robustness for AT models

We now present the ℓ_2 certification results using the randomized smoothing framework as the backbone, as proposed in our Algorithm 1. We certify the test images with 99.9% probability. We estimate the class-label probabilities of g (Equation 4) using $100,000$ noisy samples, as in (Cohen et al., 2019; Salman et al., 2019a). We use the full test-set of $10,000$ images for CIFAR-10 and a sub-sample of 500 test images for ImageNet.

Figure 3: Certification through adaptation produces non-trivial certified robustness at various ℓ_2 radii for both **(Left)** ImageNet and **(Right)** CIFAR-10 datasets.

Non-trivial certification for AT models. In Figure 3, we first demonstrate that AT models can achieve non-trivial ℓ_2 certified robustness using our proposed certification through adaptation technique for both ImageNet and CIFAR-10 datasets. Here, we use $\text{Adv}_\infty[4/255]$ and $\text{Adv}_2[3]$ for ImageNet and $\text{Adv}_\infty[8/255]$

and $\text{Adv}_2[1]$ for CIFAR-10. We apply fixed noise levels of $\sigma = 0.5$ to certify all test examples using proposed Algorithm 1. Here, we compare with the certification results of the Baseline, Adv_∞ and Adv_2 models at $\sigma = 0.25$ in the standard settings (i.e., without adapting these models). We can see a significant boost of ℓ_2 certification results for both Adv_∞ and Adv_2 models using our proposed framework. Further, Adv_2 models consistently achieve better certification performance compared to Adv_∞. We also compare with $\text{Rand}_{\sigma=0.5}$ models at fixed $\sigma = 0.5$, as in Cohen et al. (2019). For CIFAR-10, both $\text{Adv}_\infty[8/255]$ and $\text{Adv}_2[1]$ outperform the $\text{Rand}_{\sigma=0.5}$ models (Cohen et al., 2019). Furthermore, for ImageNet, $\text{Adv}_2[3]$ achieves better certified accuracy compared to $\text{Rand}_{\sigma=0.5}$ beyond ℓ_2-radii of 1.5. Please refer to Table 3 and 4 (Appendix) for detailed comparisons of different models, trained using different specifications.

Figure 4: CIFAR-10: AT models, trained using larger threat boundaries, produces better certification results for higher ℓ_2 radii. Here, we apply our proposed certification through adaptation with fixed noise-level $\sigma = 0.5$. (c) Comparison of Adv_2 models with SmoothAdv (Salman et al., 2019a), trained and certified using $\sigma = 0.5$.

Larger Threat Boundary for Better Certification. Learning AT models at a higher threat boundary produces better certified robustness at higher ℓ_2 radii. Figure 4(a) and 4(b) demonstrate this phenomena for CIFAR-10 on both Adv_∞ and Adv_2 models respectively .

Figure 4(c) also compares the certified accuracy of Adv_2 models with the existing state-of-the-art *SmoothAdv* models (Salman et al., 2019a). SmoothAdv utilizes adversarial training using an adaptive attack with an ℓ_2 threat boundary of ϵ and Gaussian noises, $\mathcal{N}(0, \sigma^2 I)$ (See details in Appendix A.2). We set the noise to $\sigma = 0.5$ and vary ϵ for their training to compare with different SmoothAdv models in Figure 4(c). As we can see that by adapting Adv_2 models at $\sigma = 0.5$ using our proposed Algorithm 1, we can already achieve similar performance as SmoothAdv. Next, we demonstrate that our proposed *Auto-Noise* technique further improves the performance of both AT models and existing randomized smoothing based models.

Figure 5: Auto-Noise (denoted as "auto") vs. fixed noise at $\sigma = 0.5$ (denoted as "fixed") for ℓ_2 certification on (a) ImageNet and (b) CIFAR-10 datasets for AT models. (c) SmoothAdv vs Adv_2 models for CIFAR-10 using Auto-Noise technique. Here, we only present the results with the best ACR scores.

4.3 Auto-Noise: Flexibility of choosing appropriate σ for certification.

In Table 2, we can see that the classification models remain robust only for a few test examples under higher Gaussian noise. It suggests that the optimal noise levels for certifying different test examples may vary significantly, indicating the importance of our proposed Auto-Noise technique.

Auto-Noise for AT models. Figure 5(a) and 5(b) present the certification performance of AT models as we apply both certification through adaptation (Algorithm 1) and Auto-Noise technique for for ImageNet and CIFAR-10 datasets respectively. We compare their performance by certifying using a fixed noise level, $\sigma = 0.5$. We can see that the Auto-Noise technique can significantly improve the performance to achieve 1.148 and 1.102 ACR scores for the best AT models on ImageNet and CIFAR-10 datasets. Figure 5(c) demonstrates that the Auto-Noise technique also improves the performance of the best SmoothAdv model to an ACR score of 0.965 for CIFAR-10. However, our *Certification through Adaptation* together with *Auto-Noise* technique for $Adv_2[3]$ model outperforms the best SmoothAdv model for CIFAR-10.

(a) $Rand_{\sigma=0.5}$ (ImageNet)   (b) $Rand_{\sigma=0.5}$ (CIFAR-10)   (c) SmoothAdv (CIFAR-10)

Figure 6: Effect of adaptation and Auto-Noise technique for existing randomized smoothing based models.

Certification through Adaptation along with Auto-Noise for existing models. In Figure 6, we compare the performance of existing randomized smoothing based models as we adapt their base models using Algorithm 1 followed by Auto-Noise technique. We can see in Figure 6(a) that incorporating adaptation using Algorithm 1 improves the $Rand_{\sigma=0.5}$ model to achieve ACR score of 1.095 on ImageNet dataset. In contrast, the certification performance for both $Rand_{\sigma=0.5}$ and SmoothAdv models degrades for CIFAR-10 datasets (Figure 6(b) and Figure 6(c)). Hence, we do not include these models in Figure 5 (c) to compare with AT models.

(a) Adv_∞ models   (b) Adv_2 models

Figure 7: CIFAR-10: Certification performance degrades for over-fitted AT models when trained without applying early-stopping criteria (Rice et al., 2020). The over-fitted models are denoted as $Adv^{overfit}$.

4.4 Over-fitted AT models degrades certification

Rice et al. (2020) demonstrate that AT models *overfit* when trained without *early stopping* criteria. It degrades their empirical robustness against adversarial attacks. Figure 7 compares with the certification

results of such *overfitted* AT models, denoted as $\text{Adv}^{overfit}$. We observe that $\text{Adv}^{overfit}$ models also degrade the certified robustness compared to their corresponding AT models, trained with early stopping criteria. In particular, the difference in their certification performance is more prominent at higher ℓ_2 radii. Hence, these results as well as our results in Figure 5 indicate that empirical and certified robustness are closely related. In particular, *improving the empirical robustness for a model also allows to provide better certified robustness.*

5   Conclusion

We propose a novel *certification through adaptation* algorithm that transforms the AT models into a randomized smoothing classifier to provide certified robustness for ℓ_2 norm. We also propose *Auto-Noise* to efficiently approximate the appropriate noise levels to certify different test examples. Empirically we improve the performance of both AT models and existing randomized smoothing-based models on CIFAR-10 and ImageNet datasets using the Auto-Noise technique. Further, our *Certification through Adaptation* together with *Auto-Noise* technique significantly improves the ACR scores using AT models. Notably, our framework does not affect the empirical robustness or benign accuracy of an AT model to provide these non-trivial ℓ_2 certification results. Hence, our paper is a step towards bridging the gap between current research of empirical and certified robustness against adversarial examples.

Broader Impact Statement

Improving empirical robustness against adversarial examples along with certification guarantees is an important problem to enhance the reliability of a DNN model for sensitive real-world applications. However, the current state-of-the-art defense methods against adversarial examples typically focus on improving either empirical or certified robustness. In this paper, we aim to bridge this gap by significantly improving the certification performance of AT models without affecting the benign accuracy or reducing their state-of-the-art empirical robustness.

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A Appendix

A.1 Detailed Certification results for different models using proposed method

Model	Noise-level	ℓ_2 Radius													ACR
		0.0	0.25	0.5	0.75	1.0	1.25	1.5	1.75	2.0	2.25	2.5	2.75	3.0	
Baseline	$\sigma = 0.25$	13.6	7.8	4.8	3.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.055
Baseline	Auto-Noise	52.4	36.8	5.0	3.2	0.6	0.6	0.4	0.4	0.4	0.4	0.4	0.4	0.4	0.194
Baseline + Adaptation	Auto-Noise	57.4	25.8	4.6	1.8	0.4	0.2	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.15
$\text{Adv}_\infty[4/255]$	Auto-Noise	34.6	31.2	4.0	3.8	0.6	0.6	0.4	0.4	0.2	0.2	0.0	0.0	0.0	0.169
$\text{Adv}_\infty[4/255]$ + Adaptation	$\sigma = 0.5$	47.4	43.6	39.4	35.8	31.4	27.6	23.4	18.2	0.0	0.0	0.0	0.0	0.0	0.609
$\text{Adv}_\infty[4/255]$ + Adaptation	Auto-Noise	65.6	59.4	50.6	46.6	38.0	33.2	26.2	20.8	12.0	8.6	6.0	4.0	1.6	0.859
$\text{Adv}_2[3.0]$	Auto-Noise	44.0	41.6	11.8	11.2	2.8	2.6	0.4	0.4	0.0	0.0	0.0	0.0	0.0	0.261
$\text{Adv}_2[3.0]$ + Adaptation	$\sigma = 0.5$	50.2	47.0	43.0	39.0	36.4	32.8	30.8	27.0	0.0	0.0	0.0	0.0	0.0	0.711
$\text{Adv}_2[3.0]$ + Adaptation	Auto-Noise	66.6	63.8	58.6	55.4	45.6	**41.0**	**35.8**	**32.4**	**23.6**	**18.6**	**15.0**	**12.8**	**7.4**	**1.148**
$\text{Rand}_{\sigma=0.5}$	$\sigma = 0.50$	68.2	60.8	54.4	47.8	38.8	33.8	28.6	23.4	0.0	0.0	0.0	0.0	0.0	0.811
$\text{Rand}_{\sigma=0.5}$	Auto-Noise	71.4	65.6	58.8	51.4	42.8	37.0	28.8	23.8	2.6	1.6	0.2	0.2	0.2	0.88
$\text{Rand}_{\sigma=0.5}$ + Adaptation	Auto-Noise	**74.8**	**69.8**	**64.4**	**56.6**	**47.8**	40.0	34.4	27.4	20.2	15.8	10.4	6.4	3.2	1.095

Table 3: ImageNet: Certified top-1 accuracy at various ℓ_2 radii as we vary σ for BN adaptation and certification along with average certified radii (ACR). We use ResNet50 for ImageNet.

		ImageNet												
Model	Noise-level	ℓ_2 Radius												ACR
		0.0	0.25	0.5	0.75	1.0	1.25	1.5	1.75	2.0	2.25	2.5	2.75	3.0	
Baseline	$\sigma = 0.25$	10.49	6.96	2.04	0.09	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.035
Baseline	Auto-Noise	33.57	18.56	10.25	4.44	0.83	0.07	0.01	0.0	0.0	0.0	0.0	0.0	0.0	0.124
Baseline + Adaptation	Auto-Noise	59.64	21.66	7.81	3.97	1.28	0.36	0.07	0.0	0.0	0.0	0.0	0.0	0.0	0.154
$\text{Adv}_\infty[4/255]$	Auto-Noise	73.71	63.04	28.75	23.91	17.96	14.19	10.12	7.08	4.99	4.14	3.24	2.49	1.84	0.57
$\text{Adv}_\infty[4/255]$ + Adaptation	$\sigma = 0.5$	63.23	47.34	31.83	18.78	9.98	4.44	1.62	0.28	0.0	0.0	0.0	0.0	0.0	0.361
$\text{Adv}_\infty[4/255]$ + Adaptation	Auto-Noise	85.53	76.02	49.42	36.23	21.05	13.4	8.7	5.58	3.15	1.69	0.66	0.19	0.07	0.654
$\text{Adv}_\infty[8/255]$	Auto-Noise	74.46	66.57	36.32	30.15	18.87	13.71	8.7	5.29	2.89	1.88	1.17	0.75	0.46	0.578
$\text{Adv}_\infty[8/255]$ + Adaptation	$\sigma = 0.5$	64.2	53.65	42.91	32.58	22.68	14.24	7.88	2.94	0.0	0.0	0.0	0.0	0.0	0.52
$\text{Adv}_\infty[8/255]$ + Adaptation	Auto-Noise	79.69	71.78	53.76	43.61	29.68	20.87	14.04	9.08	5.53	3.33	1.71	0.81	0.35	0.741
$\text{Adv}_\infty[12/255]$	Auto-Noise	69.46	63.12	35.73	30.63	17.54	14.78	10.27	9.16	8.01	7.2	6.21	5.31	3.78	0.649
$\text{Adv}_\infty[12/255]$ + Adaptation	$\sigma = 0.5$	59.19	51.53	43.94	36.41	28.69	21.25	14.53	8.03	0.0	0.0	0.0	0.0	0.0	0.583
$\text{Adv}_\infty[12/255]$ + Adaptation	Auto-Noise	70.75	64.54	50.63	43.38	32.5	24.43	18.05	12.2	8.31	5.37	3.36	1.96	1.23	0.76
$\text{Adv}_\infty[16/255]$	Auto-Noise	58.47	53.41	31.48	26.76	16.68	14.04	10.89	9.17	7.42	5.62	3.81	2.43	1.53	0.55
$\text{Adv}_\infty[16/255]$ + Adaptation	$\sigma = 0.5$	53.8	48.07	42.51	36.54	30.55	24.68	18.49	12.11	0.0	0.0	0.0	0.0	0.0	0.599
$\text{Adv}_\infty[16/255]$ + Adaptation	Auto-Noise	61.07	56.01	45.76	40.29	31.6	24.53	18.73	14.23	10.39	7.37	5.05	3.36	2.13	0.731
$\text{Adv}_2[0.5]$	Auto-Noise	71.6	61.2	22.17	17.64	12.26	10.97	10.17	9.76	9.48	9.12	8.53	7.52	6.61	0.603
$\text{Adv}_2[0.5]$ + Adaptation	$\sigma = 0.5$	63.77	48.81	33.82	20.95	11.5	5.64	2.29	0.62	0.0	0.0	0.0	0.0	0.0	0.386
$\text{Adv}_2[0.5]$ + Adaptation	Auto-Noise	86.26	77.52	61.25	46.44	23.42	16.22	11.55	9.2	7.62	6.47	5.07	3.81	2.51	0.796
$\text{Adv}_2[1.0]$	Auto-Noise	81.08	71.0	43.82	34.77	17.25	11.15	6.19	3.68	1.76	1.02	0.52	0.27	0.15	0.608
$\text{Adv}_2[1.0]$ + Adaptation	$\sigma = 0.5$	66.05	56.45	46.24	35.6	26.89	18.73	11.37	5.41	0.0	0.0	0.0	0.0	0.0	0.582
$\text{Adv}_2[1.0]$ + Adaptation	Auto-Noise	82.34	75.38	64.53	53.8	36.04	27.55	19.53	12.61	7.29	4.33	2.39	1.21	0.67	0.871
$\text{Adv}_2[1.25]$	Auto-Noise	78.32	72.56	44.86	39.13	25.98	21.02	16.31	12.17	8.18	5.18	2.25	1.25	0.66	0.741
$\text{Adv}_2[1.25]$ + Adaptation	$\sigma = 0.5$	66.22	57.73	48.8	39.64	31.07	22.61	15.82	8.96	0.0	0.0	0.0	0.0	0.0	0.644
$\text{Adv}_2[1.25]$ + Adaptation	Auto-Noise	80.52	74.25	64.95	56.56	40.81	32.71	24.96	17.87	11.5	8.07	5.88	4.05	2.59	0.972
$\text{Adv}_2[1.5]$	Auto-Noise	75.26	69.75	48.42	41.73	26.44	20.82	14.12	10.14	6.87	4.75	3.02	1.81	0.87	0.733
$\text{Adv}_2[1.5]$ + Adaptation	$\sigma = 0.5$	63.67	56.55	49.19	41.72	34.47	27.36	20.23	12.98	0.0	0.0	0.0	0.0	0.0	0.687
$\text{Adv}_2[1.5]$ + Adaptation	Auto-Noise	76.22	70.47	62.39	55.91	42.45	35.79	29.01	21.71	14.23	10.04	6.51	4.07	2.29	0.99
$\text{Adv}_2[2.5]$	Auto-Noise	61.2	57.42	42.26	38.0	26.56	21.41	14.21	10.34	7.33	4.96	3.24	2.06	1.07	0.662
$\text{Adv}_2[2.5]$ + Adaptation	$\sigma = 0.5$	54.73	50.53	46.26	41.84	37.74	33.2	28.69	23.34	0.0	0.0	0.0	0.0	0.0	0.726
$\text{Adv}_2[2.5]$ + Adaptation	Auto-Noise	63.36	59.53	54.68	50.3	42.95	38.62	33.97	29.42	23.03	19.22	15.3	11.34	7.51	1.073
$\text{Adv}_2[3.0]$	Auto-Noise	64.45	60.57	45.73	41.06	28.48	22.92	15.1	10.77	7.23	4.8	2.77	1.67	1.1	0.702
$\text{Adv}_2[3.0]$ + Adaptation	$\sigma = 0.5$	53.75	49.41	45.57	41.52	37.43	33.37	28.82	23.65	0.0	0.0	0.0	0.0	0.0	0.721
$\text{Adv}_2[3.0]$ + Adaptation	Auto-Noise	61.96	58.58	53.64	49.67	42.76	38.69	34.54	30.36	24.65	20.77	17.09	13.66	9.18	1.102
$\text{Rand}_{\sigma=0.5}$	$\sigma = 0.5$	62.13	51.68	40.38	30.25	20.81	13.36	7.71	3.38	0.0	0.0	0.0	0.0	0.0	0.494
$\text{Rand}_{\sigma=0.5}$	Auto-Noise	79.48	71.75	60.23	48.72	35.97	25.16	15.09	10.13	6.98	5.58	4.18	2.94	1.76	0.821
$\text{Rand}_{\sigma=0.5}$ + Adaptation	Auto-Noise	78.27	69.51	57.16	44.73	31.19	19.27	10.4	4.25	1.65	0.57	0.14	0.01	0.0	0.695
$\text{SmoothAdv}_{\sigma=0.5,\epsilon=0.25}$	$\sigma = 0.5$	67.35	57.8	47.63	37.41	27.88	20.33	13.53	8.03	0.0	0.0	0.0	0.0	0.0	0.614
$\text{SmoothAdv}_{\sigma=0.5,\epsilon=0.25}$	Auto-Noise	72.88	65.23	55.25	44.87	34.93	24.79	16.44	9.17	4.92	1.91	0.73	0.21	0.07	0.737
$\text{SmoothAdv}_{\sigma=0.5,\epsilon=0.25}$ + Adaptation	Auto-Noise	74.45	65.68	54.28	42.59	31.76	21.61	13.19	7.16	3.41	1.43	0.52	0.16	0.05	0.697
$\text{SmoothAdv}_{\sigma=0.5,\epsilon=0.5}$	$\sigma = 0.5$	67.21	58.82	49.68	40.35	31.93	24.18	17.05	10.57	0.0	0.0	0.0	0.0	0.0	0.665
$\text{SmoothAdv}_{\sigma=0.5,\epsilon=0.5}$	Auto-Noise	71.85	65.28	56.41	48.2	39.47	29.82	21.44	13.55	7.54	3.45	1.35	0.41	0.12	0.807
$\text{SmoothAdv}_{\sigma=0.5,\epsilon=0.5}$ + Adaptation	Auto-Noise	73.54	66.14	56.81	47.04	37.2	26.99	18.46	10.78	5.67	2.6	1.0	0.44	0.13	0.773
$\text{SmoothAdv}_{\sigma=0.5,\epsilon=1.0}$	$\sigma = 0.5$	63.95	56.53	49.53	41.38	34.63	27.81	21.22	14.41	0.0	0.0	0.0	0.0	0.0	0.694
$\text{SmoothAdv}_{\sigma=0.5,\epsilon=1.0}$	Auto-Noise	67.91	62.28	55.36	48.41	41.14	33.57	26.27	18.42	11.87	6.1	2.64	0.95	0.32	0.854
$\text{SmoothAdv}_{\sigma=0.5,\epsilon=1.0}$ + Adaptation	Auto-Noise	69.6	63.04	55.52	47.65	38.93	30.7	22.57	15.34	9.21	4.51	2.02	0.9	0.33	0.813
$\text{SmoothAdv}_{\sigma=0.5,\epsilon=2.0}$	$\sigma = 0.5$	57.59	52.82	47.67	42.68	37.55	32.64	27.52	22.42	0.0	0.0	0.0	0.0	0.0	0.733
$\text{SmoothAdv}_{\sigma=0.5,\epsilon=2.0}$	Auto-Noise	61.27	57.27	52.52	48.17	43.49	38.02	33.15	27.47	21.86	15.81	9.5	4.97	2.01	0.965
$\text{SmoothAdv}_{\sigma=0.5,\epsilon=2.0}$ + Adaptation	Auto-Noise	61.23	56.9	51.33	46.44	41.05	35.65	30.11	24.35	18.48	12.8	7.76	4.27	2.3	0.908

Table 4: CIFAR-10: Certified top-1 accuracy at various ℓ_2 radii as we vary σ for test-time BN adaptation along with average certified radii (ACR) for individual settings.

A.2 Implementation Details

We present our experimental results on CIFAR-10 (Krizhevsky et al., 2009) and ImageNet (Deng et al., 2009) datasets. The descriptions of different models and training hyper-parameters are provided in the following:

A.2.1 CIFAR-10.

We use pre-activation ResNet18 architecture (He et al., 2016b) for our experiments on CIFAR-10. We apply the SGD optimizer with a batch size of 128. We execute a total of 200 training epochs and apply a step-wise learning rate decay set initially at 0.1 and divided by 10 at 100 and 150 epochs, and weight decay 5×10^{-4}.

AT models (Madry et al., 2018; Rice et al., 2020): Unless and otherwise specified, our AT models are learned using early stopping criteria as described in (Rice et al., 2020). We learn several AT models with different threat boundaries for our experiments. We denote them by specifying their corresponding

threat model and threat boundaries. For example, $\text{Adv}_2[1.5]$ denotes an AT model that is learned using PGD adversary with ℓ_2 threat model and a threat boundary of $\epsilon = 1.5$, along with *early-stopping criteria* (Rice et al., 2020). We also learn AT models *without* using early-stopping criteria, as in (Madry et al., 2018) for our comparison in Figure 7. These models are denoted as $\text{Adv}^{overfit}$.

We use *projected gradient descent (PGD)* adversarial attack (Madry et al., 2018) to train these AT models as follows: For Adv_∞, we use 10 iterations and an ℓ_∞ step size of $\epsilon/4$. For Adv_2, we use 10 iterations and an ℓ_2 step size of $\epsilon/8.5$. This is the same experimental setup as in (Rice et al., 2020)). We choose a small set of $1,000$ images from the CIFAR-10 test set for our validation. We apply the PGD attack with the same hyper-parameters for our validation during training. We save the best model using the *early-stopping* criteria (Rice et al., 2020).

Randomized smoothing model by Cohen et al. (2019): We also train $\text{Rand}_{\sigma=0.5}$ by training with augmented random noise, sampled from an isotropic Gaussian distribution $\mathcal{N}(0, \sigma^2 I)$ with $\sigma = 0.5$. Here, we keep the same model architecture, learning rates, batch sizes, and other hyper-parameters as used to learn the AT models.

Randomized smoothing model by Salman et al. (2019a): We also compare with the state-of-the-art certification models, called 'SmoothAdv', by Salman et al. (2019a) for our experiments on ℓ_2 certification We train the SmoothAdv models by choosing random noise vectors followed by an adaptive adversarial attack with specified ℓ_2 threat boundary of ϵ at each iteration. The noise vectors are sampled from an isotropic Gaussian distribution $\mathcal{N}(0, \sigma^2 I)$.

We note that the training hyper-parameter ϵ has the most significant impact on the certification curve for a SmoothAdv model (please refer to Table 7-15 of (Salman et al., 2019a) for more details). For our experiments, we train 4 different SmoothAdv models with $\epsilon = \{0.25, 0.5, 1, 2\}$ and $\sigma = 0.5$ using adaptive PGD attack with 10 steps. We denote them as $\text{SmoothAdv}_{\sigma=0.5,\epsilon=0.25}$, $\text{SmoothAdv}_{\sigma=0.5,\epsilon=0.5}$, $\text{SmoothAdv}_{\sigma=0.5,\epsilon=1}$ and $\text{SmoothAdv}_{\sigma=0.5,\epsilon=2}$ respectively. We use the same training set-up and other hyper-parameters as specified in their Github: https://github.com/Hadisalman/smoothing-adversarial.

A.2.2 ImageNet.

We use ResNet50 architecture (He et al., 2016a) for ImageNet. We obtain the Baseline and $\text{Rand}_{\sigma=0.5}$ models from (Cohen et al., 2019)[2]. These models are trained using Gaussian augmented noises, sampled from isotropic Gaussian distribution $\mathcal{N}(0, \sigma^2 I)$ with $\sigma = 0.0$ (i.e., no noise) and $\sigma = 0.5$ respectively.

The AT models i.e., $\text{Adv}_\infty[4/255]$ and $\text{Adv}_2[3.0]$ are learned for ℓ_∞ and ℓ_2 threat models with threat boundary of $4/255$ and 3, respectively. We use the publicly available models provided by Rice et al. (2020) [3]. These models are fine-tuned using PGD-based adversarial training with early stopping criteria, originally provided by Engstrom et al. (2019) [4].

We resize the input images to 256×265 pixels and crop 224×224 pixels from the center. For our experiments on certification, we use a set of 500 test images by choosing at most 1 sample for each class.

A.3 Choice of Adaptive BN hyper-parameters

BN adaptation technique is controlled by two hyper-parameters, i.e., the *test batch-size* and *momentum* (ρ) (see Equation 2) to update the statistics of the batch-normalization layers. Assuming that the test images are obtained independently from the same test distribution, we can efficiently compute the BN statistics from these images. The hyper-parameter $\rho \in [0, 1]$ controls the tread-off between pre-computed training statistics and test statistics. We can obtain a better estimation of the test distribution from a large test batch. Hence, we can choose a higher value of ρ.

Here, we compare the top-1 test accuracy of AT models under Gaussian augmented noise with $\sigma = 0.5$ for different choices of ρ and the batch size. We skip the standard baseline models from our analysis and

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[2]https://github.com/locuslab/smoothing
[3]https://github.com/locuslab/robust_overfitting
[4]https://github.com/MadryLab/robustness

refer to the previous works (Schneider et al., 2020; Nado et al., 2020) that analyzed the effects of these hyper-parameters for the standard baseline DNN classifiers.

(a) ImageNet				(b) CIFAR-10		
ρ	Adv_∞	Adv_2		ρ	Adv_∞	Adv_2
0.0 (No adaptation)	$0.4_{\pm 0.01}$	$0.9_{\pm 0.01}$		0.0 (No adaptation)	$16.1_{\pm 7.85}$	$21.5_{\pm 7.79}$
0.1	$2.1_{\pm 0.04}$	$7.7_{\pm 0.09}$		0.1	$45.1_{\pm 0.49}$	$46.9_{\pm 0.48}$
0.3	$20.6_{\pm 0.16}$	$36.6_{\pm 0.09}$		0.3	$59.2_{\pm 0.42}$	$60.8_{\pm 0.33}$
0.5	$41.1_{\pm 0.09}$	$45.5_{\pm 0.13}$		0.5	$62.4_{\pm 0.27}$	$64.4_{\pm 0.6}$
0.7	$43.5_{\pm 0.14}$	$46.7_{\pm 0.13}$		0.7	$62.8_{\pm 0.52}$	$64.9_{\pm 0.31}$
0.9	$44.2_{\pm 0.12}$	$46.8_{\pm 0.13}$		0.9	$62.8_{\pm 0.71}$	$64.9_{\pm 0.31}$
1.0 (Full adaptation)	$44.8_{\pm 0.13}$	$47.2_{\pm 0.14}$		1.0 (Full adaptation)	$62.4_{\pm 0.64}$	$64.9_{\pm 0.73}$

Table 5: Top-1 accuracy using fixed test batch-size = 512 for AT models under Gaussian augmented noise with $\sigma = 0.5$ for different choices of momentum, ρ during inference. We randomly shuffle the test images to report $(mean + 2 \times sd)$ of 5 different runs.

Momentum (ρ). We first investigate the effect of momentum (ρ) as we choose a large batch size of 512. In Table 5, we present the performance of AT models for different values of ρ. Recall that, $\rho = 1$ denotes *full adaptation* (Equation 2). Here, we completely ignore the training statistics and recompute the BN statistics using the test batches. In contrast, $\rho = 0$ represents *no adaptation*, i.e., the same as the standard 'deterministic' inference setup. In this case, we use the previously computed BN statistics obtained during training.

We observe that for ImageNet (Table 5 [Left]) the performance started converging at $\rho = 0.7$. For CIFAR-10 (Table 5 [Right]), the convergence started even earlier at $\rho = 0.5$.

(a) ImageNet				(b) CIFAR-10		
Batch Size	Adv_∞	Adv_2		Batch Size	Adv_∞	Adv_2
w/o BN adapt	$0.4_{\pm 0.01}$	$0.9_{\pm 0.01}$		w/o BN adapt	$16.1_{\pm 7.85}$	$21.5_{\pm 7.79}$
8	$11.5_{\pm 0.22}$	$9.1_{\pm 0.15}$		8	$57.2_{\pm 1.23}$	$59.5_{\pm 0.38}$
16	$28.1_{\pm 0.22}$	$26.7_{\pm 0.14}$		16	$60.2_{\pm 0.79}$	$62.3_{\pm 0.87}$
32	$37.1_{\pm 0.24}$	$37.6_{\pm 0.2}$		32	$61.5_{\pm 0.46}$	$63.6_{\pm 0.55}$
64	$41.4_{\pm 0.26}$	$42.9_{\pm 0.12}$		64	$62.3_{\pm 0.5}$	$64.0_{\pm 0.38}$
128	$43.3_{\pm 0.15}$	$45.4_{\pm 0.13}$		128	$62.7_{\pm 0.68}$	$64.4_{\pm 0.53}$
256	$44.4_{\pm 0.21}$	$46.7_{\pm 0.07}$		256	$62.7_{\pm 0.68}$	$64.9_{\pm 0.48}$
512	$44.8_{\pm 0.13}$	$47.2_{\pm 0.14}$		512	$62.4_{\pm 0.64}$	$64.9_{\pm 0.73}$

Table 6: Top-1 accuracy using fixed $\rho = 1$ for AT models under Gaussian augmented noise with $\sigma = 0.5$ for different size of test batches during inference. We randomly shuffle the test images to report $(mean + 2 \times s.d.)$ of 5 different runs.

Batch Size. Next, we investigate the minimum size of the test batches to choose $\rho = 1$ (i.e., full-adaptation). In Table 6, we fix $\rho = 1$ and vary the test batch sizes as we evaluate these AT models. We observe that the performance of these models started improving even when we are using the test batches of size 8. The performance further improves as we choose larger sizes of test batches. We can see that their performance started converging as we choose the test batches of size 64 for ImageNet. On the other hand, the convergence started much earlier for CIFAR-10.

A.4 Performance against different corruptions

We mainly focus on ℓ_2 certification using Gaussian noise in this paper. However, we note that randomized smoothing techniques have been also applied to provide certifications for other perturbation types as well (e.g., random uniform noise for ℓ_1 norm (Yang et al., 2020)). Consequently, we can apply our proposed Algorithm 1 to adapt an AT model for any given perturbation types without any additional training for different applications.

Further, Hendrycks & Dietterich (2019) recently introduced ImageNet-C and CIFAR10-C datasets by *algorithmically generated random corruptions* from *noise*, *blur*, *weather*, and *digital* categories with 5 different severity levels for each corruption. Several recent works demonstrated that adaptive BN techniques can significantly improve the performance of any classifier (including AT models) against different random corruptions. Further, – also demonstrated the effectiveness of AT models even without applying any adaptation. Hence, our proposed certification framework for AT models is a step forward towards further improving the reliability of sensitive real-world applications.