Certified Adversarial Robustness via Randomized Smoothing

Jeremy Cohen ¹ Elan Rosenfeld ¹ J. Zico Kolter ¹²

Abstract

We show how to turn any classifier that classifies well under Gaussian noise into a new classifier that is certifiably robust to adversarial perturbations under the ℓ_2 norm. This "randomized smoothing" technique has been proposed recently in the literature, but existing guarantees are loose. We prove a tight robustness guarantee in ℓ_2 norm for smoothing with Gaussian noise. We use randomized smoothing to obtain an ImageNet classifier with e.g. a certified top-1 accuracy of 49% under adversarial perturbations with ℓ_2 norm less than 0.5 (=127/255). No certified defense has been shown feasible on ImageNet except for smoothing. On smaller-scale datasets where competing approaches to certified ℓ_2 robustness are viable, smoothing delivers higher certified accuracies. Our strong empirical results suggest that randomized smoothing is a promising direction for future research into adversarially robust classification. Code and models are available at http: //github.com/locuslab/smoothing.

1. Introduction

Modern image classifiers achieve high accuracy on i.i.d. test sets but are not robust to small, adversarially-chosen perturbations of their inputs (Szegedy et al., 2014; Biggio et al., 2013). Given an image x correctly classified by, say, a neural network, an adversary can usually engineer an adversarial perturbation δ so small that $x+\delta$ looks just like x to the human eye, yet the network classifies $x+\delta$ as a different, incorrect class. Many works have proposed heuristic methods for training classifiers intended to be robust to adversarial perturbations. However, most of these heuristics have been subsequently shown to fail against suitably powerful adversaries (Carlini & Wagner, 2017; Athalye et al., 2018; Uesato et al., 2018). In response, a line of work on

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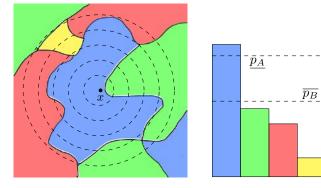


Figure 1. Evaluating the smoothed classifier at an input x. Left: the decision regions of the base classifier f are drawn in different colors. The dotted lines are the level sets of the distribution $\mathcal{N}(x,\sigma^2I)$. Right: the distribution $f(\mathcal{N}(x,\sigma^2I))$. As discussed below, $\underline{p_A}$ is a lower bound on the probability of the top class and $\overline{p_B}$ is an upper bound on the probability of each other class. Here, g(x) is "blue."

certifiable robustness studies classifiers whose prediction at any point x is verifiably constant within some set around x (Wong & Kolter, 2018; Raghunathan et al., 2018a, e.g.). In most of these works, the robust classifier takes the form of a neural network. Unfortunately, all existing approaches for certifying the robustness of neural networks have trouble scaling to networks that are large and expressive enough to solve problems like ImageNet.

One workaround is to look for robust classifiers that are not neural networks. Recently, two papers (Lecuyer et al., 2019; Li et al., 2018) showed that an operation we call *randomized smoothing*¹ can transform any arbitrary base classifier f into a new "smoothed classifier" g that is certifiably robust in ℓ_2 norm. Let f be an arbitrary classifier which maps inputs \mathbb{R}^d to classes \mathcal{Y} . For any input x, the smoothed classifier's prediction g(x) is defined to be the class which f is most likely to classify the random variable $\mathcal{N}(x,\sigma^2I)$ as. That is, g(x) returns the most probable prediction by f of random Gaussian corruptions of x.

If the base classifier f is most likely to classify $\mathcal{N}(x,\sigma^2I)$ as x's correct class, then the smoothed classifier g will be

¹Carnegie Mellon University ²Bosch Center for AI. Correspondence to: Jeremy Cohen < jeremycohen@cmu.edu>.

¹Smoothing was proposed under the name "PixelDP" (for differential privacy). We use a different name since our improved analysis does not involve differential privacy.

correct at x. But the smoothed classifier g will also possess a desirable property that the base classifier may lack: one can verify that g's prediction is constant within an ℓ_2 ball around any input x, simply by estimating the probabilities with which f classifies $\mathcal{N}(x,\sigma^2I)$ as each class. The higher the probability with which f classifies $\mathcal{N}(x,\sigma^2I)$ as the most probable class, the larger the ℓ_2 radius around x in which g provably returns that class.

Lecuyer et al. (2019) proposed randomized smoothing as a provable adversarial defense, and used it to train the first certifiably robust classifier for ImageNet. Subsequently, Li et al. (2018) proved a stronger robustness guarantee. However, both of these guarantees are loose, in the sense that the smoothed classifier g is provably always more robust than the guarantee indicates. In this paper, we prove the first tight robustness guarantee for randomized smoothing. Our analysis reveals that smoothing with Gaussian noise naturally induces certifiable robustness under the ℓ_2 norm. We suspect that other, as-yet-unknown noise distributions might induce robustness to other perturbation sets such as general ℓ_p norm balls.

Randomized smoothing has one major drawback. If f is a neural network, it is not possible to *exactly* compute the probabilities with which f classifies $\mathcal{N}(x,\sigma^2I)$ as each class. Therefore, it is not possible to exactly evaluate g's prediction at any input x, or to exactly compute the radius in which this prediction is certifiably robust. Instead, we present Monte Carlo algorithms for both tasks that are guaranteed to succeed with arbitrarily high probability.

Despite this drawback, randomized smoothing enjoys several compelling advantages over other certifiably robust classifiers proposed in the literature: it makes no assumptions about the base classifier's architecture, it is simple to implement and understand, and, most importantly, it permits the use of arbitrarily large neural networks as the base classifier. In contrast, other certified defenses do not cur-

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

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





Figure 2. The smoothed classifier's prediction at an input x (left) is defined as the most likely prediction by the base classifier on random Gaussian corruptions of x (right; $\sigma=0.5$). Note that this Gaussian noise is much larger in magnitude than the adversarial perturbations to which g is provably robust. One interpretation of randomized smoothing is that these large random perturbations "drown out" small adversarial perturbations.

rently scale to large networks. Indeed, smoothing is the only certified adversarial defense which has been shown feasible on the full-resolution ImageNet classification task.

We use randomized smoothing to train state-of-the-art certifiably ℓ_2 -robust ImageNet classifiers; for example, one of them achieves 49% provable top-1 accuracy under adversarial perturbations with ℓ_2 norm less than 127/255 (Table 1). We also demonstrate that on smaller-scale datasets like CIFAR-10 and SHVN, where competing approaches to certified ℓ_2 robustness are feasible, randomized smoothing can deliver better certified accuracies, both because it enables the use of larger networks and because it does not constrain the expressivity of the base classifier.

2. Related Work

Many works have proposed classifiers intended to be robust to adversarial perturbations. These approaches can be broadly divided into *empirical* defenses, which empirically seem robust to known adversarial attacks, and *certified* defenses, which are *provably* robust to certain kinds of adversarial perturbations.

Empirical defenses The most successful empirical defense to date is *adversarial training* (Goodfellow et al., 2015; Kurakin et al., 2017; Madry et al., 2018), in which adversarial examples are found during training (often using projected gradient descent) and added to the training set. Unfortunately, it is typically impossible to tell whether a prediction by an empirically robust classifier is truly robust to adversarial perturbations; the most that can be said is that a specific attack was unable to find any. In fact, many heuristic defenses proposed in the literature were later "broken" by stronger adversaries (Carlini & Wagner, 2017; Athalye et al., 2018; Uesato et al., 2018; Athalye & Carlini, 2018).

Aiming to escape this cat-and-mouse game, a growing body of work has focused on defenses with formal guarantees.

Certified defenses A classifier is said to be *certifiably robust* if for any input x, one can easily obtain a guarantee that the classifier's prediction is constant within some set around x, often an ℓ_2 or ℓ_∞ ball. In most work in this area, the certifiably robust classifier is a neural network. Some works propose algorithms for certifying the robustness of generically trained networks, while others (Wong & Kolter, 2018; Raghunathan et al., 2018a) propose both a robust training method and a complementary certification mechanism.

Certification methods are either exact (a.k.a "complete") or conservative (a.k.a "sound but incomplete"). In the context of ℓ_p norm-bounded perturbations, exact methods take a classifier g, input x, and radius r, and report whether or not there exists a perturbation δ within $\|\delta\| \leq r$ for which $q(x) \neq q(x+\delta)$. In contrast, conservative methods either certify that no such perturbation exists or decline to make a certification; they may decline even when it is true that no such perturbation exists. Exact methods are usually based on Satisfiability Modulo Theories (Katz et al., 2017; Carlini et al., 2017; Ehlers, 2017; Huang et al., 2017) or mixed integer linear programming (Cheng et al., 2017; Lomuscio & Maganti, 2017; Dutta et al., 2017; Fischetti & Jo, 2018; Bunel et al., 2018). Unfortunately, no exact methods have been shown to scale beyond moderate-sized (100,000 activations) networks (Tjeng et al., 2019), and networks of that size can only be verified when they are trained in a manner that impairs their expressivity.

Conservative certification is more scalable. Some conservative methods bound the global Lipschitz constant of the neural network (Gouk et al., 2018; Tsuzuku et al., 2018; Anil et al., 2019; Cisse et al., 2017), but these approaches tend to be very loose on expressive networks. Others measure the *local* smoothness of the network in the vicinity of a particular input x. In theory, one could obtain a robustness guarantee via an upper bound on the local Lipschitz constant of the network (Hein & Andriushchenko, 2017), but computing this quantity is intractable for general neural networks. Instead, a panoply of practical solutions have been proposed in the literature (Wong & Kolter, 2018; Wang et al., 2018a;b; Raghunathan et al., 2018a;b; Wong et al., 2018; Dvijotham et al., 2018b;a; Croce et al., 2019; Gehr et al., 2018; Mirman et al., 2018; Singh et al., 2018; Gowal et al., 2018; Weng et al., 2018a; Zhang et al., 2018). Two themes stand out. Some approaches cast verification as an optimization problem and import tools such as relaxation and duality from the optimization literature to provide conservative guarantees (Wong & Kolter, 2018; Wong et al., 2018; Raghunathan et al., 2018a;b; Dvijotham et al., 2018b;a). Others step through the network layer by layer, maintaining at each layer an outer approximation of the set of activations

reachable by a perturbed input (Mirman et al., 2018; Singh et al., 2018; Gowal et al., 2018; Weng et al., 2018a; Zhang et al., 2018). None of these local certification methods have been shown to be feasible on networks that are large and expressive enough to solve modern machine learning problems like the ImageNet classification task. Also, all either assume specific network architectures (e.g. ReLU activations or a layered feedforward structure) or require extensive customization for new network architectures.

Related work involving noise Prior works have proposed using a network's robustness to Gaussian noise as a proxy for its robustness to adversarial perturbations (Weng et al., 2018b; Ford et al., 2019), and have suggested that Gaussian data augmentation could supplement or replace adversarial training (Zantedeschi et al., 2017; Kannan et al., 2018). Smilkov et al. (2017) observed that averaging a classifier's input gradients over Gaussian corruptions of an image yields very interpretable saliency maps. The robustness of neural networks to random noise has been analyzed both theoretically (Fawzi et al., 2016; Franceschi et al., 2018) and empirically (Dodge & Karam, 2017). Finally, Webb et al. (2019) proposed a statistical technique for estimating the noise robustness of a classifier more efficiently than naive Monte Carlo simulation; we did not use this technique since it appears to lack formal high-probability guarantees. While these works hypothesized relationships between a neural network's robustness to random noise and the same network's robustness to adversarial perturbations, randomized smoothing instead uses a classifier's robustness to random noise to create a new classifier robust to adversarial perturbations.

Randomized smoothing Randomized smoothing has been studied previously for adversarial robustness. Several works (Liu et al., 2018; Cao & Gong, 2017) proposed similar techniques as heuristic defenses, but did not prove any guarantees. Lecuyer et al. (2019) used inequalities from the differential privacy literature to prove an ℓ_2 and ℓ_1 robustness guarantee for smoothing with Gaussian and Laplace noise, respectively. Subsequently, Li et al. (2018) used tools from information theory to prove a stronger ℓ_2 robustness guarantee for Gaussian noise. However, all of these robustness guarantees are loose. In contrast, we prove a tight robustness guarantee in ℓ_2 norm for randomized smoothing with Gaussian noise.

3. Randomized smoothing

Consider a classification problem from \mathbb{R}^d to classes \mathcal{Y} . As discussed above, randomized smoothing is a method for constructing a new, "smoothed" classifier g from an arbitrary base classifier f. When queried at x, the smoothed classifier g returns whichever class the base classifier f is most likely

to return when x is perturbed by isotropic Gaussian noise:

$$g(x) = \operatorname*{arg\,max}_{c \in \mathcal{Y}} \mathbb{P}(f(x + \varepsilon) = c) \tag{1}$$
 where $\varepsilon \sim \mathcal{N}(0, \sigma^2 I)$

An equivalent definition is that g(x) returns the class c whose pre-image $\{x' \in \mathbb{R}^d : f(x') = c\}$ has the largest probability measure under the distribution $\mathcal{N}(x, \sigma^2 I)$. The noise level σ is a hyperparameter of the smoothed classifier g which controls a robustness/accuracy tradeoff; it does not change with the input x. We leave undefined the behavior of g when the argmax is not unique.

We will first present our robustness guarantee for the smoothed classifier g. Then, since it is not possible to exactly evaluate the prediction of g at x or to certify the robustness of g around x, we will give Monte Carlo algorithms for both tasks that succeed with arbitrarily high probability.

3.1. Robustness guarantee

Suppose that when the base classifier f classifies $\mathcal{N}(x,\sigma^2I)$, the most probable class c_A is returned with probability p_A , and the "runner-up" class is returned with probability p_B . Our main result is that smoothed classifier g is robust around x within the ℓ_2 radius $R = \frac{\sigma}{2}(\Phi^{-1}(p_A) - \Phi^{-1}(p_B))$, where Φ^{-1} is the inverse of the standard Gaussian CDF. This result also holds if we replace p_A with a lower bound $\underline{p_A}$ and we replace p_B with an upper bound $\overline{p_B}$.

Theorem 1. Let $f: \mathbb{R}^d \to \mathcal{Y}$ be any deterministic or random function, and let $\varepsilon \sim \mathcal{N}(0, \sigma^2 I)$. Let g be defined as in (1). Suppose $c_A \in \mathcal{Y}$ and $\underline{p_A}, \overline{p_B} \in [0, 1]$ satisfy:

$$\mathbb{P}(f(x+\varepsilon)=c_A) \ge \underline{p_A} \ge \overline{p_B} \ge \max_{c \ne c_A} \mathbb{P}(f(x+\varepsilon)=c)$$
 (2)

Then $g(x + \delta) = c_A$ for all $\|\delta\|_2 < R$, where

$$R = \frac{\sigma}{2} (\Phi^{-1}(\underline{p_A}) - \Phi^{-1}(\overline{p_B})) \tag{3}$$

We now make several observations about Theorem 1²

- Theorem 1 assumes nothing about f. This is crucial since it is unclear which well-behavedness assumptions, if any, are satisfied by modern deep architectures.
- The certified radius R is large when: (1) the noise level σ is high, (2) the probability of the top class c_A is high, and (3) the probability of each other class is low.

• The certified radius R goes to ∞ as $\underline{p_A} \to 1$ and $\overline{p_B} \to 0$. This should sound reasonable: the Gaussian distribution is supported on all of \mathbb{R}^d , so the only way that $f(x+\varepsilon)=c_A$ with probability 1 is if $f=c_A$ almost everywhere.

Both Lecuyer et al. (2019) and Li et al. (2018) proved ℓ_2 robustness guarantees for the same setting as Theorem 1, but with different, smaller expressions for the certified radius. However, our ℓ_2 robustness guarantee is *tight*: if (2) is all that is known about f, then it is impossible to certify an ℓ_2 ball with radius larger than R. In fact, it is impossible to certify any superset of the ℓ_2 ball with radius R:

Theorem 2. Assume $\underline{p_A} + \overline{p_B} \leq 1$. For any perturbation δ with $\|\delta\|_2 > R$, there exists a base classifier f consistent with the class probabilities (2) for which $g(x + \delta) \neq c_A$.

Theorem 2 shows that Gaussian smoothing naturally induces ℓ_2 robustness: if we make no assumptions on the base classifier beyond the class probabilities (2), then the set of perturbations to which a Gaussian-smoothed classifier is provably robust is *exactly* an ℓ_2 ball.

The complete proofs of Theorems 1 and 2 are in Appendix A. We now sketch the proofs in the special case when there are only two classes.

Theorem 1 (binary case). Suppose $\underline{p_A} \in (\frac{1}{2}, 1]$ satisfies $\mathbb{P}(f(x+\varepsilon) = c_A) \geq \underline{p_A}$. Then $g(x+\delta) = c_A$ for all $\|\delta\|_2 < \sigma\Phi^{-1}(p_A)$.

Proof sketch. Fix a perturbation $\delta \in \mathbb{R}^d$. To guarantee that $g(x+\delta)=c_A$, we need to show that f classifies the translated Gaussian $\mathcal{N}(x+\delta,\sigma^2I)$ as c_A with probability $>\frac{1}{2}$. However, all we know about f is that f classifies $\mathcal{N}(x,\sigma^2I)$ as c_A with probability $\geq \underline{p_A}$. This raises the question: out of all possible base classifiers f which classify $\mathcal{N}(x,\sigma^2I)$ as c_A with probability $\geq \underline{p_A}$, which one f^* classifies $\mathcal{N}(x+\delta,\sigma^2I)$ as c_A with the smallest probability? One can show using an argument similar to the Neyman-Pearson lemma (Neyman & Pearson, 1933) that this "worst-case" f^* is a linear classifier whose decision boundary is normal to the perturbation δ (Figure 3):

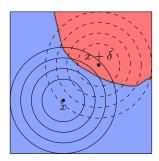
$$f^*(x') = \begin{cases} c_A & \text{if } \delta^T(x' - x) \le \sigma \|\delta\|_2 \Phi^{-1}(\underline{p_A}) \\ c_B & \text{otherwise} \end{cases}$$
 (4)

This "worst-case" f^* classifies $\mathcal{N}(x+\delta,\sigma^2I)$ as c_A with probability $\Phi\left(\Phi^{-1}(\underline{p_A})-\frac{\|\delta\|_2}{\sigma}\right)$. Therefore, to ensure that even the "worst-case" f^* classifies $\mathcal{N}(x+\delta,\sigma^2I)$ as c_A with probability $>\frac{1}{2}$, we solve for those δ for which

$$\Phi\left(\Phi^{-1}(\underline{p_A}) - \frac{\|\delta\|_2}{\sigma}\right) > \frac{1}{2}$$

which is equivalent to the condition $\|\delta\|_2 < \sigma\Phi^{-1}(p_A)$. \square

²After the dissemination of this work, a more general result was published in Levine et al. (2019); Salman et al. (2019): if $h: \mathbb{R}^d \to [0,1]$ is a function and \hat{h} is the "smoothed" version $\hat{h}(x) = \mathbb{E}_{\varepsilon \sim \mathcal{N}(0,\sigma^2I)}[h(x+\varepsilon)]$, then the function $x \mapsto \Phi^{-1}(\hat{h}(x))$ is $1/\sigma$ -Lipschitz. Theorem 1 can be proved by applying this result to the functions $f_c(x) = \mathbf{1}[f(x) = c]$ for each class c.



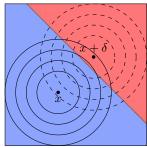


Figure 3. Illustration of f^* in two dimensions. The concentric circles are the density contours of $\mathcal{N}(x,\sigma^2I)$ and $\mathcal{N}(x+\delta,\sigma^2I)$. Out of all base classifiers f which classify $\mathcal{N}(x,\sigma^2I)$ as c_A (blue) with probability $\geq \underline{p_A}$, such as both classifiers depicted above, the "worst-case" f^* —the one which classifies $\mathcal{N}(x+\delta,\sigma^2I)$ as c_A with minimal probability—is depicted on the right: a linear classifier with decision boundary normal to the perturbation δ .

Theorem 2 is a simple consequence: for any δ with $\|\delta\|_2 > R$, the base classifier f^* defined in (4) is consistent with (2); yet if f^* is the base classifier, then $g(x + \delta) = c_B$.

Figure 5 (left) plots our ℓ_2 robustness guarantee against the guarantees derived in prior work. Observe that our R is much larger than that of Lecuyer et al. (2019) and moderately larger than that of Li et al. (2018). Appendix I derives the other two guarantees using this paper's notation.

Linear base classifier A two-class linear classifier $f(x) = \mathrm{sign}(w^Tx + b)$ is already certifiable: the distance from any input x to the decision boundary is $|w^Tx + b|/||w||_2$, and no perturbation δ with ℓ_2 norm less than this distance can possibly change f's prediction. In Appendix B we show that if f is linear, then the smoothed classifier g is identical to the base classifier f. Moreover, we show that our bound (3) will certify the true robust radius $|w^Tx + b|/||w||$, rather than a smaller, overconservative radius. Therefore, when f is linear, there always exists a perturbation δ just beyond the certified radius which changes g's prediction.

Noise level can scale with image resolution Since our expression (3) for the certified radius does not depend explicitly on the data dimension d, one might worry that randomized smoothing is less effective for images of higher resolution — certifying a fixed ℓ_2 radius is "less impressive" for, say, a 224×224 image than for a 56×56 image. However, as illustrated by Figure 4, images in higher resolution can tolerate higher levels σ of isotropic Gaussian noise before their class-distinguishing content gets destroyed. As a consequence, in high resolution, smoothing can be performed with a larger σ , leading to larger certified radii. See Appendix G for a more rigorous version of this argument.

3.2. Practical algorithms

We now present practical Monte Carlo algorithms for evaluating g(x) and certifying the robustness of g around x. More details can be found in Appendix C.

3.2.1. PREDICTION

Evaluating the smoothed classifier's prediction g(x) requires identifying the class c_A with maximal weight in the categorical distribution $f(x+\varepsilon)$. The procedure described in pseudocode as PREDICT draws n samples of $f(x+\varepsilon)$ by running n noise-corrupted copies of x through the base classifier. Let \hat{c}_A be the class which appeared the largest number of times. If \hat{c}_A appeared much more often than any other class, then PREDICT returns \hat{c}_A . Otherwise, it abstains from making a prediction. We use the hypothesis test from Hung & Fithian (2019) to calibrate the abstention threshold so as to bound by α the probability of returning an incorrect answer. PREDICT satisfies the following guarantee:

Proposition 1. With probability at least $1 - \alpha$ over the randomness in PREDICT, PREDICT will either abstain or return g(x). (Equivalently: the probability that PREDICT returns a class other than g(x) is at most α .)

The function SAMPLEUNDERNOISE $(f, x, \text{num}, \sigma)$ in the pseudocode draws num samples of noise, $\varepsilon_1 \dots \varepsilon_{\text{num}} \sim \mathcal{N}(0, \sigma^2 I)$, runs each $x + \varepsilon_i$ through the base classifier f, and returns a vector of class counts. BINOMPVALUE $(n_A, n_A + n_B, p)$ returns the p-value of the two-sided hypothesis test that $n_A \sim \text{Binomial}(n_A + n_B, p)$.

Even if the true smoothed classifier g is robust at radius R, PREDICT will be vulnerable in a certain sense to adversarial perturbations with ℓ_2 norm slightly less than R. By engineering a perturbation δ for which $f(x+\delta+\varepsilon)$ puts mass just over $\frac{1}{2}$ on class c_A and mass just under $\frac{1}{2}$ on class c_B , an adversary can force PREDICT to abstain at a high rate. If this scenario is of concern, a variant of Theorem 1 could be proved to certify a radius in which $\mathbb{P}(f(x+\delta+\varepsilon)=c_A)$ is larger by some margin than $\max_{c\neq c_A} \mathbb{P}(f(x+\delta+\varepsilon)=c)$.

3.2.2. CERTIFICATION

Evaluating and certifying the robustness of g around an input x requires not only identifying the class c_A with maximal weight in $f(x + \varepsilon)$, but also estimating a lower bound



Figure 4. Left to right: clean 56 x 56 image, clean 224 x 224 image, noisy 56 x 56 image ($\sigma=0.5$), noisy 224 x 224 image ($\sigma=0.5$).

Pseudocode for certification and prediction

evaluate g at x

else return ABSTAIN

```
\begin{array}{l} \textbf{function} \ \mathsf{PREDICT}(f,\sigma,x,n,\alpha) \\ \ \mathsf{counts} \leftarrow \mathsf{SAMPLEUNDERNOISE}(f,x,n,\sigma) \\ \hat{c}_A, \hat{c}_B \leftarrow \mathsf{top} \ \mathsf{two} \ \mathsf{indices} \ \mathsf{in} \ \mathsf{counts} \\ n_A, n_B \leftarrow \mathsf{counts}[\hat{c}_A], \ \mathsf{counts}[\hat{c}_B] \\ \ \mathsf{if} \ \mathsf{BINOMPVALUE}(n_A,n_A+n_B,0.5) \leq \alpha \ \mathsf{return} \ \hat{c}_A \\ \ \mathsf{else} \ \mathsf{return} \ \mathsf{ABSTAIN} \\ \\ \# \ \mathit{certify} \ \mathit{the} \ \mathit{robustness} \ \mathit{of} \ \mathit{g} \ \mathit{around} \ \mathit{x} \\ \ \mathsf{function} \ \mathsf{Certify}(f,\sigma,x,n_0,n,\alpha) \\ \ \mathsf{counts}0 \leftarrow \mathsf{SAMPLEUNDERNOISE}(f,x,n_0,\sigma) \\ \hat{c}_A \leftarrow \mathsf{top} \ \mathsf{index} \ \mathsf{in} \ \mathsf{counts}0 \\ \ \mathsf{counts} \leftarrow \mathsf{SAMPLEUNDERNOISE}(f,x,n,\sigma) \\ \ \mathit{p}_A \leftarrow \mathsf{LowerConfBound}(\mathsf{counts}[\hat{c}_A],n,1-\alpha) \\ \end{array}
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 $\overline{\mathbf{if}} p_A > \frac{1}{2}$ return prediction \hat{c}_A and radius $\sigma \Phi^{-1}(p_A)$

 $\underline{p_A}$ on the probability that $f(x+\varepsilon)=c_A$ and an upper bound $\overline{p_B}$ on the probability that $f(x+\varepsilon)$ equals any other class. Doing all three of these at the same time in a statistically correct manner requires some care. One simple solution is presented in pseudocode as CERTIFY: first, use a small number of samples from $f(x+\varepsilon)$ to take a guess at c_A ; then use a larger number of samples to estimate $\underline{p_A}$; then simply take $\overline{p_B}=1-p_A$.

Proposition 2. With probability at least $1 - \alpha$ over the randomness in CERTIFY, if CERTIFY returns a class \hat{c}_A and a radius R (i.e. does not abstain), then g predicts \hat{c}_A within radius R around x: $g(x + \delta) = \hat{c}_A \ \forall \|\delta\|_2 < R$.

The function LOWERCONFBOUND $(k, n, 1-\alpha)$ in the pseudocode returns a one-sided $(1-\alpha)$ lower confidence interval for the Binomial parameter p given a sample $k \sim \text{Binomial}(n, p)$.

Certifying large radii requires many samples Recall from Theorem 1 that R approaches ∞ as $\underline{p_A}$ approaches 1. Unfortunately, it turns out that $\underline{p_A}$ approaches 1 so slowly with n that R also approaches ∞ very slowly with n. Consider the most favorable situation: $f(x) = c_A$ everywhere. This means that g is robust at radius ∞ . But after observing n samples of $f(x+\varepsilon)$ which all equal c_A , the tightest (to our knowledge) lower bound would say that with probability least $1-\alpha$, $p_A \geq \alpha^{(1/n)}$. Plugging $\underline{p_A} = \alpha^{(1/n)}$ and $\overline{p_B} = 1 - \underline{p_A}$ into (3) yields an expression for the certified radius as a function of n: $R = \sigma \Phi^{-1}(\alpha^{1/n})$. Figure 5 (right) plots this function for $\alpha = 0.001$, $\sigma = 1$. Observe that certifying a radius of 4σ with 99.9% confidence would require $\approx 10^5$ samples.

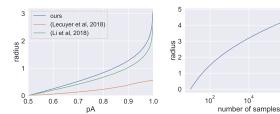


Figure 5. Left: Certified radius R as a function of $\underline{p_A}$ (with $\overline{p_B}=1-\underline{p_A}$ and $\sigma=1$) under all three randomized smoothing bounds. Right: A plot of $R=\sigma\Phi^{-1}(\alpha^{1/n})$ for $\alpha=0.001$ and $\sigma=1$. The radius we can certify with high probability grows slowly with the number of samples, even in the *best* case where $f(x)=c_A$ everywhere.

3.3. Training the base classifier

Theorem 1 holds regardless of how the base classifier f is trained. However, in order for g to classify the labeled example (x, c) correctly and robustly, f needs to consistently classify $\mathcal{N}(x, \sigma^2 I)$ as c. In high dimension, the Gaussian distribution $\mathcal{N}(x, \sigma^2 I)$ places almost no mass near its mode x. As a consequence, when σ is moderately high, the distribution of natural images has virtually disjoint support from the distribution of natural images corrupted by $\mathcal{N}(0, \sigma^2 I)$; see Figure 2 for a visual demonstration. Therefore, if the base classifier f is trained via standard supervised learning on the data distribution, it will see no noisy images during training, and hence will not necessarily learn to classify $\mathcal{N}(x,\sigma^2 I)$ with x's true label. Therefore, in this paper we follow Lecuyer et al. (2019) and train the base classifier with Gaussian data augmentation at variance σ^2 . A justification for this procedure is provided in Appendix F. However, we suspect that there may be room to improve upon this training scheme, perhaps by training the base classifier so as to maximize the smoothed classifier's certified accuracy at some tunable radius r.

4. Experiments

In adversarially robust classification, one metric of interest is the *certified test set accuracy* at radius r, defined as the fraction of the test set which g classifies correctly with a prediction that is certifiably robust within an ℓ_2 ball of radius r. However, if g is a randomized smoothing classifier, computing this quantity exactly is not possible, so we instead report the *approximate certified test set accuracy*, defined as the fraction of the test set which CERTIFY classifies correctly (without abstaining) and certifies robust with a radius $R \geq r$. Appendix D shows how to convert the approximate certified accuracy that holds with high probability over the randomness in CERTIFY. However Appendix H.2 demonstrates that when

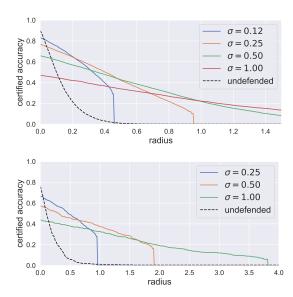


Figure 6. Approximate certified accuracy attained by randomized smoothing on CIFAR-10 (top) and ImageNet (bottom). The hyperparameter σ controls a robustness/accuracy tradeoff. The dashed black line is an upper bound on the empirical robust accuracy of an undefended classifier with the base classifier's architecture.

 α is small, the difference between these two quantities is negligible. Therefore, in our experiments we omit the step for simplicity and report approximate certified accuracies.

In all experiments, unless otherwise stated, we ran CERTIFY with $\alpha=0.001$, so there was at most a 0.1% chance that CERTIFY returned a radius in which g was not truly robust. Unless otherwise stated, when running CERTIFY we used $n_0=100$ Monte Carlo samples for selection and n=100,000 samples for estimation.

In the figures above that plot certified accuracy as a function of radius r, the certified accuracy always decreases gradually with r until reaching some point where it plummets to zero. This drop occurs because for each noise level σ and number of samples n, there is a hard upper limit to the radius we can certify with high probability, achieved when all n samples are classified by f as the same class.

ImageNet and CIFAR-10 results We applied randomized smoothing to CIFAR-10 (Krizhevsky, 2009) and ImageNet (Deng et al., 2009). On each dataset we trained several smoothed classifiers, each with a different σ . On CIFAR-10 our base classifier was a 110-layer residual network; certifying each example took 15 seconds on an NVIDIA RTX 2080 Ti. On ImageNet our base classifier was a ResNet-50; certifying each example took 110 seconds. We also trained a neural network with the base classifier's architecture on clean data, and subjected it to a DeepFool ℓ_2 adversarial attack (Moosavi-Dezfooli et al., 2016), in order

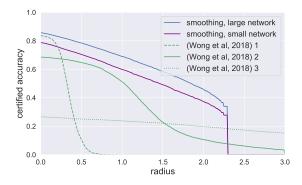
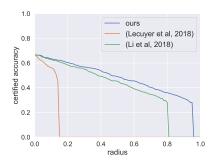


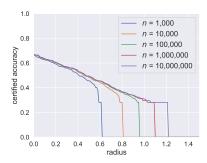
Figure 7. Comparison betwen randomized smoothing and Wong et al. (2018). Each green line is a small resnet classifier trained and certified using the method of Wong et al. (2018) with a different setting of its hyperparameter ϵ . The purple line is our method using the same small resnet architecture as the base classifier; the blue line is our method with a larger neural network as the base classifier. Wong et al. (2018) gives deterministic robustness guarantees, whereas smoothing gives high-probability guaranatees; therefore, we plot here the certified accuracy of Wong et al. (2018) against the "approximate" certified accuracy of smoothing.

to obtain an empirical upper bound on its robust accuracy. We certified the full CIFAR-10 test set and a subsample of 500 examples from the ImageNet test set.

Figure 6 plots the certified accuracy attained by smoothing with each σ . The dashed black line is the empirical upper bound on the robust accuracy of the base classifier architecture; observe that smoothing improves substantially upon the robustness of the undefended base classifier architecture. We see that σ controls a robustness/accuracy tradeoff. When σ is low, small radii can be certified with high accuracy, but large radii cannot be certified. When σ is high, larger radii can be certified, but smaller radii are certified at a lower accuracy. This observation echoes the finding in Tsipras et al. (2019) that adversarially trained networks with higher robust accuracy tend to have lower standard accuracy. Tables of these results are in Appendix E.

Figure 8 (**left**) plots the certified accuracy obtained using our Theorem 1 guarantee alongside the certified accuracy obtained using the analogous bounds of Lecuyer et al. (2019) and Li et al. (2018). Since our expression for the certified radius R is greater (and, in fact, tight), our bound delivers higher certified accuracies. Figure 8 (**middle**) projects how the certified accuracy would have changed had CERTIFY used more or fewer samples n (under the assumption that the relative class proportions in counts would have remained constant). Finally, Figure 8 (**right**) plots the certified accuracy as the confidence parameter α is varied. Observe that the certified accuracy is not very sensitive to α .





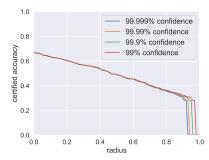


Figure 8. Experiments with randomized smoothing on ImageNet with $\sigma=0.25$. Left: certified accuracies obtained using our Theorem 1 versus those obtained using the robustness guarantees derived in prior work. Middle: projections for the certified accuracy if the number of samples n used by CERTIFY had been larger or smaller. Right: certified accuracy as the failure probability α of CERTIFY is varied.

Comparison to baselines We compared randomized smoothing to three baseline approaches for certified ℓ_2 robustness: the duality approach from Wong et al. (2018), the Lipschitz approach from Tsuzuku et al. (2018), and the approach from Weng et al. (2018a); Zhang et al. (2018). The strongest baseline was Wong et al. (2018); we defer the comparison to the other two baselines to Appendix H.

In Figure 7, we compare the largest publicly released model from Wong et al. (2018), a small resnet, to two randomized smoothing classifiers: one which used the same small resnet architecture for its base classifier, and one which used a larger 110-layer resnet for its base classifier. First, observe that smoothing with the large 110-layer resnet substantially outperforms the baseline (across all hyperparameter settings) at all radii. Second, observe that smoothing with the small resnet also outperformed the method of Wong et al. (2018) at all but the smallest radii. We attribute this latter result to the fact that neural networks trained using the method of Wong et al. (2018) are "typically overregularized to the point that many filters/weights become identically zero," per that paper. In contrast, the base classifier in randomized smoothing is a fully expressive neural network.

Prediction It is computationally expensive to certify the robustness of g around a point x, since the value of n in CERTIFY must be very large. However, it is far cheaper to evaluate g at x using PREDICT, since n can be small. For example, when we ran PREDICT on ImageNet ($\sigma = 0.25$) using n = 100, making each prediction only took 0.15 seconds, and we attained a top-1 test accuracy of 65% (Appendix E).

As discussed earlier, an adversary can potentially force PREDICT to abstain with high probability. However, it is relatively rare for PREDICT to abstain on the actual data distribution. On ImageNet ($\sigma=0.25$), PREDICT with failure probability $\alpha=0.001$ abstained 12% of the time when n=100,4% when n=1000, and 1% when n=10,000.

Empirical tightness of bound When f is linear, there always exists a class-changing perturbation just beyond the certified radius. Since neural networks are not linear, we empirically assessed the tightness of our bound by subjecting an ImageNet smoothed classifier ($\sigma=0.25$) to a projected gradient descent-style adversarial attack (Appendix J.3). For each example, we ran CERTIFY with $\alpha=0.01$, and, if the example was correctly classified and certified robust at radius R, we tried finding an adversarial example for g within radius g. We succeeded g0 of the time at radius g1.5g1.8g2 of the time at radius g2.8g3.1g3.1g4 of the time at radius g4.1g5.1g5.1g6.1g7.1g

5. Conclusion

Theorem 2 establishes that smoothing with Gaussian noise naturally confers adversarial robustness in ℓ_2 norm: if we have no knowledge about the base classifier beyond the distribution of $f(x+\varepsilon)$, then the set of perturbations to which the smoothed classifier is provably robust is precisely an ℓ_2 ball. We suspect that smoothing with other noise distributions may lead to similarly natural robustness guarantees for other perturbation sets such as general ℓ_p norm balls.

Our strong empirical results suggest that randomized smoothing is a promising direction for future research into adversarially robust classification. Many empirical approaches have been "broken," and provable approaches based on certifying neural network classifiers have not been shown to scale to networks of modern size. It seems to be computationally infeasible to reason in any sophisticated way about the decision boundaries of a large, expressive neural network. Randomized smoothing circumvents this problem: the smoothed classifier is not itself a neural network, though it leverages the discriminative ability of a neural network base classifier. To make the smoothed classifier robust, one need simply make the base classifier classify well under noise. In this way, randomized smoothing reduces the unsolved problem of adversarially robust classification to the comparably solved domain of supervised learning.

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A. Proofs of Theorems 1 and 2

Here we provide the complete proofs for Theorem 1 and Theorem 2. We fist prove the following lemma, which is essentially a restatement of the Neyman-Pearson lemma (Neyman & Pearson, 1933) from statistical hypothesis testing.

Lemma 3 (Neyman-Pearson). Let X and Y be random variables in \mathbb{R}^d with densities μ_X and μ_Y . Let $h : \mathbb{R}^d \to \{0,1\}$ be a random or deterministic function. Then:

1. If
$$S = \left\{z \in \mathbb{R}^d : \frac{\mu_Y(z)}{\mu_X(z)} \le t\right\}$$
 for some $t > 0$ and $\mathbb{P}(h(X) = 1) \ge \mathbb{P}(X \in S)$, then $\mathbb{P}(h(Y) = 1) \ge \mathbb{P}(Y \in S)$.

2. If
$$S = \left\{z \in \mathbb{R}^d : \frac{\mu_Y(z)}{\mu_X(z)} \ge t\right\}$$
 for some $t > 0$ and $\mathbb{P}(h(X) = 1) \le \mathbb{P}(X \in S)$, then $\mathbb{P}(h(Y) = 1) \le \mathbb{P}(Y \in S)$.

Proof. Without loss of generality, we assume that h is random and write h(1|x) for the probability that h(x) = 1. First we prove part 1. We denote the complement of S as S^c .

$$\begin{split} \mathbb{P}(h(Y) = 1) - \mathbb{P}(Y \in S) &= \int_{\mathbb{R}^d} h(1|z) \, \mu_Y(z) dz - \int_S \mu_Y(z) dz \\ &= \left[\int_{S^c} h(1|z) \mu_Y(z) dz + \int_S h(1|z) \mu_Y(z) dz \right] - \left[\int_S h(1|z) \mu_Y(z) dz + \int_S h(0|z) \mu_Y(z) dz \right] \\ &= \int_{S^c} h(1|z) \mu_Y(z) dz - \int_S h(0|z) \mu_Y(z) dz \\ &\geq t \left[\int_{S^c} h(1|z) \mu_X(z) dz - \int_S h(0|z) \mu_X(z) \right] \\ &= t \left[\int_{S^c} h(1|z) \mu_X(z) dz + \int_S h(1|z) \mu_X(z) dz - \int_S h(1|z) \mu_X(z) dz - \int_S h(0|z) \mu_X(z) \right] \\ &= t \left[\int_{\mathbb{R}^d} h(1|z) \mu_X(z) dz - \int_S \mu_X(z) dz \right] \\ &= t \left[\mathbb{P}(h(X) = 1) - \mathbb{P}(X \in S) \right] \\ &\geq 0 \end{split}$$

The inequality in the middle is due to the fact that $\mu_Y(z) \le t \, \mu_X(z) \, \forall z \in S$ and $\mu_Y(z) > t \, \mu_X(z) \, \forall z \in S^c$. The inequality at the end is because both terms in the product are non-negative by assumption.

The proof for part 2 is virtually identical, except both "\ge " become "\le ."

Remark: connection to statistical hypothesis testing. Part 2 of Lemma 3 is known in the field of statistical hypothesis testing as the Neyman-Pearson Lemma (Neyman & Pearson, 1933). The hypothesis testing problem is this: we are given a sample that comes from one of two distributions over \mathbb{R}^d : either the null distribution X or the alternative distribution Y. We would like to identify which distribution the sample came from. It is worse to say "Y" when the true answer is "Y." Therefore we seek a (potentially randomized) procedure $h: \mathbb{R}^d \to \{0,1\}$ which returns "Y" when the sample really came from X with probability no greater than some failure rate α . In particular, out of all such rules h, we would like the *uniformly most powerful* one h^* , i.e. the rule which is most likely to correctly say "Y" when the sample really came from Y. Neyman & Pearson (1933) showed that h^* is the rule which returns "Y" deterministically on the set $S^* = \{z \in \mathbb{R}^d : \frac{\mu_Y(z)}{\mu_X(z)} \ge t\}$ for whichever t makes $\mathbb{P}(X \in S^*) = \alpha$. In other words, to state this in a form that looks like Part 2 of Lemma 3: if h is a different rule with $\mathbb{P}(h(X) = 1) \le \alpha$, then h^* is more powerful than h, i.e. $\mathbb{P}(h(Y) = 1) \le \mathbb{P}(Y \in S^*)$.

Now we state the special case of Lemma 3 for when X and Y are isotropic Gaussians.

Lemma 4 (Neyman-Pearson for Gaussians with different means). Let $X \sim \mathcal{N}(x, \sigma^2 I)$ and $Y \sim \mathcal{N}(x + \delta, \sigma^2 I)$. Let $h : \mathbb{R}^d \to \{0, 1\}$ be any deterministic or random function. Then:

1. If
$$S = \{z \in \mathbb{R}^d : \delta^T z \leq \beta\}$$
 for some β and $\mathbb{P}(h(X) = 1) \geq \mathbb{P}(X \in S)$, then $\mathbb{P}(h(Y) = 1) \geq \mathbb{P}(Y \in S)$

$$2. \ \text{ If } S = \left\{z \in \mathbb{R}^d : \delta^T z \geq \beta \right\} \text{ for some } \beta \text{ and } \mathbb{P}(h(X) = 1) \leq \mathbb{P}(X \in S) \text{, then } \mathbb{P}(h(Y) = 1) \leq \mathbb{P}(Y \in S)$$

Proof. This lemma is the special case of Lemma 3 when X and Y are isotropic Gaussians with means x and $x + \delta$.

By Lemma 3 it suffices to simply show that for any β , there is some t > 0 for which:

$$\{z: \delta^T z \le \beta\} = \left\{z: \frac{\mu_Y(z)}{\mu_X(z)} \le t\right\} \quad \text{and} \quad \{z: \delta^T z \ge \beta\} = \left\{z: \frac{\mu_Y(z)}{\mu_X(z)} \ge t\right\}$$
 (5)

The likelihood ratio for this choice of X and Y turns out to be:

$$\frac{\mu_Y(z)}{\mu_X(z)} = \frac{\exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^d (z_i - (x_i + \delta_i))^2)\right)}{\exp\left(-\frac{1}{2\sigma^2} \sum_{i=1}^d (z_i - x_i)^2\right)}$$
$$= \exp\left(\frac{1}{2\sigma^2} \sum_{i=1}^d 2z_i \delta_i - \delta_i^2 - 2x_i \delta_i\right)$$
$$= \exp(a\delta^T z + b)$$

where a>0 and b are constants w.r.t z, specifically $a=\frac{1}{\sigma^2}$ and $b=\frac{-(2\delta^T x+\|\delta\|^2)}{2\sigma^2}$.

Therefore, given any β we may take $t = \exp(a\beta + b)$, noticing that

$$\delta^T z \le \beta \iff \exp(a\delta^T z + b) \le t$$

 $\delta^T z \ge \beta \iff \exp(a\delta^T z + b) \ge t$

Finally, we prove Theorem 1 and Theorem 2.

Theorem 1 (restated). Let $f: \mathbb{R}^d \to \mathcal{Y}$ be any deterministic or random function. Let $\varepsilon \sim \mathcal{N}(0, \sigma^2 I)$. Let $g(x) = \arg\max_{\varepsilon} \mathbb{P}(f(x+\varepsilon) = c)$. Suppose that for a specific $x \in \mathbb{R}^d$, there exist $c_A \in \mathcal{Y}$ and $p_A, \overline{p_B} \in [0,1]$ such that:

$$\mathbb{P}(f(x+\varepsilon) = c_A) \ge \underline{p_A} \ge \overline{p_B} \ge \max_{c \ne c_A} \mathbb{P}(f(x+\varepsilon) = c)$$
 (6)

Then $g(x + \delta) = c_A$ for all $\|\delta\|_2 < R$, where

$$R = \frac{\sigma}{2} (\Phi^{-1}(\underline{p_A}) - \Phi^{-1}(\overline{p_B})) \tag{7}$$

Proof. To show that $g(x + \delta) = c_A$, it follows from the definition of g that we need to show that

$$\mathbb{P}(f(x+\delta+\varepsilon)=c_A) > \max_{c_B \neq c_A} \mathbb{P}(f(x+\delta+\varepsilon)=c_B)$$

We will prove that $\mathbb{P}(f(x+\delta+\varepsilon)=c_A)>\mathbb{P}(f(x+\delta+\varepsilon)=c_B)$ for every class $c_B\neq c_A$. Fix one such class c_B without loss of generality.

For brevity, define the random variables

$$X := x + \varepsilon = \mathcal{N}(x, \sigma^2 I)$$
$$Y := x + \delta + \varepsilon = \mathcal{N}(x + \delta, \sigma^2 I)$$

In this notation, we know from (6) that

$$\mathbb{P}(f(X) = c_A) \ge p_A \quad \text{and} \quad \mathbb{P}(f(X) = c_B) \le \overline{p_B}$$
 (8)

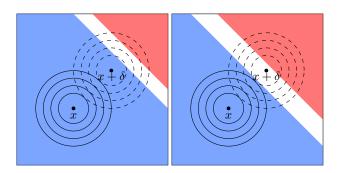


Figure 9. Illustration of the proof of Theorem 1. The solid line concentric circles are the density level sets of $X := x + \varepsilon$; the dashed line concentric circles are the level sets of $Y := x + \delta + \varepsilon$. The set A is in blue and the set B is in red. The figure on the left depicts a situation where $\mathbb{P}(Y \in A) > \mathbb{P}(Y \in B)$, and hence $g(x + \delta)$ may equal c_A . The figure on the right depicts a situation where $\mathbb{P}(Y \in A) < \mathbb{P}(Y \in B)$ and hence $g(x + \delta) \neq c_A$.

and our goal is to show that

$$\mathbb{P}(f(Y) = c_A) > \mathbb{P}(f(Y) = c_B) \tag{9}$$

Define the half-spaces:

$$A := \{ z : \delta^T(z - x) \le \sigma \| \delta \| \Phi^{-1}(\underline{p_A}) \}$$

$$B := \{ z : \delta^T(z - x) \ge \sigma \| \delta \| \Phi^{-1}(1 - \overline{p_B}) \}$$

Algebra (deferred to the end) shows that $\mathbb{P}(X \in A) = \underline{p_A}$. Therefore, by (8) we know that $\mathbb{P}(f(X) = c_A) \geq \mathbb{P}(X \in A)$. Hence we may apply Lemma 4 with $h(z) := \mathbf{1}[f(z) = \overline{c_A}]$ to conclude:

$$\mathbb{P}(f(Y) = c_A) \ge \mathbb{P}(Y \in A) \tag{10}$$

Similarly, algebra shows that $\mathbb{P}(X \in B) = \overline{p_B}$. Therefore, by (8) we know that $\mathbb{P}(f(X) = c_B) \leq \mathbb{P}(X \in B)$. Hence we may apply Lemma 4 with $h(z) := \mathbf{1}[f(z) = c_B]$ to conclude:

$$\mathbb{P}(f(Y) = c_B) \le \mathbb{P}(Y \in B) \tag{11}$$

To guarantee (9), we see from (10, 11) that it suffices to show that $\mathbb{P}(Y \in A) > \mathbb{P}(Y \in B)$, as this step completes the chain of inequalities

$$\mathbb{P}(f(Y) = c_A) \ge \mathbb{P}(Y \in A) > \mathbb{P}(Y \in B) \ge \mathbb{P}(f(Y) = c_B) \tag{12}$$

We can compute the following:

$$\mathbb{P}(Y \in A) = \Phi\left(\Phi^{-1}(\underline{p_A}) - \frac{\|\delta\|}{\sigma}\right) \tag{13}$$

$$\mathbb{P}(Y \in B) = \Phi\left(\Phi^{-1}(\overline{p_B}) + \frac{\|\delta\|}{\sigma}\right) \tag{14}$$

Finally, algebra shows that $\mathbb{P}(Y \in A) > \mathbb{P}(Y \in B)$ if and only if:

$$\|\delta\| < \frac{\sigma}{2} (\Phi^{-1}(\underline{p_A}) - \Phi^{-1}(\overline{p_B})) \tag{15}$$

which recovers the theorem statement.

We now restate and prove Theorem 2, which shows that the bound in Theorem 1 is tight. The assumption below in Theorem 2 that $\underline{p_A} + \overline{p_B} \le 1$ is mild: given any $\underline{p_A}$ and $\overline{p_B}$ which do not satisfy this condition, one could have always redefined $\overline{p_B} \leftarrow \overline{1} - \underline{p_A}$ to obtain a Theorem 1 guarantee with a larger certified radius, so there is no reason to invoke Theorem 1 unless $p_A + \overline{p_B} \le 1$.

Theorem 2 (restated). Assume $\underline{p_A} + \overline{p_B} \leq 1$. For any perturbation $\delta \in \mathbb{R}^d$ with $\|\delta\|_2 > R$, there exists a base classifier f^* consistent with the observed class probabilities (6) such that if f^* is the base classifier for g, then $g(x + \delta) \neq c_A$.

Proof. We re-use notation from the preceding proof.

Pick any class c_B arbitrarily. Define A and B as above, and consider the function

$$f^*(x) := \begin{cases} c_A & \text{if } x \in A \\ c_B & \text{if } x \in B \\ \text{other classes} & \text{otherwise} \end{cases}$$

This function is well-defined, since $A \cap B = \emptyset$ provided that $p_A + \overline{p_B} \le 1$.

By construction, the function f^* satisfies (6) with equalities, since

$$\mathbb{P}(f^*(x+\varepsilon)=c_A)=\mathbb{P}(X\in A)=p_A \qquad \mathbb{P}(f^*(x+\varepsilon)=c_B)=\mathbb{P}(X\in B)=\overline{p_B}$$

It follows from (13) and (14) that

$$\mathbb{P}(Y \in A) < \mathbb{P}(Y \in B) \iff \|\delta\|_2 > R$$

By assumption, $\|\delta\|_2 > R$, so $\mathbb{P}(Y \in A) < \mathbb{P}(Y \in B)$, or equivalently,

$$\mathbb{P}(f^*(x+\delta+\varepsilon)=c_A) < \mathbb{P}(f^*(x+\delta+\varepsilon)=c_B)$$

Therefore, if f^* is the base classifier for g, then $g(x + \delta) \neq c_A$.

A.O.1. DEFERRED ALGEBRA

Claim. $\mathbb{P}(X \in A) = p_A$

 $\textit{Proof.} \ \ \text{Recall that} \ X \sim \mathcal{N}(x, \sigma^2 I) \ \text{and} \ A = \{z: \delta^T(z-x) \leq \sigma \|\delta\|\Phi^{-1}(\underline{p_A})\}.$

$$\mathbb{P}(X \in A) = \mathbb{P}(\delta^{T}(X - x) \leq \sigma \|\delta\|\Phi^{-1}(\underline{p_{A}}))$$

$$= \mathbb{P}(\delta^{T}\mathcal{N}(0, \sigma^{2}I) \leq \sigma \|\delta\|\Phi^{-1}(\underline{p_{A}}))$$

$$= \mathbb{P}(\sigma \|\delta\|Z \leq \sigma \|\delta\|\Phi^{-1}(\underline{p_{A}}))$$

$$= \Phi(\Phi^{-1}(\underline{p_{A}}))$$

$$= p_{A}$$

$$(Z \sim \mathcal{N}(0, 1))$$

Claim. $\mathbb{P}(X \in B) = \overline{p_B}$

Proof. Recall that $X \sim \mathcal{N}(x, \sigma^2 I)$ and $B = \{z : \delta^T(z - x) \le \sigma \|\delta\|\Phi^{-1}(1 - \overline{p_B})\}.$

$$\mathbb{P}(X \in A) = \mathbb{P}(\delta^{T}(X - x) \ge \sigma \|\delta\|\Phi^{-1}(1 - \overline{p_{B}}))$$

$$= \mathbb{P}(\delta^{T}\mathcal{N}(0, \sigma^{2}I) \ge \sigma \|\delta\|\Phi^{-1}(1 - \overline{p_{B}}))$$

$$= \mathbb{P}(\sigma \|\delta\|Z \ge \sigma \|\delta\|\Phi^{-1}(1 - \overline{p_{B}}))$$

$$= \mathbb{P}(Z \ge \Phi^{-1}(1 - \overline{p_{B}}))$$

$$= 1 - \Phi(\Phi^{-1}(1 - \overline{p_{B}}))$$

$$= \overline{p_{B}}$$

$$(Z \sim \mathcal{N}(0, 1))$$

Claim.
$$\mathbb{P}(Y \in A) = \Phi\left(\Phi^{-1}(\underline{p_A}) - \frac{\|\delta\|}{\sigma}\right)$$

Proof. Recall that $Y \sim \mathcal{N}(x + \delta, \sigma^2 I)$ and $A = \{z : \delta^T(z - x) \leq \sigma \|\delta\|\Phi^{-1}(p_A)\}.$

$$\begin{split} \mathbb{P}(Y \in A) &= \mathbb{P}(\delta^{T}(Y - x) \leq \sigma \|\delta\|\Phi^{-1}(\underline{p_{A}})) \\ &= \mathbb{P}(\delta^{T}\mathcal{N}(0, \sigma^{2}I) + \|\delta\|^{2} \leq \sigma \|\delta\|\Phi^{-1}(\underline{p_{A}})) \\ &= \mathbb{P}(\sigma \|\delta\|Z \leq \sigma \|\delta\|\Phi^{-1}(\underline{p_{A}}) - \|\delta\|^{2}) \\ &= \mathbb{P}\left(Z \leq \Phi^{-1}(\underline{p_{A}}) - \frac{\|\delta\|}{\sigma}\right) \\ &= \Phi\left(\Phi^{-1}(\underline{p_{A}}) - \frac{\|\delta\|}{\sigma}\right) \end{split}$$

$$(Z \sim \mathcal{N}(0, 1))$$

Claim. $\mathbb{P}(Y \in B) = \Phi\left(\Phi^{-1}(\overline{p_B}) + \frac{\|\delta\|}{\sigma}\right)$

 $\textit{Proof.} \ \ \text{Recall that} \ Y \sim \mathcal{N}(x+\delta,\sigma^2 I) \ \text{and} \ B = \{z: \delta^T(z-x) \geq \sigma \|\delta\|\Phi^{-1}(1-\overline{p_B})\}.$

$$\mathbb{P}(Y \in B) = \mathbb{P}(\delta^{T}(Y - x) \ge \sigma \|\delta\|\Phi^{-1}(1 - \overline{p_{B}}))
= \mathbb{P}(\delta^{T}\mathcal{N}(0, \sigma^{2}I) + \|\delta\|^{2} \ge \sigma \|\delta\|\Phi^{-1}(1 - \overline{p_{B}}))
= \mathbb{P}(\sigma \|\delta\|Z + \|\delta\|^{2} \ge \sigma \|\delta\|\Phi^{-1}(1 - \overline{p_{B}}))
= \mathbb{P}\left(Z \ge \Phi^{-1}(1 - \overline{p_{B}}) - \frac{\|\delta\|}{\sigma}\right)
= \mathbb{P}\left(Z \le \Phi^{-1}(\overline{p_{B}}) + \frac{\|\delta\|}{\sigma}\right)
= \Phi\left(\Phi^{-1}(\overline{p_{B}}) + \frac{\|\delta\|}{\sigma}\right)$$

B. Smoothing a two-class linear classifier

In this appendix, we analyze what happens when the base classifier f is a two-class linear classifier $f(x) = \text{sign}(w^T x + b)$. To match the definition of g, we take $\text{sign}(\cdot)$ to be undefined when its argument is zero.

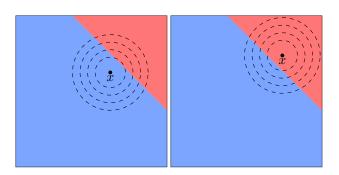


Figure 10. Illustration of Proposition 3. A binary linear classifier $f(x) = \text{sign}(w^T x + b)$ partitions \mathbb{R}^d into two half-spaces, drawn here in blue and red. An isotropic Gaussian $\mathcal{N}(x, \sigma^2 I)$ will put more mass on whichever half-space its center x lies in: in the figure on the left, x is in the blue half-space and $\mathcal{N}(x, \sigma^2 I)$ puts more mass on the blue than on red. In the figure on the right, x is in the red half-space and $\mathcal{N}(x, \sigma^2 I)$ puts more mass on red than on blue. Since the smoothed classifier's prediction g(x) is defined to be whichever half-space $\mathcal{N}(x, \sigma^2 I)$ puts more mass in, and the base classifier's prediction f(x) is defined to be whichever half-space x is in, we have that g(x) = f(x) for all x.

Our first result is that when f is a two-class linear classifier, the smoothed classifier g is identical to the base classifier f.

Proposition 3. If f is a two-class linear classifier $f(x) = sign(w^T x + b)$, and g is the smoothed version of f with any σ , then g(x) = f(x) for any x (where f is defined).

Proof. From the definition of g,

$$g(x) = 1 \iff \mathbb{P}_{\varepsilon}(f(x+\varepsilon) = 1) > \frac{1}{2}$$

$$\iff \mathbb{P}_{\varepsilon}\left(\operatorname{sign}(w^{T}(x+\varepsilon) + b) = 1\right) > \frac{1}{2}$$

$$\iff \mathbb{P}_{\varepsilon}\left(w^{T}x + w^{T}\varepsilon + b \ge 0\right) > \frac{1}{2}$$

$$\iff \mathbb{P}\left(\sigma\|w\|Z \ge -w^{T}x - b\right) > \frac{1}{2}$$

$$\iff \mathbb{P}\left(Z \le \frac{w^{T}x + b}{\sigma\|w\|}\right) > \frac{1}{2}$$

$$\iff \frac{w^{T}x + b}{\sigma\|w\|} > 0$$

$$\iff w^{T}x + b > 0$$

$$\iff f(x) = 1$$

$$(\varepsilon \sim \mathcal{N}(0, \sigma^{2}I))$$

$$(Z \sim \mathcal{N}(0, 1))$$

A similar calculation shows that $g(x) = -1 \iff f(x) = -1$.

A two-class linear classifier $f(x) = \text{sign}(w^Tx + b)$ is already certifiable: the distance from any point x to the decision boundary is $(w^Tx + b)/\|w\|_2$, and no distance with ℓ_2 norm strictly less than this distance can possibly change f's prediction. Let g be a smoothed version of f. By Proposition 3, g is identical to f, so it follows that g is truly robust around any input x within the ℓ_2 radius $(w^Tx + b)/\|w\|_2$. We now show that Theorem 1 will certify this radius, rather than a smaller, over-conservative radius.

Proposition 4. If f is a two-class linear classifier $f(x) = sign(w^T x + b)$, and g is the smoothed version of f with any σ , then invoking Theorem 1 at any x (where f is defined) with $\underline{p_A} = p_A$ and $\overline{p_B} = p_B$ will yield the certified radius $R = \frac{|w^T x + b|}{||w||}$.

Proof. In binary classification, $p_A = 1 - p_B$, so Theorem 1 returns $R = \sigma \Phi^{-1}(p_A)$.

We have:

$$\begin{aligned} p_A &= \mathbb{P}_{\varepsilon}(f(x+\varepsilon) = g(x)) \\ &= \mathbb{P}_{\varepsilon}(\operatorname{sign}(w^T(x+\varepsilon) + b) = \operatorname{sign}(w^Tx + b)) \\ &= \mathbb{P}_{\varepsilon}(\operatorname{sign}(w^Tx + \sigma || w || Z + b) = \operatorname{sign}(w^Tx + b)) \end{aligned} \tag{By Proposition 3, } g(x) = f(x))$$

There are two cases: if $w^T x + b > 0$, then

$$p_{A} = \mathbb{P}_{\varepsilon}(w^{T}x + \sigma ||w||Z + b > 0)$$

$$= \mathbb{P}_{\varepsilon} \left(Z > \frac{-w^{T}x - b}{\sigma ||w||} \right)$$

$$= \mathbb{P}_{\varepsilon} \left(Z < \frac{w^{T}x + b}{\sigma ||w||} \right)$$

$$= \Phi \left(\frac{w^{T}x + b}{\sigma ||w||} \right)$$

On the other hand, if $w^T x + b < 0$, then

$$p_A = \mathbb{P}_{\varepsilon}(w^T x + \sigma || w || Z + b < 0)$$
$$= \mathbb{P}_{\varepsilon} \left(Z < \frac{-w^T x - b}{\sigma || w ||} \right)$$
$$= \Phi \left(\frac{-w^T x - b}{\sigma || w ||} \right)$$

In either case, we have:

$$p_A = \Phi\left(\frac{|w^T x + b|}{\sigma ||w||}\right)$$

Therefore, the bound in Theorem 1 returns a radius of

$$R = \sigma \Phi^{-1}(p_A)$$
$$= \frac{|w^T x + b|}{\|w\|}$$

The previous two propositions imply that when f is a two-class linear classifier, the Theorem 1 bound is "tight" in the sense that there always exists a class-changing perturbation just beyond the certified radius.³

Proposition 5. Let f be a two-class linear classifier $f(x) = sign(w^Tx + b)$, let g be the smoothed version of f for some σ , let x be any point (where f is defined), and let R be the radius certified around x by Theorem 1. Then for any radius r > R, there exists a perturbation δ with $\|\delta\|_2 = r$ for which $g(x + \delta) \neq g(x)$.

³Note that this is a different sense of "tight" than the sense in which Theorem 2 proves that Theorem 1 is tight. Theorem 2 proves that for any fixed perturbation δ outside the radius certified by Theorem 1, there exists a base classifier f for which $g(x + \delta) \neq g(x)$. In contrast, Proposition 5 proves that for any fixed binary linear base classifier f, there exists a perturbation δ just outside the radius certified by Theorem 1 for which $g(x + \delta) \neq g(x)$.

Proof. By Proposition 3 it suffices to show that there exists some perturbation δ with $\|\delta\|_2 = r$ for which $f(x+\delta) \neq f(x)$. By Proposition 4, we know that $R = \frac{\|w^T x + b\|}{\|w\|_2}$.

If $w^Tx + b > 0$, consider the perturbation $\delta = -\frac{w}{\|w\|_2}r$. This perturbation satisfies $\|\delta\|_2 = r$ and

$$w^{T}(x+\delta) + b = w^{T}x + b + w^{T}\delta$$

$$= w^{T}x + b - ||w||_{2}r$$

$$< w^{T}x + b - ||w||_{2}R$$

$$= w^{T}x + b - |w^{T}x + b|$$

$$= w^{T}x + b - (w^{T}x + b)$$

$$= 0$$

implying that $f(x + \delta) = -1$.

Likewise, if $w^Tx+b<0$, then consider the perturbation $\delta=\frac{w}{\|w\|_2}r$. This perturbation satisfies $\|\delta\|_2=r$ and $f(x+\delta)=-1$.

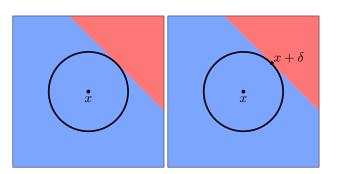


Figure 11. Left: Illustration of of Proposition 4. The red/blue half-spaces are the decision regions of both the base classifier f and the smoothed classifier g. (Since the base classifier is binary linear, g = f everywhere.) The black circle is the robustness radius R certified by Theorem 1. Right: Illustration of Proposition 5. For any r > R, there exists a perturbation δ with $\|\delta\|_2 = r$ for which $g(x + \delta) \neq g(x)$.

This special property of two-class linear classifiers is not true in general. In fact, it is possible to construct situations where g's prediction around some point x_0 is robust at radius ∞ , yet Theorem 1 only certifies a radius of τ , where τ is arbitrarily close to zero.

Proposition 6. For any $\tau > 0$, there exists a base classifier f and an input x_0 for which the corresponding smoothed classifier g is robust around x_0 at radius ∞ , yet Theorem 1 only certifies a radius of τ around x_0 .

Proof. Let $t = -\Phi^{-1}(\frac{1}{2}\Phi(\tau))$ and consider the following base classifier:

$$f(x) = \begin{cases} 1 & \text{if } x < -t \\ -1 & \text{if } -t \le x \le t \\ 1 & \text{if } x > t \end{cases}$$

Let g be the smoothed version of f with $\sigma = 1$. We will show that g(x) = 1 everywhere, implying that g's prediction is robust around $x_0 = 0$ with radius ∞ . Yet Theorem 1 only certifies a radius of τ around x_0 .

Let $Z \sim \mathcal{N}(0, 1)$. For any x, we have:

$$\begin{split} \mathbb{P}(f(x+\varepsilon) = -1) &= \mathbb{P}(-t \leq x + \varepsilon \leq t) \\ &= \mathbb{P}[-t - x \leq Z \leq t - x] \\ &\leq \mathbb{P}[-t \leq Z \leq t] \\ &= 1 - 2\Phi(-t) \\ &= 1 - \Phi(\tau) \\ &< \frac{1}{2}. \end{split} \tag{apply Lemma 5 below with } \ell = -t - x)$$

Therefore, g(x) = 1 for all x.

Meanwhile, at $x_0 = 0$, we have:

$$\mathbb{P}(f(x_0 + \varepsilon) = 1) = \mathbb{P}(f(\varepsilon) = 1)$$

$$= \mathbb{P}(Z < -t \text{ or } Z > t)$$

$$= 2\Phi(-t)$$

$$= \Phi(\tau),$$

so by Theorem 1, the certified radius around x_0 is $R = \tau$.

The proof of Proposition 6 employed the following lemma, which formalizes the visually obvious fact that out of all intervals of some fixed width 2t, the interval with maximal mass under the standard normal distribution Z is the interval [-t, t].

Lemma 5. Let $Z \sim \mathcal{N}(0,1)$. For any $\ell \in \mathbb{R}$, t > 0, we have $\mathbb{P}(\ell \le Z \le \ell + 2t) \le \mathbb{P}(-t \le Z \le t)$.

Proof. Let ϕ be the PDF of the standard normal distribution. Since ϕ is symmetric about the origin (i.e. $\phi(x) = \phi(-x) \ \forall x$),

$$\mathbb{P}(-t \le Z \le t) = 2 \int_0^t \phi(x) dx.$$

There are two cases to consider:

Case 1: The interval $[\ell, \ell+2t]$ is entirely positive, i.e. $\ell \geq 0$, or $[\ell, \ell+2t]$ is entirely negative, i.e. $\ell+2t \leq 0$.

First, we use the fact that ϕ is symmetric about the origin to rewrite $\mathbb{P}(\ell \leq Z \leq \ell + 2t)$ as the probability that Z falls in a non-negative interval [a, a + 2t] for some a.

Specifically, if $\ell \geq 0$, then let $a = \ell$. Else, if $\ell + 2t \leq 0$, then let $a = -(\ell + 2t)$. We therefore have:

$$\mathbb{P}(\ell \le Z \le \ell + 2t) = \mathbb{P}(a \le Z \le a + 2t).$$

Therefore:

$$\mathbb{P}(-t \le Z \le t) - \mathbb{P}(\ell \le Z \le \ell + 2t) = \int_0^t \phi(x) dx - \int_a^{a+t} \phi(x) dx + \int_0^t \phi(x) dx - \int_{a+t}^{a+2t} \phi(x) dx$$

$$= \int_a^{a+t} \phi(x-a) dx - \int_a^{a+t} \phi(x) dx + \int_{a+t}^{a+2t} \phi(x-a-t) dx - \int_{a+t}^{a+2t} \phi(x) dx$$

$$= \int_a^{a+t} \left[\phi(x-a) - \phi(x) \right] dx + \int_{a+t}^{a+2t} \left[\phi(x-a-t) - \phi(x) \right] dx$$

$$\ge \int_a^{a+t} 0 dx + \int_{a+t}^{a+2t} 0 dx$$

$$= 0$$

where the inequality is because ϕ is monotonically decreasing on $[0, \infty)$.

Case 2: I is partly positive, partly negative, i.e. $\ell < 0 < \ell + 2t$.

First, we use the fact that ϕ is symmetric about the origin to rewrite $\mathbb{P}(\ell \leq Z \leq \ell + 2t)$ as the sum of the probabilities that Z falls in two non-negative intervals [0,a] and [0,b] for some a,b.

Specifically, let $a = \min(-\ell, \ell + 2t)$ and $b = \max(-\ell, \ell + 2t)$. We therefore have:

$$\mathbb{P}(\ell \le Z \le \ell + 2t) = \mathbb{P}(0 \le Z \le a) + \mathbb{P}(0 \le Z \le b).$$

Note that by construction, a + b = 2t, and $0 \le a \le t$ and $t \le b \le 2t$.

We have:

$$\mathbb{P}(-t \le Z \le t) - \mathbb{P}(\ell \le Z \le \ell + 2t) = \left(\int_0^t \phi(x)dx - \int_0^a \phi(x)dx\right) - \left[\int_0^b \phi(x)dx - \int_0^t \phi(x)dx\right)$$

$$= \int_a^t \phi(x)dx - \int_t^b \phi(x)dx$$

$$= \int_a^t \phi(x)dx - \int_t^{2t-a} \phi(x)dx$$

$$= \int_a^t \phi(x)dx - \int_a^t \phi(x-a+t)dx$$

$$= \int_a^t (\phi(x) - \phi(x-a+t))dx$$

$$\ge \int_a^t 0 dx$$

$$= 0$$

where the inequality is again because ϕ is monotonically decreasing on $[0, \infty)$.

C. Practical algorithms

In this appendix, we elaborate on the prediction and certification algorithms described in Section 3.2. The pseudocode in Section 3.2 makes use of several helper functions:

- SAMPLEUNDERNOISE $(f, x, \text{num}, \sigma)$ works as follows:
 - 1. Draw num samples of noise, $\varepsilon_1 \dots \varepsilon_{\text{num}} \sim \mathcal{N}(0, \sigma^2 I)$.
 - 2. Run the noisy images through the base classifier f to obtain the predictions $f(x + \varepsilon_1), \dots, f(x + \varepsilon_{\text{num}})$.
 - 3. Return the counts for each class, where the count for class c is defined as $\sum_{i=1}^{\text{num}} \mathbf{1}[f(x+\varepsilon_i)=c]$.
- BINOMPVALUE $(n_A, n_A + n_B, p)$ returns the p-value of the two-sided hypothesis test that $n_A \sim \text{Binomial}(n_A + n_B, p)$. Using scipy.stats.binom_test, this can be implemented as: binom_test (nA, nA + nB, p).
- LOWERCONFBOUND $(k, n, 1 \alpha)$ returns a one-sided (1α) lower confidence interval for the Binomial parameter p given that $k \sim \text{Binomial}(n, p)$. In other words, it returns some number \underline{p} for which $\underline{p} \leq p$ with probability at least 1α over the sampling of $k \sim \text{Binomial}(n, p)$. Following Lecuyer et al. (2019), we chose to use the Clopper-Pearson confidence interval, which inverts the Binomial CDF (Clopper & Pearson, 1934). Using statsmodels.stats.proportion.proportion_confint, this can be implemented as

```
proportion_confint(k, n, alpha=2*alpha, method="beta")[0]
```

C.1. Prediction

The randomized algorithm given in pseudocode as PREDICT leverages the hypothesis test given in Hung & Fithian (2019) for identifying the top category of a multinomial distribution. PREDICT has one tunable hyperparameter, α . When α is small, PREDICT abstains frequently but rarely returns the wrong class. When α is large, PREDICT usually makes a prediction, but may often return the wrong class.

We now prove that with high probability, PREDICT will either return g(x) or abstain.

Proposition 1 (restated). With probability at least $1 - \alpha$ over the randomness in PREDICT, PREDICT will either abstain or return g(x). (Equivalently: the probability that PREDICT returns a class other than g(x) is at most α .)

Proof. For notational convenience, define $p_c = \mathbb{P}(f(x+\varepsilon)=c)$. Let $c_A = \max_c p_c$. Notice that by definition, $g(x) = c_A$. We can describe the randomized procedure PREDICT as follows:

- 1. Sample a vector of class counts $\{n_c\}_{c\in\mathcal{V}}$ from Multinomial $(\{p_c\}_{c\in\mathcal{V}}, n)$.
- 2. Let $\hat{c}_A = \arg \max_c n_c$ be the class whose count is largest. Let n_A and n_B be the largest count and the second-largest count, respectively.
- 3. If the p-value of the two-sided hypothesis test that n_A is drawn from Binom $(n_A + n_B, \frac{1}{2})$ is less than α , then return \hat{c}_A . Else, abstain.

The quantities c_A and the p_c 's are fixed but unknown, while the quantities \hat{c}_A , the n_c 's, n_A , and n_B are random.

We'd like to prove that the probability that PREDICT returns a class other than c_A is at most α . PREDICT returns a class other than c_A if and only if (1) $\hat{c}_A \neq c_A$ and (2) PREDICT does not abstain.

We have:

```
\begin{split} \mathbb{P}(\text{PREDICT returns class } \neq c_A) &= \mathbb{P}(\hat{c}_A \neq c_A, \text{PREDICT does not abstain}) \\ &= \mathbb{P}(\hat{c}_A \neq c_A) \; \mathbb{P}(\text{PREDICT does not abstain} | \hat{c}_A \neq c_A) \\ &\leq \mathbb{P}(\text{PREDICT does not abstain} | \hat{c}_A \neq c_A) \end{split}
```

Recall that PREDICT does not abstain if and only if the p-value of the two-sided hypothesis test that n_A is drawn from $\operatorname{Binom}(n_A+n_B,\frac{1}{2})$ is less than α . Theorem 1 in Hung & Fithian (2019) proves that the conditional probability that this event occurs given that $\hat{c}_A \neq c_A$ is exactly α . That is,

$$\mathbb{P}(\text{PREDICT does not abstain}|\hat{c}_A \neq c_A) = \alpha$$

Therefore, we have:

$$\mathbb{P}(\text{PREDICT returns class } \neq c_A) \leq \alpha$$

C.2. Certification

The certification task is: given some input x and a randomized smoothing classifier described by (f, σ) , return both (1) the prediction g(x) and (2) a radius R in which this prediction is certified robust. This task requires identifying the class c_A with maximal weight in $f(x+\varepsilon)$, estimating a lower bound $\underline{p_A}$ on $p_A := \mathbb{P}(f(x+\varepsilon) = c_A)$ and estimating an upper bound $\overline{p_B}$ on $p_B := \max_{c \neq c_A} \mathbb{P}(f(x+\varepsilon) = c)$ (Figure 1).

Suppose for simplicity that we already knew c_A and needed to obtain \underline{p}_A . We could collect n samples of $f(x+\varepsilon)$, count how many times $f(x+\varepsilon)=c_A$, and use a Binomial confidence interval to obtain a lower bound on p_A that holds with probability at least $1-\alpha$ over the n samples.

However, estimating $\underline{p_A}$ and $\overline{p_B}$ while simultaneously identifying the top class c_A is a little bit tricky, statistically speaking. We propose a simple two-step procedure. First, use n_0 samples from $f(x+\varepsilon)$ to take a guess \hat{c}_A at the identity of the top class c_A . In practice we observed that $f(x+\varepsilon)$ tends to put most of its weight on the top class, so n_0 can be set very small. Second, use n samples from $f(x+\varepsilon)$ to obtain some $\underline{p_A}$ and $\overline{p_B}$ for which $\underline{p_A} \leq p_A$ and $\overline{p_B} \geq p_B$ with probability at least $1-\alpha$. We observed that it is much more typical for the mass of $f(x+\varepsilon)$ not allocated to c_A to be allocated entirely to one runner-up class than to be allocated uniformly over all remaining classes. Therefore, the quantity $1-\underline{p_A}$ is a reasonably tight upper bound on p_B . Hence, we simply set $\overline{p_B} = 1 - p_A$, so our bound becomes

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

The full procedure is described in pseudocode as CERTIFY. If $\underline{p_A} < \frac{1}{2}$, we abstain from making a certification; this can occur especially if $\hat{c}_A \neq g(x)$, i.e. if we misidentify the top class using the first n_0 samples of $f(x + \varepsilon)$.

Proposition 2 (restated). With probability at least $1 - \alpha$ over the randomness in CERTIFY, if CERTIFY returns a class \hat{c}_A and a radius R (i.e. does not abstain), then we have the robustness guarantee

$$g(x + \delta) = \hat{c}_A$$
 whenever $\|\delta\|_2 < R$

Proof. From the contract of LOWERCONFBOUND, we know that with probability at least $1-\alpha$ over the sampling of $\varepsilon_1 \dots \varepsilon_n$, we have $\underline{p_A} \leq \mathbb{P}[f(x+\varepsilon) = \hat{c}_A]$. Notice that CERTIFY returns a class and radius only if $\underline{p_A} > \frac{1}{2}$ (otherwise it abstains). If $\underline{p_A} \leq \mathbb{P}[f(x+\varepsilon) = \hat{c}_A]$ and $\frac{1}{2} < \underline{p_A}$, then we can invoke Theorem 1 with $\overline{p_B} = 1 - \underline{p_A}$ to obtain the desired guarantee.

D. Estimating the certified test-set accuracy

In this appendix, we show how to convert the "approximate certified test accuracy" considered in the main paper into a lower bound on the true certified test accuracy that holds with high probability over the randomness in CERTIFY.

Consider a classifier g, a test set $S = \{(x_1, c_1) \dots (x_m, c_m)\}$, and a radius r. For each example $i \in [m]$, let z_i indicate whether g's prediction at x_i is both correct and robust at radius r, i.e.

$$z_i = \mathbf{1}[g(x_i + \delta) = c_i \ \forall ||\delta||_2 < r]$$

The certified test set accuracy of g at radius r is defined as $\frac{1}{m}\sum_{i=1}^m z_i$. If g is a randomized smoothing classifier, we cannot compute this quantity exactly, but we can estimate a lower bound that holds with arbitrarily high probability over the randomness in CERTIFY. In particular, suppose that we run CERTIFY with failure rate α on each example x_i in the test set. Let the Bernoulli random variable Y_i denote the event that on example i, CERTIFY returns the correct label $c_A=c_i$ and a certified radius R which is greater than r. Let $Y=\sum_{i=1}^m Y_i$. In the main paper, we referred to Y/m as the "approximate certified accuracy." It is "approximate" because $Y_i=1$ does not mean that $z_i=1$. Rather, from Proposition 2, we know the following: if $z_i=0$, then $\mathbb{P}(Y_i=1)\leq \alpha$. We now show how to exploit this fact to construct a one-sided confidence interval for the unobserved quantity $\frac{1}{m}\sum_{i=1}^m z_i$ using the observed quantities Y and m.

Theorem 6. For any $\rho > 0$, with probability at least $1 - \rho$ over the randomness in CERTIFY,

$$\frac{1}{m} \sum_{i=1}^{m} z_i \ge \frac{1}{1-\alpha} \left(\frac{Y}{m} - \alpha - \sqrt{\frac{2\alpha(1-\alpha)\log(1/\rho)}{m}} - \frac{\log(1/\rho)}{3m} \right) \tag{16}$$

Proof. Let $m_{\text{good}} = \sum_{i=1}^m z_i$ and $m_{\text{bad}} = \sum_{i=1}^m (1-z_i)$ be the number of test examples on which $z_i = 1$ or $z_i = 0$, respectively. We model $Y_i \sim \text{Bernoulli}(p_i)$, where p_i is in general unknown. Let $Y_{\text{good}} = \sum_{i:z_i=1} Y_i$ and $Y_{\text{bad}} = \sum_{i:z_i=0} Y_i$. The quantity of interest, the certified accuracy $\frac{1}{m} \sum_{i=1}^m z_i$, is equal to m_{good}/m . However, we only observe $Y = Y_{\text{good}} + Y_{\text{bad}}$.

Note that if $z_i = 0$, then $p_i \le \alpha$, so we have $\mathbb{E}[Y_i] = p_i \le \alpha$ and assuming $\alpha \le \frac{1}{2}$, we have $\text{Var}[Y_i] = p_i (1 - p_i) \le \alpha (1 - \alpha)$.

Since Y_{bad} is a sum of m_{bad} independent random variables each bounded between zero and one, with $\mathbb{E}[Y_{\text{bad}}] \leq \alpha m_{\text{bad}}$ and $\text{Var}(Y_{\text{bad}}) \leq m_{\text{bad}}\alpha(1-\alpha)$, Bernstein's inequality (Blanchard, 2007) guarantees that with probability at least $1-\rho$ over the randomness in CERTIFY,

$$Y_{\text{bad}} \le \alpha m_{\text{bad}} + \sqrt{2m_{\text{bad}}\alpha(1-\alpha)\log(1/\rho)} + \frac{\log(1/\rho)}{3}$$

From now on, we manipulate this inequality — remember that it holds with probability at least $1 - \rho$.

Since $Y = Y_{good} + Y_{bad}$, may write

$$Y_{\text{good}} \ge Y - \alpha m_{\text{bad}} - \sqrt{2m_{\text{bad}}\alpha(1-\alpha)\log(1/\rho)} - \frac{\log(1/\rho)}{3}$$

Since $m_{\text{good}} \geq Y_{\text{good}}$, we may write

$$m_{\text{good}} \ge Y - \alpha m_{\text{bad}} - \sqrt{2m_{\text{bad}}\alpha(1-\alpha)\log(1/\rho)} - \frac{\log(1/\rho)}{3}$$

Since $m_{good} + m_{bad} = m$, we may write

$$m_{\mathrm{good}} \geq \frac{1}{1-lpha} \left(Y - lpha \, m - \sqrt{2m_{\mathrm{bad}}lpha(1-lpha)\log(1/
ho)} - \frac{\log(1/
ho)}{3}
ight)$$

Finally, in order to make this confidence interval depend only on observables, we use $m_{\text{bad}} \leq m$ to write

$$m_{\rm good} \geq \frac{1}{1-\alpha} \left(Y - \alpha \, m - \sqrt{2m\alpha(1-\alpha)\log(1/\rho)} - \frac{\log(1/\rho)}{3} \right)$$

Dividing both sides of the inequality by m recovers the theorem statement.

E. ImageNet and CIFAR-10 Results

E.1. Certification

Tables 2 and 3 show the approximate certified top-1 test set accuracy of randomized smoothing on ImageNet and CIFAR-10 with various noise levels σ . By "approximate certified accuracy," we mean that we ran CERTIFY on a subsample of the test set, and for each r we report the fraction of examples on which CERTIFY (a) did not abstain, (b) returned the correct class, and (c) returned a radius R greater than r. There is some probability (at most α) that any example's certification is inaccurate. We used $\alpha=0.001$ and n=100000. On CIFAR-10 our base classifier was a 110-layer residual network and we certified the full test set; on ImageNet our base classifier was a ResNet-50 and we certified a subsample of 500 points. Note that the certified accuracy at r=0 is just the standard accuracy of the smoothed classifier. See Appendix J for more experimental details.

	r = 0.0	r = 0.5	r = 1.0	r = 1.5	r = 2.0	r = 2.5	r = 3.0
$\sigma = 0.25$							
$\sigma = 0.50$	0.57	0.46	0.37	0.29	0.00	0.00	0.00
$\sigma = 1.00$	0.44	0.38	0.33	0.26	0.19	0.15	0.12

Table 2. Approximate certified test accuracy on ImageNet. Each row is a setting of the hyperparameter σ , each column is an ℓ_2 radius. The entry of the best σ for each radius is bolded. For comparison, random guessing would attain 0.001 accuracy.

	r = 0.0	r = 0.25	r = 0.5	r = 0.75	r = 1.0	r = 1.25	r = 1.5
$\sigma = 0.12$	0.83	0.60	0.00	0.00	0.00	0.00	0.00
$\sigma = 0.25$	0.77	0.61	0.42	0.25	0.00	0.00	0.00
$\sigma = 0.50$	0.66	0.55	0.43	0.32	0.22	0.14	0.08
$\sigma = 1.00$	0.47	0.41	0.34	0.28	0.22	0.17	0.14

Table 3. Approximate certified test accuracy on CIFAR-10. Each row is a setting of the hyperparameter σ , each column is an ℓ_2 radius. The entry of the best σ for each radius is bolded. For comparison, random guessing would attain 0.1 accuracy.

E.2. Prediction

Table 4 shows the performance of PREDICT as the number of Monte Carlo samples n is varied between 100 and 10,000. Suppose that for some test example (x, c), PREDICT returns the label \hat{c}_A . We say that this prediction was *correct* if $\hat{c}_A = c$ and we say that this prediction was *accurate* if $\hat{c}_A = g(x)$. For example, a prediction could be correct but inaccurate if g is wrong at x, yet PREDICT accidentally returns the correct class. Ideally, we'd like PREDICT to be both correct and accurate.

With n=100 Monte Carlo samples and a failure rate of $\alpha=0.001$, PREDICT is cheap to evaluate (0.15 seconds on our hardware) yet it attains relatively high top-1 accuracy of 65% on the ImageNet test set, and only abstains 12% of the time. When we use n=10,000 Monte Carlo samples, PREDICT takes longer to evaluate (15 seconds), yet only abstains 4% of the time. Interestingly, we observe from Table 4 that most of the abstentions when n=100 were for examples on which g was wrong, so in practice we would lose little accuracy by taking n to be as small as 100.

	CORRECT, ACCURATE	CORRECT, INACCURATE	INCORRECT, ACCURATE	INCORRECT, INACCURATE	ABSTAIN
N					
100	0.65	0.00	0.23	0.00	0.12
1000	0.68	0.00	0.28	0.00	0.04
10000	0.69	0.00	0.30	0.00	0.01

Table 4. Performance of PRECICT as n is varied. The dataset was ImageNet and $\sigma=0.25$, $\alpha=0.001$. Each column shows the fraction of test examples which ended up in one of five categories; the prediction at x is "correct" if PREDICT returned the true label, while the prediction is "accurate" if PREDICT returned g(x). Computing g(x) exactly is not possible, so in order to determine whether PREDICT was accurate, we took the gold standard to be the top class over n=100,000 Monte Carlo samples.

F. Training with Noise

As mentioned in section 3.3, in the experiments for this paper, we followed Lecuyer et al. (2019) and trained the base classifier by minimizing the cross-entropy loss with Gaussian data augmentation. We now provide some justification for this idea

Let $\{(x_1, c_1), \dots, (x_n, c_n)\}$ be a training dataset. We assume that the base classifier takes the form $f(x) = \arg\max_{c \in \mathcal{V}} f_c(x)$, where each f_c is the scoring function for class c.

Suppose that our goal is to maximize the sum of of the log-probabilities that f will classify each $x_i + \varepsilon$ as c_i :

$$\sum_{i=1}^{n} \log \mathbb{P}_{\varepsilon}(f(x_i + \varepsilon) = c_i) = \sum_{i=1}^{n} \log \mathbb{E}_{\varepsilon} \mathbf{1} \left[\arg \max_{c} f_c(x_i + \varepsilon) = c_i \right]$$
(17)

Recall that the softmax function can be interpreted as a continuous, differentiable approximation to arg max:

$$\mathbf{1}\left[\arg\max_{c} f_c(x_i + \varepsilon) = c_i\right] \approx \frac{\exp(f_{c_i}(x_i + \varepsilon))}{\sum_{c \in \mathcal{V}} \exp(f_c(x_i + \varepsilon))}$$

Therefore, our objective is approximately equal to:

$$\sum_{i=1}^{n} \log \mathbb{E}_{\varepsilon} \left[\frac{\exp(f_{c_i}(x_i + \varepsilon))}{\sum_{c \in \mathcal{Y}} \exp(f_c(x_i + \varepsilon))} \right]$$
 (18)

By Jensen's inequality and the concavity of log, this quantity is lower-bounded by:

$$\sum_{i=1}^{n} \mathbb{E}_{\varepsilon} \left[\log \frac{\exp(f_{c_i}(x_i + \varepsilon))}{\sum_{c \in \mathcal{Y}} \exp(f_c(x_i + \varepsilon))} \right]$$

which is the negative of the cross-entropy loss under Gaussian data augmentation.

Therefore, minimizing the cross-entropy loss under Gaussian data augmentation will maximize (18), which will approximately maximize (17).

G. Noise Level can Scale with Input Resolution

Since our robustness guarantee (3) in Theorem 1 does not explicitly depend on the data dimension d, one might worry that randomized smoothing is less effective for images in high resolution — certifying a fixed ℓ_2 radius is "less impressive" for, say, 224×224 image than for a 56×56 image. However, it turns out that in high resolution, images can be corrupted with larger levels of isotropic Gaussian noise while still preserving their content. This fact is made clear by Figure 12, which shows an image at high and low resolution corrupted by Gaussian noise with the same variance.full The class ("hummingbird") is easy to discern from the high-resolution noisy image, but not from the low-resolution noisy image. As a consequence, in high resolution one can take σ to be larger while still being able to obtain a base classifier that classifies noisy images accurately. Since our Theorem 1 robustness guarantee scales linearly with σ , this means that in high resolution one can certify larger radii.

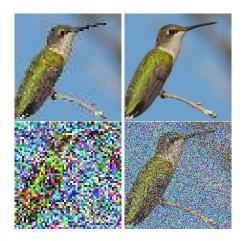


Figure 12. **Top**: An ImageNet image from class "hummingbird" in resolutions 56x56 (left) and 224x224 (right). **Bottom**: the same images corrupted by isotropic Gaussian noise at $\sigma = 0.5$. On noiseless images the class is easy to distinguish no matter the resolution, but on noisy data the class is much easier to distinguish when the resolution is high.

The argument above can be made rigorous, though we first need to decide what it means for two images to be high- and low-resolution versions of each other. Here we present one solution:

Let \mathcal{X} denote the space of "high-resolution" images in dimension $2k \times 2k \times 3$, and let \mathcal{X}' denote the space of "low-resolution" images in dimension $k \times k \times 3$. Let AVGPOOL: $\mathcal{X} \to \mathcal{X}'$ be the function which takes as input an image x in dimension $2k \times 2k \times 3$, averages together every 2x2 square of pixels, and outputs an image in dimension $k \times k \times 3$.

Equipped with these definitions, we can say that $(x, x') \in \mathcal{X} \times \mathcal{X}'$ are a high/low resolution image pair if x' = AVGPOOL(x).

Proposition 7. Given any smoothing classifier $g': \mathcal{X}' \to \mathcal{Y}$, one can construct a smoothing classifier $g: \mathcal{X} \to \mathcal{Y}$ with the following property: for any $x \in \mathcal{X}$ and $x' = \mathsf{AVGPOOL}(x)$, g predicts the same class at x that g' predicts at x', but is certifiably robust at twice the radius.

Proof. Given some smoothing classifier $g'=(f',\sigma')$ from \mathcal{X}' to \mathcal{Y} , define g to be the smoothing classifier (f,σ) from \mathcal{X} to \mathcal{Y} with noise level $\sigma=2\sigma'$ and base classifier $f(x)=f'(\operatorname{AVGPOOL}(x))$. Note that the average of four independent copies of $\mathcal{N}(0,(2\sigma)^2)$ is distributed as $\mathcal{N}(0,\sigma^2)$. Therefore, for any high/low-resolution image pair $x'=\operatorname{AVGPOOL}(x)$, the random variable $\operatorname{AVGPOOL}(x+\varepsilon)$, where $\varepsilon\sim\mathcal{N}(0,(2\sigma)^2I_{2k\times 2k\times 3})$, is equal in distribution to the random variable $x'+\varepsilon'$, where $\varepsilon'\sim\mathcal{N}(0,\sigma^2I_{k\times k\times 3})$. Hence, $f(x+\varepsilon)=f'(\operatorname{AVGPOOL}(x+\varepsilon))$ has the same distribution as $f'(x'+\varepsilon')$. By the definition of g, this means that g(x)=g'(x'), Additionally, by Theorem 1, since $\sigma=2\sigma'$, this means that g's prediction at x is certifiably robust at twice the radius as g''s prediction at x'.

H. Additional Experiments

H.1. Comparisons to baselines

Figure 13 compares the certified accuracy of a smoothed 20-layer resnet to that of the released models from two recent works on certified ℓ_2 robustness: the Lipschitz approach from Tsuzuku et al. (2018) and the approach from Zhang et al. (2018). Note that in these experiments, the base classifier for smoothing was larger than the networks of competing approaches. The comparison to Zhang et al. (2018) is on CIFAR-10, while the comparison to Tsuzuku et al. (2018) is on SVHN. Note that for each comparison, we preprocessed the dataset to follow the preprocessing used when the baseline was trained; therefore, the radii reported for CIFAR-10 here are not comparable to the radii reported elsewhere in this paper. Full experimental details are in Appendix J.

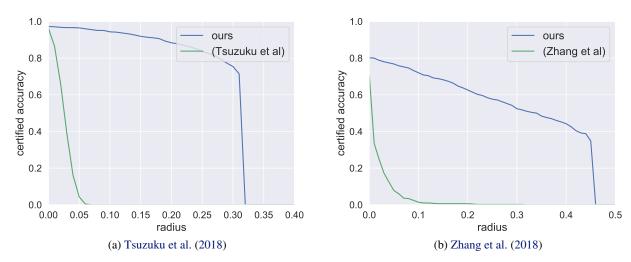


Figure 13. Randomized smoothing with a 20-layer resnet base classifier attains higher certified accuracy than the released models from two recent works on certified ℓ_2 robustness.

H.2. High-probability guarantees

Appendix D details how to use CERTIFY to obtain a lower bound on the certified test accuracy at radius r of a randomized smoothing classifier that holds with high probability over the randomness in CERTIFY. In the main paper, we declined to do this and simply reported the approximate certified test accuracy, defined as the fraction of test examples for which CERTIFY gives the correct prediction and certifies it at radius r. Of course, with some probability (guaranteed to be less than α), each of these certifications is wrong.

However, we now demonstrate empirically that there is a negligible difference between a proper high-probability lower bound on the certified accuracy and the approximate version that we reported in the paper. We created a randomized smoothing classifier g on ImageNet with a ResNet-50 base classifier and noise level $\sigma=0.25$. We used CERTIFY with $\alpha=0.001$ to certify a subsample of 500 examples from the ImageNet test set. From this we computed the approximate certified test accuracy at each radius r. Then we used the correction from Appendix D with $\rho=0.001$ to obtain a lower bound on the certified test accuracy at r that holds pointwise with probability at least $1-\rho$ over the randomness in CERTIFY. Figure 14 plots both quantities as a function of r. Observe that the difference is so negligible that the lines almost overlap.

H.3. How much noise to use when training the base classifier?

In the main paper, whenever we created a randomized smoothing classifier g at noise level σ , we always trained the corresponding base classifier f with Gaussian data augmentation at noise level σ . In Figure 15, we show the effects of training the base classifier with a different level of Gaussian noise. Observe that g has a lower certified accuracy if f was trained using a different noise level. It seems to be worse to train with noise $< \sigma$ than to train with noise $> \sigma$.

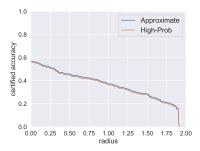


Figure 14. The difference between the approximate certified accuracy, and a high-probability lower bound on the certified accuracy, is negligible.

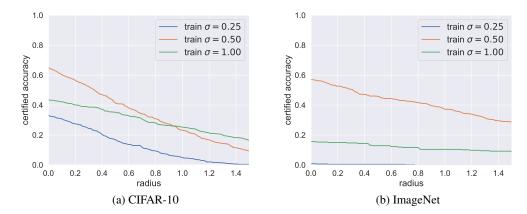


Figure 15. Vary training noise while holding prediction noise fixed at $\sigma = 0.50$.

I. Derivation of Prior Randomized Smoothing Guarantees

In this appendix, we derive the randomized smoothing guarantees of Lecuyer et al. (2019) and Li et al. (2018) using the notation of our paper. Both guarantees take same general form as ours, except with a different expression for R:

Theorem (generic guarantee): Let $f: \mathbb{R}^d \to \mathcal{Y}$ be any deterministic or random function, and let $\varepsilon \sim \mathcal{N}(0, \sigma^2 I)$. Let g be defined as in (1). Suppose $c_A \in \mathcal{Y}$ and $\underline{p_A}, \overline{p_B} \in [0, 1]$ satisfy:

$$\mathbb{P}(f(x+\varepsilon)=c_A) \ge \underline{p_A} \ge \overline{p_B} \ge \max_{c \ne c_A} \mathbb{P}(f(x+\varepsilon)=c)$$
(19)

Then $g(x + \delta) = c_A$ for all $\|\delta\|_2 < R$.

For convenience, define the notation $X \sim \mathcal{N}(x, \sigma^2 I)$ and $Y \sim \mathcal{N}(x + \delta, \sigma^2 I)$.

I.1. Lecuyer et al. (2019)

Lecuyer et al. (2019) proved a version of the generic robustness guarantee in which

$$R = \sup_{0<\beta \leq \min\left(1,\frac{1}{2}\log\frac{\overline{p_A}}{\overline{p_B}}\right)} \frac{\sigma\beta}{\sqrt{2\log\left(\frac{1.25(1+\exp(\beta))}{\underline{p_A}-\exp(2\beta)\overline{p_B}}\right)}}$$

Proof. In order to avoid notation that conflicts with the rest of this paper, we use β and γ where Lecuyer et al. (2019) used ϵ and δ .

Suppose that we have some $0 < \beta \le 1$ and $\gamma > 0$ such that

$$\sigma^2 = \frac{\|\delta\|^2}{\beta^2} 2\log\frac{1.25}{\gamma} \tag{20}$$

The "Gaussian mechanism" from differential privacy guarantees that:

$$\mathbb{P}(f(X) = c_A) \le \exp(\beta)\mathbb{P}(f(Y) = c_A) + \gamma \tag{21}$$

and, symmetrically,

$$\mathbb{P}(f(Y) = c_B) \le \exp(\beta)\mathbb{P}(f(X) = c_B) + \gamma \tag{22}$$

See Lecuyer et al. (2019), Lemma 2 for how to obtain this form from the standard form of the (β, γ) DP definition.

Fix a perturbation δ . To guarantee that $g(x + \delta) = c_A$, we need to show that $\mathbb{P}(f(Y) = c_A) > \mathbb{P}(f(Y) = c_B)$ for each $c_B \neq c_A$.

Together, (21) and (22) imply that to guarantee $\mathbb{P}(f(Y) = c_A) > \mathbb{P}(f(Y) = c_B)$ for any c_B , it suffices to show that:

$$\mathbb{P}(f(X) = c_A) > \exp(2\beta)\mathbb{P}(f(X) = c_B) + \gamma(1 + \exp(\beta)) \tag{23}$$

Therefore, in order to guarantee that $\mathbb{P}(f(Y) = c_A) > \mathbb{P}(f(Y) = c_B)$ for each $c_B \neq c_A$, by (19) it suffices to show:

$$p_A > \exp(2\beta)\overline{p_B} + \gamma(1 + \exp(\beta))$$
 (24)

Now, inverting (20), we obtain:

$$\gamma = 1.25 \exp\left(-\frac{\sigma^2 \beta^2}{2\|\delta\|^2}\right) \tag{25}$$

Plugging (25) into (24), we see that to guarantee $\mathbb{P}(f(Y) = c_A) \geq \mathbb{P}(f(Y) = c_B)$ it suffices to show that:

$$\underline{p_A} > \exp(2\beta)\overline{p_B} + 1.25 \exp\left(-\frac{\sigma^2 \beta^2}{2\|\delta\|^2}\right) (1 + \exp(\beta)) \tag{26}$$

which rearranges to:

$$\frac{\underline{p_A} - \exp(2\beta)\overline{p_B}}{1.25(1 + \exp(\beta))} > \exp\left(-\frac{\sigma^2 \beta^2}{2\|\delta\|^2}\right) \tag{27}$$

Since the RHS is always positive, and the denominator on the LHS is always positive, this condition can only possibly hold if the numerator on the LHS is positive. Therefore, we need to restrict β to

$$0 < \beta \le \min\left(1, \frac{1}{2}\log\frac{p_A}{\overline{p_B}}\right) \tag{28}$$

The condition (27) is equivalent to:

$$\|\delta\|^2 \log \frac{1.25(1 + \exp(\beta))}{p_A - \exp(2\beta)\overline{p_B}} < \frac{\sigma^2 \beta^2}{2}$$
 (29)

Since $\underline{p_A} \le 1$ and $\overline{p_B} \ge 0$, the denominator in the LHS is ≤ 1 which is in turn \le the numerator on the LHS. Therefore, the term inside the log in the LHS is greater than 1, so the log term on the LHS is greater than zero. Therefore, we may divide both sides of the inequality by the log term on the LHS to obtain:

$$\|\delta\|^2 < \frac{\sigma^2 \beta^2}{2\log\left(\frac{1.25(1+\exp(\beta))}{\underline{p_A}-\exp(2\beta)\overline{p_B}}\right)}$$
(30)

Finally, we take the square root and maximize the bound over all valid β (28) to yield:

$$\|\delta\| < \sup_{0 < \beta \le \min\left(1, \frac{1}{2}\log\frac{\overline{P_A}}{\overline{P_B}}\right)} \frac{\sigma\beta}{\sqrt{2\log\left(\frac{1.25(1 + \exp(\beta))}{\overline{P_A} - \exp(2\beta)\overline{P_B}}\right)}}$$
(31)

Figure 16a plots this bound at varying settings of the tuning parameter β , while Figure 16c plots how the bound varies with β for a fixed p_A and $\overline{p_B}$.

I.2. Li et al. (2018)

Li et al. (2018) proved a version of the generic robustness guarantee in which

$$R = \sup_{\alpha > 0} \sigma \sqrt{-\frac{2}{\alpha} \log \left(1 - \underline{p_A} - \overline{p_B} + 2\left(\frac{1}{2}(\underline{p_A}^{1-\alpha} + \overline{p_B}^{1-\alpha})^{1-\alpha}\right)\right)}$$

Proof. A generalization of KL divergence, the α -Renyi divergence is an information theoretic measure of distance between two distributions. It is parameterized by some $\alpha > 0$. The α -Renyi divergence between two discrete distributions P and Q is defined as:

$$D_{\alpha}(P||Q) := \frac{1}{\alpha - 1} \log \left(\sum_{i=1}^{k} \frac{p_i^{\alpha}}{q_i^{\alpha - 1}} \right)$$
(32)

In the continuous case, this sum is replaced with an integral. The divergence is undefined when $\alpha=1$ since a division by zero occurs, but the limit of $D_{\alpha}(P||Q)$ as $\alpha \to 1$ is the KL divergence between P and Q.

Li et al. (2018) prove that if P is a discrete distribution for which the highest probability class has probability $\geq \underline{p_A}$ and all other classes have probability $\leq \overline{p_B}$, then for any other discrete distribution Q for which

$$D_{\alpha}(P||Q) < -\log\left(1 - \underline{p_A} - \overline{p_B} + 2\left(\frac{1}{2}(\underline{p_A}^{1-\alpha} + \overline{p_B}^{1-\alpha})^{1-\alpha}\right)\right)$$
(33)

the highest-probability class in Q is guaranteed to be the same as the highest-probability class in P.

We now apply this result to the discrete distributions P = f(X) and Q = f(Y). If $D_{\alpha}(f(X)||f(Y))$ satisfies (33), then it is guaranteed that $g(x) = g(x + \delta)$.

The data processing inequality states that applying a function to two random variables can only decrease the α -Renyi divergence between them. In particular,

$$D_{\alpha}(f(X)||f(Y)) < D_{\alpha}(X||Y) \tag{34}$$

There is a closed-form expression for the α -Renyi divergence between two Gaussians:

$$D_{\alpha}(X||Y) = \frac{\alpha \|\delta\|^2}{2\sigma^2} \tag{35}$$

Therefore, we can guarantee that $g(x + \delta) = c_A$ so long as

$$\frac{\alpha \|\delta\|^2}{2\sigma^2} < -\log\left(1 - \underline{p_A} - \overline{p_B} + 2\left(\frac{1}{2}(\underline{p_A}^{1-\alpha} + \overline{p_B}^{1-\alpha})^{1-\alpha}\right)\right) \tag{36}$$

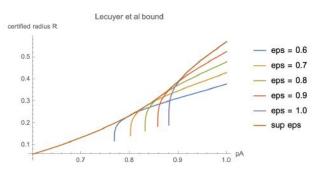
which simplifies to

$$\|\delta\| < \sigma \sqrt{-\frac{2}{\alpha} \log \left(1 - \underline{p_A} - \overline{p_B} + 2\left(\frac{1}{2}(\underline{p_A}^{1-\alpha} + \overline{p_B}^{1-\alpha})^{1-\alpha}\right)\right)}$$
 (37)

Finally, since this result holds for any $\alpha > 0$, we may maximize over α to obtain the largest possible certified radius:

$$\|\delta\| < \sup_{\alpha > 0} \sigma \sqrt{-\frac{2}{\alpha} \log \left(1 - \underline{p_A} - \overline{p_B} + 2\left(\frac{1}{2}(\underline{p_A}^{1-\alpha} + \overline{p_B}^{1-\alpha})^{1-\alpha}\right)\right)}$$
 (38)

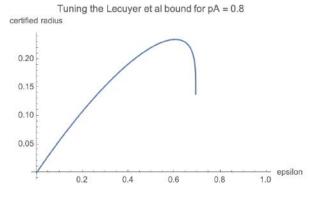
Figure 16b plots this bound at varying settings of the tuning parameter α , while figure 16d plots how the bound varies with α for a fixed p_A and $\overline{p_B}$.

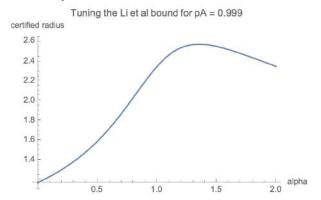


- alpha = 0.5
- alpha = 0.5
- alpha = 0.9
- alpha = 1.1
- alpha = 4.0
- sup alpha
- sup alpha

(a) The Lecuyer et al. (2019) bound over several settings of β . The brown line is the pointwise supremum over all eligible β , computed numerically.

(b) The Li et al. (2018) bound over several settings of α . The purple line is the pointwise supremum over all eligible α , computed numerically.





(c) Tuning the Lecuyer et al. (2019) bound wrt β when $\underline{p_A}=0.8, \overline{p_B}=0.2$

(d) Tuning the Li et al. (2018) bound wrt α when $\underline{p_A}=0.999, \overline{p_B}=0.0001$

J. Experiment Details

J.1. Comparison to baselines

We compared randomized smoothing against three recent approaches for ℓ_2 -robust classification (Tsuzuku et al., 2018; Wong et al., 2018; Zhang et al., 2018). Tsuzuku et al. (2018) and Wong et al. (2018) propose both a robust training method and a complementary certification mechanism, while Zhang et al. (2018) propose a method to certify generically trained networks. In all cases we compared against networks provided by the authors. We compared against Wong et al. (2018) and Zhang et al. (2018) on CIFAR-10, and we compared against Tsuzuku et al. (2018) on SVHN.

In image classification it is common practice to preprocess a dataset by subtracting from each channel the mean over the dataset, and dividing each channel by the standard deviation over the dataset. However, we wanted to report certified radii in the original image coordinates rather than in the standardized coordinates. Therefore, throughout most of this work we *first* added the Gaussian noise, and *then* standardized the channels, before feeding the image to the base classifier. (In the practical PyTorch implementation, the first layer of the base classifier was a layer that standardized the input.) However, all of the baselines we compared against provided pre-trained networks which assumed that the dataset was first preprocessed in a specific way. Therefore, when comparing against the baselines we also preprocessed the datasets first, so that we could report certified radii that were directly comparable to the radii reported by the baseline methods.

Comparison to Wong et al. (2018) Following Wong et al. (2018), the CIFAR-10 dataset was preprocessed by subtracting (0.485, 0.456, 0.406) and dividing by (0.225, 0.225, 0.225).

While the body of the Wong et al. (2018) paper focuses on ℓ_{∞} certified robustness, their algorithm naturally extends to ℓ_2 certified robustness, as developed in the appendix of the paper. We used three ℓ_2 -trained residual networks publicly released by the authors, each trained with a different setting of their hyperparameter $\epsilon \in \{0.157, 0.628, 2.51\}$. We used code publicly released by the authors at https://github.com/locuslab/convex_adversarial/blob/master/

examples/cifar_evaluate.py to compute the robustness radius of test images. The code accepts a radius and returns TRUE (robust) or FALSE (not robust); we incorporated this subroutine into a binary search procedure to find the largest radius for which the code returned TRUE.

For randomized smoothing we used $\sigma=0.6$ and a 20-layer residual network base classifier. We ran CERTIFY with $n_0=100$, n=100,000 and $\alpha=0.001$.

For both methods, we certified the full CIFAR-10 test set.

Comparison to Tsuzuku et al. (2018) Following Tsuzuku et al. (2018), the SVHN dataset was not preprocessed except that pixels were divided by 255 so as to lie within [0, 1].

We compared against a pretrained network provided to us by the authors in which the hyperparameter of their method was set to c = 0.1. The network was a wide residual network with 16 layers and a width factor of 4. We used the authors' code at https://github.com/ytsmiling/lmt to compute the robustness radius of test images.

For randomized smoothing we used $\sigma=0.1$ and a 20-layer residual network base classifier. We ran CERTIFY with $n_0=100$, n=100,000 and $\alpha=0.001$.

For both methods, we certified the whole SVHN test set.

Comparison to Zhang et al. (2018) Following Zhang et al. (2018), the CIFAR-10 dataset was preprocessed by subtracting 0.5 from each pixel.

We compared against the cifar_7_1024_vanilla network released by the authors, which is a 7-layer MLP. We used the authors' code at https://github.com/IBM/CROWN-Robustness-Certification to compute the robustness radius of test images.

For randomized smoothing we used $\sigma=1.2$ and a 20-layer residual network base classifier. We ran CERTIFY with $n_0=100$, n=100,000 and $\alpha=0.001$.

For randomized smoothing, we certified the whole CIFAR-10 test set. For Zhang et al. (2018), we certified every fourth image in the CIFAR-10 test set.

J.2. ImageNet and CIFAR-10 Experiments

Our code is available at http://github.com/locuslab/smoothing.

In order to report certified radii in the original coordinates, we *first* added Gaussian noise, and *then* standardized the data. Specifically, in our PyTorch implementation, the first layer of the base classifier was a normalization layer that performed a channel-wise standardization of its input. For CIFAR-10 we subtracted the dataset mean (0.4914, 0.4822, 0.4465) and divided by the dataset standard deviation (0.2023, 0.1994, 0.2010). For ImageNet we subtracted the dataset mean (0.485, 0.456, 0.406) and divided by the standard deviation (0.229, 0.224, 0.225).

For both ImageNet and CIFAR-10, we trained the base classifier with random horizontal flips and random crops (in addition to the Gaussian data augmentation discussed explicitly in the paper). On ImageNet we trained with synchronous SGD on four NVIDIA RTX 2080 Ti GPUs; training took approximately three days.

On ImageNet our base classifier used the ResNet-50 architecture provided in torchvision. On CIFAR-10 we used a 110-layer residual network from https://github.com/bearpaw/pytorch-classification.

On ImageNet we certified every 100-th image in the validation set, for 500 images total. On CIFAR-10 we certified the whole test set.

In Figure 8 (**middle**) we fixed $\sigma=0.25$ and $\alpha=0.001$ while varying the number of samples n. We did not actually vary the number of samples n that we simulated: we kept this number fixed at 100,000 but varied the number that we fed the Clopper-Pearson confidence interval.

In Figure 8 (**right**), we fixed $\sigma = 0.25$ and n = 100,000 while varying α .

J.3. Adversarial Attacks

As discussed in Section 4, we subjected smoothed classifiers to a projected gradient descent-style adversarial attack. We now describe the details of this attack.

Let f be the base classifier and let σ be the noise level. Following Li et al. (2018), given an example $(x, c) \in \mathbb{R}^d \times \mathcal{Y}$ and a radius r, we used a projected gradient descent style adversarial attack to optimize the objective:

$$\underset{\delta:\|\delta\|_{2} < r}{\arg\max} \ \mathbb{E}_{\varepsilon \sim \mathcal{N}(0,\sigma^{2}I)} \left[\ell(f(x+\delta+\varepsilon),c) \right]$$
(39)

where ℓ is the softmax loss function. (Breaking notation with the rest of the paper in which f returns a class, the function f here refers to the function that maps an image in \mathbb{R}^d to a vector of classwise scores.)

At each iteration of the attack, we drew k samples of noise, $\varepsilon_1 \dots \varepsilon_k \sim \mathcal{N}(0, \sigma^2 I)$, and followed the stochastic gradient $g_t = \sum_{i=1}^k \nabla_{\delta_t} \ell(f(x+\delta_t+\varepsilon_k), c)$.

As is typical (Kolter & Madry, 2018), we used a "steepest ascent" update rule, which, for the ℓ_2 norm, means that we normalized the gradient before applying the update. The overall PGD update is: $\delta_{t+1} = \operatorname{proj}_r\left(\delta_t + \eta \frac{g_t}{\|g_t\|}\right)$ where the function proj_r that projects its input onto the ball $\{z: \|z\|_2 \le r\}$ is given by $\operatorname{proj}_r(z) = \frac{rz}{\max(r, \|z\|_2)}$. We used a constant step size η and a fixed number T of PGD iterations.

In practice, our step size was $\eta=0.1$, we used T=20 steps of PGD, and we computed the stochastic gradient using k=1000 Monte Carlo samples.

Unfortunately, the objective we optimize (39) is not actually the attack objective of interest. To force a misclassification, an attacker needs to find some perturbation δ with $\|\delta\|_2 < r$ and some class c_B for which

$$\mathbb{P}_{\varepsilon \sim \mathcal{N}(0, \sigma^2 I)}(f(x + \delta + \varepsilon) = c_B) \ge \mathbb{P}_{\varepsilon \sim \mathcal{N}(0, \sigma^2 I)}(f(x + \delta + \varepsilon) = c)$$

Effective adversarial attacks against randomized smoothing are outside the scope of this paper.

K. Examples of Noisy Images

We now show examples of CIFAR-10 and ImageNet images corrupted with varying levels of noise.

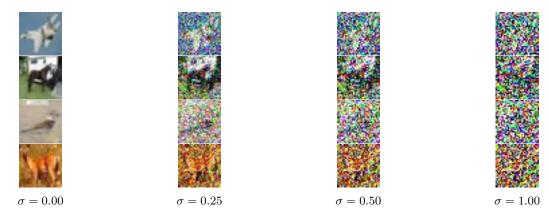


Figure 17. CIFAR-10 images additively corrupted by varying levels of Gaussian noise $\mathcal{N}(0, \sigma^2 I)$. Pixel values greater than 1.0 (=255) or less than 0.0 (=0) were clipped to 1.0 or 0.0.

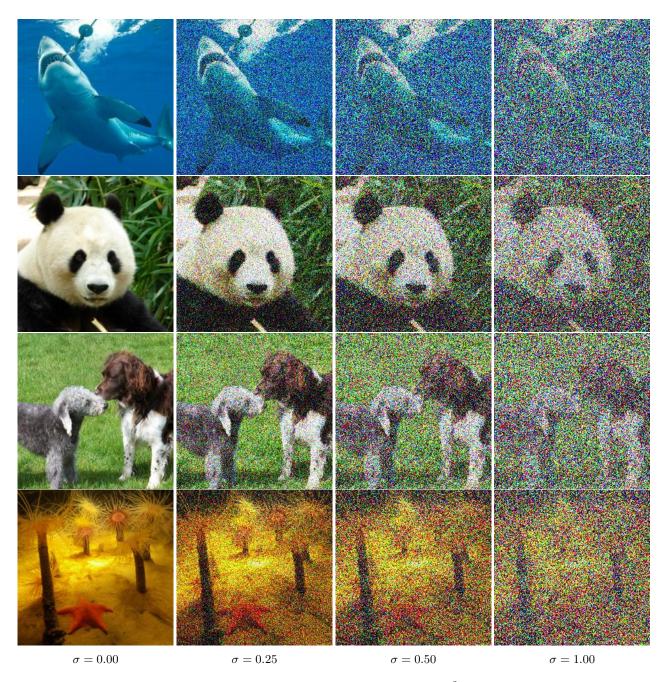


Figure 18. ImageNet images additively corrupted by varying levels of Gaussian noise $\mathcal{N}(0, \sigma^2 I)$. Pixel values greater than 1.0 (=255) or less than 0.0 (=0) were clipped to 1.0 or 0.0.