GSmooth: Certified Robustness against Semantic Transformations via Generalized Randomized Smoothing

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Abstract

Certified defenses such as randomized smoothing have shown promise towards building reliable machine learning systems against $\ell_p$-norm bounded attacks. However, existing methods are insufficient or unable to provably defend against semantic transformations, especially those without closed-form expressions (such as defocus blur and pixelate), which are more common in practice and often unrestricted. To fill up this gap, we propose generalized randomized smoothing (GSmooth), a unified theoretical framework for certifying robustness against general semantic transformations via a novel dimension augmentation strategy. Under the GSmooth framework, we present a scalable algorithm that uses a surrogate image-to-image network to approximate the complex transformation. The surrogate model provides a powerful tool for studying the properties of semantic transformations and certifying robustness. Experimental results on several datasets demonstrate the effectiveness of our approach for robustness certification against multiple kinds of semantic transformations and corruptions, which is not achievable by the alternative baselines.

1. Introduction

Deep learning models are vulnerable to adversarial examples (Biggio et al., 2013; Szegedy et al., 2014; Goodfellow et al., 2015) as well as semantic transformations (Engstrom et al., 2019; Hendrycks & Dietterich, 2019), which can limit their applications in various security-sensitive tasks. For example, a small adversarial patch on the road markings can mislead the autonomous driving system (Jing et al., 2021), which raises severe safety concerns. Compared with the $\ell_p$-norm bounded adversarial examples, semantic transformations can occur more naturally in real-world scenarios and are often unrestricted, including image rotation, translation, blur, weather, etc., most of which are common corruptions (Hendrycks & Dietterich, 2019). Such transformations do not damage the semantic features of images that can still be recognized by humans, but they degrade the performance of deep learning models significantly. Therefore, it is imperative to improve model robustness against these semantic transformations.

Although various methods (Wang et al., 2019; Hendrycks et al., 2020; Xie et al., 2020; Calian et al., 2021) can empirically improve model robustness against semantic transfor-
mations on typical benchmarks (evaluated in average-case), these methods often fail to defend against adaptive attacks by generating adversarial semantic transformations (Hosseini & Poovendran, 2018; Engstrom et al., 2019; Wong et al., 2019), which are optimized over the parameter space of transformations for the worst-case. In contrast, the certified defenses aim to provide a certified region where the model is theoretically robust under any attack or perturbation (Wong & Kolter, 2018; Cohen et al., 2019; Gowal et al., 2018; Zhang et al., 2019). As an example in Fig. 1, we might encounter any levels and types of complex semantic transformations for autonomous driving cars in practice. An ideal safe model should tell users its safe regions that the model is certifiably robust under different transformations.

Several recent studies (Fischer et al., 2020; Mohapatra et al., 2020; Li et al., 2021) have attempted to extend the certified defenses to simple semantic transformations with good mathematical properties like translation and Gaussian blur. However, these methods are neither scalable nor capable of certifying robustness against complex image corruptions and transformations, especially the non-resolvable ones (Li et al., 2021). Typically, many non-resolvable transformations, such as zoom blur and pixelate, do not have closed-form expressions. This makes the theoretical analyses of these transformations difficult and sometimes impossible with the existing methods, although they are common in real-world scenarios. Therefore, it remains highly challenging to certify robustness against these complex and realistic semantic transformations.

In this paper, we propose generalized randomized smoothing (GSmooth), a novel unified theoretical framework for certified robustness against general semantic transformations, including both the resolvable ones (e.g., translation) and non-resolvable ones (e.g., rotational blur). Specifically, we propose to use an image-to-image translation neural network to approximate these transformations. Due to the strong capacity of neural networks, our method is flexible and scalable for modeling these complex non-resolvable semantic transformations. Then, we can theoretically provide the certified radius for the proxy neural networks by introducing new augmented noise in the layers of the surrogate model, which can be used for certifying the original transformations. We further provide a theoretical analysis and an error bound for the approximation, which shows that the impact of the approximation error on the certified bound can be ignored in practice. Finally, we validate the effectiveness of our methods on several publicly available datasets. The results demonstrate that our method is effective for certifying complex semantic transformations. Our GSmooth achieves state-of-the-art performance in both certified accuracy and empirical accuracy for different types of blur or image quality corruptions.

2. Related Work

2.1. Robustness under Semantic Transformations

Unlike an $\ell_p$ perturbation adding a small amount of noise to an image, semantic attacks are usually unrestricted. Representative works include the adversarial patches (Brown et al., 2017; Song et al., 2018), the manipulation based on spatial transformations such as rotation or translation (Xiao et al., 2018; Engstrom et al., 2019). Recently, Hendrycks & Dietterich (2019) show that a wide variety of image corruptions and perturbations degrade the performance of many deep learning models. Most of them such as types of blur, pixelate are hard to be analyzed mathematically, such that defending against them is highly challenging. Various data augmentation techniques (Cubuk et al., 2019; Hendrycks et al., 2020; 2021; Robey et al., 2020) have been developed to enhance robustness under semantic perturbations. Also, Calian et al. (2021) propose adversarial data augmentation that can be viewed as adversarial training for defending against semantic perturbations.

2.2. Certified Defense against Semantic Transformations

Beyond empirical defenses, several works (Singh et al., 2019; Balunović et al., 2019; Mohapatra et al., 2020) have attempted to certify some simple geometric transformations. However, these are deterministic certification approaches and their performance on realistic datasets is unsatisfactory. Randomized smoothing is a novel certification method that originated from differential privacy (Lecuyer et al., 2019). Cohen et al. (2019) then improve the certified bound and apply it to realistic settings. Yang et al. (2020) exhaustively analyze the bound by using different noise distributions and norms. Hayes (2020) and Yang et al. (2020) point out that randomized smoothing suffers from the curse of dimensionality for the $\ell_{\infty}$ norm. Fischer et al. (2020) and Li et al. (2021) extend randomized smoothing to certify some simple semantic transformations, e.g., image translation and rotation. They show that randomized smoothing could be used to certify attacks beyond $\ell_p$ norm. However, their methods are limited to simple semantic transformations, which are easy to analyze due to their resolvable mathematical properties. Scalable algorithms for certifying most non-resolvable and complex semantic transformations remain unexplored.

3. Proposed Method

In this section, we present generalized randomized smoothing (GSmooth) with theoretical analyses.
3.1. Problem Formulation

We first introduce the notations and problem formulation. Given the input \( x \in \mathbb{R}^n \) and the label of \( \mathcal{Y} = \{1, 2, \ldots, K\} \), we denote the classifier as \( f(x) : \mathbb{R}^n \to [0, 1]^K \), which outputs predicted probabilities over all \( K \) classes. The prediction of \( f \) is \( \arg \max_{y \in \mathcal{Y}} f(x)_i \), where \( f(\cdot) \) denotes the \( i \)-th element of \( f(\cdot) \). We denote \( \tau(\theta, x) : \mathbb{R}^m \times \mathbb{R}^n \to \) to be a semantic transformation of the raw input \( x \) with parameter \( \theta \in \mathbb{R}^m \). We define the smoothed classifier \( G(x) \) as

\[
G(x) = \mathbb{E}_{\theta \sim P(\theta)}[f(\tau(\theta, x))],
\]

which is the average prediction for the samples under a smooth distribution \( g(\theta) \propto \exp(-\psi(\theta)) \), here \( \psi : \mathbb{R}^m \to \mathbb{R} \) is a smooth function. We let \( y_A \) be the predicted label of the smoothed classifier \( G(x) \) for a clean image, and we use \( G(x)_A \) to denote the probability of the top-1 class \( y_A \) in the rest of the paper as follows. Similarly, we can define \( y_B \) as the runner-up class of the smoothed classifier \( G(x) \).

\[
y_A \triangleq \arg \max_{i \in \mathcal{Y}} G(x)_i, \quad y_B \triangleq \arg \max_{i \in \mathcal{Y}\setminus y_A} G(x)_i, \tag{2}
\]

and we use \( G(x)_B \) to denote the probability of class \( y_B \).

A classifier has a certified robust radius \( R \) if it satisfies that for any perturbation \( \|\xi\| \leq R \) where \( \|\cdot\| \) is any \( L_p \) norm without specification, we have

\[
\arg \max_{i \in \mathcal{Y}} G(\tau(\xi, x))_i = y_A. \tag{3}
\]

In this paper, we categorize semantic transformations into two classes: resolvable and non-resolvable. A semantic transformation is resolvable if the composition of two transformations with parameters belonging to a perturbation set \( \theta, \xi \in P \subset \mathbb{R}^m \), is still a transformation with a new parameter \( \gamma = \gamma(\theta, \xi) \in P \subset \mathbb{R}^m \), here \( \gamma(\cdot, \cdot) : P \times P \to P \) is a function depending on these parameters, i.e., satisfying

\[
\tau(\theta, \tau(\xi, x)) = \tau(\gamma(\theta, \xi), x). \tag{4}
\]

Otherwise, it is non-resolvable, e.g., zoom blur and pixelate. The theoretical properties of resolvable transformations make it much easier to derive the certified bound. Therefore, in next two subsections, we will discuss resolvable and non-resolvable cases in turn under a unified framework.

3.2. Certified Bound for Resolvable Transformations

We first discuss a class of transformations that are resolvable. We introduce a function \( \Phi(\cdot) \) which will be used in the certified bound. For any vector \( u \) with unit norm, i.e., \( \|u\| = 1 \), we set \( \gamma_u \triangleq \langle u, \nabla \psi(\theta) \rangle \) as a random variable, where \( \delta \sim g(\cdot) \) and \( \nabla \) is the gradient operator. We further define the complementary Cumulative Distribution Function (CDF) of \( \gamma_u \) as \( \Phi_u(c) = \mathbb{P}[\gamma_u > c] \) and the inverse complementary CDF of \( \gamma_u \) as \( \Phi_u^{-1}(p) = \inf \{ c | \mathbb{P}[\gamma_u > c] \leq p \} \). Following Yang et al. (2020), we define a function \( \Phi \) as

\[
\Phi(p) = \max_{\|u\|=1} \mathbb{E}[\gamma_u | \gamma_u > \Phi_u^{-1}(p)]. \tag{5}
\]

For resolvable semantic transformations, we have the following theorem.

**Theorem 1 (Certified bound for Resolvable Transformations)**: Let \( f(x) \) be a classifier with a certified certified robust radius \( R \), we define the smoothed classifier \( G \) as

\[
G(x) = \mathbb{E}_{\theta \sim P(\theta)}[f(\tau(\theta, x))],
\]

and there exist two constants \( p_A, p_B \) satisfying

\[
G(x)_A \geq p_A \geq p_B \geq G(x)_B,
\]

then

\[
\arg \max_{i \in \mathcal{Y}} G(\tau(\xi, x))_i = y_A \tag{6}
\]

and

\[
R = \frac{1}{2M^*} \int_{p_B}^{p_A} \frac{1}{P(\Phi(p))} \, dp, \tag{7}
\]

where \( \Phi \) is the inverse CDF of the standard Gaussian distribution. These two kinds of transformations include image translation and Gaussian blur, which are basic semantic transformations and the results are consistent with previous work (Li et al., 2021; Fischer et al., 2020). The certification of these simple transformations only requires applying translation or Gaussian blur to the sample and we obtain the average classification score under the noise distribution.

3.3. Certified Bound for General Transformations

Translation and Gaussian blur are two special cases of semantic transformations. In practice, most semantic transformations are not commutable or even not resolvable. Therefore, we need to develop better methods for certifying more
Figure 2. A graphical illustration of our GSmooth. We use a surrogate image-to-image translation network to accurately fit a semantic transformation. Then we add new augmented noise into the surrogate model and construct the GSsmooth classifier. The augmented noise is sampled to ensure that the transformation is resolvable in the semantic space. We theoretically calculate the certified bound for the surrogate model to certify the original transformation.

types of semantic transformations. However, the existing methods like Semanify-NN (Mohapatra et al., 2020), based on convex relaxation, and TSS (Li et al., 2021), based on randomized smoothing, require developing a specific algorithm or bound for each individual semantic transformation. This is not scalable and might be infeasible for more complicated transformations without explicit mathematical forms.

To address this challenge, we draw inspiration from the fact that neural networks are able to approximate functions including a complex and unknown semantic transformation (Zhu et al., 2017). Specifically, we propose to use a surrogate image-to-image translation network to accurately fit the semantic transformation. We theoretically prove that, by introducing an augmented noise in the layer of the surrogate model, as shown in Fig. 2, randomized smoothing can be extended to handle these transformations. Specifically, we define the surrogate model as the following form that will lead to a simple certified bound, as we shall see:

$$
\tau(\theta, x) = H(F_1(\theta) + F_2(x)),
$$

where $F_1(\cdot)$, $F_2(\cdot)$, and $H(\cdot)$ are three individual neural networks. $F_1(\cdot)$ and $F_2(\cdot)$ are encoders for transformation parameters and images respectively, and their encodings are added together in the semantic space, which is critical for the theoretical certification. We find that the surrogate neural network is much easier to analyze and can be certified by introducing a dimension augmentation strategy for both noise parameters and input images.

As illustrated in Fig. 2, the augmented noise is added to the semantic layer $H(\cdot)$ in the surrogate model. Our key insight is that the transformation can be viewed as the superposition of a resolvable part and a non-resolvable residual part in the augmented semantic space. Then, we can use the augmented noise to control the non-resolvable residual part of the augmented dimension $d \geq m + n$. This dimension augmentation is the key step in our method. The augmentation for noise is from $\mathbb{R}^m$ to $\mathbb{R}^d$. To keep the dimension consistent, we also augment data $x$ to $\mathbb{R}^d$ by padding 0 entries. By certifying the transformation using the surrogate model, we are able to certify the original transformation if the approximation error is within an acceptable region (details are in Theorem 3). Our method is flexible and scalable because the surrogate neural network has a uniform mathematical form for theoretical analysis and is trained automatically. Next, we discuss the details of GSsmooth.

Specifically, we introduce the augmented data $\tilde{x} \in \mathbb{R}^d$ and the augmented parameter $\tilde{\theta} \in \mathbb{R}^d$ as

$$
\tilde{x} = \left( \begin{array} {c} 0_{d-n} \\ x \end{array} \right), \quad \tilde{\theta} = \left( \begin{array} {c} \theta \\ \theta' \end{array} \right),
$$

where the additional parameters $\theta' \in \mathbb{R}^n$ are sampled from $g'(\theta')$, and the joint distribution of $\theta'$ and $\theta$ is $\tilde{g} = \tilde{g}(\theta, \theta')$. We define the generalized smoothed classifier as

$$
\tilde{G}(\tilde{x}) = \mathbb{E}_{\tilde{g} \sim \tilde{g}(\cdot)} \left[ \tilde{f}(\tilde{\theta}, \tilde{x}) \right],
$$

where $\tilde{f}$ is the “augmented target classifier” that is equivalent to the original classifier when constrained on the original input $x$, which means $\tilde{f}(\tilde{x}) = f(x)$. Note that now all the functions are augmented for a $d$-dimensional input. We further augment our surrogate neural network to represent the augmented transformation $\tilde{\tau} : \mathbb{R}^d \rightarrow \mathbb{R}^d$ as

$$
\tilde{\tau}(\tilde{\theta}, \tilde{x}) = \tilde{H}(\tilde{F}_1(\tilde{\theta}) + \tilde{F}_2(\tilde{x})),
$$

where $\tilde{H}(\cdot)$, $\tilde{F}_1(\cdot)$, $\tilde{F}_2(\cdot) : \mathbb{R}^d \rightarrow \mathbb{R}^d$ are parts of the augmented surrogate model. By carefully designing the interaction between the augmented parameters and the original parameters, we could turn the transformation to a resolvable one. It does not change the original surrogate model when
constraining to the original input $x$ and $\theta$. Specifically, we design $\tilde{F}_1$, $\tilde{F}_2$ and $\tilde{H}$ as follows:

$$
\tilde{F}_1(\tilde{\theta}) = \begin{pmatrix} \theta \\ F_1(\theta) + \theta' \end{pmatrix}, \quad \tilde{F}_2(\tilde{x}) = \begin{pmatrix} 0_{d-n} \\ F_2(x) \end{pmatrix},
$$

$$
\tilde{H}(\tilde{x}) = \begin{bmatrix} I_{d-n} \\ H(x) \end{bmatrix}.
$$

Before stating our main theorem, to simplify the notations, we set

$$
\tilde{z}_\xi = \tilde{F}_1(\tilde{\xi}) + \tilde{F}_2(\tilde{x}), \quad \tilde{z}_\theta = \tilde{F}_1(\tilde{\theta}) + \tilde{F}_2(\tilde{x}),
$$

$$
\tilde{y}_\xi = (y'_\xi, y_\xi)^T = \tilde{H}(\tilde{F}_1(\tilde{\xi}) + \tilde{F}_2(\tilde{x})), \quad \tilde{y}_\theta = (y'_\theta, y_\theta)^T = \tilde{H}(\tilde{F}_1(\tilde{\theta}) + \tilde{F}_2(\tilde{x})).
$$

Then we provide our main theoretical result below, i.e., the GSmooth classifier is certifiably robust within a given range.

**Theorem 2 (Certified bound for Non-resolvable Transformations)**, proof in Appendix A.2. For any classifier $f(x)$, let $\tilde{G}(\tilde{x})$ be the smoothed classifier defined in Eq. (10). If there exist $p_A$ and $p_B$ satisfying

$$
\tilde{G}(\tilde{x})_A \geq p_A \geq p_B \geq \tilde{G}(\tilde{x})_B,
$$

then

$$
\arg \max_{i \in Y} \tilde{G}(\tilde{\xi}(\tilde{x}), \tilde{\xi}))_i = y_A \text{ holds for any } \|\xi\|_2 \leq R, \text{ where}
$$

$$
R = \frac{1}{2M^*} \int_{p_B} \frac{1}{\Phi(p)} dp,
$$

and the coefficient $M^*$ is defined as

$$
M^* = \max_{\xi, \theta \in P} \sqrt{1 + \left\| \frac{\partial F_2(y_\xi)}{\partial \xi} - \frac{\partial F_1(\theta)}{\partial \theta} \right\|_2^2}.
$$

We have several observations from the theorem. First, it is noted that the certified radius is similar to the result in Theorem 1. Second, compared with resolvable transformations, we need to introduce a new type of noise when constructing the GSsmooth classifier. This isotropic noise has the same dimension as the data and is added to the intermediate layers of surrogate neural networks. The theoretical explanation behind this is that this isotropic noise allows the Jacobian matrix of the semantic transformation to be invertible, which is crucial for the proof. Third, we find that the coefficient $M^*$ depends on the norm of the difference of two Jacobian matrices and is independent of the target classifier. Later we will discuss the meaning of this term in detail.

Before diving into our theoretical insight and proof of the theorem, we introduce a specific case of Theorem 2 which is convenient for practical usage. We empirically found that taking a linear transformation as $F_1(\theta) = A_1 \theta + b_1$ where $A_1 \in \mathbb{R}^{n \times n}$, $b_1 \in \mathbb{R}^n$ does not sacrifice the precision of the surrogate network. So, we have $\frac{\partial F_1(\theta)}{\partial \theta} = A_1$.

After substituting the term in Eq. (15), we only need to optimize $\xi$ to calculate $M^*$ which can make the bound tighter. Additionally, we use two Gaussian distributions as the noise distribution and the augmented noise distribution, i.e., $g(\theta') = N(0, \sigma_1^2 I)$ and $g'(\theta') = N(0, \sigma_2^2 I)$. Formally, we have the following corollary.

**Corollary 1.** Suppose $f(x)$ is a classifier and $\tilde{G}(\tilde{x})$ is the smoothed classifier defined in Eq. (10). If the layer $F_1(\theta)$ in the surrogate network has the following form:

$$
F_1(\theta) = A_1 \theta + b_1,
$$

where $A_1 \in \mathbb{R}^{d \times m}$, $b_1 \in \mathbb{R}^d$ are the parameters. We empirically found

$$
\tilde{G}(\tilde{x})_A \geq p_A \geq p_B \geq \tilde{G}(\tilde{x})_B,
$$

then

$$
\arg \max_{i \in Y} \tilde{G}(\tilde{\xi}(\tilde{x}), \tilde{\xi}))_i = y_A \text{ for any } \|\xi\|_2 \leq R,
$$

where

$$
R = \frac{1}{2M^*} \left( \Psi (p_A) - \Psi (p_B) \right),
$$

where $\Psi(\cdot)$ is the inverse CDF of the standard Gaussian distribution, and the coefficient $M^*$ is defined as

$$
M^* = \max_{\xi, \theta \in P} \sqrt{1 + \left\| \frac{\partial F_2(y_\xi)}{\partial \xi} - \frac{\partial F_1(\theta)}{\partial \theta} \right\|_2^2}.
$$

4. Proof Sketch and Theoretical Analysis

In this section, we briefly summarize the main idea for proving Theorem 2 and provide the theoretical insights for our GSmooth further. More details of the proof can be found in Appendix A.2.

4.1. Proof Sketch of Theorem 2

The key idea is to prove that the gradient of the smoothed classifier can be bounded by a function of the classification confidence and the parameters of the noise distribution. Formally, we calculate the gradient to the perturbation parameter $\xi$ for our augmented smoothed classifier as

$$
\nabla_\xi \tilde{G}(\tilde{\xi}(\tilde{x})) = \nabla_\xi \mathbb{E}_{\tilde{\theta} \sim \tilde{g}(\tilde{\theta})} [\tilde{f}(\tilde{\theta}, \tilde{\xi}(\tilde{x}))].
$$

We further expand the expectation into an integral and find that

$$
\nabla_\xi \tilde{G}(\tilde{\xi}(\tilde{x})) = \int_{\mathbb{R}^d} \frac{\partial \tilde{f}(\tilde{\theta}, \tilde{y}_\xi)}{\partial \xi} \tilde{g}(\tilde{\theta}) d\tilde{\theta}.
$$

The key step is to eliminate the gradient of $\frac{\partial \tilde{f}(\tilde{\theta}, \tilde{y}_\xi)}{\partial \xi}$ and replace it with $\frac{\partial \tilde{f}(\tilde{\theta}, \tilde{y}_\xi)}{\partial \theta}$. Then we integrate it by parts to get the following objective:

$$
\nabla_\xi \tilde{G}(\tilde{\xi}(\tilde{x})) = - \int_{\mathbb{R}^d} \tilde{F}(\tilde{\theta}, \tilde{y}_\xi) \frac{\partial M(\tilde{\xi}, \tilde{\theta}) \tilde{g}(\tilde{\theta})}{\partial \theta} d\tilde{\theta}.
$$
After that, we can bound the gradient of the GSmooth classifier by using a technique similar to randomized smoothing (Yang et al., 2020).

4.2. Theoretical Insights

Next, we provide some theoretical insights for our augmentation scheme on transformation parameters.

- **Transformation space expansion.** The key purpose of the augmented noise is to construct a closed subspace using additional dimensions. In the augmented space, the Jacobian matrix of the semantic transformation becomes invertible, which is crucial for our proof.

- **Decomposition of the non-resolvable transformations.** As we can see in Eq. (18), \( M^* \) is influenced by two factors. One is the standard deviation of the two noise distributions. The other is the norm of the Jacobian matrix \( \frac{\partial F_2(y)}{\partial \xi} - A_1 \), which can be viewed as the residual of the non-resolvable part of the transformation. Along these lines, our method decomposes the unknown semantic transformation into a resolvable part and a residual part. The non-resolvable residual part can be handled by introducing an additional noise with standard deviation \( \sigma_2 \).

4.3. Error Analysis for Surrogate Model Approximation

In this subsection, we theoretically analyze the effectiveness of certifying a real semantic transformation due to the existence of approximation error of surrogate neural networks.

**Theorem 3 (Error Analysis, proof in Appendix A.3).** Suppose the simulation of the semantic transformation has a small enough error

\[
\|\tilde{\tau}(\hat{\xi}, \hat{x}) - \tau(\xi, x)\|_2 < \epsilon,
\]

where \( \tau(\xi, x) \) is the real semantic transformation. Then there exists a constant ratio

\[
A = A(\|F_1'(\hat{\xi})\|_2, \|F_2'(\hat{y}_\xi)\|_2, \|F_2'(\hat{z}_\xi)\|_2) > 0,
\]

which does not depend on the target classifier. The certified radius for the real semantic transformation satisfies:

\[
R_r > R(1 - A\epsilon),
\]

where \( R \) is the certified radius in Eq. (14) for the surrogate neural network in Theorem 2.

We find that the reduction of the certified radius is influenced by two factors. The first one is the approximation error \( \epsilon \) between the surrogate transformation and the real semantic transformation. The second one, the ratio \( A \), is about the norm of the Jacobian matrix for some layers of the surrogate model. This is also an inherent property of the semantic transformation itself and does not depend on the target classifier.

5. Experiments

In this section, we conduct extensive experiments to show the effectiveness of our GSmooth on various types of semantic transformations.

5.1. Experimental Setup and Evaluation Metrics

We use MNIST (Lecun et al., 1998), CIFAR-10, and CIFAR-100 (Krizhevsky et al., 2009) datasets to verify our methods. We train a ResNet with 110 layers (He et al., 2016a) from scratch. Similar to prior work, we apply moderate data augmentation (Cohen et al., 2019) to improve the generalization of the classifier. For the surrogate image-to-image translation model for simulating semantic transformations, we adopt the U-Net architecture (Ronneberger et al., 2015) for \( \tilde{H}(\cdot) \) and several simple convolutional or linear layers for \( \tilde{F}_1(\cdot) \) and \( \tilde{F}_2(\cdot) \). All models are trained by using an Adam optimizer (Kingma & Ba, 2015) with an initial learning rate of 0.001 that decays every 50 epochs until convergence.

The evaluation metric is the certified accuracy, which is the percentage of samples that are correctly classified with a larger certified radius than the given range. We use \( \|\alpha\| \) to indicate the preset certified radius. The results are evaluated on the real semantic transformations after considering the error correction in Theorem 3.

5.2. Main Results for Certified Robustness

To demonstrate the effectiveness of our GSmooth on certifying complex semantic transformations, we compare the results of our GSmooth with several baselines, including randomized smoothing for some simple semantic transformations of TSS (Li et al., 2021) and IndivSPT/distSPT (Fischer et al., 2020). Our GSmooth is a natural and powerful extension of their methods. We also compare our method with deterministic certification approaches, including DeepG (Balunović et al., 2019), which uses linear relaxations similar to Wong & Kolter (2018), Interval (Singh et al., 2019), which is based on interval bound propagation, VeriVis (Pei et al., 2017), which enumerates all possible outcomes for semantic transformations with finite values of parameters, and Semanify-NN (Mohapatra et al., 2020), which uses a new preprocessing layer to turn the problem into a \( \ell_p \) norm certification.

We measure the certified robust accuracy for different se-
Table 1. Our main results of certified robust accuracy on several datasets and multiple types of semantic transformations. – or 0.0% means the method fails to certify this type of semantic transformation.

| Transformation | Type     | Dataset          | Certified Radius | GSmooth (Ours) | TSS | DeepG Interval | VeriVis | Semanify-NN | IndivSPT/ distSPT |
|---------------|----------|------------------|------------------|----------------|-----|----------------|---------|-------------|-------------------|
| Gaussian Blur | Additive | MNIST            | [α]2 < 6         | 91.0           | 90.6 | –              | –       | –           | –                 |
|               |          | CIFAR-10         | [α]2 < 4         | 67.4           | 63.6 | –              | –       | –           | –                 |
|               |          | CIFAR-100        | [α]2 < 4         | 22.1           | 21.0 | –              | –       | –           | –                 |
| Translation   | Additive | MNIST            | [α]2 < 8         | 98.7           | 99.6 | 0.0            | 0.0     | 98.8        | 98.8              |
|               |          | CIFAR-10         | [α]2 < 20        | 82.2           | 80.8 | 0.0            | 0.0     | 65.0        | 65.0              |
|               |          | CIFAR-100        | [α]2 < 20        | 42.2           | 41.3 | –              | –       | 24.2        | 24.2              |
| Brightness    | Resolvable| MNIST          | [α]∞ < 0.5       | 97.7           | 97.6 | ≤0.4           | 0.0     | –           | ≤14.1             |
|               |          | CIFAR-10         | [α]∞ < 0.4       | 82.5           | 82.4 | 0.0            | 0.0     | –           | –                 |
|               |          | CIFAR-100        | [α]∞ < 0.4       | 42.3           | 41.4 | 0.0            | 0.0     | –           | –                 |
| Rotation      | Non-resolvable | MNIST    | [α]2 < 50°       | 95.7           | 97.4 | ≤85.8          | ≤6.0    | –           | ≤92.48            |
|               |          | CIFAR-10         | [α]2 < 10°       | 65.6           | 70.6 | 62.5           | 20.2    | –           | ≤49.37            |
|               |          | CIFAR-100        | [α]2 < 10°       | 33.2           | 36.7 | 0.0            | 0.0     | –           | ≤21.7             |
| Scaling       | Non-resolvable | MNIST    | [α]2 < 0.3       | 95.9           | 97.2 | 85.0           | 16.4    | –           | –                 |
|               |          | CIFAR-10         | [α]2 < 0.3       | 54.3           | 58.8 | 0.0            | 0.0     | –           | –                 |
|               |          | CIFAR-100        | [α]2 < 0.3       | 31.2           | 37.8 | 0.0            | 0.0     | –           | –                 |
| Rotational Blur| Non-resolvable | MNIST  | [α]2 < 10        | 95.9           | 97.2 | –              | –       | –           | –                 |
|               |          | CIFAR-10         | [α]2 < 10        | 39.7           | 39.7 | –              | –       | –           | –                 |
|               |          | CIFAR-100        | [α]2 < 10        | 27.2           | 27.2 | –              | –       | –           | –                 |
| Defocus Blur  | Non-resolvable | MNIST  | [α]2 < 5         | 89.2           | 89.2 | –              | –       | –           | –                 |
|               |          | CIFAR-10         | [α]2 < 5         | 89.2           | 89.2 | –              | –       | –           | –                 |
|               |          | CIFAR-100        | [α]2 < 5         | 25.0           | 25.0 | –              | –       | –           | –                 |
|               |          |               | [α]2 < 5         | 13.1           | 13.1 | –              | –       | –           | –                 |
| Zoom Blur     | Non-resolvable | MNIST  | [α]2 < 0.5       | 93.9           | 93.9 | –              | –       | –           | –                 |
|               |          | CIFAR-10         | [α]2 < 0.5       | 44.6           | 44.6 | –              | –       | –           | –                 |
|               |          | CIFAR-100        | [α]2 < 0.5       | 14.2           | 14.2 | –              | –       | –           | –                 |
| Pixelate      | Non-resolvable | MNIST  | [α]2 < 0.5       | 87.1           | 87.1 | –              | –       | –           | –                 |
|               |          | CIFAR-10         | [α]2 < 0.5       | 45.3           | 45.3 | –              | –       | –           | –                 |
|               |          | CIFAR-100        | [α]2 < 0.5       | 30.2           | 30.2 | –              | –       | –           | –                 |

Table 2. Results of empirical accuracy under adaptive attack on CIFAR-10 (PGD using EqT). For comparison, we also list the results of the corresponding certified accuracy in Table 1.

| Type          | Certified Acc. (%) | Adaptive Attack Acc. (%) |
|---------------|--------------------|-------------------------|
|               | GSmooth            | Vanilla                 |
| Gaussian blur | 67.4               | 68.1                    |
|               | 3.4                | 3.4                     |
| Translation   | 82.2               | 87.5                    |
|               | 4.2                | 4.2                     |
| Brightness    | 82.5               | 85.9                    |
|               | 9.6                | 9.6                     |
| Rotation      | 65.6               | 68.4                    |
|               | 65.4               | 65.4                    |
| Rotational blur| 39.7               | 45.0                    |
|               | 33.1               | 33.1                    |
| Defocus blur  | 25.0               | 25.5                    |
|               | 16.6               | 16.6                    |
| Pixelate      | 45.3               | 49.2                    |
|               | 38.2               | 38.2                    |

To demonstrate that the certified radius is tight enough for real applications, we conduct empirical robustness experiments by testing our method under two types of corruptions. First, we apply project gradient descent (PGD) (Madry et al., 2018) using Expectation over Transformation (EqT) (Athalye et al., 2018) and evaluate the accuracy under adversarial examples on CIFAR-10. Second, we measure the empirical performance of GSmooth under common image corruptions such as CIFAR-10-C (Hendrycks & Dietterich, 2019). We choose AugMix (Hendrycks et al., 2020) and TSS (Li et al., 2021) as baselines. For evaluation, we choose subsets of CIFAR-10-C that are attacked by deterministic corruptions.
### Table 3. Results of ablation study on the influence of standard deviation of smoothing distributions, i.e., transformation noise $\sigma_1$ and augmented noise $\sigma_2$ for certification accuracy on rotational blur.

| Cert Acc. (%) | CIFAR-10 | CIFAR-100 |
|---------------|----------|-----------|
|               | $\sigma_2$ |          | $\sigma_2$ |          |
|               | 0.05 | 0.10 | 0.15 | 0.25 | 0.05 | 0.10 | 0.15 | 0.20 |
| Rotational Blur | 0.1 | 44.3 | 46.4 | 35.5 | 16.1 | 0.1 | 23.1 | 26.2 | 17.2 | 10.4 |
|               | 0.25 | 45.7 | 47.1 | 38.3 | 18.9 | 0.25 | 23.2 | 27.2 | 20.3 | 11.3 |
|               | 0.5  | 46.5 | 48.4 | 38.8 | 18.3 | 0.5  | 22.2 | 26.1 | 18.6 | 11.8 |
|               | 0.75 | 42.1 | 45.5 | 36.6 | 17.0 | 0.75 | 24.0 | 25.5 | 18.3 | 13.2 |

### Table 4. Empirical accuracy (%) on subsets of CIFAR-10-C. Results with the best performance are bolded.

| Type          | AugMix | TSS   | GSmooth |
|---------------|--------|-------|---------|
| Gaussian blur | 67.4   | 75.8  | 76.0    |
| Brightness    | 82.4   | 71.8  | 72.1    |
| Defocus blur  | 72.2   | 75.6  | 76.8    |
| Zoom blur     | 70.8   | 75.2  | 77.1    |
| Motion blur   | 68.6   | 70.2  | 70.5    |
| Pixelate      | 50.9   | 76.0  | 76.7    |

The performance under adaptive attack is shown in Table 2. From the results, we find that the empirical accuracy is always higher than the certified accuracy, which indicates the tightness of the certified bound for GSmooth. Additionally, GSmooth also serves as a strong empirical defense compared with a vanilla neural network. The results on CIFAR-10-C are listed in Table 4. We see that our method achieves improvement on most types of corruptions. Since the corruptions in CIFAR-10-C are randomly produced and model-agnostic, the overall performance is better than adaptive attacks. In summary, these empirical results show that the certified bound is tight enough and that GSmooth can also be used as a strong empirical defense method.

### 5.4. Ablation Studies

**Ablation study on the influence of noise distribution.** The choice of noise distribution is important for randomized smoothing based methods. Since our GSmooth can certify different types of semantic transformations that exhibit different properties, it is necessary to understand the influence of different smoothing distributions for different semantic transformations. We choose (folded) Gaussian, uniform, and exponential distribution and compare the certified accuracy on zoom blur transformation for both CIFAR-10 and CIFAR-100 datasets. As shown in Fig. 3, we found that the impact of smoothing distributions depends on the dataset. On average, uniform distribution is better for small radius certification, while exponential distribution is more suitable for certifying a large radius.

**Ablation study on the influence of noise variance for certification.** Since our GSmooth contains two different variances for controlling the resolvable part and the residual part for a non-resolvable semantic transformation, here we investigate the effect of different noise variance on the certified accuracy. The results are shown in Table 3. We found that using medium transformation noise and augmented noise achieves the best certified accuracy. This fact is consistent with results in Cohen et al. (2019). An explanation is that there is a trade-off: higher noise variance decreases the coefficient $M^*$, but it might also degrade the clean accuracy.

**Visualization experiments: comparison between augmented semantic noise and image noise.** Our GSmooth needs to add a new noise in the semantic layers of the surrogate model. Here we compare the difference between these two types of noise and visualize them. We randomly sample images from CIFAR-10 and add Gaussian noise with $\sigma = 0.2$ to both the semantic layer of the surrogate model simulating zoomed blur transformation and raw images. Results are shown in Fig. 4. Both types of noise severely blur the images. But we found that the augmented semantic noise is more placid, which can therefore keep the holistic semantic features better, e.g., as shapes.
6. Conclusion

In this paper, we proposed a generalized randomized smoothing framework (GSmooth) for certifying robustness against general semantic transformations. Considering that it is nontrivial to conduct theoretical analysis for non-resolvable transformations, we proposed a novel method using a surrogate neural network to fit semantic transformations. Then we theoretically provide a tight certified robustness bound for the surrogate model, which can be used for certifying semantic transformations. Extensive experiments on publicly available datasets verify the effectiveness of our method by achieving state-of-the-art performance on various types of semantic transformations especially for those complex transformations such as zoom blur or pixelate.

Acknowledgments

This work was supported by the National Key Research and Development Program of China (2020AAA0106000, 2020AAA0104304, 2020AAA0106302, 2017YFA0700904), NSFC Projects (Nos. 62061136001, 61621136008, 62076147, U19B2034, U19A2081, U1811461), the major key project of PCL (No. PCL2021A12), Tsinghua-Alibaba Joint Research Program, Tsinghua-OPPO Joint Research Center, and Tiangong Institute for Intelligent Computing. NVIDIA NVAIL Program and the High Performance Computing Center, Tsinghua University.

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A. Proofs of Theorems

In this section, we will provide detailed proofs of theorems in our paper.

First, we restate the theorem of randomized smoothing for additive noise and binary classifiers \( f : \mathbb{R}^n \rightarrow [0, 1] \).

**Theorem 4.** Let \( f(x) \) be any classifier and \( G(x) \) be the smoothed classifier defined as

\[
G(x) = \mathbb{E}_{\theta \sim g}[f(x + \theta)],
\]

if \( G(x) < \frac{1}{2} \), then \( G(x + \delta) < \frac{1}{2} \) holds for any

\[
\|\delta\| < \int_{G(x)}^{\frac{1}{2}} \frac{1}{\Phi(p)} \, dp,
\]

where \( \Phi(\cdot) \) is a function about smoothing distribution defined in Eq. (5).

**Proof.** We first calculate the gradient of the smoothed classifier as

\[
\nabla G(x) = \frac{\partial}{\partial x} \int_{\mathbb{R}^n} f(x + \theta) g(\theta) \, d\theta \\
= \int_{\mathbb{R}^n} \frac{\partial}{\partial x} f(x + \theta) g(\theta) \, d\theta \\
= \int_{\mathbb{R}^n} \left( \frac{\partial}{\partial \theta} f(x + \theta) \right) g(\theta) \, d\theta.
\]

Then we multiple any vector with unit norm \( u \in \mathcal{B}_n(1) = \{ u : \|u\| = 1, u \in \mathbb{R}^n \} \),

\[
|\langle \nabla G(x), u \rangle| = \left| \int_{\mathbb{R}^n} \left( \frac{\partial}{\partial \theta} f(x + \theta) \right) g(\theta) \, d\theta, u \right| \\
= \left| \int_{\mathbb{R}^n} \left( \frac{\partial}{\partial \theta} f(x + \theta), u \right) g(\theta) \, d\theta \right| \\
= \left| \sum_i \int_{\mathbb{R}^n} \frac{\partial f(x + \theta)}{\partial \theta_i} u_i g(\theta) \, d\theta \right| \\
= \left| \sum_i \int_{\mathbb{R}^n} \left( \int_{-\infty}^{+\infty} \frac{\partial f(x + \theta)}{\partial \theta_i} u_i g(\theta) \, d\theta \right) \prod_{j \neq i} d\theta_j \right| \\
\leq 1 \sum_i \int_{\mathbb{R}^n} \left( \int_{-\infty}^{+\infty} f(x + \theta) \frac{\partial g(\theta)}{\partial \theta_i} \, d\theta \right) \prod_{j \neq i} d\theta_j \\
= \left| \sum_i \int_{\mathbb{R}^n} f(x + \theta) \frac{\partial g(\theta)}{\partial \theta_i} u_i \, d\theta \right| \\
= \left| \int_{\mathbb{R}^n} f(x + \theta) \langle \nabla g(\theta), u \rangle \, d\theta \right| \\
= \left| \int_{\mathbb{R}^n} f(x + \theta) g(\theta) \langle \nabla \psi(\theta), u \rangle \, d\theta \right| \\
= |\mathbb{E}_{\theta \sim g}[f(x + \theta) \langle \nabla \psi(\theta), u \rangle]|,
\]

here equation 1 holds because of integration by parts. To bound the gradient of the smoothed classifier, we use the following inequality,

\[
|\langle \nabla G(x), u \rangle| \leq \sup_{f : G(x) = G(x)} \mathbb{E}_{\theta \sim g} \left[ \hat{f}(x + \theta) \langle \nabla \psi(\theta), u \rangle \right].
\]
GSmooth: Certified Robustness against Semantic Transformations via Generalized Randomized Smoothing

As shown in Yang et al. (2020), the optimal $\hat{f}(x)$ achieves at,
\[
\hat{f}(x + \theta) = \begin{cases} 
1, & \text{if } \langle u, \nabla \psi(\theta) \rangle > \varphi_u^{-1}(G(x)) \\
0, & \text{else}.
\end{cases}
\] (27)

Then, we have
\[
\mathbb{E}_{\theta \sim g} \left[ \hat{f}(x + \theta) \langle u, \nabla \psi(\theta) \rangle \right] = \mathbb{E}_{\gamma_u \sim \gamma} \mathbb{E}_{\theta \sim g} \left[ \gamma_u \mathbb{1}_{\langle u, \nabla \psi(\theta) \rangle > \varphi_u^{-1}(G(x))} \right] \leq \Phi(G(x)),
\] (28)

which means that,
\[
|\langle \nabla G(x), u \rangle| \leq \Phi(G(x)).
\] (29)

Since it holds for all $u \in B(n)$, i.e., $\|u\| \leq 1$, we have,
\[
\max_{u \in B(n)} \langle \nabla G(x), u \rangle \leq \Phi(G(x)).
\] (30)

Consider a path from $\xi_t : [0, \|\delta\|] \to \mathbb{R}^d$ with $\xi_0 = x$, $\xi_t = x + \delta$ and $\xi'_t = \frac{\delta}{\|\delta\|}$, we have
\[
\frac{dG(\xi_t)}{dt} = \langle \nabla G(\xi_t), u \rangle \leq \Phi(G(\xi_t)).
\] (31)

If the norm of $\delta$ satisfies that,
\[
\|\delta\| < \int_{G(x)}^{1/2} \frac{1}{\Phi(p)} dp.
\] (32)

If the right hand side of eq (32) exists, we name it $\|\delta_0\| = \int_{G(x)}^{1/2} 1/\Phi(p) dp$. WLOG, we assume that $G(\xi_t)$ is increasing in $t$, then we could calculate the minimal $t$ when $G(\xi_t)$ increase to $1/2$,
\[
T = \int_{G(x)}^{1/2} \frac{1}{\Phi(p)} dp = \|\delta_0\|.
\] (33)

By the generality of $\delta$ we have $G(x + \delta) < 1/2$ holds for any $\delta < \|\delta_0\|$. \qed

This theorem can be naturally extended to problems with $p > 2$ classes by considering the two top classes which are $G(x)_A$ and $G(x)_B$. This turns the problem into a binary classification problem.

A.1. The Proof of Theorem 1

In this part, we will prove Theorem 1.

**Theorem 1.** For any classifier $f(x)$, let $G(x)$ be the smoothed classifier defined in Eq. (1). If there exists a function $M(\cdot, \cdot) : P \times P \to \mathbb{R}$ satisfying
\[
\frac{\partial \gamma(\theta, \xi)}{\partial \xi} = M(\theta, \xi),
\]
and there exist two constants $p_A, p_B$ satisfying
\[
G(x)_A \geq p_A \geq p_B \geq G(x)_B,
\]
then $y_A = \arg\max_{i \in Y} G(\gamma(\xi, x))$, holds for any $\|\xi\| \leq R$, where
\[
R = \frac{1}{2M^*} \int_{p_B}^{p_A} \frac{1}{\Phi(p)} dp,
\] (34)

and $M^* = \max_{\xi, \theta \in P} \|M(\xi, \theta)\|$.

Proof. WLOG, we only prove it for binary cases that \( f(\cdot) : \mathbb{R}^n \to [0, 1] \). Recall that \( G(x) = \mathbb{E}_{\theta \sim g}[f(\tau(\theta, x))] \), we have

\[
\nabla_{\xi} G(\gamma(\theta, \xi), x) = \int \frac{\partial f(\tau(\theta, \xi), x)}{\partial \tau(\theta, \xi)} \frac{\partial \gamma(\theta, \xi)}{\partial \xi} g(\theta) d\theta \\
= \int \frac{\partial f(\tau(\theta, \xi), x)}{\partial \gamma(\theta, \xi)} \frac{\partial \gamma(\theta, \xi)}{\partial \xi} g(\theta) d\theta \\
= \int \frac{\partial f(\tau(\theta, \xi), x)}{\partial \gamma(\theta, \xi)} \frac{\partial f(\gamma(\theta, \xi), x)}{\partial \theta} \partial \gamma(\theta, \xi) \theta, \xi \partial \xi M(\theta, \xi) g(\theta) d\theta \\
= \int \frac{\partial f(\tau(\theta, \xi), x)}{\partial \gamma(\theta, \xi)} \partial \gamma(\theta, \xi) \partial \xi M(\theta, \xi) g(\theta) d\theta.
\]

For any \( u \in \mathbb{R}^d \) satisfying \( \|u\| = 1 \), we have

\[
|\langle \nabla_{\xi} G(\gamma(\xi, x)), u \rangle| = \left| \int \frac{\partial f(\gamma(\theta, \xi), x)}{\partial \theta} M(\theta, \xi) u g(\theta) d\theta \right| \\
\leq M^* \max_{\|v\|=1} \left| \int \frac{\partial f(\gamma(\theta, \xi), x)}{\partial \theta} v g(\theta) d\theta \right| \\
\frac{1}{M^*} \max_{\|v\|=1} \left| \int f(\gamma(\theta, \xi), x) \frac{\partial g(\theta)}{\partial \theta} v d\theta \right|.
\]

Here \( M^* = \max_{\theta, \xi} \|M(\theta, \xi)\| \) and equality 1 holds because of partial integral. Moreover, we assume that \( g(\theta) = \exp(-\psi(\theta)) \) and can further prove that

\[
|\langle \nabla_{\xi} G(\gamma(\xi, x)), u \rangle| \leq M^* \max_{\|v\|=1} \left| \int f(\gamma(\theta, \xi), x) \frac{\partial g(\theta)}{\partial \theta} v d\theta \right| \\
= M^* \max_{\|v\|=1} \left| \int f(\gamma(\theta, \xi), x) g(\theta) \nabla \psi(\theta) v d\theta \right| \\
= M^* \max_{\|v\|=1} \mathbb{E}_{\theta \sim g} \left[ f(\gamma(\theta, \xi), x) (\nabla \psi(\theta), v) \right] \\
\leq M^* \sup_{\|v\|=1} \mathbb{E}_{\theta \sim g} \left[ \hat{f}(\gamma(\theta, \xi), x) (\psi(\theta), u) \right].
\]

Similar with the proof of Theorem 4, the optimal \( \hat{f} \) achieves at

\[
\hat{f}(\gamma(\theta, \xi), x) = \begin{cases} 
1, & \text{if } (\psi(\theta), u) > \varphi_u^{-1}(G(\gamma(\xi, x))), \\
0, & \text{else}.
\end{cases}
\]

Then we have

\[
|\langle \nabla_{\xi} G(\gamma(\xi, x)), u \rangle| \leq \Phi(G(\gamma(\xi, x))).
\]

Consider a path from \( \xi : [0, \|\delta\|] \to \mathbb{R}^d \) with \( \xi_0 = x, \|\xi\| = \tau(\xi, x) \) and \( \xi' = \frac{\delta}{\|\delta\|} \), we have

\[
\frac{dG(\xi)}{dt} = (\nabla G(\xi), u) \leq \Phi(G(\xi)).
\]

The last part of the proof is the same with Theorem 4. \( \square \)

A.2. The proof of Theorem 2

In this part, we will prove Theorem 2, which is the main result in this paper.

**Theorem 2.** Suppose \( f(x) \) is any classifier and \( \tilde{G}(\tilde{x}) \) is the smoothed classifier defined in Eq. (10), if there exists \( p_A, p_B \) that satisfies that

\[
\tilde{G}x_A > p_A > p_B > \tilde{G}x_B,
\]

then \( y_A = \arg \max_{i \in Y} \tilde{G}(\gamma(\xi, \tilde{x})) \) for any \( \|\xi\|_2 \leq R \) where

\[
R = \frac{1}{2M^*} \int_{\Phi(A)}^{1} \frac{1}{\Phi(p)} dp,
\]
and the coefficient $M^*$ is defined as

$$M^* = \max_{\xi, \theta \in P} \sqrt{1 + \left\| \frac{\partial F_2(y_\xi)}{\partial \xi} - \frac{\partial F_1(\theta)}{\partial \theta} \right\|_2^2}. \quad (47)$$

**Proof.** WLOG, we prove it for binary cases where $f(\cdot) : \mathbb{R}^n \rightarrow [0, 1]$. First, we will calculate the gradient of $\tilde{G}(\tilde{\xi}, \tilde{x})$ to $\xi$ as

$$\nabla_\xi \tilde{G}(\tilde{\xi}, \tilde{x}) = \nabla_\xi \mathbb{E}_{\tilde{\theta} \sim \mathbb{G}(\tilde{\theta})} \left[ \tilde{f}(\tilde{\theta}, \tilde{\xi}, \tilde{x}) \right]. \quad (48)$$

We expand the expectation into integral and use chain rule to see that

$$\nabla_\xi \tilde{G}(\tilde{\xi}, \tilde{x}) = \int_{\mathbb{R}^{n+d}} \frac{\partial \tilde{f}(\tilde{\theta}, \tilde{y}_\xi)}{\partial \tilde{\theta}} \frac{\partial \tilde{\xi}(\tilde{\theta}, \tilde{y}_\xi)}{\partial \tilde{\xi}} \frac{\partial \tilde{y}_\xi}{\partial \xi} \tilde{g}(\tilde{\theta}) d\tilde{\theta}. \quad (49)$$

Similar to previous proof, the key step is to eliminate the gradient of $\frac{\partial f(\tilde{\theta}, \tilde{y}_\xi)}{\partial \tilde{\theta}}$ and replace it with $\frac{\partial f(\tilde{\theta}, \tilde{y}_\xi)}{\partial \tilde{y}_\xi}$. Since

$$\frac{\partial \tilde{\xi}(\tilde{\theta}, \tilde{y}_\xi)}{\partial \tilde{\theta}} = \begin{bmatrix} \sigma_1'(z_\theta) \\ \sigma_2'(z_\theta) \end{bmatrix} \begin{bmatrix} F'_{21}(y_\xi) \\ F'_{22}(y_\xi) \end{bmatrix},$$

$$\frac{\partial \tilde{y}_\xi}{\partial \xi} = \begin{bmatrix} H_1'(z_\xi) \\ H_2'(z_\xi) \end{bmatrix} \begin{bmatrix} I_d \\ F'_1(\xi) \end{bmatrix} I_n, \quad (50)$$

We have

$$\nabla_\xi \tilde{G}(\tilde{\xi}, \tilde{x}) = \int_{\mathbb{R}^{n+d}} \frac{\partial \tilde{F}(\tilde{\theta}, \tilde{y}_\xi)}{\partial \tilde{\theta}} \begin{bmatrix} H_1'(z_\theta) \\ H_2'(z_\theta) \end{bmatrix} \begin{bmatrix} I_d \\ F'_1(\xi) \end{bmatrix} I_n \tilde{g}(\tilde{\theta}) d\tilde{\theta}, \quad (52)$$

$$\begin{aligned}
\nabla_\xi \tilde{G}(\tilde{\xi}, \tilde{x}) &= \int_{\mathbb{R}^{n+d}} \frac{\partial \tilde{F}(\tilde{\theta}, \tilde{y}_\xi)}{\partial \tilde{\theta}} \left[ \begin{bmatrix} H_1'(z_\theta) \\ H_2'(z_\theta) \end{bmatrix} \begin{bmatrix} I_d \\ F'_1(\xi) \end{bmatrix} I_n \tilde{\theta} \right] \tilde{g}(\tilde{\theta}) d\tilde{\theta} \\
&= \int_{\mathbb{R}^{n+d}} \frac{\partial \tilde{F}(\tilde{\theta}, \tilde{y}_\xi)}{\partial \theta} \begin{bmatrix} H_1'(z_\theta) \\ H_2'(z_\theta) \end{bmatrix} \begin{bmatrix} I_d \\ F'_1(\xi) \end{bmatrix} I_n \tilde{g}(\tilde{\theta}) d\tilde{\theta} \quad (53) \\
&= \int_{\mathbb{R}^{n+d}} \frac{\partial \tilde{F}(\tilde{\theta}, \tilde{y}_\xi)}{\partial \theta} \begin{bmatrix} I_d \\ -F'_1(\theta) \end{bmatrix} I_n \begin{bmatrix} F'_{21}(y_\xi) \\ F'_{22}(y_\xi) \end{bmatrix} \tilde{g}(\tilde{\theta}) d\tilde{\theta} \quad (54) \\
&= \int_{\mathbb{R}^{n+d}} \frac{\partial \tilde{F}(\tilde{\theta}, \tilde{y}_\xi)}{\partial \theta} \begin{bmatrix} I_d \\ F'_1(\xi) \end{bmatrix} I_n \tilde{g}(\tilde{\theta}) d\tilde{\theta} \quad (55)
\end{aligned}$$

here we define

$$\tilde{M}(\tilde{\xi}, \tilde{\theta}) \triangleq \begin{bmatrix} I_d \\ -F'_1(\theta) \end{bmatrix} I_n \begin{bmatrix} F'_{21}(y_\xi) \\ F'_{22}(y_\xi) \end{bmatrix} \begin{bmatrix} H_1'(z_\theta) \\ H_2'(z_\theta) \end{bmatrix} \begin{bmatrix} I_d \\ F'_1(\xi) \end{bmatrix} I_n. \quad (56)$$

We consider the unit enlargement, which means that

$$H_1(z') = z', \quad F_21(x') = x', \quad (57)$$

thus we have

$$\tilde{M}(\tilde{\xi}, \tilde{\theta}) = \begin{bmatrix} I_d \\ F'_{21}(y_\xi) - F'_1(\theta) \end{bmatrix} \begin{bmatrix} O_{d \times n} \\ F'_{22}(y_\xi) H'_2(z_\xi) \end{bmatrix}. \quad (58)$$
Since \( \theta' \) is the virtual parameter introduced, which can be taken as 0 in case of actual disturbance. Thus we only need to consider the projection of \( \nabla \tilde{G}(\tilde{\eta}_\xi) \) in the space of \( \xi \), i.e., we set
\[
\tilde{u} = \begin{pmatrix} u \\ O_{n \times 1} \end{pmatrix},
\]
where \( u \in \mathbb{R}^d \) satisfying \( \|u\| = 1 \). Assume
\[
\tilde{g}(\tilde{\theta}) = \exp(-\tilde{\psi}(\tilde{\theta})),
\]
\[
\frac{\partial \tilde{g}(\tilde{\theta})}{\partial \theta} = -\tilde{g}(\tilde{\theta})\nabla \tilde{\psi}(\tilde{\theta}).
\]
And we have
\[
\left| \nabla \tilde{G}(\tilde{\eta}_\xi), \tilde{u} \right| = \int_{\mathbb{R}^{n+d}} \frac{\partial \tilde{f}(\tilde{\tau}(\tilde{\theta}, \tilde{\eta}_\xi))}{\partial \theta} M(\tilde{\xi}, \tilde{\theta}) \tilde{u} \tilde{g}(\tilde{\theta}) d\tilde{\theta}
\]
\[
= \int_{\mathbb{R}^{n+d}} \frac{\partial \tilde{f}(\tilde{\tau}(\tilde{\theta}, \tilde{\eta}_\xi))}{\partial \theta} \left[ \begin{array}{cc} I_d, & O_{d \times n} \\ F_{22}'(y_\xi) - F_1'(\theta), & O_{n \times n} \end{array} \right] \tilde{u} \tilde{g}(\tilde{\theta}) d\tilde{\theta}
\]
\[
= \int_{\mathbb{R}^{n+d}} \frac{\partial \tilde{f}(\tilde{\tau}(\tilde{\theta}, \tilde{\eta}_\xi))}{\partial \theta} M(\xi, \theta) \tilde{u} \tilde{g}(\tilde{\theta}) d\tilde{\theta}
\]
\[
\leq M^* \max_{\|v\|_2 = 1} \left| \int_{\mathbb{R}^{n+d}} \frac{\partial \tilde{f}(\tilde{\tau}(\tilde{\theta}, \tilde{\eta}_\xi))}{\partial \theta} \tilde{g}(\tilde{\theta}) d\tilde{\theta} \right|
\]
\[
= \frac{1}{M^*} \max_{\|v\|_2 = 1} \left| \int_{\mathbb{R}^{n+d}} \tilde{f}(\tilde{\tau}(\tilde{\theta}, \tilde{\eta}_\xi)) \frac{\partial \tilde{g}(\tilde{\theta})}{\partial \theta} \tilde{g}(\tilde{\theta}) d\tilde{\theta} \right|
\]
\[
= M^* \max_{\|v\|_2 = 1} \left| \mathbb{E}_{\tilde{g} \sim g} \left[ \tilde{f}(\tilde{\tau}(\tilde{\theta}, \tilde{\eta}(\tilde{\xi}, x))) \langle \nabla \tilde{\psi}(\tilde{\theta}), \tilde{v} \rangle \right] \right|
\]
here equality 1 holds because of partial integral. Moreover, we can bound the right hand side by
\[
\left| \nabla \tilde{G}(\tilde{\eta}_\xi), \tilde{u} \right| \leq \sup_{\tilde{f} : \tilde{G}(\tau(\xi, x)) = G(\tau(\xi, x))} M^* \max_{\|v\|_2 = 1} \left| \mathbb{E}_{\tilde{g} \sim g} \left[ \tilde{f}(\tilde{\tau}(\tilde{\theta}, \tilde{\tau}(\tilde{\xi}, x))) \langle \nabla \tilde{\psi}(\tilde{\theta}), \tilde{v} \rangle \right] \right|
\]
and the optimal \( \tilde{f} \) is
\[
\tilde{f}(\tilde{\tau}(\tilde{\theta}, \tilde{\tau}(\tilde{\xi}, x)) = \begin{cases} 1, & \text{if } (\tilde{\psi}(\tilde{\theta}), \tilde{u}) > \varphi^{-1}_a(\tilde{G}(\tilde{\tau}(\tilde{\xi}, x))) \\ 0, & \text{else} \end{cases}
\]
here
\[
M(\xi, \theta) = \left[ \begin{array}{cc} I_d, & O_{d \times n} \\ F_{22}'(y_\xi) - F_1'(\theta), & O_{n \times n} \end{array} \right]
\]
and \( M^* \) is
\[
M^* = \max_{\xi, \theta \in P} \left\| \left[ \begin{array}{cc} I_d, & O_{d \times n} \\ F_{22}'(y_\xi) - F_1'(\theta), & O_{n \times n} \end{array} \right] \right\|_2
\]
\[
= \max_{\xi, \theta \in P} \left\| \left[ \begin{array}{ccc} \frac{\partial F_{22}(y_\xi)}{\partial \xi} - \frac{\partial F_1(\theta)}{\partial \theta} \end{array} \right] \right\|_2
\]
\[
= \max_{\xi, \theta \in P} \sqrt{1 + \left\| \left( \frac{\partial F_{22}(y_\xi)}{\partial \xi} - \frac{\partial F_1(\theta)}{\partial \theta} \right) \right\|_2^2}.
\]
Notice that here $F_{22} \cdot \cdot \cdot$ is the same as $F_{2} \cdot \cdot \cdot$ in the main text. Then we could apply the techniques used in Theorem 1 and Theorem 4 here and have:

$$
R = \frac{1}{2M^2} \int_{p_1}^{p_2} \frac{1}{\Phi(p)} dp.
$$

(72)

Thus we have proven this theorem.

A3. The Proof of Theorem 3

In this part, we will prove Theorem 3.

**Theorem 3.** Suppose the simulation of the semantic transformation has a small enough error

$$
\| \hat{\tau}(\xi, \tilde{x}) - \tau(\xi, \tilde{x}) \|_2 < \varepsilon,
$$

where $\tau(\xi, \tilde{x})$ is the real semantic transformation. Then there exists a constant ratio

$$
A = A(||F_{1}'(\hat{\xi})||_2, ||F_{2}'(\tilde{y}_\xi)||_2, ||F_{2}'(\tilde{z}_\xi)||_2) > 0,
$$

which does not depend on the target classifier. The certified radius for the real semantic transformation satisfies:

$$
R_r > R(1 - A\varepsilon),
$$

(73)

where $R$ is the certified radius in Eq. (14) for the surrogate neural network in Theorem 2.

**Proof.** We set

$$
\tilde{u} = \begin{pmatrix} u \\ 0_{n \times 1} \end{pmatrix},
$$

(74)

here $u \in \mathbb{R}^d$ satisfying $\|u\| = 1$. Then we have

$$
\left\langle \nabla_\xi \hat{G}(\hat{\tau}(\xi, \tilde{x})), \nabla_\xi \hat{G}(\bar{\tau}(\bar{\xi}, \bar{\tilde{x}})), \tilde{u} \right\rangle = \int \left( \frac{\partial \hat{f}(\hat{\theta}, \hat{\tau}(\hat{\xi}, \tilde{x})))}{\partial \hat{\xi}} - \frac{\partial \hat{f}(\hat{\theta}, \bar{\tau}(\bar{\xi}, \bar{\tilde{x}})))}{\partial \hat{\xi}} \right) \hat{\theta} \hat{\theta} d\hat{\theta}
$$

$$
= \int (\hat{\tau}(\hat{\xi}, \tilde{x}) - \bar{\tau}(\bar{\xi}, \bar{\tilde{x}})) \frac{\partial^2 \hat{f}(\hat{\theta}, \hat{\tau}(\hat{\xi}, \tilde{x})))}{\partial \hat{\xi} \partial \hat{\tau}} \hat{\theta} \hat{\theta} d\hat{\theta}.
$$

(75)

Set $L = \frac{\partial^2 f(\hat{\theta}, \hat{\tau}(\hat{\xi}, \tilde{x})))}{\partial \hat{\xi} \partial \hat{\tau}}$, and we have

$$
L = \frac{\partial}{\partial \hat{\xi}} \left( \frac{\partial \hat{f}(\hat{\theta}, \hat{\tau}(\hat{\xi}, \tilde{x})))}{\partial \hat{\tau}} \right) = \frac{\partial}{\partial \hat{\xi}} \left( \frac{\partial \hat{f}(\hat{\theta}, \hat{\tau}(\hat{\xi}, \tilde{x})))}{\partial \hat{\tau}} \frac{\partial \hat{\tau}(\hat{\theta}, \hat{\tau}(\hat{\xi}, \tilde{x})))}{\partial \hat{\tau}} \right).
$$

(76)

Set $y_{\xi} = \hat{\tau}(\hat{\xi}, \tilde{x})$, and we have:

$$
\frac{\partial \hat{\tau}(\hat{\theta}, \hat{\tau}(\hat{\xi}, \tilde{x})))}{\partial \hat{\tau}} = \frac{\partial \hat{H}(\hat{F}_1(\hat{\theta}) + F_2(\hat{\tau}(\hat{\xi}, \tilde{x})))}{\partial \hat{\tau}}
$$

$$
= \hat{H}' (\hat{F}_1(\hat{\theta}) + F_2(\hat{\tau}(\hat{\xi}, \tilde{x}))) \frac{\partial \hat{F}_2(\hat{\tau}(\hat{\xi}, \tilde{x})))}{\partial \hat{\tau}}
$$

$$
= \hat{H}' (\hat{F}_1(\hat{\theta}) + F_2(\hat{\tau}(\hat{\xi}, \tilde{x}))) \left[ \begin{array}{c} I_d \\ F_2(\hat{\tau}(\hat{\xi}, \tilde{x})) \end{array} \right] \left[ \begin{array}{c} I_d \\ F_2(\hat{\tau}(\hat{\xi}, \tilde{x})) \end{array} \right] \frac{\partial \hat{F}_2(\hat{\tau}(\hat{\xi}, \tilde{x})))}{\partial \hat{\tau}}
$$

$$
= \frac{\partial \hat{\tau}(\hat{\theta}, \hat{\tau}(\hat{\xi}, \tilde{x})))}{\partial \hat{\theta}} \left[ \begin{array}{c} I_d \\ -F_2(\hat{\tau}(\hat{\xi}, \tilde{x})) \end{array} \right] \hat{F}_2(\hat{\tau}(\hat{\xi}, \tilde{x}))
$$

$$
= \frac{\partial \hat{\tau}(\hat{\theta}, \hat{\tau}(\hat{\xi}, \tilde{x})))}{\partial \hat{\theta}} A_1,
$$

(77)
here \( A_1 = \begin{bmatrix} Ld & -F'_1(\theta) \\ -F'_1(\theta) & I_n \end{bmatrix} \). By the proof above, we have \( \frac{\partial}{\partial \xi} = \frac{\partial}{\partial \xi} A_2 \), thus we have

\[
L = \frac{\partial}{\partial \xi} \left( \frac{\partial \tilde{f}(\tilde{\theta}, \tilde{\tau}(\tilde{\xi}, \tilde{x}))}{\partial \tilde{\tau}} \right) \frac{\partial \tilde{\tau}(\tilde{\theta}, \tilde{\tau}(\tilde{\xi}, \tilde{x}))}{\partial \tilde{\tau}} A_2 = \frac{\partial}{\partial \theta} \left( \frac{\partial \tilde{f}(\tilde{\theta}, \tilde{\tau}(\tilde{\xi}, \tilde{x}))}{\partial \tilde{\tau}} \right) A_2 \tag{78}
\]

Furthermore, we can prove that

\[
\langle \nabla_\xi \tilde{G}(\tilde{\tau}(\tilde{\xi}, \tilde{x})), \nabla_\xi \tilde{G}(\tilde{\tau}(\tilde{\xi}, \tilde{x})), \tilde{u} \rangle \\
= \int \left( \tilde{\tau}(\tilde{\xi}, \tilde{x}) - \tilde{\tau}(\tilde{\xi}, \tilde{x}) \right) \frac{\partial^2 \tilde{f}(\tilde{\theta}, \tilde{\tau}(\tilde{\xi}, \tilde{x}))}{\partial \xi \partial \tilde{\tau}} \tilde{u} \tilde{g}(\tilde{\theta}) d\tilde{\theta} \\
= \int \left( \tilde{\tau}(\tilde{\xi}, \tilde{x}) - \tilde{\tau}(\tilde{\xi}, \tilde{x}) \right) \frac{\partial \tilde{f}(\tilde{\theta}, \tilde{\tau}(\tilde{\xi}, \tilde{x}))}{\partial \tilde{\theta}} A_2 \tilde{u} \tilde{g}(\tilde{\theta}) d\tilde{\theta} \tag{79}
\]

where \( \tilde{\theta} \) is a constant depending on \( \| F'_1(\tilde{\xi}) \|, \| F'_2(\tilde{\xi}) \| \) and \( \| F'_2(\tilde{\xi}) \| \). Then there exists \( A \) and we have

\[
R_e \geq R(1 - \epsilon A), \tag{80}
\]

where

\[
R = \frac{1}{2M^\epsilon} \int_{p_{1n}} \frac{1}{\Phi(p)} dp.
\]

Thus we have proven this theorem. \( \square \)

**B. Implementation Details and Experimental Settings**

**B.1. Practical Algorithms for Calculating \( M^* \)**

For resolvable transformations in Theorem 1, the \( M^* \) is defined as

\[
M^* = \max_{\xi, \theta \in \mathcal{D}} \| M(\xi, \theta) \|. \tag{81}
\]

Since if we have verified that the semantic transformation is resolvable, most of time we have a closed form of \( M^* \) like contrast/brightness transformation and we are able to calculate it analytically as shown in Li et al. (2021).

For non-resolvable transformations in Corollary 1, \( M^* \) is defined as

\[
M^* = \max_{\xi \in \mathcal{D}} \sqrt{\frac{1}{\sigma_1^2} + \frac{1}{\sigma_2^2}} \left\| \frac{\partial F_2(y_{\xi})}{\partial \xi} - A_1 \right\|_{2}^2. \tag{82}
\]

This ratio is similar with the Lipschitz bound for a semantic transformation in Li et al. (2021). For low dimensional semantic transformations, we are able to interpolate the domain to find a maximum \( M^* \) and corresponding \( \xi \). But this remains a challenge for high dimensional semantic transformations. Specifically, for a given \( \xi \), we need to compute the norm of \( \frac{\partial F_2(y_{\xi})}{\partial \xi} - A_1 \). The Jacobian matrix is \( n \times n \). Calculating it requires \( n \) times of backpropagation. Thus it is inefficient to store the matrix or directly compute its norm. To solve the problem, we notice that

\[
\left\| \frac{\partial F_2(y_{\xi})}{\partial \xi} - A_1 \right\|_{2}^2 = \max_{\|u\|_{2} = 1} \left\| \left( \frac{\partial F_2(y_{\xi})}{\partial \xi} - A_1 \right) u \right\|_{2}^2. \tag{83}
\]
And then we have
\[
\left( \frac{\partial F_2(y_\xi)}{\partial \xi} - A_1 \right)^T u = \frac{\partial}{\partial \xi} (F_2(y_\xi) - A_1, u) .
\] (84)

Since tranposing a matrix does not change its norm, we could calculate its norm by optimizing \( u \) that,
\[
\max_{\|u\|_2 = 1} \left\| \frac{\partial}{\partial \xi} (F_2(y_\xi) - A_1, u) \right\|_2^2 .
\] (85)

Using this formulation, we only need to multiply the output with an unit vector and perform one backpropagation. This is a simple convex optimization problem. Then we could use any iterative algorithm to find its solution which is very fast to compute. This trick is crucial and it makes the matrix norm computation to be scalable in practice.

### B.2. Other Experimental Details

Our GSmooth requires to train two neural networks. First we randomly generate corrupted images to train a image-to-image neural network. The training process of classifiers and certification for semantic transformations are done on 2080Ti GPUs. We use a U-Net (Ronneberger et al., 2015) for the surrogate model and replace all BatchNorm layers with GroupNorm (Wu & He, 2018) since we might use the model in low batchsize settings. The U-Net could be replace by other networks used in image segmentation or superresolution like Res-UNet (Diakogiannis et al., 2020) or EDSR (Lim et al., 2017). We use L1-loss to train the surrogate model which achieves better accuracy than others which is also reported (Lim et al., 2017).

After training a surrogate model to simulate the semantic transformation, we then train the base classifier for certification with a moderate data augmentation (Li et al., 2021; Cohen et al., 2019) to ensure that training and testing of the classifier is performed on the same distribution. There are two types of data augmentation, one is the semantic transformation and the other is the augmented noise introduced only in our work. Data augmentation based semantic transformation could be done using both the surrogate model or the raw semantic transformation. We can only use the surrogate model to add the augmented noise because this noise is a type of semantic noise in the layers of surrogate model. In our experiments the standard deviation of the augmented noise is chosen from \( 0.1 \sim 0.4 \) depending on the performance. The basic network architectures for these datasets are kept the same with Li et al. (2021). On CIFAR-100 datsets, we use a PreResNet (He et al., 2016b) re-implement the method by Li et al. (2021). We also adopt the progressive sampling trick mentioned in TSS (Li et al., 2021) which is useful to reduce computational cost and certify larger radius. The details could also be found in Li et al. (2021).