Robust Deep Learning Ensemble against Deception

Wenqi Wei, Student member, IEEE, and Ling Liu, Fellow, IEEE

Abstract—Deep neural network (DNN) models are known to be vulnerable to maliciously crafted adversarial examples and to out-of-distribution inputs drawn sufficiently far away from the training data. How to protect a machine learning model against deception of both types of destructive inputs remains an open challenge. This paper presents XEnsemble, a diversity ensemble verification methodology for enhancing the adversarial robustness of DNN models against deception caused by either adversarial examples or out-of-distribution inputs. XEnsemble by design has three unique capabilities. First, XEnsemble builds diverse input denoising verifiers by leveraging different data cleaning techniques. Second, XEnsemble develops a disagreement-diversity ensemble learning methodology for guarding the output of the prediction model against deception. Third, XEnsemble provides a suite of algorithms to combine input verification and output verification to protect the DNN prediction models from both adversarial examples and out of distribution inputs. Evaluated using eleven popular adversarial attacks and two representative out-of-distribution datasets, we show that XEnsemble achieves a high defense success rate against adversarial examples and a high detection success rate against out-of-distribution data inputs, and outperforms existing representative defense methods with respect to robustness and defensibility.

Index Terms—Deep learning, adversarial attack and defense, ensemble method

1 INTRODUCTION

Deep learning has achieved unparalleled success across a variety of machine learning tasks, e.g., image classification and speech recognition. However, deep neural network (DNN) models are also known to be vulnerable to deceptive inputs that are either adversarial examples or out-of-distribution examples. Adversarial examples [1] are malicious inputs crafted covertly over benign examples to fool deep learning models to misclassify without being detected by the human, and out-of-distribution examples [2] are query inputs whose distribution differs from the training distribution. Both problems pose potential threats to many mission-critical systems and applications that use deep learning as a primary decision-making component, such as real-time object recognition, self-driving cars and voice command recognition.

The robustness of a DNN model depends on its capability to survive from the deception vulnerabilities due to both maliciously crafted adversarial inputs and out-of-distribution inputs. Both types of deceptive inputs are attributed to the same problem: the input to the prediction model has been altered maliciously. Existing defense methods against adversarial examples do not generalize over different attack algorithms [3]. Different defense methods tend to have different robustness under either different attack algorithms or different settings of attack parameters of the same attack algorithm [4]. Meanwhile, existing out-of-distribution defenses either have a limited defense success rate [5] on the adversarial example or fail miserably [6]. In this paper, we make two arguments. First, a robust defense of a privately trained DNN model against deception should be capable of shielding the well-trained prediction model from intentional manipulation with either maliciously patched inputs or out-of-distribution inputs. Second, a robust defense solution should be independent of attacks and should generalize well across different attacks, different datasets, and different DNN algorithms.

Bearing these problems in mind, we develop a diversity ensemble verification methodology, called XEnsemble, to maximize the adversarial robustness of DNN models against deception. The design of XEnsemble leverages two unique properties of deceptive inputs: (1) if an ensemble consists of only weak models whose prediction accuracy is lower than the victim target model, which we aim to protect, then we show that such an ensemble of weak models will be a poor ensemble choice for defending against deceptive inputs. (2) Not all ensemble teams from well-trained models can be effective against deception. We show that only those ensembles that have high fault tolerance in terms of disagreement diversity and respond to negative examples very differently are the ensemble teams of high robustness. A distinct property of high disagreement-diversity ensembles is that their member models tend to have very different gradient information. This contrasting gradient information tends to cause the same adversarial examples to have highly divergent and inconsistent behavior across their member models. Furthermore, this conflicting gradient information provides a distinctive opportunity for a disagreement diversity ensemble to integrate diverse decision boundaries from its member models to infer the ensemble decision boundary, which consequently reduces the attack transferability [7] of both adversarial and out-of-distribution inputs.

In summary, XEnsemble by design is capable of auto-verifying any input to the prediction model to minimize the detrimental effects due to malicious and erroneous data inputs. Consider that adversarial examples are typically generated from their corresponding benign examples, XEnsemble should be capable of auto-repairing the adverse effects caused by adversarial examples generated by different attack methods, aiming to maximize the repairing rate for adversarial examples and to achieve a high prevention success rate (PSR). For those adversarial examples that escape from the auto-repairing process, we seek to auto-detect them and filter them out. At the same time, since the out-of-distribution inputs are drawn far away from the class distribution of a trained prediction model and are outliers to the prediction tasks, the defense should maximize the detection success rate (TSR) for identifying as many out-of-distribution examples as possible and prune them out.

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In summary, XEnsemble by design is capable of auto-verifying any input to the prediction model to minimize the detrimental effects due to malicious and erroneous data inputs. Consider that adversarial examples are typically generated from their corresponding benign examples, XEnsemble should be capable of auto-repairing the adverse effects caused by adversarial examples generated by different attack methods, aiming to maximize the repairing rate for adversarial examples and to achieve a high prevention success rate (PSR). For those adversarial examples that escape from the auto-repairing process, we seek to auto-detect them and filter them out. At the same time, since the out-of-distribution inputs are drawn far away from the class distribution of a trained prediction model and are outliers to the prediction tasks, the defense should maximize the detection success rate (TSR) for identifying as many out-of-distribution examples as possible and prune them out.
Adversarial attacks can be formulated as $\min ||x - x'||_p$ s.t. $f(x') = y^*$, $f(x') \neq f(x)$, where $y^*$ denotes the target class label for targeted attacks or any label other than the correct class for untargeted attacks. $p$ is the distance norm, such as $L_0$, $L_2$, and $L_\infty$. For a given adversarial input $x_{\text{adv}}$ of a benign image $x$, $L_0$ norm indicates the number of pixels of $x$ that are changed in $x_{\text{adv}}$. $L_2$ norm is the Euclidean distance between $x$ and $x_{\text{adv}}$, and $L_\infty$ norm denotes the maximum change to any pixel of benign input $x$ in $x_{\text{adv}}$.

This paper makes three novel contributions. First, the proposed XEnsemble approach is attack-independent. It verifies the input to the prediction model by using multiple diverse input data cleansing techniques to denoise primarily the adversarial inputs. Then it verifies the output of the attack target model by creating multiple failure-independent model verifiers that have high disagreement-diversity. Second, the proposed XEnsemble approach can effectively increase the adversarial robustness of the attack target DNN model by maximizing the number of adversarial inputs that can be auto-repaired and maximizing the number of out-of-distribution inputs that can be detected. Third but not the least, our XEnsemble algorithms for auto-verification, auto-repairing, and auto-detection can generalize well across attack methods since XEnsemble algorithms do not require re-training the DNN model under protection using existing attack algorithms, and can be easily implemented on modern neural network architectures and used as a plug-in by the state of the art deep learning software frameworks. Evaluated using eleven popular adversarial attacks and two representative out-of-distribution datasets, we show that XEnsemble approach can effectively strengthen the robustness of a DNN model under protection in terms of high attack prevention success rate (PSR) for adversarial examples and high attack detection success rate (TSR) for out-of-distribution input when comparing to existing representative defense techniques. It is also worth noting that the DNN model under the protection of XEnsemble can further improve its prediction accuracy in the presence of no attacks.

2 OVERVIEW AND PROBLEM STATEMENT

2.1 Deceptive Input Artifacts

**Adversarial Examples** are the input artifacts that are created from benign inputs by adding adversarial distortions, aiming to cause the target model to misclassify with high confidence [8]. Adversarial example generation process can be formulated as

$$\min ||x - x'||_p \quad \text{s.t.} \quad f(x') = y^*, \quad f(x') \neq f(x),$$

where $y^*$ denotes the target class label for targeted attacks or any label other than the correct class for untargeted attacks. $p$ is the distance norm, such as $L_0$, $L_2$, and $L_\infty$. For a given adversarial input $x_{\text{adv}}$ of a benign image $x$, $L_0$ norm indicates the number of pixels of $x$ that are changed in $x_{\text{adv}}$, $L_2$ norm is the Euclidean distance between $x$ and $x_{\text{adv}}$, and $L_\infty$ norm denotes the maximum change to any pixel of benign input $x$ in $x_{\text{adv}}$.

For targeted attacks, we consider two targets representing two ends of the attack spectrum: the most-likely attack class in the prediction target model has 94.8% benign test accuracy. The OODs are either classified as an airplane with some attacks at high confidence of 1. adversarial example generated by one of the 11 attacks causes the benign horse input is a horse with 0.983 confidence. Each adversarial example generated by one of the 11 attacks causes the target model to misclassify the horse image into either a bird or an airplane, with some attacks at high confidence of 1.

**Out-of-Distribution (OOD) Inputs** are the artifacts of abnormal inputs drawn from a completely different distribution than the domain of the learning task. OOD inputs can be easily utilized by an adversary to launch malicious attacks because when deploying neural networks in real-world applications, there is often very little control over the test data distribution [2]. Figure 1a provides a visualization of adversarial perturbation attack to a DenseNet classifier well-trained on CIFAR-10. Its prediction on the benign horse input is a horse with a 0.983 confidence. Each adversarial example generated by one of the 11 attacks causes the target model to misclassify the horse image into either a bird or an airplane, with some attacks at high confidence of 1.
learning against deception.

2.2 Adversarial Attack Algorithms

Let $x$ and $x_{adv}$ be a benign input and its adversarial example respectively, $f(x; \theta)$ denote the prediction model with $\theta$ representing the neural network parameters, and $f(x; \tau)$ takes an input query example $x$ and outputs $\hat{y}$ and $y$ as the prediction vector and predicted class for the benign input $x$ respectively. During the model training phase, $f(x, C_x; \theta)$ is iteratively learned over the fixed training dataset of $\{x, C_x\}$, where $C_x$ denotes the class label given for training input $x$. The model parameters $\theta$ are updated through gradient descent optimization using back-propagation on a loss function, denoted by $J(h_i(x), C_y)$ where $h_i(x)$ is the intermediate result at the $i$th iteration and the training completes when the convergence condition of the iterative training is met, which produces $f(x; \theta)$ as the resulting prediction model. At the prediction phase, the prediction model $f(x; \theta)$ takes any query input $x$ and produces the prediction output denoted by $\hat{y}$ and $y$.

When adversarial examples are sent to a prediction model, the goal of untargeted attack [4] is to cause the prediction model to misclassify. Thus, with $x_{adv} = x + \Delta_x$, the attack objective is to perturb the benign input $x$ with small $\Delta_x$ to increase the loss function value $J(h(x + \Delta_x), y_x)$ such that the prediction result will be altered from the correct class label $y_x$ of its benign input $x$. By gradient ascent, the attacker needs to decrease the value of $x$ when the partial gradient is below 0 or to increase the value of $x$ when the partial gradient is above 0, which will result in increasing the loss value of $J(h(x + \Delta_x), y_x)$.

For targeted attacks, the goal of the attacker is changed to minimize the value of the loss function $J(h(x + \Delta_x), y_t)$ where $y_t$ denotes the attack target class label. Thus, the attacker needs to decrease the pixel value of benign example $x$ when the partial gradient is above 0 or to increase the pixel value of $x$ when the partial gradient is below 0, which will cause to the value of the loss function $J(h(x + \Delta_x), y_t)$ to decrease.

White-box attack v.s. Black-box attack. White-box attacks refer to adversarial examples generated by attackers who have full knowledge of the prediction model. All attacks that manipulate the gradient Information are white-box attacks since attackers use the gradient information of the attack objective to guide the learning of adversarial perturbation in terms of where (location) and how much (amount) noise should be injected to a benign input $x$. Black-box attacks refer to adversarial examples that are generated from a surrogate model that an attack generates, which can be viewed as a shadow model of the private attack target model. By the transferability of adversarial examples [7, 15], one can launch black-box attacks using such adversarial examples. One approach to generating the surrogate model for any privately held prediction model is to utilize query probing through the model prediction API and the membership inference [16].

To measure and compare the adverse effect and cost of adversarial examples generated by different attack algorithms, we introduce the following six attack evaluation metrics.

**Attack Success Rate (ASR)** indicates the percentage of all attack inputs that are successful adversarial examples. An adversarial example is successful when the attack goal is achieved: misclassification in untargeted attacks or reaching the target label in targeted attacks.

**Misclassification Rate (MR)** is the percentage of adversarial attack inputs that are misclassified. MR equals to ASR in untargeted attacks (UA) and may be larger than ASR in targeted attacks (TA). A targeted attack example may fail being classified as the target label and land on a misclassified label.

**Mean confidence on adversarial class (AdvConf)** is the mean confidence on the adversarial class of successful adversarial examples: $\frac{1}{n} \sum_{i=1}^{n} p^*$, where * denotes the misclassified class in UA and the target class in TA.

**Perturbation Distance Cost (Perturb)** is measured by the root mean square deviation: $\sqrt{\frac{1}{n} \sum_{i=1}^{n} ||x_{adv} - x||^2}$ for successful adversarial examples.

**Perception Distance Cost (Percept)** is the human perception distance metrics [7] on successful adversarial examples. Let $V_i$ be the pixel value for pixel $i$. $S_i$ be the 9 or 4 (corner) or 6 (edge)-pixel neighbors of pixel $i$ and $\mu$ be the mean value. Then the Standard Deviation of the patch area (PSTD) around pixel $i$ is $\sqrt{\sum_{V_{i\in S_i}} \sum_{V \neq \mu} (V - \mu)^2}$. The sensitivity ($Sen$) of pixel $i$ is then computed as $Sen(i) = \left\{ \begin{array}{ll} 1 & \text{PSTD}(i) \leq \frac{1}{n} \sum_{i=1}^{n} |\delta | \middle| Sen(S_i) \right\}$. Where we compute DistPercept by $\frac{1}{n} \sum_{i} |\delta v | Sen(S_i)$. $\delta v$ denotes the perturbation on pixel $i$.

**Time cost (Time)** measures the average generation time of a single adversarial example and is measured in seconds.

We evaluate eleven adversarial attacks on CIFAR-10 and ImageNet in Table 1 using the above metrics. Consider that some attacks are expensive in per-example time cost, we select the first 100 correctly predicted benign examples in the test set to generate attack examples. For FGSM, $\theta$ is set to 0.0156 for CIFAR-10 and 0.0078 for ImageNet, since with such a small $\theta$ it is sufficient to cause a high attack success rate. For BIM, the per iteration $\theta$ is 0.0012 and 0.002, and the maximum $\theta$ is 0.008 and 0.004 for CIFAR-10 and ImageNet respectively. For CW attacks, the attack confidence is set to 5 for both CIFAR-10 and ImageNet, and the maximum optimization iteration is set to 1000 since this setting is sufficient for CW algorithms to achieve 100% attack success rate. The adversarial example is fed into the target ML model every 100 iterations of optimization to check if the attack is successful. For JSMA, the maximum distortion of the image is set to 10% instead of 15%, the maximum default in paper [12].

| Attack | Time | ASR | MR | AdvConf | Perturb | Percept | Times (s) |
|--------|------|-----|----|---------|---------|---------|-----------|
| FGSM   | 91.8 | 0.95 | 0.95 | 0.95 | 0.95 | 0.95 | 0.95 |
| BIM    | 92.0 | 0.92 | 0.92 | 0.92 | 0.92 | 0.92 | 0.92 |
| PGD    | 92.1 | 0.92 | 0.92 | 0.92 | 0.92 | 0.92 | 0.92 |
| CW∞    | 92.1 | 0.92 | 0.92 | 0.92 | 0.92 | 0.92 | 0.92 |
| CWx    | 92.1 | 0.92 | 0.92 | 0.92 | 0.92 | 0.92 | 0.92 |
| CWy    | 92.1 | 0.92 | 0.92 | 0.92 | 0.92 | 0.92 | 0.92 |
| JSMA   | 92.1 | 0.92 | 0.92 | 0.92 | 0.92 | 0.92 | 0.92 |

**TABLE 1: Evaluation of adversarial attacks.**
Adversarial training defense techniques retrain the attack target model by using both benign training set and adversarial examples generated using known attack algorithms [1], [18] in order to improve the generalization of the target model in the presence of adversarial attacks. PGD adversarial training with random restart [10] and multi-model-training on adversarial examples [19] are the two most recent and more advanced adversarial training algorithms. Adversarial training can be seen as giving the target model a set of flu-shots, one per attack algorithm, and thus, adversarial training defense can be effective against known attacks. However, it also suffers from the attack-dependent training and fails to generalize and against other attacks.

Gradient masking defense techniques add an additional layer of training to reduce the sensitivity of a trained model in response to small changes in input data. The main idea is to obfuscate the gradient information or use a near-zero gradient to off-set or minimize the impact of gradient information manipulation performed by an adversary. [20] adds a gradient penalty term in the model training objective, which is a summation of the layer-wise Frobenius norm of the Jacobian matrix. The gradient penalty makes the target model less sensitive to small perturbations in input, but notably reduces the accuracy and learning effectiveness of the target model. Defensive distillation [21] replaces the last layer with a defensive softmax function and a temperature knob to control the extent of distillation after training.

Input transformation applying careful input manipulation techniques to the input data before sending it to the target prediction model. Some popular image processing techniques like binary filters and median smoothing filters are employed in [22] to perform feature squeezing on input data. Other input transformation solutions include PixelDefend [23], information encoding [24], image quilting and total variation minimization [25], randomness [26] or region sampling [27]. The dimension reduction techniques include the PCA projection of benign training data with the top $k$ principle axes [28] and the DNN denoising autoencoders [20], [29], [30], which learns the latent space representation on training data and leverages the latent patterns to detect adversarial inputs.

Defense on OOD Inputs. The first out-of-distribution detection method, proposed by the work [14], adds small perturbations to the input data by softmax-controlled input preprocessing and is often referred to as the baseline. One way to improve the baseline method is to combine the input noise injection with output temperature scaling by distillation temperature control [6]. However, both detection methods rely on a proper setting of the input noise amount parameter and the output temperature parameter, which are dataset-specific. Another proposal utilizes the Mahalanobis distance with respect to the closest class conditional distribution to flag both out-of-distribution examples and adversarial perturbed examples [5]. Other methods include training robust classifier against out-of-distribution data [31], GAN-based detection [32] and semantic representation [33].

Limitations of Existing Defenses. (1) Existing defense methods are sensitive to certain magic parameters inherent in their design, such as the percentage of adversarial examples in a batch in adversarial training, the temperature in Defensive Distillation, the detection threshold trained on benign dataset and adversarial inputs in both input transformation and denoising auto-encoder detector defense. Such dataset-specific and/or attack algorithm-specific control parameters make the defense methods non-adaptive [34]. (2) Existing detection only defenses are either limited to either out-of-distribution inputs or adversarial examples, whereas other defense methods can only defend adversarial examples but not able to detect OOD input. We argue that a defense system is practical if it is attack-independent and can generalize over attack algorithms. A robust defense approach should not depend on finding the attack-specific or dataset-specific control knob (threshold) to distinguish the adversarial inputs from the benign inputs and to detect and flag those out of distribution inputs. XEnsemble is developed to promote high robustness and high defensibility of the DNN model against both adversarial examples and out-of-distribution inputs.

3 XEnsemble Solution Approach

3.1 Overview

During the prediction phase, adversarial examples are sent to the prediction APIs to cause misclassification. Our past work [4] identified that different DNN models tend to have different gradient information and thus an adversarial example is often misclassified inconsistently across the different models. For untargeted attacks, such adversarial divergence is reflected by different attack destination classes of the same input. For targeted attacks, the same adversarial example often results in different most-likely and least-likely attack target classes under different prediction models. Although adversarial examples are transferable from one model to another [7], the transferability across different DNN models is not consistent, and the transferability is relatively more severe for untargeted attacks but less so for targeted attacks. For the same adversarial example, the probability of being misclassified by different models to the same wrong class label is not high. Meanwhile, different inputs from the same class also demonstrate some inconsistency under a single model: different destination labels in untargeted attacks and different most-likely and least-likely attack labels in targeted attacks [4]. For OOD inputs, we observe that the provided wrongly-predicted label, even under noise with the same distribution and different appearance, is different due to the exhibited uncertainty [35]. Since both adversarial example and OOD input cause misclassification and both have a low probability of being misclassified to the same wrong class, such prediction discrepancy can be utilized to build a robust prediction model to defend the out-of-distribution input.

Motivated by the characterization of adversarial examples [4], we argue that a robust defense should meet the following two design objectives simultaneously: (1) It should provide a uniform defense architecture that can generalize over both attack algorithms and datasets, and be capable of defending against both adversarial examples and out-of-distribution examples simultaneously. (2) It should be capable of distinguishing the adversarial examples that can be repaired from those that cannot, aiming to maximize the auto-repairing effectiveness. It should also be capable of maximizing the detection rate on the out-of-distribution examples to reduce or minimize the misclassification rate.

We propose to develop XEnsemble, an input-output model verification ensemble defense methodology. XEnsemble is by design unique in two aspects. First, it promotes the composition of disagreement diversity ensembles using high accuracy base models instead of weak models. Second, it combines input verification with output verification using ensemble techniques based on both denoising and failure independent redundancy. XEnsemble can protect a well trained DNN model at the prediction phase without re-training the model using adversarial examples. XEnsemble can be easily added as a plug-in to existing modern...
neural network architecture. Figure 2 shows an architectural sketch of
the XEnsemble system. It combines diverse input denoising techniques with
disagreement diversity output verification techniques. An input \( x \) submitted to a DNN model under protection (target model) is first processed by \( k \) diverse input denoising techniques, denoted by \( input\_{df1}, input\_{df2}, \ldots, input\_{dfk} \) \((k \geq 3)\). We require to choose only those techniques such that both the target model and the ensemble member models have high test accuracy, on par with their accuracy performance on the original dataset. Second, for each of the \( k \) denoising input versions of \( x \), say \( x_q \), it will be sent to the output-verification ensemble layer, which will select \( n \) model verifiers, denote by \( output\_{mg1}, output\_{mg2}, \ldots, output\_{mgn} \) \((n \geq 3)\) for output
model verification. XEnsemble will verify, repair and output the defense-approved prediction outcome of the target model, denoted by \( ST\text{-}\text{def}-\text{out}(x) \). The two ensemble size parameters \( k \) and \( n \) for input denoising process and output model verification are chosen either randomly or by using specific diversity ranking criteria [35]. Consider output model verification, we first constructed a pool of base models that have diverse network structure or backbone algorithm compared to the target model. This base model pool can be obtained by training new models from scratch or by leveraging the model zoo of pre-trained models for the same task [22]. Then, we compute the ensemble diversity score for each combination of ensemble teams of size 2 or larger from the base model pool. For a base model pool of size \( M=3, 5 \) or 10, we will have a total of 3, 26, 1013 ensemble teams. In our first prototype of XEnsemble, we use the \( \kappa \) method [37] to compute the \( \kappa \) value for each team as the prediction disagreement measure. Third, upon receiving multiple versions of the input \( x \) from the input denoising layer, we select an ensemble team from the list of top-ranked ensembles by their ensemble diversity scores, we send each of the \( k \) input versions to the chosen diversity ensemble and collect the total of \( k \times n \) prediction results. We combine these results by ranking them against a pre-defined confidence level and output the verified prediction results if the degree of the prediction agreement is higher than the pre-defined confidence level, and otherwise, we flag the input (when the agreement is below the threshold). Algorithm 1 provides a procedural sketch of the XEnsemble method.

We would like to note that the concept of input denoising and the ensemble diversity are general and applicable to different data modalities, such as image, audio, and text. For example, quantization, filtering, and Gaussian smoothing can be applied to image data; spectral subtraction and Wiener filtering are effective for audio data. In the rest of the paper, we describe in detail our prototype implementation system using the image classification learning as an example application domain. Hence, the input denoising ensemble methods and the output verification ensemble methods are tailored accordingly. We consider three threat scenarios for XEnsemble when an adversary attacks victim model (target model) based on the level of knowledge about the XEnsemble defense system: (1) zero knowledge (black-box threat model), (2) partial knowledge (gray-box threat model), and (3) full knowledge (insider adversary) (white box threat model). We first show that when attackers can launch white box attack to the target model but have no prior knowledge of XEnsemble protection. This is the common scenario that is used in the literature for defense proposals. We will also discuss the scenario where attackers have partial (gray box threat) or full knowledge (white box threat) of XEnsemble defense in addition to the target victim model.

### 3.2 Input Verification Ensemble

The main goal of input verification is to apply multiple data modality-specific input noise reduction techniques to clean the input and produce denoised versions of the input, aiming to remove adversarial perturbations or detect the out of distribution inputs and to make the first attempt to prevent adversarial misclassification. While the benign input and their denoised version are prone to be correctly classified, Our work [4] shows that the adversarial example and its denoised counterparts will demonstrate prediction discrepancy. While the location of the attack perturbation is carefully chosen and the amount is minimized to meet the imperceptibility, input denoising is applied uniformly on the entire image and is by design to preserve the semantic and visualization quality of the input image. We argue that the input noise reduction techniques should be chosen to preserve certain verifiable properties, such as the test accuracy of the target model on benign inputs, while capable of removing the adverse effect from an adversarial input.

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**Algorithm 1: Workflow of XEnsemble**

1. **Inputs:**
   - \( x_0 \): query data, \( m_{g0} \): target prediction model, \( k \): number of input-denoising modules, \( n \): number of output verification models, \( T \): \( L_1 \) ranking confidence level
2. **ensemble preparation**
   - select \( k \) input-denoising methods \( df_1, df_2, \ldots, df_k \) with expertise in processing different kinds of noise.
3. **generate a base model pool according to the target model and the prediction task**
4. **from the base model pool, create a diversity ensemble model pool using \( \kappa \) metric or other diversity metrics.**
5. **given the diversity ensemble model pool, get top \( n \) model ensembles with \( n \): models: \{\( mg_1, mg_2, \ldots, mg_n \}\}_{1,…,m}**
6. **ensemble prediction**
   - generate multiple denoised version of query: \( x_1, \ldots, x_k \) from \( x_0 \) via different noise reduction techniques \( df_1, df_2, \ldots, df_k \).
   - feed \( x_0, x_1, \ldots, x_k \) to all models in the selected ensembles \{\( mg_1, mg_2, \ldots, mg_n \}\}_{1,…,m} and get ensemble prediction results
7. **ranking prediction made by**
   - \{\( mg_1(x_0), mg_2(x_0), \ldots, mg_n(x_0) \)\}_{1,…,m} and get ensemble prediction results
8. **if \( L_1 \) distance ranking of the selected ensemble < ranking confidence level then**
9. **output XEnsemble verified prediction results**
10. **else**
    - flag the deception input and output a watchout alert.
11. **end if**

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Figure 2: Architecture of the XEnsemble defense system.
| Attack | benign | FGSM | BiM | CW∞ | CW2 | CW0 | JSMA | average |
|--------|--------|------|-----|------|------|------|------|---------|
| no defense | 0.9484 | 0.18 | 0.08 | 0.00 | 0.00 | 0.00 | 0.00 | 0.021 |
| quan-1-bit | 0.2111 | 0.17 | 0.14 | 0.15 | 0.17 | 0.16 | 0.14 | 0.16 | 0.163 |
| quan-4-bit | 0.9514 | 0.21 | 0.17 | 0.45 | 0.53 | 0.54 | 0.82 | 0.08 | 0.3 | 0.2 | 0.345 |
| medfilter-2*2 | 0.9879 | 0.08 | 0.35 | 0.84 | 0.79 | 0.86 | 0.96 | 0.09 | 0.79 | 0.79 |
| medFilter-3*3 | 0.7502 | 0.42 | 0.63 | 0.66 | 0.69 | 0.69 | 0.72 | 0.73 | 0.77 | 0.75 | 0.626 |
| NLM-11-3-2 | 0.9421 | 0.2 | 0.25 | 0.36 | 0.74 | 0.38 | 0.78 | 0.0 | 0.01 | 0.22 | 0.12 | 0.339 |
| NLM-11-3-4 | 0.9178 | 0.27 | 0.46 | 0.35 | 0.57 | 0.85 | 0.9 | 0.05 | 0.11 | 0.46 | 0.32 | 0.453 |
| NLM-13-3-2 | 0.9418 | 0.19 | 0.26 | 0.35 | 0.37 | 0.38 | 0.81 | 0.85 | 0.1 | 0.01 | 0.22 | 0.12 | 0.356 |
| NLM-13-3-4 | 0.9083 | 0.27 | 0.45 | 0.35 | 0.59 | 0.85 | 0.86 | 0.87 | 0.05 | 0.13 | 0.47 | 0.32 | 0.453 |
| rotation-12 | 0.8353 | 0.53 | 0.52 | 0.35 | 0.61 | 0.73 | 0.65 | 0.76 | 0.3 | 0.47 | 0.34 | 0.523 |
| rotation-9 | 0.8529 | 0.28 | 0.5 | 0.51 | 0.64 | 0.79 | 0.67 | 0.82 | 0.45 | 0.39 | 0.36 | 0.329 |
| rotation-3 | 0.8575 | 0.27 | 0.35 | 0.35 | 0.55 | 0.84 | 0.86 | 0.87 | 0.05 | 0.13 | 0.47 | 0.32 | 0.453 |
| rotation-6 | 0.8493 | 0.26 | 0.41 | 0.30 | 0.57 | 0.7 | 0.62 | 0.72 | 0.22 | 0.47 | 0.32 | 0.453 |
| med_2*2, rot_12, NLM-13-3-4 | 0.8927 | 0.38 | 0.60 | 0.67 | 0.72 | 0.89 | 0.79 | 0.81 | 0.36 | 0.39 | 0.47 | 0.32 |

Table 2: Defense accuracy of different feature denoising techniques for MNIST, CIFAR-10, and ImageNet.

For image classifiers, image smoothing and image augmentation techniques are popular for image noise reduction [38]. The former includes pixel quantization by color bit depth reduction, local spatial smoothing, and non-local spatial smoothing. The latter include image rotation, image cropping, and rescaling, image quilting and compression. Although these techniques are not designed to remove the injected noise directly, they can be utilized to make the perturbation less or no longer effective. In the first implementation of XEnsemble, four techniques are implemented using the Scipy library [39] and OpenCV [40].

**Rotation** method is a standard image geometric transformation technique provided in SciPy library, rotation preserves the geometric distance of the image and does not change the neighborhood information for most of the pixels except for the corner cases. In our prototype defense, the rotation degree is varied from -12 to 12 with an interval of 3 degree.

**The Color-depth reduction** is another technique that reduces the color depth of 8 bits (2^8 = 256 values) to i bits (2^i values). If i = 1, then the bit quantization will replace the [0,255] space to 1-bit encoding with 2 values: it takes 0 when the nearby pixel value is smaller than 127 and takes 1 when pixel values are in the range of [128, 255]. We use quan-i-bit to denote the quantization of the input image from the original 8-bit encoded color depth to i-bit (1 ≤ i ≤ 8).

The local spatial smoothing technique uses nearby pixels to smooth each pixel, with Gaussian, mean or median smoothing. A median filter runs a sliding window over each pixel of the image, where the center pixel is replaced by the median value of the neighboring pixels within the window. The size of the window is a configurable parameter, ranging from 1 up to the image size.

The **non-local spatial smooth (NLM)** technique smooths over similar pixels by exploring a larger neighborhood (11 × 11 search window) instead of just nearby pixels and replaces the center patch (size of 3 × 3) with the (Gaussian) weighted average of those similar patches in the search window. NLM-a-b-c denotes non-local means smoothing filter with searching window size k × k. A square shape window size, e.g., 2 × 2 or 3 × 3, is often used with reflect padding.

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Table 2 shows the results of input-denoising layer. In this set of experiments, we feed each denoised version to the target model and we show the performance of individual denoising technique and one example denoising ensemble for CIFAR-10 and ImageNet respectively. We make several interesting observations. First, employing an input noise reduction technique can always improve the robustness of the target model compared to the no-defense scenario. However, there is no single input denoising method that is effective across all 11 attacks. Each technique is good at removing some types of noise but not the other. Second, not all noise reduction techniques exhibit consistent performance across different datasets trained with different models (e.g., CIFAR-10 with DenseNet and ImageNet with MobileNet as shown in Table 3). Another interesting observation is that the least-likely attacks are relatively easier to defend than the most-likely attacks.
One reason could be that the perturbation in the least-likely attacks is larger and the denoising techniques may work more effectively. In comparison, removing the carefully injected tiny noise in the most-likely attacks may become harder. Finally, we observe that the input denoising ensemble (see last row of each dataset) show stronger defense compared to individual technique alone, while offering competitive benign test accuracy and providing significantly improved robustness under all 11 attacks. Figure 5 shows an intuitive illustration for CIFAR-10.

3.3 Output Verification Ensemble

Ensemble Diversity. We define ensemble diversity in terms of both model structure-based diversity and model disagreement-based diversity [41]. We say that an ensemble meets the structural diversity if the member models of an ensemble are trained using different training process, such as varying training dataset, initial weight filters, neural network structure, neural network algorithm employed (e.g., LeNet, VGG, MobileNet, ResNet-50, ResNet-101, ResNet-152), or by using different settings of hyperparameters (e.g., feature vector size, mini-batch size, # epochs, # iterations, learning rate functions, optimization algorithms). Thus, the structural diversity of ensemble is related to the diversity inherent in the algorithms and the hyperparameter settings used for the DNN model training. The disagreement diversity of an ensemble is related to the outputs of the DNN ensemble, which promotes the failure independence of ensemble member models and increases the overall predictive performance (accuracy).

Several popular diversity metrics, e.g., kappa statistics [37], Q statistic [42], correlation coefficient, fail/non-fail disagreement measure [43], double-fault measure [44] can be used for selecting most disagreement-diverse models from the N out baseline candidate models trained over the same benign training set. In the first prototype of Xensemble, we use the Kappa κ statistics, a pairwise metric, to measure the diversity degree between two models using negative examples. Let N denote the number of prediction results, K denote the number of classes, Ni,j denote the number of instances labeled as class i by one model and as class j by the other model. The κ metric is defined by

$$f_κ = \frac{\sum_{i=1}^{K} \frac{N_{i,i} - \sum_{k=1}^{K} \left(N_{i,k} - \frac{N_{i} \cdot N_{k}}{N}\right)}{1 - \sum_{i=1}^{K} \left(N_{i,k} - \frac{N_{i} \cdot N_{k}}{N}\right)}}$$

(1)

In Equation 1, the first term computes the percentage of agreement made by the two classifiers i and j under the same series of queries, the second term computes the chance of agreement in which the * is any label in the output space. κ value is closer to 1 when two models have more agreements, and is closer to 0 if there is more discrepancy. The disagreement diversity of an ensemble team of size M is computed by averaging all pairwise κ values of its member models.

Creating Diversity Ensemble. We develop a two-step diversity ensemble creation algorithm: First, we create a pool of candidate ensemble member models, or so-called base models. Each base model should meet the following two criteria: (1) the structure-based ensemble diversity, and (2) the high benign test accuracy comparable to that of the target model. For benchmark datasets like CIFAR-10, CIFAR-100, ImageNet-1000, instead of training N redundant DNN models, one can also collect those pre-trained DNN models on these benchmark datasets from the public domain. Although generating a pool of base models for datasets in some application domain can be potentially expensive, there are several recent efforts [45], [49] present encouraging mechanisms to create multiple base models conveniently, such as within a single training phase using Snapshots. Second, we need to create disagreement-based ensemble teams from the base model pool. This can be carried out by finding all the subsets of the base model pool of size P, which meet the following two constraints: (i) we want to include the target model in every defense ensemble; and (ii) we want to remove all ensemble teams of size 2. Thus, instead of considering 2P subsets, we only need to consider 2P−2 subsets to create the pool of disagreement-based diversity ensemble teams from a base model pool of size P. We refer to those subsets as the ensemble candidate teams. For each candidate teams, we compute its ensemble disagreement score based on the chosen diversity metric, such as the Kappa κ value. Then we rank all 2P−2 candidate ensemble teams by their κ scores and form a pool of κ ensembles by selecting the top-ranked ensemble teams whose κ values are lower than the system-defined κ diversity threshold. The lower the κ value of an ensemble, the higher the disagreement-based ensemble diversity.

Defense with Output Verification Ensemble. The output verification ensemble defense involves two problems: (1) We need to develop robust ensemble consensus methods, which can effectively combine, rank, and integrate predictions from members of an ensemble committee to produce the ensemble prediction output with high accuracy, aiming to improve the robustness of the target model under protection against in adversarial examples and out-of-distribution examples. (2) At prediction phase, for each query input, one ensemble team should be chosen randomly from the disagreement diversity ranked pool of ensemble teams as the chosen output verification team to verify and repair the prediction of the target model by simply providing the ensemble recommendation as the verified output of the target model.

There are several consensus methods for combining the outputs of multiple models in an ensemble of size M. For example, an ensemble output can be created by aggregating the outputs from its M member DNN models via simple averaging (or sum, max, median, min) or a weighted averaging method. The weighted averaging embraces the relative accuracy of the ensemble member DNN classifiers, e.g., the confidence of the top-1 class label. In general, averaging and weighted averaging are popular aggregation methods for the linear opinion pools. Voting is a representative non-linear combining method, which combines the individual votes from M member models using rank-based information. The majority voting is the simplest method, which chooses the classification made by more than half of the DNN member classifiers. When there is no agreement among more than 50% of the DNN member models, the ensemble result is considered an error. The downside of the majority is the scenario where 50% of an ensemble committee misclassify, and a majority voting, in this case, results in ensemble error. The plurality voting method improves the majority in the sense that the collective decision is the classification reached by more DNN classifiers than any other. A correct decision by the majority is inevitably a correct decision by plurality, but not vice versa [41].

We illustrate the model verification ensemble defense against adversarial examples and out-of-distribution attacks in Figure 4.
ensemble teams of structure diversity by simply choosing a subset of size 3 or larger from the base model pool, which we refer to as the Kappa \( \kappa \) ensemble. We highlight those examples that are correctly repaired in green by the random ensemble of a selection of base models and by the Kappa \( \kappa \) ranked ensemble team and highlight those that are detected as deceptive inputs in red, which are either OOD inputs or adversarial examples that cannot be repaired by the chosen ensemble team. We observe that the random ensemble is less diverse compared to the Kappa \( \kappa \) ranked ensemble team.

For instance, two verifiers out of the random ensemble of three models and by the Kappa \( \kappa \) selected ensemble team. We observe that the random ensemble is less diverse compared to the Kappa \( \kappa \) ranked ensemble team. We highlight those examples that are correctly repaired in green by the random ensemble of a selection of base models and by the Kappa \( \kappa \) ranked ensemble team and highlight those that are detected as deceptive inputs in red, which are either OOD inputs or adversarial examples that cannot be repaired by the chosen ensemble team. We observe that the random ensemble is less diverse compared to the Kappa \( \kappa \) ranked ensemble team.

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Table 4: $\kappa$ value and the benign ensemble accuracy of Top 3 ranked $\kappa$ ensemble teams of different sizes for CIFAR-10 and ImageNet.

| Model  | C10 | I100 |
|--------|-----|------|
| #model | 2   | 3    | 4    | 5    | 3    | 4    | 4    | 4    | 4    |
| acc    | 0.408 | 0.43 | 0.44 1 | 0.43 | 0.453 | 0.48 | 1    | 0.43 | 0.408 |
| $\kappa$ | 1,3  | 1,3,4 | 1,2,3,5 | 1,2,3,5  | 0.8928 | 0.9048 | 0.8836 | 0.755  | 0.318 |
| acc    | 0.9285 | 0.9684 | 0.9365 | 0.9585 | 0.775 | 0.755 | 0.805 | -     | -     |

4.2 Defense Evaluation Metrics

We evaluate the effectiveness of our model verification ensemble defense approach and compare it with other existing defenses by a number of cost and effect metrics.

**Defense Success Rate (DSR).** DSR measures the success rate of the defense system by verifying, repairing and flagging adversarial examples and out-of-distribution examples.

**Prevention Success Rate (PSR).** PSR measures the percentage of adversarial examples and out-of-distribution examples that are repaired and correctly classified by the defense.

**Detection Success Rate (TSR).** TSR measures the percentage of adversarial examples and out-of-distribution examples that cannot be repaired but are flagged by the defense.

When adversarial examples and out-of-distribution examples are presented as threats to a target DNN model, the defense success rate (DSR) is the sum of PSR and TSR, i.e., DSR = PSR + TSR. Since there is no correct label for the out-of-distribution input in a trained model, the PSR for OOD is 0 and DSR equals to TSR. To better measure the detection performance of XEnsemble, we also use the following common metrics to evaluate the effectiveness of model verification ensemble defense for detecting out-of-distribution examples in addition to TSR.

**Detection error (DError)** measures the error made both on out-of-distribution and in-distribution data. It is computed by $\beta(1-\text{TPR})+(1-\beta)\text{FPR}$. TPR is computed by TP / (TP+FN), where TP denotes the portion of correctly detected out-of-distribution examples and FN denotes the portion of OOD inputs that are considered as in-distribution data. FPR is computed by FP/(FP+TN), where FP is the proportion of in-distribution inputs that are identified as out-of-distribution inputs and TN is the proportion of in-distribution data that are identified correctly. We set $\beta = 0.5$.

**AUROC** is a threshold-independent metric that measures the tradeoff between (1-TPR) and TPR. The range of AUROC is [0,1]. It can be interpreted as the probability that a positive example is assigned a higher detection score than a negative example. The better the detection performance is, the larger the AUROC will be.

4.3 Defending Adversarial Attacks on CIFAR-10

We evaluate the effectiveness of XEnsemble defense for verifying and repairing the prediction decision made by the target model in the presence of adversarial examples. This set of experiments compares three different model verification ensemble defense options: XEnsemble-rand, XEnsemble-$\kappa$-rand, and XEnsemble-best-$\kappa$. XEnsemble-rand is an ensemble created from the base model pool with structure-based diversity. XEnsemble-$\kappa$-rand is an ensemble with disagreement diversity, selected randomly from the Kappa ranked list of ensembles whose Kappa ensemble diversity measure is above the system-defined diversity threshold. XEnsemble-best-$\kappa$ is the ensemble with the highest diversity in the Kappa ranked list of ensembles. For CIFAR-10, the XEnsemble-best-$\kappa$ ensemble is VM 1,3,4. We provide the defense performance measurement in Table 5. We observe three interesting facts: (1) XEnsemble strategy is always beneficial regardless whether it is the random ensemble from the baseline verification model pool, or the random $\kappa$ ensemble from the pool of $\kappa$ ranked ensemble list, or the best $\kappa$ ensemble. (2) the best $\kappa$ model ensemble is the most effective over all 11 attacks in terms of average defense success rate (prediction accuracy). (3) When defending adversarial example, the model verification ensemble defense is capable of repairing most of the adversarial perturbed input with high PSR. In particular, as shown in Table 6 DSR is further improved by TSR when the verification cannot agree with each other.

**Improvement with Input-Model Ensemble.** In Table 6 we also show the improvement of defense performance when we combine the output model verification layer with the input defense layer and build the input-model verification diversity ensemble. In our prototype, we apply a median filter with window size 2x2, a rotation with -12 degree, and a non-local mean filter NLM 13-3-4 to the CIFAR-10 input and then feed the processed input to multiple models. There can be other ways to combine the diverse input processing techniques with diverse output models and we consider it as future work. The input-model verification XEnsembles improves the model XEnsemble defense significantly.

**Effect of Transferability.** The transferability of adversarial examples is widely reported in literature [7]. An immediate
question one would ask is how the XEnsemble of multiple model verifiers will copes with the transferability of adversarial examples. Due to the limitation of space, we report the attack transferability experiments only on the CIFAR-10 dataset. For CIFAR-10, we measured the transferability of adversarial examples from the target model (TM) on all 7 defense models and the Best $\kappa$ ensemble (TM, VM 1,3,4) (recall Table 6). The results are shown in Table 7. In the ensemble, we measure transferability basing on the following criteria. For untargeted attacks, we consider cases where multiple models agree on the same wrong prediction as untargeted transferability since strong prediction discrepancy will be captured by the proposed defense and the query will subsequently be flagged. For targeted attacks, we consider an adversarial example is transferable only when it is being misclassified to the same target label by other models. We observe three interesting facts. (1) The untargeted attack (by FGSM or BIM) is less effectively mitigated if we only use one defense model due to transferability. (2) For all targeted attacks, one additional DM model can reasonably reduce the transferability. (3) The transferability to the Best$\kappa$ ensemble becomes very small and mostly negligible. Combining the defense success rate result for the Best$\kappa$ ensemble in Table 7 and the transferability results for the Best$\kappa$ ensemble in Table 7, low transferability does not necessarily mean that the adversarial example is correctly classified, leaving us the space to further improve the performance of XEnsemble. These observations are consistent with the result in [7], which shows the existence of many weak transferability scenarios across classifiers.

**Comparison Study.** We further strengthen the robustness performance of XEnsemble with the input augmentation ensemble and output model verification ensemble imaging smoothing. We compare the effectiveness of input-model verification XEnsemble solutions with 9 existing defense approaches from two categories: defense with no detection and defense with only detection. The former focuses on providing the correct prediction label for adversarial examples and does not integrate the detection function. Therefore, DSR= PSR and TSR=0. We consider Adversarial Training (AdvTrain [1]), Ensemble Adversarial Training (En'

### Table 5: Measurement of the Defense Success Rate on base models and XEnsemble on CIFAR-10

| CIFAR-10 | test acc | output verification ensemble (DSR/PSR/TSR) | input-output verification ensemble (DSR/PSR/TSR) |
|----------|----------|---------------------------------------------|-----------------------------------------------|
|          |          | XEnsemble-rand | XEnsemble-best-$\kappa$ | XEnsemble-rand | XEnsemble-best-$\kappa$ |
|          |          | VM 1,3,5 | VM 1,3,4 | VM 1 | VM 1 | VM 1,3,5 | VM 1,3,4 |
| no attack | 0.95 | 0.92/0.88/0.02 | 0.99/0.85/0.14 | 0.91/0.84/0.07 | 0.91/0.82/0.12 | 0.91/0.89/0.06 | 0.91/0.88/0.10 |
| FGSM | 0.15 | 0.71/0.68/0.03 | 0.76/0.70/0.07 | 0.72/0.69/0.04 | 0.85/0.75/0.12 | 0.91/0.77/0.14 | 0.91/0.79/0.12 |
| BIM | 0.08 | 0.22/0.11/0.03 | 0.22/0.11/0.03 | 0.22/0.11/0.03 | 0.22/0.11/0.03 | 0.22/0.11/0.03 | 0.22/0.11/0.03 |
| PGD | 0.14 | 0.86/0.81/0.03 | 0.91/0.80/0.03 | 0.91/0.80/0.03 | 0.91/0.80/0.03 | 0.91/0.80/0.03 | 0.91/0.80/0.03 |
| CW$_\infty$ | most | 0 | 0.90/0.87/0.03 | 0.91/0.87/0.03 | 0.92/0.89/0.03 | 0.92/0.89/0.03 | 0.92/0.89/0.03 |
| CW$_1$ | most | 0 | 0.91/0.88/0.03 | 0.92/0.89/0.03 | 0.92/0.89/0.03 | 0.92/0.89/0.03 | 0.92/0.89/0.03 |
| CW$_\infty$ | most | 0 | 0.91/0.87/0.04 | 0.92/0.87/0.04 | 0.93/0.88/0.04 | 0.93/0.88/0.04 | 0.93/0.88/0.04 |
| JSMA | most | 0 | 0.72/0.69/0.04 | 0.73/0.69/0.05 | 0.74/0.69/0.06 | 0.74/0.69/0.06 | 0.74/0.69/0.06 |

### Table 6: Defense success measurements in DSR/PSR/TSR for alternative XEnsemble algorithms on CIFAR-10

| attack model | FGSM | BIM | PGD | CW$_\infty$ | CW$_1$ | CW$_\infty$ | JSMA | model average |
|--------------|------|-----|-----|------------|--------|-------------|------|--------------|
| TM           | 1    | 0.353 | 0.412 | 0.424 | 0.436 | 0.424 | 0.235 | 0.127 | 0.133 | 0.135 | 0.160 | 0.152 | 0.044 |
| VM 1         | 1    | 0.918 | 0.64 | 0.77 | 0.86 | 0.79 | 0.76 | 0.8 | 0.83 | 0.59 | 0.53 | 0.6 | 0.33 | 0.682 |
| VM 2         | 0.923 | 0.6 | 0.75 | 0.84 | 0.76 | 0.73 | 0.8 | 0.78 | 0.66 | 0.58 | 0.35 | 0.674 |
| VM 3         | 0.924 | 0.59 | 0.73 | 0.83 | 0.73 | 0.75 | 0.77 | 0.77 | 0.56 | 0.5 | 0.61 | 0.35 | 0.648 |
| VM 4         | 0.928 | 0.59 | 0.7 | 0.81 | 0.77 | 0.73 | 0.81 | 0.74 | 0.59 | 0.42 | 0.56 | 0.32 | 0.64 |
| VM 5         | 0.926 | 0.62 | 0.72 | 0.84 | 0.78 | 0.77 | 0.82 | 0.79 | 0.59 | 0.49 | 0.62 | 0.39 | 0.675 |
| XEnsemble-rand | 0.8928 | 0.71 | 0.82 | 0.86 | 0.9 | 0.88 | 0.91 | 0.91 | 0.91 | 0.73 | 0.79 | 0.82 | 0.65 | 0.837 |
| XEnsemble-best-$\kappa$ | 0.9604 | 0.73 | 0.85 | 0.91 | 0.97 | 0.95 | 0.97 | 0.94 | 0.73 | 0.87 | 0.91 | 0.75 | 0.871 |

### Table 7: Transferability of adversarial examples to five CIFAR-10 verification models and the best ensemble team.

| attack model | TM          | VM 1        | VM 2        | VM 3        | VM 4        | VM 5        | Best ensemble |
|--------------|-------------|-------------|-------------|-------------|-------------|-------------|---------------|
| FGSM         | 1           | 0.353       | 0.412       | 0.424       | 0.436       | 0.424       | 0.235         |
| BIM          | 1           | 0.196       | 0.217       | 0.235       | 0.263       | 0.261       | 0.129         |
| PGD          | 1           | 0.116       | 0.128       | 0.139       | 0.174       | 0.139       | 0.066         |
| CW$_\infty$  | most        | 0           | 0.09        | 0.11        | 0.12        | 0.15        | 0.13          |
| CW$_1$       | most        | 0.0         | 0.0         | 0.0         | 0.0         | 0.0         | 0.0           |
| CW$_\infty$  | most        | 0.0         | 0.0         | 0.0         | 0.0         | 0.0         | 0.0           |
| JSMA         | most        | 0.1         | 0.1         | 0.1         | 0.1         | 0.1         | 0.1           |
| model average| 0.127       | 0.133       | 0.135       | 0.160       | 0.152       | 0.044       |               |
of surviving the ML component for its routine function under attack. While defense with only detection methods can be useful in sensitive applications like malware detection, such defenses are not suitable for mission-critical systems that cannot tolerate real-time interruptions. Our method can achieve comparable defense success rate and perform extremely well on the OOD input. (3) the best $\kappa$ ensemble is effective across all 11 attacks and the winner for all 8 targeted attacks. Another merit of the input-model verification $\text{XEnsemble}$ is that many of the augmentation techniques are non-differentiable. Therefore, the input ensemble cannot be jointly optimized with multiple models to perform the cross-layer attack.

### 4.4 Defending Adversarial Attacks on ImageNet

We next evaluate the effectiveness of $\text{XEnsemble}$ on ImageNet and provide the results in Table 8. For ImageNet models, the $\text{XEnsemble}$-$\kappa$ ensemble consists of the target model the VM 1,2,3,4 and provides the best defense for 8 out of 9 attacks. Although the single-model accuracy of ImageNet is not as high as CIFAR-10, the discrepancy between models plays an important role in the proposed model verification ensemble defense when auto-verifying the input. Particularly as shown in Table 8, the defense success rate on ImageNet not only comes from the competitive prediction accuracy (around 70%) of the individual model but also results from the highly diverse predictions of the same input under different models. Ensemble of these verification models brings a prediction accuracy over 80% on the selected 100 attack inputs for each attack while flagged inputs contribute to an additional 10% TSR to the DSR. Meanwhile, Table 9 also shows the robustness improvement brought by the input defense layer. Note that the JSMA attack is not included for ImageNet due to its overwhelming overhead on the heuristic search of the pixel space in high-resolution images during the attack generation. We also observe that the benign test accuracy of all three $\text{XEnsemble}$ ensembles and the input transformation ensemble defense are higher than that of the target model, showing the power of ensemble learning over individual members of the ensemble. Another merit of the proposed defense is that it does not require a modification nor re-training of the target DNN model under protection, which can be very expensive for large-scale images such as ImageNet.

The experiments also indicate that the ensemble defense success rate does not have a high correlation with the size of the ensemble, thus high diversity ensemble of one size may have a high accuracy comparable with those ensembles of other ensemble sizes. Although the effects and benefits of diversity ensemble is witnessed in our experiment and many other researches, there are many issues worth further investigation, including the quantification of ensemble diversity with theoretical formulation and the

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**TABLE 8:** Comparison of $\text{XEnsemble}$ with existing defenses on CIFAR-10. DSR=$\text{PR}+\text{TSR}$, TSR=0 for the defenses with only detection (highlight the best in bold for each category).

| CIFAR-10 | defense | benign | $\text{FGSM}_\infty$ | $\text{BIM}_\infty$ | $\text{PGD}_\infty$ | $\text{CW}_\infty$ | $\text{CW}_2$ | $\text{JSMA}_\infty$ | OOD | avg DSR |
|----------|---------|--------|----------------------|----------------------|----------------------|------------------|------------------|------------------|------|---------|
| no defense | $\text{TM}$ | 0.9484 | 0.15 | 0.08 | 0.14 | 0 | 0 | 0 | 0 | 0.028 |
| Defense with no detection | $\text{Adversain}$ | 0.879 | 0.64 | 0.58 | 0.83 | 0.68 | 0.77 | 0.75 | 0.79 | 0.44 | 0.48 | 0.5 | 0.45 | 0 | 0 | 0.516 |
| | $\text{EnsTrain}$ | 0.8895 | 0.69 | 0.61 | 0.67 | 0.71 | 0.80 | 0.81 | 0.82 | 0.55 | 0.59 | 0.60 | 0.59 | 0 | 0 | 0.571 |
| | $\text{PGD-defense}$ | 0.9128 | 0.76 | 0.68 | 0.86 | 0.76 | 0.84 | 0.78 | 0.86 | 0.55 | 0.59 | 0.61 | 0.64 | 0 | 0 | 0.61 |
| | $\text{DefDistill}$ | 0.9118 | 0.6 | 0.65 | 0.64 | 0.79 | 0.88 | 0.86 | 0.90 | 0.60 | 0.69 | 0.70 | 0.47 | 0 | 0 | 0.598 |
| | $\text{EnsTrans}$ | 0.8014 | 0.23 | 0.4 | 0.51 | 0.56 | 0.61 | 0.57 | 0.61 | 0.19 | 0.34 | 0.45 | 0.41 | 0 | 0 | 0.375 |
| Defense with only detection | $\text{PS}$ | 0.894 | 0.133 | 0.55 | 0.067 | 0.64 | 1 | 0.85 | 1 | 0.75 | 0.1 | 0.041 | 0.298 | 0.802 | 0.174 | 0 | 0.051 |
| | $\text{MagNet}$ | 0.873 | 0.92 | 1 | 1 | 0.94 | 1 | 0.97 | 1 | 0.75 | 0.95 | 0.85 | 0.96 | 0.928 | 0.968 | 0.941 |
| | $\text{NIC}$ | 0.912 | 1 | 1 | 1 | 1 | 0.94 | 1 | 0.95 | 1 | 0.90 | 0.99 | 0.905 | 0.921 | 0.969 |
| | $\text{LID}$ | 0.944 | 0.53 | 0.52 | 0.69 | 0.69 | 0.84 | 0.67 | 0.85 | 0.73 | 0.82 | 0.76 | 0.69 | 0.877 | 0.949 | 0.733 |
| Prevention | $\text{XEnsemble}$-$\kappa$ | 0.9186 | 0.85 | 0.91 | 0.96 | 0.92 | 0.92 | 0.92 | 0.99 | 0.97 | 0.99 | 0.98 | 0.996 | 0.998 | 0.993 |
| | $\text{XEnsemble}$-$\kappa$ | 0.9153 | 0.91 | 0.94 | 0.93 | 0.94 | 0.94 | 0.94 | 0.94 | 0.94 | 0.94 | 0.94 | 0.94 | 0.998 | 0.992 | 0.943 |
| | $\text{XEnsemble}$-$\kappa$ | 0.9446 | 0.93 | 0.99 | 0.95 | 0.97 | 0.98 | 0.97 | 0.99 | 0.98 | 0.97 | 0.98 | 0.998 | 0.996 | 0.997 |

**TABLE 9:** Defense Success Rate measurement of ImageNet under adversarial attacks.

| ImageNet | combo | benign | $\text{FGSM}_\infty$ | $\text{BIM}_\infty$ | $\text{PGD}_\infty$ | $\text{CW}_\infty$ | $\text{CW}_2$ | $\text{JSMA}_\infty$ | OOD | average |
|----------|-------|-------|----------------------|----------------------|----------------------|------------------|------------------|------------------|------|---------|
| $\text{TM}$ (no defense) | 0.959 | 0.01 | 0 | 0 | 0.04 | 0 | 0.06 | 0 | 0 | 0.014 |
| $\text{VM}$ | 0.67 | 0.73 | 0.77 | 0.84 | 0.81 | 0.81 | 0.81 | 0.82 | 0.79 | 0.793 |
| $\text{VM}$ | 0.68 | 0.7 | 0.78 | 0.85 | 0.83 | 0.83 | 0.84 | 0.84 | 0.81 | 0.76 | 0.799 |
| $\text{VM}$ | 0.67 | 0.78 | 0.84 | 0.83 | 0.85 | 0.83 | 0.84 | 0.84 | 0.83 | 0.825 |
| $\text{VM}$ | 0.735 | 0.86 | 0.85 | 0.85 | 0.92 | 0.85 | 0.92 | 0.85 | 0.889 | 0.889 |
| $\text{XEnsemble}$-$\kappa$ | 0.775 | 0.92 | 0.92 | 0.92 | 0.99 | 0.98 | 0.97 | 0.99 | 0.94 | 0.925 |
| $\text{XEnsemble}$-$\kappa$ | 0.755 | 0.83 | 0.9 | 0.89 | 0.92 | 0.91 | 0.92 | 0.89 | 0.894 | 0.894 |
| $\text{XEnsemble}$-$\kappa$ | 0.805 | 0.94 | 0.93 | 0.92 | 0.96 | 0.96 | 0.95 | 0.91 | 0.97 | 0.943 |

**TABLE 10:** Defense details of $\text{XEnsemble}$ on ImageNet. Number measured in DSR/PSR/TSR.
4.5 Effectiveness of Detecting OOD Inputs

We perform the out-of-distribution input detection experiment on both CIFAR-10 and CIFAR-100. We use the DenseNet CIFAR-100 model with 76.65% benign accuracy as the target model and create the ensemble pool for verification ensembles in a similar manner as those in the previous set of experiments on CIFAR-10 and ImageNet. The CIFAR-100 model pool consists of a number of Wide-ResNet models: WRN-28-10 with 80.75% benign accuracy, WRN-28-10-dropout with 81.15% accuracy, WRN-40-4 with 79.27% accuracy, and WRN-40-10 with 81.7% accuracy. The first parameter is the model depth and the second parameter is the number of Wide-ResNet models: WRN-28-10 with 80.75% benign accuracy, WRN-28-10-dropout with 81.15% accuracy, WRN-40-4 with 79.27% accuracy, and WRN-40-10 with 81.7% accuracy.

The first parameter is the model depth and the second parameter is the number of Wide-ResNet models: WRN-28-10 with 80.75% benign accuracy, WRN-28-10-dropout with 81.15% accuracy, WRN-40-4 with 79.27% accuracy, and WRN-40-10 with 81.7% accuracy. The first parameter is the model depth and the second parameter is the number of Wide-ResNet models: WRN-28-10 with 80.75% benign accuracy, WRN-28-10-dropout with 81.15% accuracy, WRN-40-4 with 79.27% accuracy, and WRN-40-10 with 81.7% accuracy.

We have demonstrated that the XEnsemble is effective against adversarial examples and out-of-distribution inputs under the black-box defense threat model in which the adversary has no knowledge of the composition of the defense system (recall Section 3.1). In this section, we evaluate the insider attack scenarios, in which the adversary has partial or full knowledge of the XEnsemble system. We refer to these two threat scenarios as grey box threats and white box threats as defined in Section 3.1. As reported in [3], [5], existing defenses fail to generalize over black box threats in the sense that some defense methods work well for certain set of attacks but fail under other types of attacks. Moreover, most existing defenses are broken under the white box threat model in which the attacker has full knowledge of the target system (both the target victim model (TM), and the composition of the defense ensemble). In this section, we evaluate the limitation of the proposed XEnsemble approach: When and how it may be broken by the cross-model ensemble attacks when a partial knowledge (grey-box) or the full knowledge (white-box) of the defense system is exposed to the adversary, such as insider snooping.

Experiment Setup. For grey-box attacks, we consider two kinds of the adversaries: (1) the attacker knows some of the models in the entire ensemble team of models and the ensemble is fixed (grey-fix); and (2) the attacker knows some of the models in the entire base model pool and the ensemble is randomly selected for every query (grey-rand). Similarly, we consider two kinds of white-box adversaries: (3) the attacker knows all of the base models in the defense system and the ensemble team used for prediction is fixed (white-fix); and (4) the attacker knows all of the baseline models and the ensemble team is randomly selected for every query (white-rand). We conduct the ensemble CW attack on
TABLE 12: Defense success rate under model verification ensemble CW attack on CIFAR-10.

We did not incorporate the input-denoising layer ensemble, which introduces additional robustness to the XEnsemble framework against insider attacks under grey box and white box threat models to defense systems. (2) We plan to extend the XEnsemble approach to other modalities, such as video, audio, and text against adversarial attacks, as well as different out-of-distribution datasets. Evaluated over eleven attack algorithms and two out-of-distribution datasets, we show that XEnsemble can achieve a high defense success rate on both adversarial and OOD inputs.

Our research continues along two directions: (1) We plan to introduce randomization in both input denoising ensemble layer and output model verification layer to add additional robustness to the XEnsemble framework against insider attacks under grey box and white box threat models to defense systems. (2) We plan to extend the XEnsemble approach to other modalities, such as video, audio, and text against adversarial attacks, as well as different out-of-distribution datasets. Evaluated over eleven attack algorithms and two out-of-distribution datasets, we show that XEnsemble can achieve a high defense success rate on both adversarial and OOD inputs.

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