ENHANCING THE RELIABILITY OF OUT-OF-DISTRIBUTION IMAGE DETECTION IN NEURAL NETWORKS

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ABSTRACT

We consider the problem of detecting *out-of-distribution* images in neural networks. We propose *ODIN*, a simple and effective method that does not require any change to a pre-trained neural network. Our method is based on the observation that using temperature scaling and adding small perturbations to the input can separate the softmax score distributions of in- and out-of-distribution images, allowing for more effective detection. We show in a series of experiments that *ODIN* is compatible with diverse network architectures and datasets. It consistently outperforms the baseline approach (Hendrycks & Gimpel, 2017) by a large margin, establishing a new state-of-the-art performance on this task. For example, *ODIN* reduces the false positive rate from the baseline 34.7% to 4.3% on the DenseNet (applied to CIFAR-10) when the true positive rate is 95%.

1 INTRODUCTION

Modern neural networks are known to generalize well when the training and testing data are sampled from the same distribution (Krizhevsky et al., 2012; Simonyan & Zisserman, 2015; He et al., 2016; Cho et al., 2014; Zhang et al., 2017). However, when deploying neural networks in real-world applications, there is often very little control over the testing data distribution. Recent works have shown that neural networks tend to make high confidence predictions even for completely unrecognizable (Nguyen et al., 2015) or irrelevant inputs (Hendrycks & Gimpel, 2017; Szegedy et al., 2014; Moosavi-Dezfooli et al., 2017). For example, a neural network trained for classifying handwritten digits can assign high confidence labels to images of animal. This has raised great concerns in AI Safety (Amodei et al., 2016), in particular how can classifiers obtain awareness of uncertainty when shown new kinds of inputs, i.e., **out-of-distribution** examples. Therefore, being able to accurately detect out-of-distribution examples can be practically important for visual recognition tasks (Krizhevsky et al., 2012; Farabet et al., 2013; Ji et al., 2013).

To make accurate detections, a seemingly straightforward approach is to enlarge and re-train the neural network on both the in- and out-of-distribution examples. However, the number of out-of-distribution examples can be infinitely many, making the re-training approach computationally expensive and intractable. Moreover, to ensure that a neural network accurately classifies in-distribution samples into correct classes while correctly detecting out-of-distribution samples, one might need to employ exceedingly large neural network architectures, which further complicates the training process.

Hendrycks & Gimpel (2017) proposed a baseline method to detect out-of-distribution examples without further re-training networks, but the performance is limited. The method is based on an observation that a well-trained neural network tends to assign higher softmax scores to in-distribution examples than out-of-distribution examples. In this paper, we go further. We observe that after using temperature scaling in the softmax function (Hinton et al., 2015; Pereyra et al., 2017) and adding small controlled perturbations to inputs, the softmax score gap between in - and out-of-distribution examples is further enlarged. We will show that the combination of these two techniques (temperature scaling and input perturbation) can lead to better detection performance. For example, provided with a pre-trained DenseNet (Huang et al., 2016) on CIFAR-10 dataset (positive samples), we test against images from TinyImageNet dataset (negative samples). Our method dramatically reduces the False Positive Rate (FPR), i.e., the fraction of misclassified out-of-distribution samples, from

34.7% to 4.3%, when 95% of in-distribution images are correctly classified. We summarize the main contributions of this paper as the following

- We propose a simple and effective method to detect out-of-distribution examples in neural networks. Our method does not require re-training the neural network and is easily implementable on any modern neural architecture.
- We test the proposed method on state-of-the-art network architectures (e.g., DenseNet (Huang et al., 2016) and Wide ResNet (Zagoruyko & Komodakis, 2016)) under a diverse set of in- and out-distribution dataset pairs. We show our method can significantly improve the detection performance, and consistently outperforms the baseline (state-of-the-art method) (Hendrycks & Gimpel, 2017) by a large margin.
- We empirically analyze how parameter settings affect the performance, and further provide theoretical intuition behind.

The outline of this paper is as follows. In Section 2, we present necessary definitions and the problem statement. In Section 3, we introduce ODIN and present performance results in Section 4. We experimentally analyze the proposed method and provide theoretical intuitions in Section 5. We summarize the related works and future directions in Section 6 and conclude the paper in Section 7.

2 Problem Statement

In this paper, we consider the problem of distinguishing in- and out-of-distribution images on a pre-trained neural network. Let $P_{\boldsymbol{X}}$ and $Q_{\boldsymbol{X}}$ denote two distinct data distributions defined on the image space $\mathcal{X}$. Assume that a neural network $\boldsymbol{f}$ is trained on a dataset drawn from the distribution $P_{\boldsymbol{X}}$. Thus, we call $P_{\boldsymbol{X}}$ the **in-distribution** and $Q_{\boldsymbol{X}}$ the **out-distribution**, respectively. In detection, we draw new images from a mixture distribution $\mathbb{P}_{\boldsymbol{X}\times Z}$ defined on $\mathcal{X} \times \{0, 1\}$, where the conditional probability distributions $\mathbb{P}_{\boldsymbol{X}|Z=0} = P_{\boldsymbol{X}}$ and $\mathbb{P}_{\boldsymbol{X}|Z=1} = Q_{\boldsymbol{X}}$ denote in- and out-distribution respectively. Now we focus on the following problem: Given an image $\boldsymbol{X}$ drawn from the mixture distribution $\mathbb{P}_{\boldsymbol{X}\times Z}$, *can we distinguish whether the image is from in-distribution $P_{\boldsymbol{X}}$ or not*?

In this paper, we focus on detecting out-of-distribution images. However, it is equally important to correctly classify an image into the right class if it is an in-distribution image. But this can be easily done: once it has been detected than an image comes from the in-distribution, we can simply use the original image and run it through the neural network to classify it. Thus, we do not change the performance of the neural network for in-distribution images and only focus on improving the detection performance for out-of-distribution images.

3 ODIN: Out-of-distribution Detector

In this section, we present our method, ODIN, for detecting out-of-distribution samples. The detector is built on two essential techniques: temperature scaling and input preprocessing. We describe the details of both components below.

Temperature Scaling. Assume that the neural network $\boldsymbol{f} = (f_1, ..., f_N)$ is trained to classify N classes. For each input $\boldsymbol{x}$, the neural network assigns a label $\hat{y}(\boldsymbol{x}) = \arg\max_i S_i(\boldsymbol{x}; T)$ by computing the softmax output for each class. Specifically,

$$S_i(\boldsymbol{x}; T) = \frac{\exp\left(f_i(\boldsymbol{x})/T\right)}{\sum_{j=1}^{N} \exp\left(f_j(\boldsymbol{x})/T\right)}, \tag{1}$$

where $T \in \mathbb{R}^+$ is the temperature scaling parameter and set to 1 during the training. For a given input $\boldsymbol{x}$, we call the maximum softmax probability, i.e., $S_{\hat{y}}(\boldsymbol{x}; T) = \max_i S_i(\boldsymbol{x}; T)$ the **softmax score**. In this paper, we use notations $S_{\hat{y}}(\boldsymbol{x}; T)$ and $S(\boldsymbol{x}; T)$ interchangeably. Prior works have established to use temperature scaling to distill the knowledge in neural networks (Hinton et al., 2015) and calibrate the prediction confidence in classification tasks (Guo et al., 2017). As we shall see later, a good manipulation of temperature T can push the softmax scores of in- and out-of-distribution images further apart from each other, making the out-of-distribution images distinguishable.

Input Preprocessing. Before feeding the image $\boldsymbol{x}$ into the neural network, we preprocess the input by adding small perturbations. The preprocessed image is given by

$$\tilde{\boldsymbol{x}} = \boldsymbol{x} - \varepsilon \text{sign}(-\nabla_{\boldsymbol{x}} \log S_{\hat{y}}(\boldsymbol{x}; T)), \tag{2}$$

where the parameter ε can be interpreted as the perturbation magnitude. The method is inspired by the idea of Goodfellow et al. (2015), where small perturbations are added to decrease the softmax score for the true label and force the neural network to make a wrong prediction. Here, our goal and setting is rather different: we aim to increase the softmax score of any given input, without the need for a class label at all. As we shall see later, the perturbation can have stronger effect on the in-distribution images than that on out-of-distribution images, making them more separable. Note that the perturbations can be easily computed by back-propagating the gradient of the cross-entropy loss w.r.t the input.

Out-of-distribution Detector. The proposed approach, ODIN, works as follows. For each image $\boldsymbol{x}$, we first calculate the preprocessed image $\tilde{\boldsymbol{x}}$ according to the equation (2). Next, we feed the preprocessed image $\tilde{\boldsymbol{x}}$ into the neural network, calculate its softmax score $S(\tilde{\boldsymbol{x}}; T)$ and compare the score to the threshold δ. We say that the image $\boldsymbol{x}$ is an in-distribution example if the softmax score is above the threshold and that the image $\boldsymbol{x}$ is an out-of-distribution example, otherwise. Therefore, the out-of-distribution detector is given by

$$g(\boldsymbol{x}; \delta, T, \varepsilon) = \begin{cases} 1 & \text{if} \max_i p(\tilde{\boldsymbol{x}}; T) \leq \delta, \\ 0 & \text{if} \max_i p(\tilde{\boldsymbol{x}}; T) > \delta. \end{cases}$$

The **detection error** $P_e(T, \varepsilon)$ under temperature T and perturbation magnitude ε is defined as

$$P_e(T, \varepsilon) = \min_{\delta} \mathbb{P}_{\boldsymbol{X} \times Z}(g(\boldsymbol{X}; \delta, T, \varepsilon) \neq Z), \tag{3}$$

representing the minimum misclassification probability over all thresholds.

4 EXPERIMENTS

In this section, we demonstrate the effectiveness of ODIN on several computer vision benchmark datasets. We run all experiments with PyTorch[1] and we will release the code to reproduce all experimental results[2].

4.1 TRAINING SETUP

Architectures and training configurations. We adopt two state-of-the-art neural network architectures, including *DenseNet* (Huang et al., 2016) and *Wide ResNet* (Zagoruyko & Komodakis, 2016). For DenseNet, our model follows the same setup as in (Huang et al., 2016), with depth $L = 100$, growth rate $k = 12$ (Dense-BC) and dropout rate 0. In addition, we evaluate the method on a Wide ResNet, with depth 28, width 10 (WRN-28-10) and dropout rate 0. Furthermore, in Appendix A.1, we provide additional experimental results on another Wide ResNet with depth 40, width 4 (WRN-40-4), which is as well used by Hendrycks & Gimpel (2017). The hyper-parameters of neural networks are set identical to the original Wide ResNet (Zagoruyko & Komodakis, 2016) and DenseNet (Huang et al., 2016) implementations. All neural networks are trained with stochastic gradient descent with Nesterov momentum (Duchi et al., 2011; Kingma & Ba, 2014). Specifically, we train Dense-BC for 300 epochs with batch size 64 and momentum 0.9; and Wide ResNet for 200 epochs with batch size 128 and momentum 0.9. The learning rate starts at 0.1, and is dropped by a factor of 10 at 50% and 75% of the training progress, respectively.

Accuracy. Each neural network architecture is trained on CIFAR-10 (C-10) and CIFAR-100 (C-100) datasets (Krizhevsky & Hinton, 2009), respectively. CIFAR-10 and CIFAR-100 images are drawn from 10 and 100 classes, respectively. Both datasets consist of 50,000 training images and 10,000 test images. The test error on CIFAR datasets are summarized in Table 1.

Architecture	**C-10**	**C-100**
Dense-BC	4.81	22.37
WRN-28-10	3.71	19.86

Table 1: Test error rates on CIFAR-10 and CIFAR-100 datasets.

[1] http://pytorch.org

[2] https://anonymous_for_review

4.2 OUT-OF-DISTRIBUTION DATASETS

At test time, the test images from CIFAR-10 (CIFAR-100) datasets can be viewed as the in-distribution (positive) examples. For out-of-distribution (negative) examples, we follow the setting in (Hendrycks & Gimpel, 2017) and test on several different natural image datasets and synthetic noise datasets. All the datasets considered are listed below.

(1) **TinyImageNet.** The Tiny ImageNet dataset[3] consists of a subset of ImageNet images (Deng et al., 2009). It contains 10,000 test images from 200 different classes. We construct two datasets, *TinyImageNet (crop)* and *TinyImageNet (resize)*, by either randomly cropping image patches of size 32×32 or downsampling each image to size 32×32.

(2) **LSUN.** The Large-scale Scene UNderstanding dataset (LSUN) has a testing set of 10,000 images of 10 different scenes (Yu et al., 2015). Similar to TinyImageNet, we construct two datasets, *LSUN (crop)* and *LSUN (resize)*, by randomly cropping and downsampling the LSUN testing set, respectively.

(3) **iSUN.** The iSUN (Xu et al., 2015) consists of a subset of SUN images. We include the entire collection of 8925 images in iSUN and downsample each image to size 32 by 32.

(4) **Gaussian Noise.** The synthetic Gaussian noise dataset consists of 10,000 random 2D Gaussian noise images, where each RGB value of every pixel is independently and identically sampled from a Gaussian distribution with mean 0.5 and unit variance. We further clip each pixel value into the range $[0, 1]$.

(5) **Uniform Noise.** The synthetic uniform noise dataset consists of 10,000 images where each RGB value of every pixel is independently and identically sampled from a uniform distribution on $[0, 1]$.

4.3 EVALUATION METRICS

We adopt the following four different metrics to measure the effectiveness of a neural network in distinguishing in- and out-of-distribution images.

(1) **FPR at 95% TPR** can be interpreted as the probability that a negative (out-of-distribution) example is misclassified as positive (in-distribution) when the true positive rate (TPR) is as high as 95%. True positive rate can be computed by TPR = TP / (TP+FN), where TP and FN denote true positives and false negatives respectively. The false positive rate (FPR) can be computed by FPR = FP / (FP+TN), where FP and TN denote false positives and true negatives respectively.

(2) **Detection Error**, i.e., P_e measures the minimum misclassification probability over all possible score thresholds. The definition of P_e is given in equation (3). Here, we set that both positive and negative examples have equal probability of appearing in the test set.

(3) **AUROC** is the Area Under the Receiver Operating Characteristic curve, which is also a threshold-independent metric (Davis & Goadrich, 2006). The ROC curve depicts the relationship between TPR and FPR. The AUROC can be interpreted as the probability that a positive example is assigned a higher detection score than a negative example (Fawcett, 2006). A perfect detector corresponds to an AUROC score of 100%.

(4) **AUPR** is the Area under the Precision-Recall curve, which is another threshold independent metric (Manning et al., 1999; Saito & Rehmsmeier, 2015). The PR curve is a graph showing the precision=TP/(TP+FP) and recall=TP/(TP+FN) against each other. The metric AUPR-In and AUPR-Out in Table 2 denote the area under the precision-recall curve where in-distribution and out-of-distribution images are specified as positives, respectively.

4.4 EXPERIMENTAL RESULTS

Comparison with baseline. In Figure 1, we show the ROC curves when DenseNet-BC-100 is evaluated on CIFAR-10 (positive) images against TinyImageNet (negative) test examples. The red curve corresponds to the ROC curve when using baseline method (Hendrycks & Gimpel, 2017), whereas the blue curve corresponds to our method with temperature $T = 1000$ and perturbation magnitude $\varepsilon = 0.0012$. We observe a strikingly large gap between the blue and red ROC curves. For example, when TPR$= 95\%$, the FPR can be reduced from 34% to 4.2% by using our approach.

[3] `https://tiny-imagenet.herokuapp.com`

	Out-of-distribution dataset	FPR (95% TPR) ↓	Detection Error ↓	AUROC ↑	AUPR In ↑	AUPR Out ↑
		Baseline (Hendrycks & Gimpel, 2017) / ODIN				
Dense-BC CIFAR-10	TinyImageNet (crop)	34.7/4.3	10.0/4.7	95.3/99.1	96.4/99.1	93.8/99.1
	TinyImageNet (resize)	40.8/7.5	11.5/6.1	94.1/98.5	95.1/98.6	92.4/98.5
	LSUN (crop)	39.3/8.7	10.2/6.0	94.8/98.2	96.0/98.5	93.1/97.8
	LSUN (resize)	33.6/3.8	9.7/4.4	95.4/99.2	96.4/99.3	94.0/99.2
	iSUN	37.2/6.3	10.8/5.5	94.8/98.8	95.9/98.9	93.1/98.8
	Uniform	23.5/0.0	5.3/0.5	96.5/99.9	97.8/100.0	93.0/99.9
	Gaussian	12.3/0.0	4.7/0.2	97.5/100.0	98.3/100.0	95.9/100.0
Dense-BC CIFAR-100	TinyImageNet (crop)	67.8/17.3	24.8/8.8	83.0/97.1	85.3/97.4	80.8/96.8
	TinyImageNet (resize)	82.2/44.3	35.0/17.5	70.4/90.7	71.4/91.4	68.6/90.1
	LSUN (crop)	69.4/17.6	23.9/9.4	83.7/96.8	86.2/97.1	80.9/96.5
	LSUN (resize)	83.3/44.0	35.0/16.8	70.6/91.5	72.5/92.4	68.0/90.6
	iSUN	84.8/49.5	35.2/18.0	69.9/90.1	71.9/91.1	67.0/88.9
	Uniform	88.3/0.5	20.6/2.5	83.2/99.5	88.1/99.6	73.1/99.0
	Gaussian	95.4/0.2	20.5/1.9	81.8/99.6	87.6/99.7	70.1/99.1
WRN-28-10 CIFAR-10	TinyImageNet (crop)	38.9/23.4	12.5/11.6	92.9/94.2	92.5/92.8	91.9/94.7
	TinyImageNet (resize)	45.6/25.5	14.8/13.4	91.0/92.1	89.7/89.0	89.9/93.6
	LSUN (crop)	35.0/21.8	10.8/9.8	94.5/95.9	95.1/95.8	93.1/95.5
	LSUN (resize)	35.0/17.6	11.4/9.7	93.9/95.4	93.8/93.8	92.8/96.1
	iSUN	40.6/21.3	13.2/11.5	92.5/93.7	91.7/91.2	91.5/94.9
	Uniform	1.6/0.0	3.2/0.2	99.2/100.0	99.3/100.0	98.9/100.0
	Gaussian	0.3/0.0	2.4/0.1	99.5/100.0	99.6/100.0	99.3/100.0
WRN-28-10 CIFAR-100	TinyImageNet (crop)	66.6/43.9	26.2/17.2	82.0/90.8	83.3/91.4	80.2/90.0
	TinyImageNet (resize)	79.2/55.9	33.5/23.3	72.2/84.0	70.4/82.8	70.8/84.4
	LSUN (crop)	74.0/39.6	27.6/15.6	80.3/92.0	83.4/92.4	77.0/91.6
	LSUN (resize)	82.2/56.5	31.6/21.7	73.9/86.0	75.7/86.2	70.1/84.9
	iSUN	82.7/57.3	32.8/22.6	72.8/85.6	74.2/85.9	69.2/84.8
	Uniform	98.2/0.1	16.2/2.2	84.1/99.1	89.9/99.4	71.0/97.5
	Gaussian	99.2/1.0	15.4/2.9	84.3/98.5	90.2/99.1	70.9/95.9

Table 2: Distinguishing in- and out-of-distribution test set data for image classification. All values are percentages. ↑ indicates larger value is better, and ↓ indicates lower value is better. All parameter settings are shown in Appendix A.2. Additional results on WRN-40-4 and MNIST dataset are reported in Appendix A.1.

Choosing parameters. For each out-of-distribution dataset, we randomly hold out 1,000 images for tuning the parameters T and ε. For temperature T, we select among 1, 2, 5, 10, 20, 50, 100, 200, 500, 1000; and for perturbation magnitude ε we choose from 21 evenly spaced numbers starting from 0 and ending at 0.004. The optimal parameters are chosen to minimize the detection error on the holdout set. We evaluate the our approach on the remaining test images. All parameter settings are reported in the Appendix A. We provide additional details on the effect of parameters in Section 5.

Main results. The main results are summarized in Table 2. For each in- and out-of-distribution dataset pair, we report both the performance of the baseline (Hendrycks & Gimpel, 2017) and our approach using temperature scaling and input preprocessing. In Table 2, we observed improved performances across all neural architectures and all dataset pairs. Noticeably, our method consistently outperforms the baseline by a large margin when measured by FPR at 95% TPR and detection error.

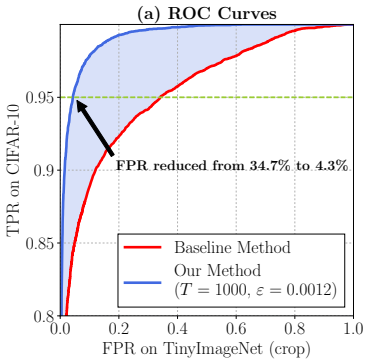

Figure 1: (a) ROC curves of baseline (red) and our method (blue) on DenseNet-BC-100 network, where CIFAR-10 and TinyImageNet (crop) are in- and out-of-distribution dataset, respectively.

4.5 Extensions

In this subsection, we analyze how the statistical distance between in- and out-of-distribution natural image dataset affects the detection performance of the proposed method.

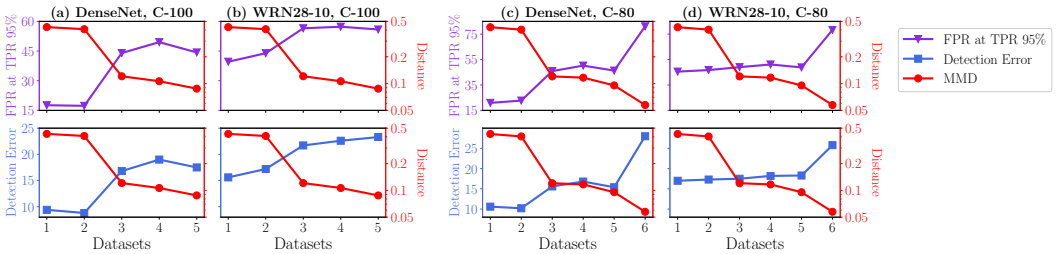

Figure 2: (a)-(d) Performances of our method vs. MMD between in- and out-of-distribution datasets. Neural networks are trained on CIFAR-100 and CIFAR-80, respectively. The out-of-distribution datasets are 1: LSUN (cop), 2: TinyImageNet (crop), 3: LSUN (resize), 4: is iSUN (resize), 5: TinyImageNet (resize) and 6: CIFAR-20.

Data distribution distance vs. Detection performance. To measure the statistical distance between in- and out-of-distribution datasets, we adopt a commonly used metric, maximum mean discrepancy (MMD) with Gaussian RBF kernel (Sriperumbudur et al., 2010; Gretton et al., 2012; Sutherland et al., 2016). Specifically, given two image sets, $V = \{v_1, ..., v_m\}$ and $W = \{w_1, ..., w_m\}$, the maximum mean discrepancy between V and Q is defined as

$$\widehat{\mathrm{MMD}}^2(V, W) = \frac{1}{\binom{m}{2}} \sum_{i \neq j} k(v_i, v_j) + \frac{1}{\binom{m}{2}} \sum_{i \neq j} k(w_i, w_j) - \frac{2}{\binom{m}{2}} \sum_{i \neq j} k(v_i, w_j),$$

where $k(\cdot, \cdot)$ is the Gaussian RBF kernel, i.e., $k(x, x') = \exp\left(-\frac{\|x - x'\|_2^2}{2\sigma^2}\right)$. We set use the same way used by Sutherland et al. (2016) to choose σ, where $2\sigma^2$ is set to the median of all Euclidean distances between all images in the aggregate set $V \cup W$.

In Figure 2 (a)(b), we show how performances of ODIN vary against the MMD distances between in- and out-of-distribution datasets[4]. The datasets (on x-axis) are ranked in the descending order of MMD distances with CIFAR datasets. There are two interesting observations can be drawn from. First, we find that the MMD distances between the cropped datasets and CIFAR-100 tend to be larger. This is likely due to the fact that cropped images only contain local image context and are thus distinct from images in CIFAR-100, while resized images contain global patterns and are thus similar to images in CIFAR-100. Second, we observe that the MMD distance tends to be negatively correlated with the detection performance. This suggests that the detection task becomes harder as in and out-of-distribution images are more similar to each other.

Same-manifold datasets. Furthermore, we investigate the extreme scenario when in- and out-of-distribution datasets are on the same manifold. In experiment, we randomly split CIFAR-100 into two disjoint datasets containing 80 and 20 classes each. We name them *CIFAR-80* and *CIFAR-20*, respectively. We train both DenseNet and Wide ResNet-28-10 on the CIFAR-80 dataset (in-distribution) and evaluate the detection performances on the CIFAR-20 dataset (out-distribution). All hyperparameters used here are exactly the same as in Section 4.1. The MMD distance between CIFAR-20 and CIFAR-80 is much smaller than other dataset pairs. In Figure 2 (c)(d), we observe that both FPR at TPR 95% and detection error become larger on the CIFAR-20 dataset. This coincides with our expectation that the detection task becomes extremely hard when in- and out-of-distribution dataset locate on the same manifold. We provide additional experimental results in Appendix A.1 and Appendix G.

5 Discussions

5.1 Effects of Parameters

In this subsection, we empirically show how temperature T and perturbation magnitude ε affect FPR at TPR 95% and AUROC on DenseNet and Wide ResNet-28-10. Additional results on other metrics and architectures are provided in Appendix B. We show the detection performances when using only the temperature scaling method (see Figure 3(a)(b), $\varepsilon = 0$), or the input preprocessing method (see Figure 3(c)(d), $T = 1$). In Figure 4, we show the detection performance w.r.t ε when T is optimal (e.g., T=1000). First, from Figure 3 (a)(b), we observe that increasing the temperature

[4] All distances are provided in Appendix G.

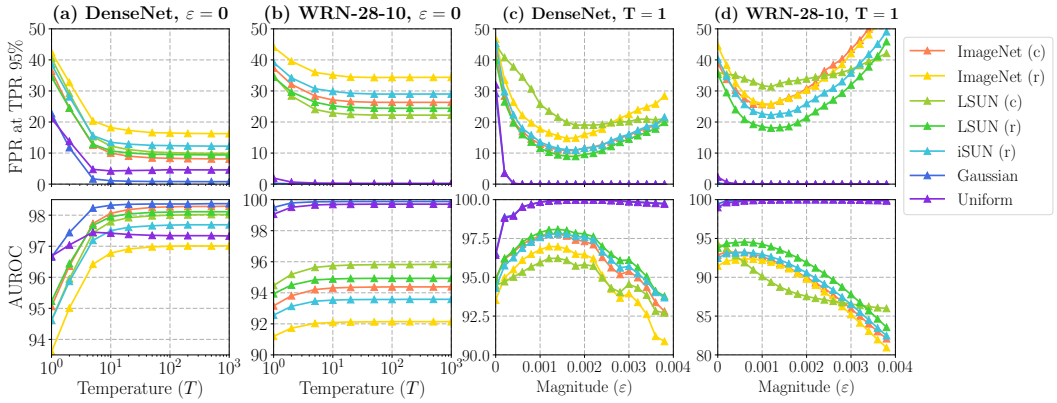

Figure 3: (a)(b) Effects of temperature T when $\varepsilon = 0$. (c)(d) Effects of perturbation magnitude ε when $T = 1$. All networks are trained on CIFAR-10 (in-distribution). Additional results on other metrics and Wide ResNet-40 are provided in Appendix B.

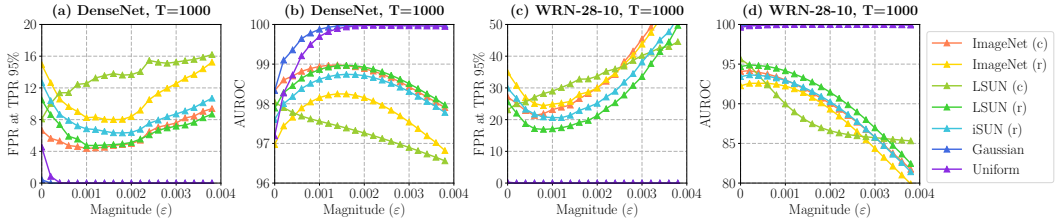

Figure 4: (a)(b) Effects of perturbation magnitude ε on DenseNet when T is large (e.g., $T = 1000$). (c)(d) Effects of perturbation magnitude of ε on Wide-ResNet-28-10 when T is large (e.g., $T = 1000$). All networks are trained on CIFAR-10. Additional results on other metrics and Wide ResNet-40 are provided in Appendix B.

can improve the detection performances, although the effects diminish when T is sufficiently large (e.g., $T > 100$). Next, from Figure 3(c)(d) and Figure 4, we observe that we can further improve the detection performances by appropriately choosing the perturbation magnitudes. We can achieve overall better performance by combining both (1) temperature scaling and (2) input preprocessing.

5.2 Analysis on Temperature Scaling

In this subsection, we analyze the effectiveness of the temperature scaling method. As shown in Figure 3 (a) and (b), we observe that a sufficiently large temperature yields better detection performance although the effects diminish when T is too large. To gain insights, we can refer to the Taylor expansion of softmax score (details provided in Appendix D). When T is sufficiently large, we have

$$S_{\hat{y}}(\boldsymbol{x};T) \approx \frac{1}{N - \frac{1}{T}\sum_i [f_{\hat{y}}(\boldsymbol{x}) - f_i(\boldsymbol{x})] + \frac{1}{2T^2}\sum_i [f_{\hat{y}}(\boldsymbol{x}) - f_i(\boldsymbol{x})]^2}, \tag{4}$$

by omitting the third and higher orders. For simplicity of notation, we define

$$U_1(\boldsymbol{x}) = \frac{1}{N-1}\sum_{i \neq \hat{y}} [f_{\hat{y}}(\boldsymbol{x}) - f_i(\boldsymbol{x})] \quad \text{and} \quad U_2(\boldsymbol{x}) = \frac{1}{N-1}\sum_{i \neq \hat{y}} [f_{\hat{y}}(\boldsymbol{x}) - f_i(\boldsymbol{x})]^2. \tag{5}$$

Interpretations of U_1 and U_2. By definition, U_1 measures the extent to which the largest unnormalized output of the neural network deviates from the remaining outputs; while U_2 measures the extent to which the remaining smaller outputs deviate from each other. We provide formal mathematical derivations in Appendix F. In Figure 5(a), we show the distribution of U_1 for each out-of-distribution dataset vs. the in-distribution dataset (in red). We observe that the largest outputs of the neural network on in-distribution images deviate more from the remaining outputs. This is likely due to the fact that neural networks tend to make more confident predictions on in-distribution images.

Further, we show in Figure 5(b) the expectation of U_2 conditioned on U_1, i.e., $E[U_2|U_1]$, for each dataset. The red curve (in-distribution images) has overall higher expectation. This indicates that, when two images have similar values on U_1, the in-distribution image tends to have a much higher

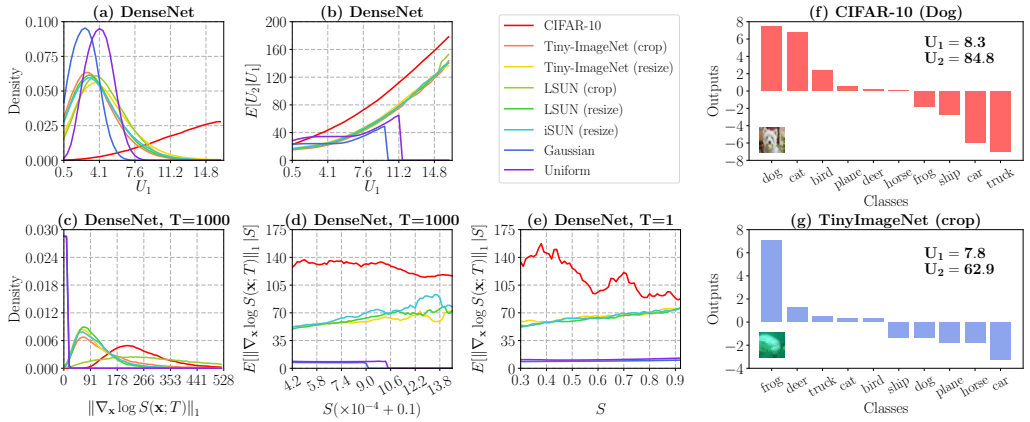

Figure 5: (a) Probability density of U_1 under different datasets on DenseNet. (b) Expectations of U_2 conditioned on U_1 on DenseNet. (c) Probability density of the norm of gradient on DenseNet under temperature $1,000$. (c)(d) Expectation of the norm of gradient conditioned on the softmax scores on DenseNet under temperature $T = 1000$ and $T = 1$, respectively. (f)(g) Outputs of DenseNet on each class for an image of dog from CIFAR-10 and an image from TinyImageNet (crop). The DenseNet is trained on CIFAR-10. Additional results on other architectures are provided in Appendix C.

value of U_2 than the out-of-distribution image. In other words, for in-distribution images, the remaining outputs (excluding the largest output) tend to be more deviated from each other compared to out-of-distribution datasets. This may happen when some classes in the in-distribution dataset share common features while others differ significantly. To illustrate this, in Figure 5 (f)(g), we show the outputs of each class using a DenseNet (trained on CIFAR-10) on a dog image from CIFAR-10, and another image from TinyImageNet (crop). For the image of dog, we can observe that the largest output for the label *dog* is close to the output for the label *cat* but is quite deviated from the outputs for the label *car* and *truck*. This is likely due to the fact that, in CIFAR-10, images of dog are very similar to the images of cat but are quite distinct from images of car and truck. For the image from TinyImageNet (crop), despite having one large output, the remaining outputs are close to each other and thus have a smaller deviation.

The effects of T. To see the usefulness of adopting a large T, we can first rewrite the softmax score function in Equation (4) as $S \propto (U_1 - U_2/2T)/T$. Hence the softmax score is largely determined by U_1 and $U_2/2T$. As noted earlier, U_1 makes in-distribution images produce larger softmax scores than out-of-distribution images since $S \propto U_1$, while U_2 has the exact opposite effect since $S \propto -U_2$. Therefore, by choosing a sufficiently large temperature, we can compensate the negative impacts of $U_2/2T$ on the detection performance, making the softmax scores between in- and out-of-distribution images more separable. Eventually, when T is sufficiently large, the distribution of softmax score is almost dominated by the distribution of U_1 and thus increasing the temperature further is no longer effective. This explains why we see in Figure 3 (a)(b) that the performance becomes unchanged when T is too large (e.g., $T > 100$). In Appendix E, we provide formal proof showing that the detection error eventually converges to a constant number when T goes to infinity.

5.3 Analysis on Input Preprocessing

As noted previously, using the temperature scaling method by itself can be effective in improving the detection performance. However, the effectiveness quickly diminishes as T becomes very large. In order to make further improvement, the input processing method can be quite complementary. This has already been seen in Figure 4, where the detection performance is improved by a large margin on most datasets when $T = 1000$, provided with an appropriately chosen perturbation magnitude ε. In this subsection, we provide insights behind this.

To explain, we can look into the first order Taylor expansion of the log-softmax function for the perturbed image $\tilde{\boldsymbol{x}}$, which can be derived as

$$\log S_{\hat{y}}(\tilde{\boldsymbol{x}}; T) = \log S_{\hat{y}}(\boldsymbol{x}; T) + \varepsilon \left\| \nabla_{\boldsymbol{x}} \log S_{\hat{y}}(\boldsymbol{x}; T) \right\|_1 + o(\varepsilon),$$

where $\boldsymbol{x}$ is the original input.

The effects of gradient. In Figure 5 (c), we present the distribution of $\|\nabla_{\boldsymbol{x}} \log S(\boldsymbol{x}; T)\|_1$ — the 1-norm of gradient of log-softmax with respect to the input $\boldsymbol{x}$ — for all datasets. A salient observation

is that CIFAR-10 images (in-distribution) tend to have larger values on the norm of gradient than most out-of-distribution images. To further see the effects of the norm of gradient on the softmax score, we provide in Figures 5 (d) the conditional expectation $E[\|\nabla_{\boldsymbol{x}} \log S(\boldsymbol{x};T)\|_1 | S]$. We can observe that, when an in-distribution image and an out-of-distribution image have the same softmax score, the value of $\|\nabla_{\boldsymbol{x}} \log S(\boldsymbol{x};T)\|_1$ for in-distribution image tends to be larger.

We illustrate the effects of the norm of gradient in Figure 6. Suppose an in-distribution image $\boldsymbol{x}_1$ (blue) and an out-of-distribution image $\boldsymbol{x}_2$ (red) have similar softmax scores, i.e., $S(\boldsymbol{x}_1) \approx S(\boldsymbol{x}_2)$. After input processing, the in-distribution image can have a much larger softmax score than the out-of-distribution image $\boldsymbol{x}_2$ since the in-distribution image $\boldsymbol{x}_1$ has a much larger value on the norm of softmax gradient than that of $\boldsymbol{x}_2$. Therefore, in- and out-of-distribution images are more separable from each other after input preprocessing[5].

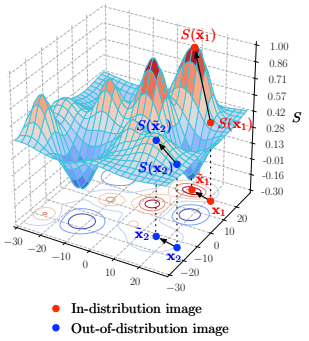

Figure 6: Illustration of effects of the input preprocessing.

The effect of ε. When the magnitude ε is sufficiently small, adding perturbations does not change the predictions of the neural network, i.e., $\hat{y}(\tilde{\boldsymbol{x}}) = \hat{y}(\boldsymbol{x})$. However, when ε is not negligible, the gap of softmax scores between in- and out-of-distribution images can be affected by $\|\nabla_{\boldsymbol{x}} \log S(\boldsymbol{x};T)\|_1$. Our observation is consistent with that in (Szegedy et al., 2014; Goodfellow et al., 2015; Moosavi-Dezfooli et al., 2017), which show that the softmax scores tend to change significantly if small perturbations are added to the in-distribution images. It is also worth noting that using a very large ε can lead to performance degradation, as seen in Figure 4. This is likely due to the fact that the second and higher order terms in the Taylor expansion are no longer insignificant when the perturbation magnitude is too large.

6 Related Works and Future Directions

The problem of detecting out-of-distribution examples in low-dimensional space has been well-studied in various contexts (see the survey by Pimentel et al. (2014)). Conventional methods such as density estimation, nearest neighbor and clustering analysis are widely used in detecting low-dimensional out-of-distribution examples (Chow, 1970; Vincent & Bengio, 2003; Ghoting et al., 2008; Devroye et al., 2013), . The density estimation approach uses probabilistic models to estimate the in-distribution density and declares a test example to be out-of-distribution if it locates in the low-density areas. The clustering method is based on the statistical distance, and declares an example to be out-of-distribution if it locates far from its neighborhood. Despite various applications in low-dimensional spaces, unfortunately, these methods are known to be unreliable in high-dimensional space such as image space (Wasserman, 2006; Theis et al., 2015). In recent years, out-of-distribution detector based on deep models have been proposed, due to their undoubtable representing power in high-dimensional space. Schlegl et al. (2017) train a generative adversarial networks to detect out-of-distribution examples in clinical scenario. Sabokrou et al. (2016) train a convolutional network to detect anomaly in scenes. Andrews et al. (2016) adopt transfer representation-learning for anomaly detection. All these works require enlarging or modifying the neural networks. In a more recent work, Hendrycks & Gimpel (2017) found that pre-trained neural networks can be overconfident to out-of-distribution example, limiting the effectiveness of detection. Our paper aims to improve the performance of detecting out-of-distribution examples, yet without requiring any change to an existing well-trained model.

Our approach leverages the following two interesting observations to help better distinguish between in- and out-of-distribution examples: (1) On in-distribution images, modern neural networks tend to produce outputs with larger variance across class labels, and (2) neural networks have larger norm of gradient when applied on in-distribution images. We believe that having a better understanding of these phenomenon can lead to further insights into this problem.

[5]Similar observation can be seen when $T = 1$, where we present the conditional expectation of the norm of softmax gradient in Figure 5 (e).

7 CONCLUSIONS

In this paper, we propose a simple and effective method to detect out-of-distribution data samples in neural networks. Our method does not require retraining the neural network and significantly improves on the baseline (state-of-the-art) on different neural architectures across various in and out-distribution dataset pairs. We empirically analyze the method under different parameter settings, and provide theoretical intuition and insights behind the approach. Future work involves exploring our method in other applications such as speech recognition and natural language processing.

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A SUPPLEMENTARY RESULTS IN SECTION 4.4

A.1 EXPERIMENTAL RESULTS

	Out-of-distribution dataset	FPR (95% TPR) ↓	Detection Error ↓	AUROC ↑	AUPR In ↑	AUPR Out ↑
		Baseline (Hendrycks & Gimpel, 2017) / Ours				
WRN-40-4 CIFAR-10	TinyImageNet (crop)	49.8/36.7	18.0/17.0	87.3/89.3	85.1/86.7	87.2/90.7
	TinyImageNet (resize)	62.3/49.1	24.4/23.8	79.3/81.6	73.5/76.9	80.6/84.8
	LSUN (crop)	34.6/23.0	11.4/10.3	93.4/95.1	93.1/94.3	92.4/95.2
	LSUN (resize)	54.5/35.1	19.4/18.3	84.7/87.0	79.8/82.6	85.3/89.7
	iSUN	58.6/41.0	21.8/20.6	82.1/84.9	76.4/80.2	83.2/87.8
	Uniform	26.6/3.2	8.1/3.8	96.1/99.2	97.0/99.2	94.8/99.2
	Gaussian	21.8/0.9	6.9/2.1	96.5/99.7	97.5/99.7	94.7/99.7
WRN-40-4 CIFAR-100	TinyImageNet (crop)	66.9/43.3	26.3/19.0	81.3/88.5	80.6/87.2	80.1/89.1
	TinyImageNet (resize)	78.1/55.1	32.4/24.7	72.6/81.6	69.4/78.0	71.6/83.4
	LSUN (crop)	74.9/35.9	28.4/16.8	79.1/90.8	81.4/89.9	76.3/91.5
	LSUN (resize)	77.9/50.0	31.0/21.5	75.2/85.6	73.1/83.5	73.3/86.4
	iSUN	79.5/52.9	31.4/22.6	74.3/84.3	72.9/81.9	71.9/85.1
	Uniform	84.7/3.3	17.5/4.0	86.3/98.8	90.5/99.1	77.0/97.9
	Gaussian	77.2/3.1	18.8/4.0	86.4/99.0	90.2/99.2	78.6/98.6
Dense-BC CIFAR-80	CIFAR-20	84.1/81.1	28.6/28.0	76.6/77.8	79.4/80.6	71.6/73.6
	TinyImageNet (crop)	72.9/22.7	23.6/10.2	83.4/96.2	86.3/96.6	79.9/95.8
	TinyImageNet (resize)	84.4/46.3	28.7/15.4	76.8/91.7	80.3/92.7	71.5/90.4
	LSUN (crop)	67.1/20.9	23.3/10.6	84.6/96.2	86.9/96.4	82.1/96.0
	LSUN (resize)	84.9/45.9	27.8/15.6	77.5/91.8	81.4/92.9	71.6/90.2
	iSUN	86.1/50.2	28.7/16.8	76.1/90.5	79.8/91.3	69.9/88.8
	Uniform	100.0/0.9	24.5/2.9	64.3/98.6	78.4/99.1	52.2/96.6
	Gaussian	98.5/1.2	21.0/2.6	80.4/99.6	86.7/99.6	68.0/99.1
WRN-28-10 CIFAR-80	CIFAR-20	80.4/78.3	26.7/25.8	79.2/80.4	81.5/82.2	74.2/76.2
	TinyImageNet (crop)	71.3/46.7	24.5/17.3	83.1/91.9	85.9/92.6	79.7/90.7
	TinyImageNet (resize)	81.0/48.8	29.0/18.3	77.1/89.2	80.0/89.5	72.6/88.5
	LSUN (crop)	74.4/45.5	25.0/17.0	82.0/92.9	84.4/93.0	78.2/91.5
	LSUN (resize)	81.9/49.0	26.8/17.5	78.8/90.1	82.2/90.8	73.4/88.8
	iSUN	82.7/51.1	27.3/18.2	78.3/89.4	81.5/90.0	72.6/88.0
	Uniform	99.6/1.4	18.3/3.2	80.6/98.9	87.7/99.2	66.8/97.6
	Gaussian	100.0/0.4	18.3/2.7	79.7/99.1	87.4/99.4	65.5/98.0
WRN-40-4 CIFAR-80	CIFAR-20	82.4/78.4	28.8/28.0	76.8/78.1	78.9/79.1	72.2/75.0
	TinyImageNet (crop)	68.3/34.3	24.3/13.9	83.6/93.4	85.9/94.0	81.2/92.5
	TinyImageNet (resize)	80.6/53.5	30.0/20.3	76.2/87.7	78.5/88.3	72.5/86.1
	LSUN (crop)	72.2/33.2	23.5/14.0	83.1/93.4	86.3/93.7	79.7/93.1
	LSUN (resize)	79.1/51.2	28.6/19.1	77.6/88.8	80.0/89.4	73.9/87.3
	iSUN	81.2/53.2	29.9/20.1	76.2/87.7	78.7/88.3	72.2/86.1
	Uniform	99.7/48.6	28.4/10.4	65.6/93.8	77.3/95.7	53.7/88.7
	Gaussian	99.7/10.7	23.5/5.4	74.3/97.7	83.0/98.4	61.2/95.2
MNIST	Omniglot	0.2/0.0	2.0/0.6	99.6/100.0	99.7/100.0	99.5/100.0
	notMNIST	10.3/8.7	6.5/6.2	97.2/98.2	97.5/98.4	97.4/98.0
	CIFAR-10bw	0.1/0.0	1.7/0.4	99.7/100.0	99.8/100.0	99.7/100.0
	Gaussian	0.0/0.0	1.3/0.3	99.7/100.0	99.8/100.0	99.7/100.0
	Uniform	0.0/0.0	0.8/0.0	99.9/100.0	99.9/100.0	99.9/100.0

Table 3: Distinguishing in- and out-of-distribution test set data for image classification. All values are percentages. ↑ indicates larger value is better, and ↓ indicates lower value is better.

MNIST: We used the same MNIST classifier used by Hendrycks & Gimpel (2017), which is a three-layer, 256 neuron-wide, fully connected network trained for 30 epochs with Adam (Kingma & Ba, 2014). The classifier achieve **99.34%** test accuracy on the MNIST test set. We compare our method with the baseline (Hendrycks & Gimpel, 2017) on five different out-of-distribution datasets: (1) Omniglot dataset (Lake et al., 2015) contains images of handwritten characters in stead of the handwritten digits in MNIST; (2) notMNIST (Bulatov, 2011) dataset contains typeface characters;

(3) CIFAR-10bw contains black and white rescaled CIFAR-10 images; (4)(5) Gaussian and Uniform image set contains the synthetic Gaussian and Uniform noise images used in Section 4.2.

Wide ResNet-40-4: We use the same architecture used by Hendrycks & Gimpel (2017) to evaluate the baseline and our method. The Wide ResNet-40-4 achieves **95.7%** test accuracy on CIFAR-10 dataset and achieve **79.27%** test accuracy on CIFAR-100.

CIFAR-80: DenseNet-BC-100 achieves **78.94%** test accuracy on CIFAR-80, while Wide ResNet-28-10 achieves **81.71%** test accuracy and Wide ResNet-40-4 achieves **79.53%** test accuracy on CIFAR-80.

A.2 Parameter Settings

For MNIST, we set $T = 1000$ and $\varepsilon = 0$. The parameter settings for other structures are shown as follows.

	DenseNet-BC-100		
Out-of-distribution datasets	**CIFAR-10**	**CIFAR-80**	**CIFAR-100**
TinyImageNet (crop)	0.0014	0.002	0.002
TinyImageNet (resize)	0.0014	0.0022	0.0022
LSUN (crop)	0	0.0036	0.0038
LSUN (resize)	0.0014	0.002	0.0018
iSUN	0.0014	0.002	0.002
Uniform	0.0014	0.0028	0.0024
Gaussian	0.0014	0.0026	0.0028
CIFAR-20	-	0.0002	-

Table 4: Optimal perturbation magnitude ε for reproducing main results in Table 2 and 3.

	DenseNet-BC-100		
Out-of-distribution datasets	**CIFAR-10**	**CIFAR-80**	**CIFAR-100**
TinyImageNet (crop)	1000	1000	1000
TinyImageNet (resize)	1000	1000	1000
LSUN (crop)	1000	1000	1000
LSUN (resize)	1000	1000	1000
iSUN	1000	1000	1000
Uniform	1000	1	1
Gaussian	1000	1	1
CIFAR-20	-	1	-

Table 5: Optimal Temperature T for reproducing main results in Table 2 and 3.

	Wide-ResNet-28-10		
Out-of-distribution datasets	**CIFAR-10**	**CIFAR-80**	**CIFAR-100**
TinyImageNet (crop)	0.0005	0.0002	0.0026
TinyImageNet (resize)	0.0011	0.0004	0.0024
LSUN (crop)	0	0.0002	0.0038
LSUN (resize)	0.0006	0.0002	0.0026
iSUN	0.0008	0.0002	0.0026
Uniform	0.0014	0.0002	0.0032
Gaussian	0.0014	0.0002	0.0032
CIFAR-20	-	5e-05	-

Table 6: Optimal perturbation magnitude ε for reproducing main results in Table 2 and 3.

	Wide-ResNet-28-10		
Out-of-distribution datasets	**CIFAR-10**	**CIFAR-80**	**CIFAR-100**
TinyImageNet (crop)	1000	1000	1000
TinyImageNet (resize)	1000	1000	1000
LSUN (crop)	1000	1000	1000
LSUN (resize)	1000	1000	1000
iSUN	1000	1000	1000
Uniform	1000	1	1000
Gaussian	1000	1	1000
CIFAR-20	-	1	-

Table 7: Optimal Temperature T for reproducing main results in Table 2 and 3.

	Wide-ResNet-40-4		
Out-of-distribution datasets	**CIFAR-10**	**CIFAR-80**	**CIFAR-100**
TinyImageNet (crop)	0.0004	0.0002	0.0014
TinyImageNet (resize)	0.0008	0.0004	0.0016
LSUN (crop)	0	0.0002	0.0038
LSUN (resize)	0.001	0.0002	0.0014
iSUN	0.0008	0.0002	0.0016
Uniform	0.0016	0.0002	0.0024
Gaussian	0.0016	0.0002	0.0026
CIFAR-20	-	0.0002	-

Table 8: Optimal perturbation magnitude ε for reproducing main results in Table 2 and 3.

	Wide-ResNet-40-4		
Out-of-distribution datasets	**CIFAR-10**	**CIFAR-80**	**CIFAR-100**
TinyImageNet (crop)	1000	1000	1000
TinyImageNet (resize)	1000	1000	1000
LSUN (crop)	1000	1000	1000
LSUN (resize)	1000	1000	1000
iSUN	1000	1000	1000
Uniform	1000	1	1000
Gaussian	1000	1	1000
CIFAR-20	-	1	-

Table 9: Optimal Temperature T for reproducing main results in Table 2 and 3.

B SUPPLEMENTARY RESULTS IN SECTION 5.1

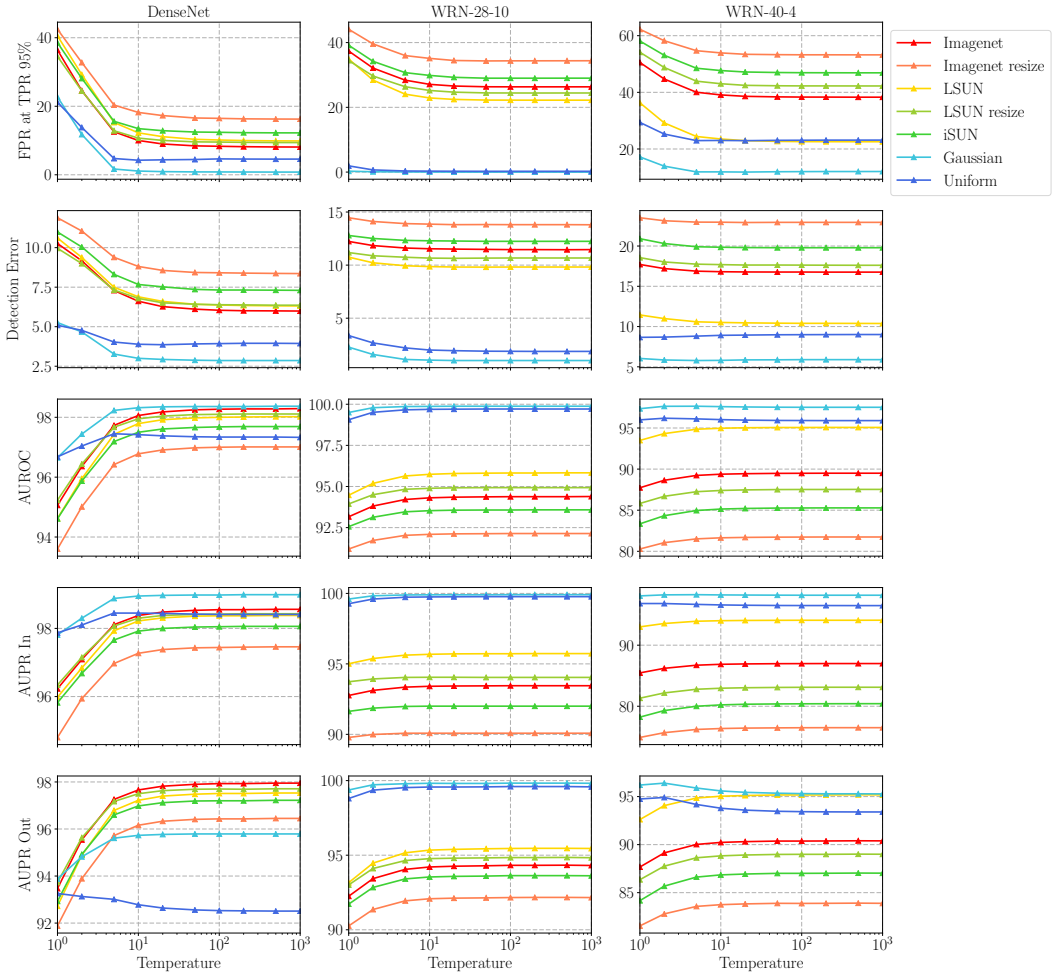

Figure 7: Detection performances on DenseNet, Wide ResNet-28-10 and Wide ResNet-40-4 under different temperature, when input preprocessing is not used, i.e., $\varepsilon = 0$. All networks are trained on CIFAR-10.

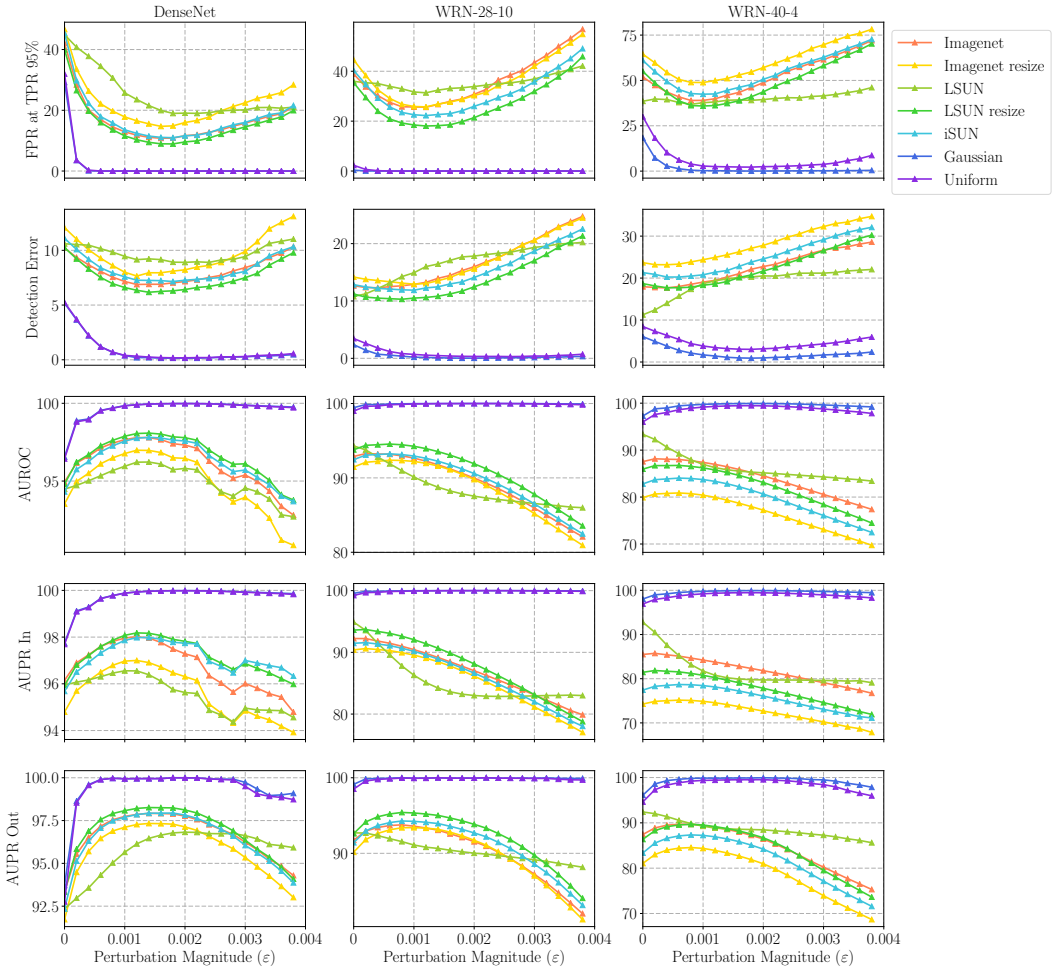

Figure 8: Detection performances on DenseNet, Wide ResNet-28-10 and Wide ResNet-40-4 under different perturbation magnitude, when temperature scaling is not used, i.e., $T = 1$. All networks are trained on CIFAR-10.

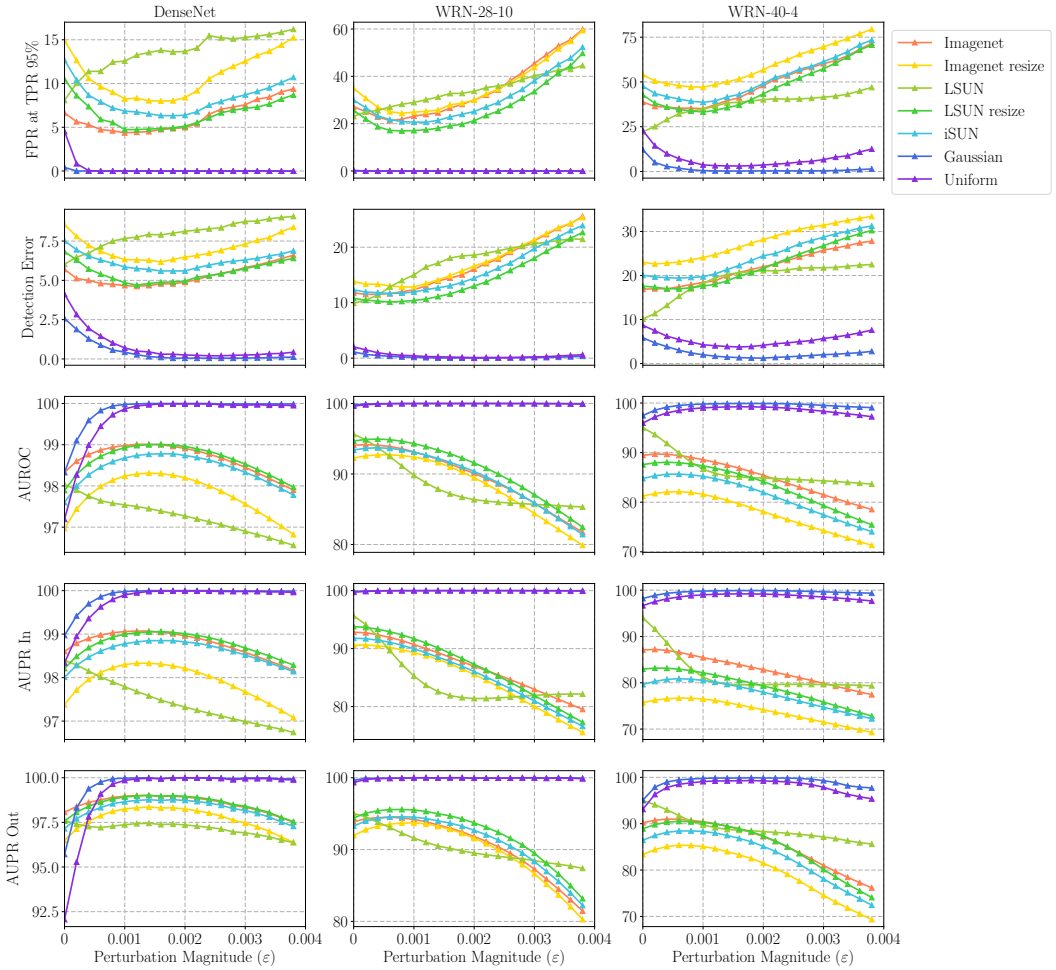

Figure 9: Detection performances on DenseNet, Wide ResNet-28-10 and Wide ResNet-40-4 under different perturbation magnitude, when the optimal temperature is used, i.e., $T = 1000$. All networks are trained on CIFAR-10.

C SUPPLEMENTARY RESULTS IN SECTION 5.2 AND 5.3

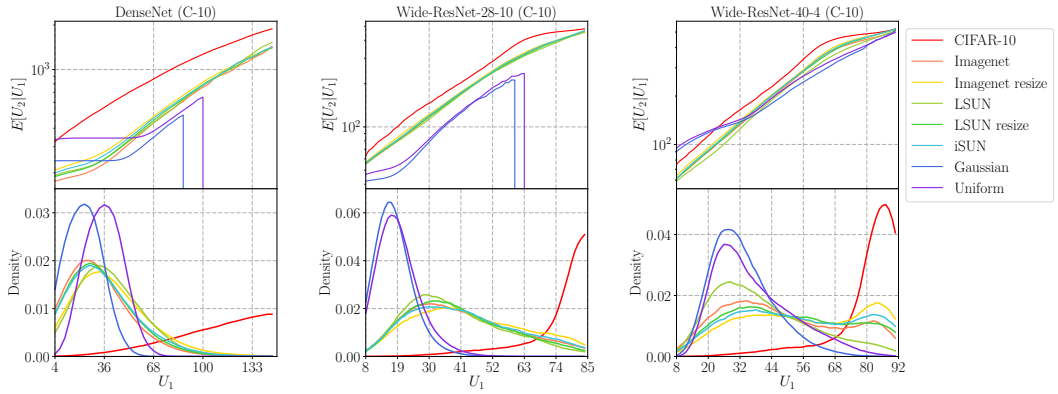

Figure 10: Expectation of the second order term U_2 conditioned on the first order term U_1 under DenseNet, Wide-ResNet-28-10 and Wide ResNet-40-4. All networks are trained on CIFAR-10.

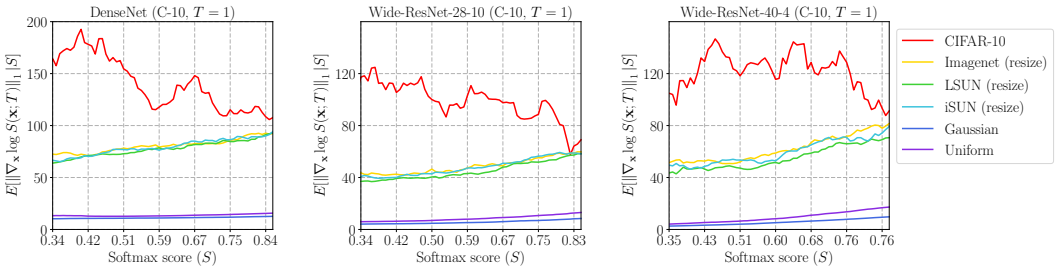

Figure 11: Expectation of gradient norms conditioned on the softmax scores under DenseNet, Wide-ResNet-28-10 and Wide ResNet-40-4, where the temperature scaling is not used. All networks are trained on CIFAR-10.

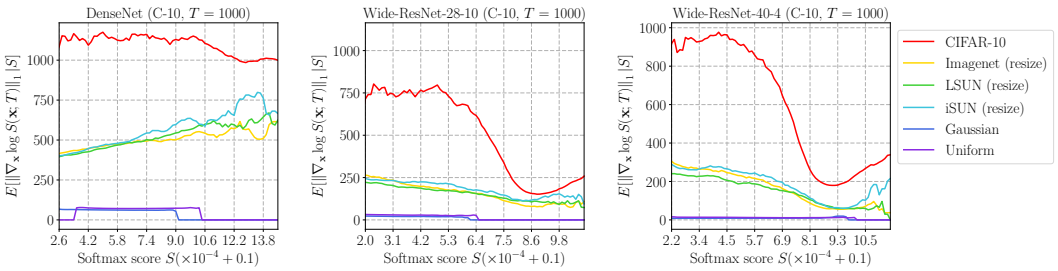

Figure 12: Expectation of gradient norms conditioned on the softmax scores under DenseNet, Wide-ResNet-28-10 and Wide ResNet-40-4, where the optimal temperature is used, i.e., $T = 1000$. All networks are trained on CIFAR-10.

D TAYLOR EXPANSION

In this section, we present the Taylor expansion of the soft-max score function:

$$
\begin{aligned}
S_{\hat{y}}(\boldsymbol{x};T) &= \frac{\exp\left(f_{\hat{y}}(\boldsymbol{x})/T\right)}{\sum_{i=1}^{N}\exp(f_i(\boldsymbol{x})/T)} \\
&= \frac{1}{\sum_{i=1}^{N}\exp\left(\frac{f_i(\boldsymbol{x})-f_{\hat{y}}(\boldsymbol{x})}{T}\right)} \\
&= \frac{1}{\sum_{i=1}^{N}\left[1+\frac{f_i(\boldsymbol{x})-f_{\hat{y}}(\boldsymbol{x})}{T}+\frac{1}{2!}\frac{(f_i(\boldsymbol{x})-f_{\hat{y}}(\boldsymbol{x}))^2}{T^2}+o\left(\frac{1}{T^3}\right)\right]} \qquad \text{by Taylor expansion} \\
&\approx \frac{1}{N-\frac{1}{T}\sum_{i=1}^{N}[f_{\hat{y}}(\boldsymbol{x})-f_i(\boldsymbol{x})]+\frac{1}{2T^2}\sum_{i=1}^{N}[f_i(\boldsymbol{x})-f_{\hat{y}}(\boldsymbol{x})]^2}
\end{aligned}
$$

E PROPOSITION 1

The following proposition 1 shows that the detection error $P_e(T,0) \approx c$ if T is sufficiently large. Thus, increasing the temperature further can only slightly improve the detection performance.

Proposition 1. *There exists a constant c only depending on function U_1, in-distribution $P_{\boldsymbol{X}}$ and out-of-distribution $Q_{\boldsymbol{X}}$ such that $\lim_{T\to\infty} P_e(T,\varepsilon) = c$, when $\varepsilon = 0$ (i.e., no input preprocessing).*

Proof. Since

$$
S_{\hat{y}}(\boldsymbol{X};T) = \frac{\exp(f_{\hat{y}}(\boldsymbol{X})/T)}{\sum_{i=1}^{N}\exp(f_i(\boldsymbol{X})/T)} = \frac{1}{1+\sum_{i\neq\hat{y}}\exp([f_i(\boldsymbol{X})-f_{\hat{y}}(\boldsymbol{X})]/T)}
$$

Therefore, for any $\boldsymbol{X}$,

$$
\begin{aligned}
\lim_{T\to\infty} T\left(-\frac{1}{S_{\hat{y}}(\boldsymbol{X};T)}+N\right) &= \lim_{T\to\infty}\sum_{i\neq\hat{y}} T\left[1-\exp\left(\frac{f_i(\boldsymbol{X})-f_{\hat{y}}(\boldsymbol{X})}{T}\right)\right] \\
&= \sum_{i\neq\hat{y}}[f_{\hat{y}}(\boldsymbol{X})-f_i(\boldsymbol{X})] = (N-1)U_1(\boldsymbol{X})
\end{aligned}
$$

This indicates that the random variable

$$
T\left(-\frac{1}{S_{\hat{y}}(\boldsymbol{X};T)}+N\right) \to (N-1)U_1(\boldsymbol{X}) \quad a.s.
$$

This means that

$$
\begin{aligned}
P_e(T,0) &= \mathbb{P}_{\boldsymbol{X}\times Z}(g(X;T,0)\neq Z) \\
&= \min_{\delta}\left\{P(Z=0)Q_{\boldsymbol{X}}(S_{\hat{y}}(\boldsymbol{X};T)>\delta)+P(Z=1)P_{\boldsymbol{X}}(S_{\hat{y}}(\boldsymbol{X};T)\leq\delta)\right\} \\
&= \min_{\delta}\left\{P(Z=0)Q_{\boldsymbol{X}}\left(T\left(N-\frac{1}{S_{\hat{y}}(\boldsymbol{X};T)}\right)>\delta\right)\right. \\
&\qquad \left.+P(Z=1)P_{\boldsymbol{X}}\left(T\left(N-\frac{1}{S_{\hat{y}}(\boldsymbol{X};T)}\right)<\delta\right)\right\} \\
&\xrightarrow{T\to\infty} \min_{\delta}\left\{P(Z=0)Q_{\boldsymbol{X}}\left((N-1)U_1(\boldsymbol{X})>\delta\right)\right. \\
&\qquad \left.+P(Z=1)P_{\boldsymbol{X}}\left((N-1)U_1(\boldsymbol{X})<\delta\right)\right\}
\end{aligned}
$$

Therefore, there exists a constant c depending on $U_1, P_{\boldsymbol{X}}, Q_{\boldsymbol{X}}$, such that

$$
\lim_{T\to\infty} P_e(T,0) = c.
$$

□

F ANALYSIS ON TEMPERATURE

For simplicity of the notations, let $\Delta_i = f_{\hat{y}} - f_i$ and thus $\Delta = \{\Delta_i\}_{i \neq \hat{y}}$. Besides, let $\bar{\Delta}$ denote the mean of the set Δ. Therefore,

$$\bar{\Delta} = \frac{1}{N-1} \sum_{i \neq \hat{y}} \Delta_i = \frac{1}{N-1} \sum_{i \neq \hat{y}} [f_{\hat{y}} - f_i] = U_1.$$

Equivalently,

$$U_1 = \text{Mean}(\Delta).$$

Next, we will show

$$U_2 = \frac{1}{N-1} \sum_{i \neq \hat{y}} [f_{\hat{y}} - f_i]^2 = \overbrace{\frac{1}{N-1} \sum_{i \neq \hat{y}} [\Delta_i - \bar{\Delta}]^2}^{\text{Variance}^2(\Delta)} + \overbrace{\bar{\Delta}^2}^{\text{Mean}^2(\Delta)}.$$

Since

$$\begin{aligned}
U_2 &= \frac{1}{N-1} \sum_{i \neq \hat{y}} \Delta_i^2 && \text{by} \Delta_i = f_{\hat{y}} - f_i \\
&= \frac{1}{N-1} \sum_{i \neq \hat{y}} (\Delta_i - \bar{\Delta} + \bar{\Delta})^2 \\
&= \frac{1}{N-1} \sum_{i \neq \hat{y}} [(\Delta_i - \bar{\Delta})^2 - 2(\Delta_i - \bar{\Delta})\bar{\Delta} + \bar{\Delta}^2] \\
&= \underbrace{\frac{1}{N-1} \sum_{i \neq \hat{y}} [\Delta_i - \bar{\Delta}]^2}_{\text{Variance}^2(\Delta)} - \underbrace{\frac{2\bar{\Delta}}{N-1} \sum_{i \neq \hat{y}} (\Delta_i - \bar{\Delta})}_{=0} + \underbrace{\bar{\Delta}^2}_{\text{Mean}^2(\Delta)}
\end{aligned}$$

then

$$U_2 = \text{Variance}^2(\Delta) + \text{Mean}^2(\Delta)$$

G ADDITIONAL RESULTS IN SECTION 4.5

Apart from the Maximum Mean Discrepancy, we as well use the Energy distance to measure the statistical distance between two datasets. Let two different distributions P and Q. Then the energy distance between distributions P and Q is defined as

$$D^2_{\text{energy}}(P, Q) = 2\mathbb{E}_{V \sim P, W \sim Q} \|X - Y\| - \mathbb{E}_{V, V' \sim P} \|X - X'\| - \mathbb{E}_{W, W' \sim Q} \|Y - Y'\|.$$

Therefore, the energy distance between two datasets $V = \{V_1, ..., V_m\} \overset{iid}{\sim} P$ and $W = \{W_1, ..., W_m\} \overset{iid}{\sim} Q$ is defined as

$$\widehat{D_{\text{energy}}}^2(P, Q) = \frac{2}{m^2} \sum_{i=1}^{m} \sum_{j=1}^{m} \|V_i - W_j\| - \frac{1}{\binom{m}{2}} \sum_{i \neq j} \|V_i - V_j\| - \frac{1}{\binom{m}{2}} \sum_{i \neq j} \|W_i - W_j\|.$$

In the experiment, we use the 2-norm $\| \cdot \|_2$.

In-distribution datasets	**Out-of-distribution Datasets**	**MMD Distance**	**Energy Distance**
CIFAR-100	Tiny-ImageNet (crop)	0.41	2.25
	LSUN (crop)	0.43	2.31
	Tiny-ImageNet (resize)	0.088	0.54
	LSUN (resize)	0.12	0.63
	iSUN (resize)	0.11	0.56
CIFAR-80	Tiny-ImageNet (crop)	0.4	2.22
	LSUN (crop)	0.43	2.29
	Tiny-ImageNet (resize)	0.095	0.57
	LSUN (resize)	0.120	0.62
	iSUN (resize)	0.116	0.61
	CIFAR-20	0.057	0.35