On the evaluation of post hoc Out-Of-Distribution detectors

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Abstract

Out-Of-Distribution (OOD) detection is becoming more and more relevant as machine learning models are deployed in the real world. This is even more important with deep neural networks as their performance get worse when used outside their training distribution. In this work, we analyze a particular scenario called post hoc, where the task is to detect OOD data using a pre-trained model trained on the In-Distribution data (ID) for a different task (in our case image classification). We consider the effect of a novel method called ReAct[22] on some of the most common scoring functions, which are softmax score, ODIN, and energy-based function. We evaluate these techniques with a wide range of models and datasets to discover their limitations and strengths. Our empirical investigation shows that ODIN with $\epsilon = 0$ is the best method in the vast majority of the cases. Additionally, we discover some failure cases and that ReAct could help fix them. The source code is available at https://github.com/tpoppo/ood-post-hoc.

1. Introduction

Nowadays, deep learning models are used in many different places and situations, even safety-critical cases, therefore, these models need to be reliable and trustworthy. For this reason, detecting Out-Of-Distribution data is a quite important problem to tackle, as most deep learning methods fail outside of their training distribution and the prediction score becomes way more unreliable[18, 14, 24]. Out-Of-Distribution detection is quite a challenging problem as it requires distinguishing whether the data comes from the training distribution or not. This problem can be divided in various subgroups[25], such as open set recognition and one-class anomaly detection. A wide range of recent and old works tried to solve these problems in many different ways[12, 6, 3] and with different assumptions and constraints. In particular, in many situations, it is not possible to train a model to specifically solve this task, as training a model to detect OOD samples can be quite complex[5]. Therefore, some works focus on post hoc OOD detection

methods, which means using a pre-trained model (e.g. on image classification) and utilizing the class scores to detect whether the data comes for the training distribution or not. Additionally, another important challenge of OOD detection is how to properly choose and evaluate the hyperparameters, for this reason, many OOD detectors are hyperparameters free or are not particularly important to tune. Our contributions are:

- 1. We implemented all the techniques considered in TensorFlow[1].
- 2. We analyzed and compared the performance of various methods on a wide range of datasets.
- 3. We found some general and practical guidelines for choosing the post hoc OOD detector.

2. Background

Firstly, we define formally the problem and then we define the mathematical notation used.

2.1. Problem

The problem of post hoc Out-Of-Distribution detection for classification is defined in the following way. Let $f: \mathcal{X} \to \mathbb{R}^K$ be the classifier (trained on the \mathcal{D}_{in} distribution), where \mathcal{X} is the sample space (in our case, it is the image space) and K is the number of output classes. Therefore, the task is to discover whether an input sample $x_0 \in \mathcal{X}$ has been generated from the \mathcal{D}_{in} In-Distribution data, which is known, or the \mathcal{D}_{out} Out-Of-Distribution data, which is unknown, by using a decision function $G(x_0; f)$ (define as in (1)).

$$G(x_0; f) = \begin{cases} 0 & \text{if } x_0 \sim \mathcal{D}_{out}, \\ 1 & \text{if } x_0 \sim \mathcal{D}_{in}. \end{cases}$$
 (1)

The difficulty in detecting OOD samples is strongly correlated with the separation between \mathcal{D}_{out} and \mathcal{D}_{in} , the less the distributions are separated, the harder the classification becomes. However, in the vast majority of the practical cases the separation between \mathcal{D}_{out} and \mathcal{D}_{in} is quite large.

In all the cases considered, the methods have a scoring function $S(x_0; f)$, which returns a large value if the sample is ID, otherwise if it is an OOD sample a small one. Therefore, to solve the initial problem we could select a threshold t and define $G(x_0; f)$ as in (2).

$$G(x_0; f) = \begin{cases} 0 & \text{if } S(x_0; f) \le t, \\ 1 & \text{if } S(x_0; f) > t. \end{cases}$$
 (2)

2.2. Notation

We will introduce some useful notations. We define $\operatorname{softmax}(x)_i = \frac{e^{x_i}}{\sum_j e^{x_j}}$, $\operatorname{sign}(x)$ is the sign function element-wise and $\operatorname{clip}(x)$ clips all the values between 0 and 1.

3. Related work

In this section, we analyze various scoring functions, which are computed from the class scores of the neural network (the output), and also we consider a novel method that injects an additional layer between the features extraction layer and the logits extraction one.

3.1. softmax score

One of the first OOD methods that tackle this problem is often called softmax score[9]. Their main claim is that correctly classified samples have a higher maximum softmax probability than the OOD samples. Thus, the resulting scoring function is shown below (3).

$$S_{MSP}(x) = \max_{k} \operatorname{softmax}(f(x))_{k} \tag{3}$$

3.2. ODIN score

The ODIN score[15] (4) was introduced as an improvement of the softmax score. They propose two addition to the softmax score which are a temperature scaling factor T and a preprocessing step that adds a small adversarial perturbation with factor ϵ (ℓ^{∞} norm of the perturbation).

$$S_{\text{ODIN}}(\tilde{x};T) = \max_{k} \text{softmax}(\frac{f(\tilde{x})}{T})_{k}$$

$$\tilde{x} = x - \epsilon \text{sign}(-\nabla \log S_{\text{ODIN}}(x))$$
(4)

The temperature scaling has been used by other methods[11] to soften the logits prediction and to better separate the in- and Out-Of-Distribution data. To obtain this effect, the hyper-parameter T is required to be a large value (generally greater than 1000). The scoring function on the original sample x is first computed to obtain $\nabla \log S_{\text{ODIN}}(x)$ and find \tilde{x} . Then the scoring function $S_{\text{ODIN}}(\tilde{x};T)$ is computed on the preprocessed sample \tilde{x} .

3.3. energy score

This method was proposed in [16], and it is based on the idea of an energy-based model. Additionally, the authors proposed not only an inference time scoring function (6), but also a regularization term in the loss (5) to increase the effectiveness of the energy score. This regularization term is added during training therefore the total loss used is $\mathcal{L}_{\text{error}} + \lambda \mathcal{L}_{\text{energy}}$, where $\mathcal{L}_{\text{error}}$ is the main loss of the problem (in most of the cases it is the cross entropy loss) and λ is an hyper-parameter that tunes the strength of the regularization. The scoring function is hyper-parameters free, while the loss term has two hyper-parameters m_{in} and m_{out} , which are the margin parameters.

$$S_{\text{energy}}(x) = -\ln \sum_{i=1}^{K} e^{f(i)_i}$$
 (5)

$$\mathcal{L}_{\text{energy}} = \mathbb{E}[\max(0, S_{\text{energy}}(x_{in}) - m_{in})] + \mathbb{E}[\max(0, m_{out}) - S_{\text{energy}}(x_{out})]$$
(6)

 x_{in} are in-distribution samples, while x_{out} are out-of-distribution samples. Therefore, the regularization loss tries to maximize the score of the ID samples and minimize the score of the OOD ones.

3.4. ReAct

In [22], they proposed ReAct an additional layer added before the last layer (before the last fully connected layer and after the last activation function) of the neural network at inference time. (7) shows how the layer behaves.

$$ReAct(x; \lambda) = \min(x, \lambda), \tag{7}$$

where min is the element-wise minimum of the two elements, $x \in \mathcal{X}$ is the input vector (the feature vector) and $\lambda \in \mathbb{R}$ is the truncation value. λ should be large enough to keep the ID distribution as close as possible to the original one, thus in practice, it is equal to the p-th percentile (generally 90%) of the ID distribution. The idea behind this new layer is tailored to the hypothesis that the OOD distribution has a positively skewed feature vector distribution, and this leads to many scoring methods to miss-classify the data from OOD to ID. The original paper dives into both a theoretical and empirical analysis of the consequences of this phenomenon.

4. Proposed approach

The main aim of our analysis is to find some useful guidelines to decide which method one should use. Overall, our discoveries suggest that:

• ODIN with $\epsilon = 0$ and T = 1000 seems a strong and simple starting choice, but it is not always optimal.

- ReAct might sometimes be useful, thus, we suggest testing with and without it. In particular, we recommend using it when the expected OOD samples are very far from the ID data.
- There is no strong correlation between the architecture and the size of the model, and the OOD detection performance.
- All the methods show good datasets transferability.

5. Methodology and Datasets

In our experiments, the main goal is to analyze the performance of various datasets and data augmentations. Throughout our work, we consider the ImageNet dataset[4] without augmentations as in-distribution, while every other case is considered out-of-distribution.

Datasets & Augmentations In order to better compare the various approaches, we used a total of 10 datasets. For the whole work, we consider the ImageNet dataset without any augmentation as the In-Distribution one, while all the other ones as Out-Of-Distribution. The main group is of 64 dataset and augmentation pairs (see Appendix A) for the full list) and it is used in all the cases where the tested model is only ResNet101, while when we compare all the models we used a reduced subset of 10 pairs (see Appendix A). The datasets and augmentations are chosen to test and compare a wide and diverse range of situations (see Appendix C for some examples).

Datasets The ImageNet dataset[4] is our In-Distribution dataset. We use a subset of iNaturalist, SUN, Places used in [22], which only includes non-overlapping categories with ImageNet. Moreover, we also consider ImageNette, ImageNet a[10], Rock Paper Scissors[17], ImageNet v2[20] datasets, and noise randomly generated from the uniform and normal distributions. ImageNette and ImageNet v2 are arguably not OOD, as the concept and categories are the same, but we prefer to consider also these less reasonable and extreme cases.

Augmentations on ImageNet Moreover, we also use a wide range of augmentations on ImageNet: Gaussian noise, blur, pixelization, perspective transformation, and JPEG encoding quality level. Most of the augmentations were done with AugLy[19]. In our work, we consider ImageNet with augmentation as OOD, this assumption is not always useful, as a really small augmentation might be reasonable and not harmful for the model.

Augmentations on other datasets We use the Fast Gradient Sign Method (FGSM)[7] (9) to create adversarial noise, a small perturbation in the input space that can lead to arbitrary changes in the resulting feature vector. These changes are nearly imperceptible for a human, but they lead the model to change the feature vector and consequently also the final logits. In this way, these experiments try to discover whether starting from an OOD sample is possible to fool the OOD detector to classify the sample as ID. Thus, to discover whether these OOD scorers are robust to weak adversarial attacks. This approach has several limitations, firstly, the adversarial noise is generally outside the scope of many OOD scorers, and secondly, the FGSM is one of the simplest and weakest adversarial attack methods. Additionally, the gradient used to generate the adversarial perturbation is computed only using the model without ReAct.

$$\mathcal{L}_{adv}(x) = \ln \sum_{i=0}^{N} e^{\operatorname{softmax}(f(x))_{k}}$$
 (8)

We decided to use the loss function of (8), which is the differentiable version of the softmax scorer. The resulting transformation is shown in (9).

$$x_{adv} = \text{clip}(x + \epsilon \text{sign}(\nabla \mathcal{L}_{adv}(x)))$$
 (9)

OOD detectors In our analysis, we used the following scoring functions: softmax, ODIN, and energy. We used two ODIN hyperparameter configurations (which were both used in the original paper), the first case is with $\epsilon=0$ and T = 1000, while the second one is with $\epsilon = 0.0014$ and T=1000. The other scoring functions are hyperparameters free. For the energy scorer, we only used the inference component and we did not train the models using the specific regularization loss, as we only compare the methods in the post hoc setting. For ReAct, we used p = 90%, which is the suggested value in the original paper. In all our experiments, we consider all the possible scoring functions with and without the ReAct layer, therefore, for a total of 8 methods. All the methods are implemented in TensorFlow and are compatible with almost all the pre-trained models available in tensorflow.keras.applications.

Models used We mainly focus our case study on ResNet101[8], which is used with the large group (see Appendix A for the full list) of dataset and augmentation pairs (if not differently stated we used this configuration). However, we also consider many other models: EfficientNetB0[23], DensetNet121[13], DenseNet169[13], DenseNet201[13], ResNet50[8], ResNet152[8], VGG16[21], VGG19[21]. These models were chosen to cover a wide range of CNN architecture and size, and because they are available on TensorFlow.

6. Experiments

In this section, we evaluate ReAct in combination with four scoring functions on a suite of OOD detection tasks.

6.1. Main results

Table 1 depicts the main datasets and augmentations of our analysis. In particular, ODIN ($\epsilon=0$) is the best method in the most important cases (e.g. iNaturalist, SUN, Places, and RockPaperScissors), however, it is worse in the toughest and arguably not even considerable OOD cases (e.g. ImageNet v2 and ImageNette), which have the same concepts of ImageNet and thus it should be nearly impossible to distinguish those as out-of-distribution. Overall, from both Table 2 and Table 1, ODIN with $\epsilon=0.0$ without the ReAct layer achieves the best results. However, the use of the ReAct layer is beneficial with softmax and ODIN.

6.2. Comparison with and without ReAct

In this subsection, we highlight the main advantages and disadvantages of adding the ReAct layer[22] with ResNet101, thus, using the set of 64 model and scoring function pairs. Overall, the ReAct method is quite useful with some scoring functions, while harmful for others. The results remain quite consistent across datasets (Table 3 and Figure 1). In particular, we can notice that while the version without ReAct completely fails (with AUC <0.5) in many cases with the ODIN and $\epsilon>0$, the version with ReAct achieves good results (see Appendix D for more details). An additional analysis of the effect of ReAct in the scores is present in the Appendix B.

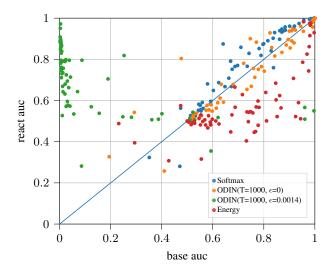


Figure 1: AUC score with and without the ReAct method across the various scoring functions. There scoring functions used are softmax (blue), $ODIN(\epsilon=0)$ (orange), $ODIN(\epsilon=0.0014)$ (green), energy (red).

The results divided per dataset show that the scoring function plays a more important role than the datasets, which means that there is good transferability across different datasets and augmentations.

6.3. The effect of augmentations

In this subsection, we analyze the effect of various augmentations and, in particular, how the OOD detectors consider the images as we increase the distortion. It is important to notice that in all the experiments we consider ImageNet without augmentation as ID, while ImageNet with augmentations as OOD.

6.3.1 Gaussian noise

Overall, all the methods follow a similar trend and can distinguish even a very small amount of noise, with the only exception of $\text{ODIN}(\epsilon=0.0014)$ without ReAct which completely fails.

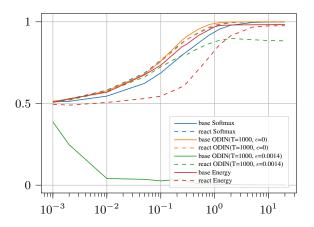


Figure 2: AUC score as the σ of the Gaussian noises changes. The ID dataset is ImageNet, while the OOD dataset is ImageNet with Gaussian noise.

6.3.2 Other augmentations

The other natural augmentations (Figure 3) show a similar picture. In particular, the $\mathtt{ODIN}(\epsilon=0.0014)$ without ReAct and the energy function with ReAct do not work properly, as both achieve an AUC smaller than 0.5 (random guessing) even in trivial cases.

6.3.3 Adversarial noise

We are not aware of any previous work on OOD detectors that analyzes the effect of adversarial noise, however, we decided to also evaluate this scenario as we consider it useful to better investigate the limitations of current methods. We used FGSM, which is one of the weakest and simplest

OOD dataset	A + +:	C+	OD TM(- 0)	OD TM(- 0.0014)	
OOD dataset	Augmentation	softmax	$ODIN(\epsilon=0)$	$ODIN(\epsilon = 0.0014)$	energy
RockPaperScissors	-	98.54/99.75	99.98 /99.82	0.40/78.12	92.46/52.22
iNaturalist	=	88.42/94.17	92.37/ 94.18	0.58/78.52	78.13/56.67
SUN	=	86.19/89.78	89.51/ 89.58	1.26/73.51	81.07/50.09
Places	=	82.86/84.14	87.09 /83.39	0.71/71.10	77.79/47.96
Gaussian Noise	-	99.84/ 100.00	100.00/100.00	0.21/90.88	98.03/97.56
Uniform Noise	-	99.85/ 100.00	100.00/100.00	0.28/95.04	95.57/98.25
ImageNet v2*	-	55.26/55.55	57.38/55.28	99.64 /54.98	57.19/48.12
ImageNette*	-	83.79 /75.92	52.58/53.93	1.06/52.70	55.34/53.00
ImageNet	$Normal(\sigma = 0.002)$	51.31/52.73	52.35/52.56	24.77/52.08	52.91 /48.98
ImageNet	$Normal(\sigma = 0.25)$	79.69/87.30	88.81 /86.97	3.77/79.54	84.82/60.31
ImageNet	$Normal(\sigma = 1.25)$	95.63/98.31	99.50 /98.77	0.49/88.71	97.77/86.15
ImageNet	Blur(r=1.0)	55.40/54.93	59.80 /54.85	40.10/53.57	58.06/46.68
ImageNet	Pixelation($r = 0.5$)	56.16/56.14	61.40 /56.30	52.21/54.30	59.16/48.24
ImageNet	JPEG(q=25)	54.37/55.26	58.53 /55.46	15.52/53.80	59.02/49.51

Table 1: AUC score without ReAct and with ReAct (in the table written as without ReAct/with ReAct) in various settings using the ResNet101 model. We consider ImageNet (without augmentations) as the ID dataset. In **bold** the best results. *ImageNet v2 and ImageNette have the same concept of ImageNet, therefore they are nearly indistinguishable from ImageNet.

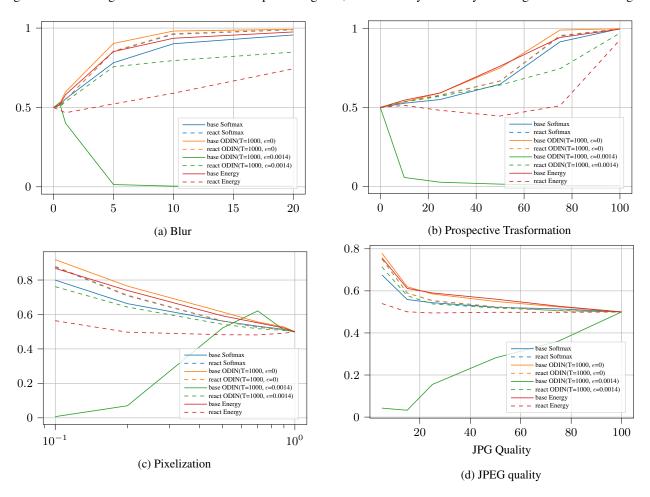


Figure 3: AUC score as a particular augmentation is used on ImageNet.

Scoring	ReAct	Avg Rank
$\overline{\text{ODIN}(\epsilon=0)}$	no	2.27
softmax	yes	2.71
$ODIN(\epsilon=0)$	yes	2.81
energy	no	4.06
softmax	no	4.52
$\texttt{ODIN}(\epsilon = 0.0014)$	yes	5.57
energy	yes	6.76
$\mathrm{ODIN}(\epsilon=0.0014)$	no	7.29

Table 2: Average ranking based on AUC score (ranked from 1 to 8, all the possible combination of scoring methods possible) for ResNet101. The lower the better.

Scoring	Better w/o	Better w/
softmax	10	54
energy	59	5
$ODIN(\epsilon=0)$	41	23
$\mathrm{ODIN}(\epsilon=0.0014)$	7	57

Table 3: It counts how many times the AUC score is better with and without ReAct.

adversarial attack techniques, and we were able to reduce the AUC score of nearly all the methods (Figure 4). The gradient is computed using the model without ReAct, thus, the reduction is more marked in these scorers. We do not show the results when evaluating the gradient with ReAct, as a similar situation is depicted just with slightly better scores, maybe because the resulting gradient is less useful[2]. Consequently, when using a weak adversarial attack (as strong adversarial attacks are able to bypass this gradient masking) the ReAct method could bring some small benefits.

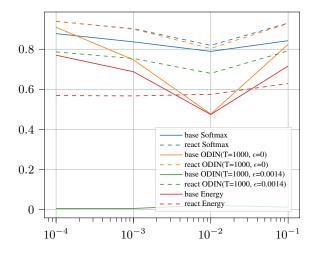


Figure 4: AUC score as the ϵ of the FGSM increases. The ID dataset is ImageNet, while the OOD dataset is iNaturalist with adversarial noise.

6.4. Comparison among models

We consider all the possible combinations of model and scoring function and for every OOD dataset we compute the AUC score between ImageNet (the ID dataset) and the OOD dataset, then we rank the model and scoring function pairs and compute the mean ranking position for each model. Figure 4 shows that ODIN ($\epsilon=0$) is overall the best method, while it is not clear whether ReAct is always better. Additionally, we notice no clear correlation between the OOD detection ability of the model and other model-specific proprieties, such as the number of parameters, kind of architecture, test accuracy, etc.

Model	Scorer	ReAct	Avg Rank
EfficientNetB0	$ODIN(\epsilon=0)$	no	1.22
ResNet50	$ODIN(\epsilon=0)$	no	1.33
DenseNet121	$ODIN(\epsilon=0)$	yes	1.44
DenseNet201	$ODIN(\epsilon=0)$	yes	1.56
VGG19	$ODIN(\epsilon=0)$	no	2.0
ResNet101	softmax	yes	2.0
ResNet101	$ODIN(\epsilon=0)$	no	2.11
ResNet151	$ODIN(\epsilon=0)$	yes	2.22
VGG16	$ODIN(\epsilon=0)$	no	2.22
VGG19	$ODIN(\epsilon=0)$	yes	2.22

Table 4: These are the 10 best model-scoring function pairs (ranks are from 1 to 64, all the combinations of the 10 models and the 8 scoring methods)

7. Conclusion

Overall, our analysis shows results similar to the ones present in the literature. However, compare with what the ReAct work suggested we found no clear performance boost and it heavily depends on many unknown and hard to analyze factors. The vast majority of the techniques analyzed are quite robust and achieve good results even in complex situations and are able to detect even small shifts in the data distribution.

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A. Full list of datasets & augmentations

The full list of datasets & augmentations used with ResNet101 (64 pairs):

- ImageNet & adversarial 0.1 softmax base
- ImageNet & adversarial 0.1 msoftmax base
- ImageNet & adversarial 0.1 softmax100 base
- ImageNet & adversarial 0.1 softmax ReAct
- ImageNet & adversarial 0.1 msoftmax ReAct
- ImageNet & adversarial 0.1 softmax100 ReAct
- ImageNet & adversarial 0.01 softmax base
- ImageNet & adversarial 0.01 msoftmax base
- ImageNet & adversarial 0.01 softmax100 base
- ImageNet & adversarial 0.01 softmax ReAct
- ImageNet & adversarial 0.01 msoftmax ReAct
- ImageNet & adversarial 0.01 softmax100 ReAct
- ImageNet a
- rock paper scissors
- ImageNet v2
- ImageNette
- iNaturalist
- SUN
- Places
- iNaturalist & adversarial 0.1 softmax base
- iNaturalist & adversarial 0.1 msoftmax base
- iNaturalist & adversarial 0.1 softmax ReAct
- iNaturalist & adversarial 0.1 msoftmax ReAct
- · Gaussian
- Uniform
- ImageNet
- ImageNet & gaussian 0.001

- ImageNet & gaussian 0.002
- ImageNet & gaussian 0.05
- ImageNet & gaussian 0.1
- ImageNet & gaussian 0.3
- ImageNet & gaussian 0.5
- ImageNet & gaussian 0.8
- ImageNet & gaussian 0.25
- ImageNet & gaussian 1.0
- ImageNet & gaussian 1.25
- ImageNet & gaussian 2.0
- ImageNet & gaussian 5.0
- ImageNet & gaussian 10.0
- ImageNet & gaussian 20.0
- ImageNet & blur 0.5
- ImageNet & blur 1.0
- ImageNet & blur 5.0
- ImageNet & blur 10.0
- ImageNet & blur 20.0
- ImageNet & pixelization 0.9
- ImageNet & pixelization 0.7
- ImageNet & pixelization 0.5
- ImageNet & pixelization 0.2
- ImageNet & pixelization 0.1
- ImageNet & perspective transform 10.0
- ImageNet & perspective transform 25.0
- ImageNet & perspective transform 50.0
- ImageNet & perspective transform 75.0
- ImageNet & perspective transform 100.0
- ImageNet & encodingquality 75
- ImageNet & encodingquality 50
- ImageNet & encodingquality 25
- ImageNet & encodingquality 15
- ImageNet & encodingquality 5
- iNaturalist & adversarial 0.01 softmax base
- iNaturalist & adversarial 0.001 softmax base
- iNaturalist & adversarial 0.0001 softmax base

The list of datasets & augmentations used for all the other models (9 pairs, that is a subset of the previous one):

- imagenet
- iNaturalist

- SUN
- Places
- ImageNet V2
- ImageNet & gaussian 0.002
- ImageNet & gaussian 0.01
- ImageNet & gaussian 0.05
- ImageNet & gaussian 0.25
- ImageNet & gaussian 1.25
- iNaturalist & adversarial 0.01 softmax base
- iNaturalist & adversarial 0.001 softmax base
- iNaturalist & adversarial 0.0001 softmax base

B. How does the score distribution change?

Figures 5 shows the score distributions in various scenarios using the scores obtained by ODIN with $\epsilon=0$ with and without the ReAct layer. The difference is quite marked even for large values of p (in our case 90%), as it reduces the variance of all the four distributions.

C. Sample Images

Figure 7 shows some sample of the images used from various augmentations and datasets.

D. Our hypothesises on why ODIN($\epsilon=0.0014$) fails

 $\mathtt{ODIN}(\epsilon=0.0014)$ without ReAct completely fails, however, if we multiply the scores by -1, it becomes one of the best methods. Unfortunately, this is true only for the version without ReAct. We were not able to explain this phenomena, our possible explanation are:

- Wrong hyper-parameters choice, generally, the ϵ is tune specifically for each model.
- Implementation bug or a minor, but fundamental, implementation detail missing.
- The use of $\epsilon > 0$ is actually harmful in some situations.

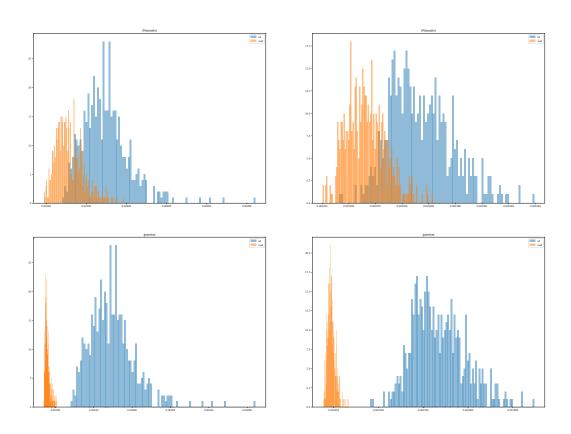


Figure 5: score distribution of the ID (light blue) and OOD dataset (orange) with the $ODIN(\epsilon=0)$ scorer. On the left with ReAct on the Right without it. In the first row the OOD dataset is iNaturalist, while in the second is the gaussian noise.

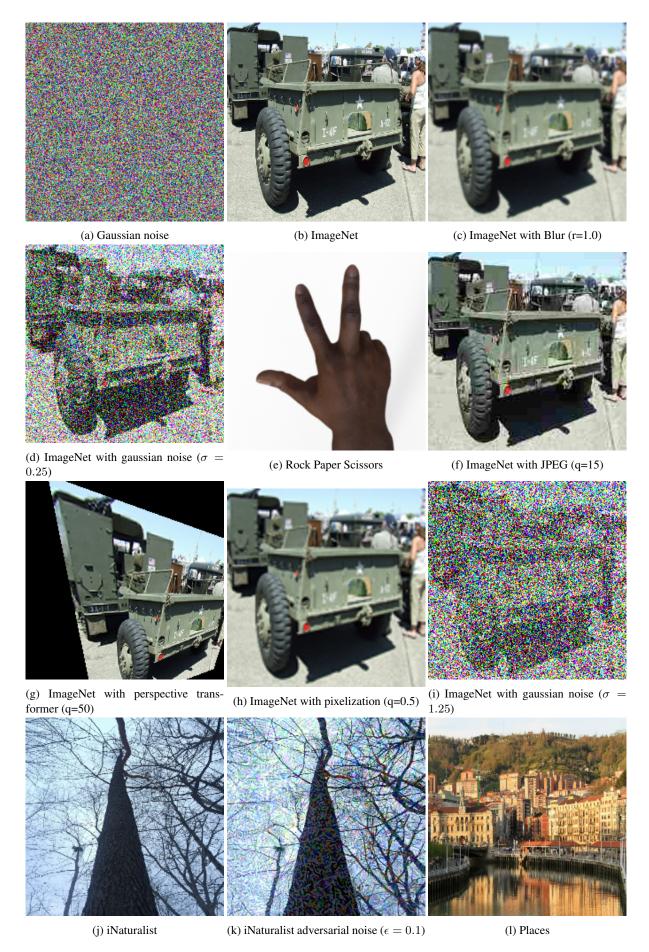


Figure 6: These are the 10 best model-scoring function pairs (ranks are from 1 to 64, all the combinations of the 10 models and the 8 scoring methods)