TEST TIME AUGMENTATIONS ARE WORTH ONE MIL-LION IMAGES FOR OUT-OF-DISTRIBUTION DETECTION

Anonymous authors

Paper under double-blind review

ABSTRACT

Out-of-distribution (OOD) detection is a major threat for deploying machine learning models in safety-critical scenarios. Data augmentations have been proven to be beneficial to OOD detection by providing diverse features. However, previous methods have only focused on the role of data augmentation in the training phase, overlooking its impact on the testing phase. In this paper, we present the first comprehensive study of the impact of test-time augmentation (TTA) on OOD detection. We find aggressive TTAs can cause distribution shifts on OOD scores of In-distribution (InD) data, whereas mild TTAs do not, resulting in the effectiveness of mild TTAs on OOD Detection. Based on the above observations, we propose a detection method that performs a K-nearest-neighbor (KNN) search on mild TTAs instead of InD data. With only 25 TTAs, our method outperforms existing methods using the entire training set (1.2 million images) on IMAGENET for OOD detection. Moreover, our approach is compatible with various model architectures and robust to adversarial examples.

023 024 025

026

000

001

002 003 004

006

008 009

010 011

012

013

014

015

016

017

018

019

021

1 INTRODUCTION

027 Deep Neural Networks (DNNs) are typi-028 cally trained in a closed-world assumption. 029 When these models encounter unfamiliar inputs from the open world, they may face out-of-031 distribution (OOD) samples, which can disrupt the system's normal operation. In safety-critical 033 applications such as autonomous driving (Kitt 034 et al., 2010) and healthcare (Schlegl et al., 2017), identifying and handling these OOD inputs is crucial. For instance, a self-driving car may fail to detect objects on the road that are not 037 included in the training set, which could lead to an accident.

To distinguish OOD samples from in-040 distribution (InD) data, a rich line of OOD 041 detection algorithms have recently been 042 developed. According to the availability 043 of OOD samples, current OOD detection 044 methodologies can be categorized into three 045 categories: OOD Exposure, InD-dependent, and 046 InD-independent (Yang et al., 2021c). OOD 047



Figure 1: OOD detection performance with different sampling ratios on IMAGENET training set. Our method is InD-independent and thus not affected by the sampling ratio. With only 25 TTAs, our method outperforms KNN (Sun et al., 2022) and VIM (Wang et al., 2022), which rely on the entire training set (1.2 million images).

Exposure involves collecting external OOD samples during training to aid the OOD detector in learning the difference between InD and OOD data. Common methods include OE (Hendrycks et al., 2018a), MCD (Yu & Aizawa, 2019), and UDG (Yang et al., 2021b). Although OOD Exposure is simple and effective, it cannot detect unseen OOD data. InD-dependent methods use known InD data as a reference set. For example, Lee et al. (2018) measure the minimum Mahalanobis distance from the class centroids; KNN (Sun et al., 2022) explores the k-th nearest neighbor distance between the input sample and the reference set; VIM (Wang et al., 2022) uses the reference set for covariance estimation. InD-dependent methods are influenced by the quantity and quality of InD data, as shown



Figure 2: The influence of IDA and OODA on the distribution Figure 3: IDA changes the heatmap of OOD, but not the InD. of OOD Score.

066 in Figure 1. In contrast, the InD-independent method designs a scoring method based on the output 067 of the model to detect OOD. MSP (Hendrycks & Gimpel, 2016) and ML (Hendrycks et al., 2019a) 068 use the maximum SoftMax and maximum Logit scores to indicate ID-ness, Energy (Liu et al., 2020) employs energy-based functions, and ODIN (Liang et al., 2017) uses temperature scaling 069 and gradient-based input perturbations. While the InD-independent method is straightforward and user-friendly, its performance requires further improvement. 071

072 Currently, numerous studies have demonstrated that data augmentation can enhance the performance 073 of OOD detection. Notable methods include Mixup (Zhang et al., 2017), CutMix (Yun et al., 2019), and PixMix (Hendrycks et al., 2022). However, these methods are mainly applied in the training 074 phase. While He et al. (2022) demonstrated that TTAs can be used for OOD detection, there is a 075 dearth of comprehensive research on the impact of TTAs on OOD detection. 076

077 In this paper, we propose an InD-independent OOD detection method based on TTA. First, we 078 present a comprehensive exploration of the effect of TTA on OOD detection. We categorize TTA 079 into In-distribution Augmentation (IDA) and Out-of-distribution Augmentation (OODA) based on their effects on image feature expression. Empirical results reveal that OODA leads to a shift in the distribution of OOD scores, rendering it ineffective for OOD detection. In contrast, IDAs are 081 favorable for OOD detection. Based on these findings, we propose an OOD detection method that boosts KNN with TTA. Specifically, we use the K-th nearest neighbor (KNN) distance between the 083 embedding of the input sample and the generated TTAs to indicate ID-ness, instead of InD data as 084 a reference set. As a non-parametric method, our method does not depend on the information of 085 external OOD data and InD data, and does not modify the model, which is a model-agnostic method. Detection results for common OOD datasets on CIFAR-10 and IMAGENET show that our method 087 outperforms existing methods. Especially for concurrent KNN (Sun et al., 2022), our method only generates 25 TTAs and outperforms the performance of KNN with 1.2 million images as the reference set on IMAGENET (as shown in Figure 1). We summarize our contributions as follows:

090 091

094

098

099

100

064

065

- 1. Our study is the first to investigate the effect of TTA on OOD detection. We classify test-time data augmentations into IDA and OODA and demonstrate that IDA can enhance OOD detection 092 performance. We believe our findings will encourage further research into TTA-based data-efficient OOD detection techniques.
- 2. We proposed an OOD detection method that employs TTA to improve KNN. Experimental results 095 show that generating as few as 25 TTA samples outperforms SOTA methods achieved by using a 096 reference set of 1.2 million images on IMAGENET.
 - 3. Our method introduces the sequential mask as TTA, and comprehensive evaluations on various OOD detection benchmarks across different model architectures show our method consistently outperforms the SOTA methods. As a plug-and-play method, our method's performance can be further enhanced by incorporating high-quality embeddings. Moreover, our method is also robust to adversarial examples that cause OOD score shifts.
- 101 102 103
- 104
- 105

A CLOSER LOOK AT TEST TIME AUGMENTATION ON OOD DETECTION 2

Geiping et al. (2022) firstly classifies data augmentation as aggressive or mild based on whether the 106 augmentation destroys image expression. Empirical results suggest that aggressive data augmentation 107 produces more diverse features, resulting in higher but unstable gains, whereas mild augmentation

123

129

130

131 132

133

134

135

136

108 Table 1: OOD Detection Performance (AUROC) of TTAs on CIFAR-10. The detection performance 109 of IDA is much higher than that of OODA, and using multiple IDAs leads to optimal performance. 110 See Appendix D for results on IMAGENET.

				0	OD Datasets			
	I IA	Cifar100	SVHN	Texture	Places365	iSUN	LSUN	Average
	Hflip	87.93	95.13	88.92	90.39	95.84	98.33	<u>92.76</u>
	Gray	86.77	92.49	87.38	88.71	93.42	96.75	90.92
	CenterMask	87.43	95.07	87.89	88.49	94.24	97.99	91.85
IDA	CenterCrop	87.17	95.27	89.10	90.24	95.77	98.06	92.60
IDA	Fourier Low Pass	87.02	94.40	89.27	90.70	96.88	98.08	92.73
	Hflip + Gray	87.63	95.21	88.93	90.24	95.71	98.43	92.69
	Hflip + Gray + CenterMask	88.37	95.24	88.97	90.11	95.48	98.37	92.76
	Hflip + Gray + CenterMask + CenterCrop	88.80	94.78	89.55	90.69	95.91	98.12	92.97
	Vflip	55.88	46.14	42.71	61.53	59.89	62.06	54.70
	Rotate	53.55	50.55	45.88	61.54	58.83	58.38	54.79
OODA	ColorJitter	65.87	61.88	61.03	70.80	69.05	70.65	66.55
	Invert	73.94	77.58	68.42	77.15	77.33	83.02	76.24
	Fourier High Pass	59.24	53.38	48.91	71.84	63.96	64.16	60.25

Table 2: LPIPS of different data augmentations: IDA generally yields lower scores than OODA, with MASK achieving the lowest LPIPS on both CIFAR-10 and IMAGENET.

 LPIPS	Hflip	Gray	Mask	Crop	Vflip	Rotate90	ColorJitter	Invert
CIFAR-10	0.048	0.1184	0.0052	0.0171	0.075	0.082	0.1618	0.2368
ImageNet	0.2961	0.2466	0.01	0.1425	0.5839	0.6312	0.4484	0.5656

leads to more stable but weaker gains. Inspired by the above observations, we also classify test-time data augmentation into In-Distribution Augmentation (IDA) and Out-of-Distribution Augmentation (OODA), and investigate its impact on OOD detection:

• **IDA**: TTAs that do not affect the expression of image features, such as horizontal flip (HFlip), gray, small-size center masking, large-size center cropping, and Fourier low-pass filtering.

• **OODA**: TTAs that drastically change the features of the image, such as vertical flip (VFlip), rotation, ColorJitter, Invert, and Fourier high-pass filtering.

137 The impact of IDA and OODA on the distribution of OOD scores. We find IDA and OODA have 138 distinct effects on the OOD score distribution. Figure 2 illustrates the shift in the distribution of OOD 139 scores (Liu et al., 2020) for both InD and OOD data resulting from IDA and OODA. Our observations 140 reveal that IDA has a negligible effect on the score distribution of InD data, while slightly modifying the distribution of OOD data. In contrast, OODA induces a distribution shift in InD data, making it 141 resemble the distribution of OOD. 142

143 The performance of IDA and OODA. Based on the above findings, we conduct a simple method 144 for OOD detection by comparing output consistency between input samples and their augmentations. 145 The results in Table 1 show that IDA can effectively detect OOD data. Moreover, using multiple 146 IDAs and selecting the one with the highest similarity can further improve the detection performance. 147 In contrast, OODA cannot be used for OOD detection, as it causes the score distribution of InD and OOD data to become similar. 148

149 How to identify IDA and OODA? According to the conclusions of Geiping et al. (2022), aug-150 mentations that have a great impact on the expression of image features are considered aggressive 151 augmentations (OODA), and vice versa, moderate augmentations (IDA). To assess how various aug-152 mentation techniques affect image representation, we computed the Learned Perceptual Image Patch Similarity (LPIPS) distances, as shown in Table 2. LPIPS quantifies the perceptual difference between 153 two images, with lower scores indicating greater similarity and thus implying less impact from the 154 augmentation method. Our analysis reveals that IDA typically yields lower LPIPS scores than OODA. 155 Interestingly, augmentations with lower LPIPS scores tend to exhibit superior performance in Table 1. 156 This correlation suggests that LPIPS can serve as an effective metric for differentiating between IDA 157 and OODA techniques. Notably, grayscale transformation is an exception to this pattern, possibly 158 due to the LPIPS model's learned sensitivity to color characteristics. 159

Why IDA is effective for OOD Detection? We provide a visual explanation of why IDA is beneficial 160 for OOD detection. We enhance Grad-CAM by modifying the weight computation of feature maps, 161 using a global average of the gradients backpropagated from the Energy score. Figure 3 illustrates



Figure 4: Overview of our method for OOD detection. We first perform a sequential mask for the input image. Next, the input image and corresponding TTAs are fed into the model to obtain embeddings. Then the k-th largest similarity between the input image and the TTAs embedding is selected as the ID score. If the score exceeds the threshold, it is detected as InD.

the visualization outcomes of InD and OOD data, as well as their IDA results. It can be observed that
the OOD heatmap is noticeably affected by IDA, while the InD heatmap remains unaffected, which
explains why IDA can be utilized for OOD detection in Table 1. See more visualization results in
Appendix E.

Takeaway: In contrast to OODA, IDA has the ability to generate distinguishable heatmap differences between InD and OOD data, making it suitable for OOD detection. Furthermore, using multiple IDAs and selecting the most similar can further improve detection performance.

3 Method

Preliminary. Let \mathcal{X} denote the input space and \mathcal{Y} denote the label space. Given a pre-trained classifier $f : \mathcal{X} \to \mathcal{Y}$, trained on InD data drawn from distribution P_{in} , the goal of OOD detection is to determine whether a test sample $x \in \mathcal{X}$ is drawn from P_{in} or from an unknown distribution P_{out} . Formally, we seek a scoring function $g : \mathcal{X} \to \mathbb{R}$ and a threshold λ such that:

191 192

173

174

175

176

181

182

183

184 185

187

188

189

190

193

194

 $h_{\lambda}(x) = \begin{cases} \text{InD,} & \text{if } g(x) \ge \lambda\\ \text{OOD,} & \text{if } g(x) < \lambda \end{cases}$ (1)

Design Objective. This work considers the classifiers trained on InD data that may encounter OOD samples. Unlike previous methods (Sun et al., 2022; Lee et al., 2018), *our goal is to design an effective OOD detection method that requires neither OOD data nor prior knowledge of InD data.*Our approach aims to explore the relationship between a sample and its TTAs, and exploit this for OOD detection. Notably, our method does not alter any component of the classifier, including the architecture and trained weights, making it a model-agnostic plug-and-play detector that can seamlessly integrate with different model architectures.

Core Idea. Our core idea is to construct a scoring function for OOD detection by utilizing the relationship between samples and their TTAs. Unlike KNN which performs a nearest neighbor search in the feature space of the entire training data, our approach focuses on searching within the local neighborhood of input samples provided by TTAs. Therefore, our method is data-efficient and InD-independent. However, our method requires some IDA that is effective for OOD detection. Therefore, selecting an appropriate TTA strategy becomes crucial for the success of our method.

208 TTA Strategy. Our findings in Sec. 2 suggest that enhancing OOD detection performance hinges 209 on identifying an array of effective IDAs. However, the repertoire of conventional IDAs is limited, 210 and combining multiple stylistically diverse augmentations doesn't necessarily improve detection 211 performance. As shown in Table 1, where the combination of Hflip and Gray underperforms 212 compared to Hflip alone. Furthermore, Table 2 reveals that masking has the least impact on image 213 features among common augmentations. Leveraging this insight, we introduce a novel Test-Time Augmentation (TTA) strategy called Sequential Mask. This approach applies masks to images in a 214 sequential manner, generating a substantial number of similar IDAs. Figure 5 shows the detection 215 performance when utilizing varying numbers of masked images as a reference set. Note that the

mask size is 8x8 on CIFAR-10 and 44x44 on IMAGENET. The results demonstrate a clear trend that
 the detection performance gradually improves with an increasing number of IDAs obtained through
 sequential mask.

219 Framework. Figure 4 depicts the overview of 220 our method. We explore the effectiveness of 221 the K-nearest neighbor search in TTAs of in-222 put samples for OOD detection. Given an input sample (x), multiple TTAs (x^*) are generated 224 by sequential mask at first. Then, both the input 225 sample and TTAs are fed into the target model, 226 obtaining embeddings for the input sample (z)and its corresponding TTAs (z^*) . Next, calcu-227 late the similarities between z and z^* . Finally, 228 the similarities are ranked and the k-th largest 229 similarity is selected to indicate ID-ness, which 230 is used to determine whether the input is OOD 231 by a threshold-based criterion as follows: 232

$$S(z,k) = \mathbf{1}\{-Sim_k(z,z^*) > \lambda\}$$
(2)

where $Sim_k(z, z^*)$ is the cosine similarity to the *k*-th nearest neighbor, and $\mathbf{1}\{\cdot\}$ is the binary indicator function. Typically, the threshold λ is selected to ensure accurate classification of the

233

234

248

249

256 257

258 259

260



Figure 5: OOD detection performance with different number of masks. x and y axes indicate the detection performance on Place365 and iNaturalist. The detection performance improves as the number of masks increases.

majority of ID data (e.g., 95%). The thresholds are independent of OOD data. The *k* is selected using the validation method in Hendrycks et al. (2018b). Compared to earlier methods, our method has several compelling advantages:

- InD Independent: Our method does not necessitate any prior knowledge of the InD data. This stands in contrast to KNN (Sun et al., 2022) and Mahalanobis distance (Lee et al., 2018), and VIM (Wang et al., 2022), which needs InD data for covariance estimation. Therefore, our method's performance remains unaffected by the InD data (see Figure 1), and it is genuinely distributional assumption-free.
 - 2. **OOD-agnostic**: Our testing process does not depend on any knowledge of the unknown data. Instead, we estimate the threshold using only the InD data.

 Model-agnostic: Our testing procedure solely requires the classifier's output and doesn't modify the classifier. This renders our method applicable to a wide range of model architectures, including convolutional neural networks (CNNs) and the more recent Transformer-based ViT model (Dosovitskiy et al., 2020). Furthermore, our method's reliance solely on input masking, ensures its adaptability across various model architectures without the need for model-specific parameter reconfiguration.

4 EXPERIMENTS

4.1 EXPERIMENTAL SETTING

ID Datasets. Following the latest OOD benchmark (Yang et al., 2022; 2021a), we chose CIFAR-10 (Krizhevsky et al., 2009) and IMAGENET (Krizhevsky et al., 2017) as the ID datasets. CIFAR-10 consists of 10 classes of 32x32 color pictures, containing a total of 60,000 images, and each class contains 6000 images. Among them, 50000 images are used as the training set and 10000 images are used as the test set. IMAGENET is a large-scale dataset with 1000 classes, its training set contains 1.2 million images and its validation set contains 50,000 images. We resize all images to 224x224.

OOD Datasets. According to the existing OOD detection benchmarks (Yang et al., 2022), we select six OOD datasets for both CIFAR-10 and IMAGENET. For CIFAR-10, the OOD datasets are Cifar100 (Krizhevsky et al., 2009), SVHN (Netzer et al., 2011), Texture (Kylberg, 2011), Places365 (Zhou et al., 2017), iSUN (Xu et al., 2015) and LSUN (Yu et al., 2015), with Cifar100

270 Table 3: Comparison with competitive OOD detection methods on CIFAR-10. A is AUROC and 271 F is FPR95, \uparrow indicates larger values are better and vice versa. The **bolded** values are the best 272 performance, and the *underlined italicized* values are the second-best performance, the same below.

273																
274		Training					_		OODE	Datasets						
217	AUC	Data	Cifa	r100	SV	HN	Tex	ture	Place	es365	iSU	JN	LS	UN	Ave	rage
275		Data	F↓	$\mathbf{A}\uparrow$	F↓	A↑										
	MSP		56.29	88.11	40.67	94.36	48.74	91.13	51.96	89.24	37.80	94.03	28.59	95.91	44.01	92.13
276	ML		49.65	88.09	28.08	95.32	41.33	91.06	42.52	89.87	26.36	95.21	13.55	97.58	33.58	92.86
077	Energy		48.09	88.18	25.63	<u>95.49</u>	39.77	91.15	<u>40.59</u>	90.02	24.34	95.38	11.85	97.79	31.71	93.00
211	ODIN		50.86	82.10	<u>23.14</u>	92.69	38.44	87.07	42.99	85.58	15.33	<u>95.82</u>	<u>10.05</u>	97.56	30.13	90.14
278	VIM	\checkmark	54.22	87.33	15.61	94.85	25.02	94.89	50.32	89.10	30.57	95.62	47.79	94.19	37.25	92.66
	KNN	\checkmark	51.90	90.27	35.32	95.31	40.30	<u>93.86</u>	45.88	<u>91.19</u>	28.86	95.70	28.23	96.00	38.42	<u>93.72</u>
279	GradNorm		73.54	60.13	65.14	68.62	73.24	57.31	68.55	66.90	62.01	70.00	41.70	82.57	64.03	67.59
280	DICE	\checkmark	53.71	83.79	26.86	93.89	40.82	89.43	47.46	85.04	30.18	93.14	8.01	98.17	34.51	90.58
200	GEN		45.21	<u>88.60</u>	27.83	95.22	40.33	91.79	36.43	91.00	24.51	95.52	12.89	97.36	<u>31.20</u>	93.25
281	NAC	\checkmark	<u>46.27</u>	88.37	32.92	94.32	<u>35.47</u>	90.37	44.82	88.83	22.18	95.55	14.36	97.27	32.67	92.45
	ASH-P		53.02	85.52	38.73	94.44	38.26	89.46	45.64	87.15	24.64	94.36	18.55	97.35	36.47	91.38
282	ASH-B		61.46	74.22	51.22	80.55	62.35	77.63	65.82	78.50	46.97	83.36	26.36	89.78	52.36	80.67
283	ASH-S		50.15	84.27	27.64	96.17	39.77	89.55	46.78	84.72	25.69	94.17	16.18	<u>98.13</u>	34.37	91.17
200	Ours		47.36	90.79	30.39	95.17	37.07	93.50	43.23	91.29	<u>17.46</u>	96.95	15.24	97.45	31.79	94.19
004																

284 285

287

286 being the near OOD and the rest being the far OOD. For IMAGENET, the OOD datasets used are NINCO (Bitterwolf et al., 2023), SSB hard (Vaze et al., 2022), iNaturalist (Van Horn et al., 2018), 288 Places365, SUN (Xiao et al., 2010), Texture, where NINCO and SSB hard are near OOD and the rest 289 are far OOD.

290 Evaluation metrics. We mainly use the following two metrics to evaluate OOD detection algorithms: 291 1) FPR95 measures the false positive rate (FPR) at which the true positive rate (TPR) is equal to 292 95%, a lower score indicates better performance. 2) AUROC measures the area under the receiver 293 operating characteristic (ROC) curve, showing the relationship between TPR and FPR. The area 294 under the ROC curve can be interpreted as the probability that a positive ID example has a higher 295 detection score than a negative OOD example, with higher scores indicating better performance. In 296 this paper, we use AUROC as the main metric.

297 Backbones. We use ResNet18 (He et al., 2016) as the backbone for CIFAR-10. The model is trained 298 for 200 epochs, with a batch size of 128. We use the cosine annealing learning rate (Loshchilov & 299 Hutter) starting at 0.1. We train the models using stochastic gradient descent with momentum 0.9, 300 and weight decay 5^{-4} . We use a ResNet50 (He et al., 2016) backbone with resolution 224x224 for 301 IMAGENET, and use the pre-trained weights from torchvision (maintainers & contributors, 2016) 302 with a 76.13% accuracy.

303 **Baseline Methods.** We compare our methods with seven baselines that do not require fine-tuning. 304 They are MSP (Hendrycks & Gimpel, 2016), MaxLogit (Hendrycks et al., 2019a), Energy (Liu 305 et al., 2020), ODIN (Liang et al., 2017), VIM (Wang et al., 2022), KNN (Sun et al., 2022) and 306 ASH (Djurisic et al.), Where ASH has three shaping algorithms (Pruning, Binary and Scale). VIM 307 and KNN require 50,000 and 200,000 InD data on CIFAR-10 and IMAGENET, respectively. See 308 Appendix A for baseline settings.

- 309
- 310 311

4.2 EVALUATION ON CIFAR-10 TASK

312 313

314 Setup. Our method is conducted on the logit space for CIFAR-10, and the mask size used is 8x8, 315 and the number of neighbors masked is 16. We use k = 2 for detection. Notably, in contrast to KNN (Sun et al., 2022), where optimal performance is highly sensitive to the choice of k-value, our 316 method demonstrates robust performance with consistently smaller k-values. The choice of space 317 source and k-value are discussed further in Sec. 4.6. 318

319 Performance. Table 3 reports the detection performance of our method and SOTA methods on 320 CIFAR-10. All methods do not use OOD data. VIM and KNN require the entire training set (50,000 321 images) as a reference set or for covariance estimation. As a SOTA method, KNN achieved an average performance of 93.72% on CIFAR-10. However, our method achieves an average performance of 322 94.19% without relying on any ID data, which outperforms existing all methods, especially on the 323 near-OOD dataset (CIFAR-100).

	Training							OODI	Datasets						
AUC	Data	NIN	1CO	SSB	-hard	iNatu	ıralist	Place	es365	SU	JN	Tex	ture	Ave	rage
	Data	F↓	A↑	F↓	A↑	F↓	A↑	F↓	A↑	F↓	A↑	F↓	A↑	F↓	Â↑
MSP		72.38	79.63	90.33	70.03	53.43	88.01	76.49	78.23	73.74	79.83	70.73	78.59	72.85	79.05
ML		69.54	79.91	89.84	70.29	48.32	91.31	73.28	81.03	66.35	84.39	60.78	84.26	68.02	81.87
Energy		70.22	79.14	93.56	69.86	50.54	90.96	74.01	80.80	65.02	84.52	58.69	84.57	68.67	81.64
ODIN		76.58	76.87	91.54	71.00	42.12	90.95	70.38	81.28	61.89	84.40	50.74	85.52	65.54	81.67
VIM	\checkmark	70.17	78.99	96.35	64.01	73.56	87.12	87.25	77.50	83.68	79.23	22.93	96.60	72.32	80.58
KNN	\checkmark	75.83	77.90	98.86	57.71	63.89	85.60	88.84	71.65	75.46	77.90	14.27	96.47	69.53	77.87
GradNorm		73.30	72.55	83.30	67.71	24.30	94.13	68.10	75.74	44.20	88.16	37.40	88.54	55.10	81.14
DICE	\checkmark	79.00	76.46	88.30	66.57	32.10	93.06	76.10	79.54	51.20	86.24	43.10	88.01	61.63	81.65
GEN		79.50	81.22	87.20	69.07	46.40	92.19	79.70	80.60	75.30	82.64	67.00	83.25	72.52	81.49
NAC	\checkmark	73.62	78.47	86.52	68.26	36.31	93.52	70.33	78.53	53.24	88.81	49.75	88.14	61.63	82.62
ASH-P		63.83	80.26	96.73	69.29	36.54	92.87	70.82	81.67	58.48	86.35	49.51	87.84	62.65	83.05
ASH-B		60.32	81.95	86.17	71.23	16.41	97.40	68.56	84.82	38.49	94.42	19.36	94.09	48.22	87.32
ASH-S		58.65	82.77	95.74	68.11	14.87	98.06	64.32	83.09	42.37	92.72	16.08	96.46	48.67	86.87
Ours		59.33	82.19	85.81	71.43	37.10	92.55	74.88	75.81	40.10	91.82	35.37	91.54	55.43	84.22

Table 4: OOD Detection Performance on IMAGENET. The labeling is the same as Table 3.

4.3 EVALUATION ON LARGE-SCALE IMAGENET TASK

Setup. The mask size used for IMAGENET is 44x44, and the number of neighbors masked is 25. We use k = 4. For space sources on IMAGENET, we found that the combination of logit and softmax can achieve the most effective results (as shown in Figure 6).

342 **Performance.** In Table 4, we compare our method with competitive methods on IMAGENET for six 343 OOD datasets. On the near-OOD dataset (NINCO and SSB-hard), we achieve the highest average 344 AUROC and the lowest average FPR95, showing the superiority of our method on hard tasks. On 345 average performance, our method achieves an average AUROC of 84.22%, which is only 2 percentage 346 points below the SOTA performance of ASH. However, Tables 3 and 4 reveal that ASH requires different shaping algorithms for various In datasets to achieve optimal performance — specifically, 347 ASH-P for CIFAR-10 and ASH-B for IMAGENET. In contrast, our method maintains consistent 348 performance across different InD datasets without such dataset-specific adaptations. 349

350 Comparison with ID-dependent Methods. Vim Wang et al. (2022) and KNN (Sun et al., 2022) 351 need ID data to calculate OOD scores, so their performance is affected by ID data. In contrast, our 352 method computes the OOD score exclusively through TTA. For each detection, KNN searches the 353 k-th nearest neighbor within the reference set (usually the entire training set), while our method only needs to perform distance calculations with generated TTAs, reducing the computational cost. 354 Only generating 25 TTAs, our method outperforms KNN with 1.2 million images as a reference set. 355 Moreover, ID-dependent methods are susceptible to unbalanced data (Mani & Zhang, 2003), while 356 ours does not. 357

Limitations. According to Table 3 and Table 4, we find that our method is weaker than SOTA methods for detecting texture whether on CIFAR-10 or IMAGENET. We think the reason is that texture images are not sensitive to masking. Hence, how to better detect OOD datasets that are not sensitive to TTA is our future work.

362 363

370

371

324

337

338 339

340

341

4.4 **BOOST BY ACTIVATION RECTIFICATION**

Our method is based on the similarity of the image with its TTAs, and Ming et al. (2023) shows that embedding quality is the key to distance-based OOD detection methods. Activation rectification (ReAct (Sun et al., 2021)) can effectively suppress the high activation values on the feature of OOD data. We combine our method with ReAct, and the results in Table 5 show that the combination achieves improved performance.

4.5 ROBUSTNESS

Azizmalayeri et al. (2022) indicates that existing OOD detection methods have made great progress,
but adversarial examples can shift the OOD score distribution. We evaluate the robustness of
different OOD detectors on three common adversarial attacks, whose hyperparameters are given in
the Appendix A. As shown in Table 6, the projected gradient descent (PGD) attack (Madry et al.,
2017) causes a shift in the OOD scores of methods based on logit and softmax outputs (MSP, ML,
Energy, and ODIN), resulting in a crash in detection performance. For distance-based (KNN) and
multi-space sources (VIM) detection methods, they detect PGD fairly well, but suffer performance

Table 6: Robustness of OOD Detection Methods on CIFAR-10.



Figure 6: Detection performance using different Figure 7: Detection performance using different space source. mask size.

degradation for the simple attack FGSM (Fast Gradient Sign Method) (Goodfellow et al., 2014).
As for our method, when using the sequential mask as the TTA, the detection performance for the C&W attack (Carlini & Wagner, 2017) is relatively low. This is possibly due to the fact that the tiny perturbation of the C&W attack is not sensitive to masking. The average detection performance is optimal when using SimCLR's combined augmentations (Chen et al., 2020). However, SimCLR is more aggressive, leading to a decrease in the detection performance of OOD.

4.6 ABLATION STUDY

378

396

397 398

399

400

401

402

403

404 405

406

Source Space. Wang et al. (2022) points out that the optimal space source for OOD Detection depends on the InD datasets and detection methods. Figure 6 shows the detection performance of our method on CIFAR-10 and IMAGENET using different spatial sources, where the red line represents the average performance for different OOD datasets. It can be seen that on CIFAR-10, logit is the optimal space source, and the combination of logit and softmax each accounting for 0.5 has the best performance on IMAGENET.

413 Mask Size. Figure 7 shows the impact of different mask sizes on detection performance, where 414 the yellow line represents the average performance for different OOD datasets. For CIFAR-10 415 and IMAGENET, the mask sizes we tested are $\{8, 6, 5, 4\}$ and $\{54, 44, 37, 32\}$ respectively, and 416 the count of generated samples are $\{16, 25, 36, 49\}$. It can be observed that the optimal count of 417 generated samples on CIFAR-10 and IMAGENET is 16 and 25, i.e., the optimal mask size is 8 and 44. Note that the choice of hyperparameters has minimal impact on the detection performance 418 of CIFAR-10. Furthermore, even when using the worst hyperparameter, our method achieves a 419 performance of over 86% on IMAGENET, surpassing the SOTA (85.54%). Therefore, our method is 420 not hyperparameter-sensitive. 421

k Value in KNN. In Figure 8, we analyze the effect of k. We vary the number of generated samples k from 1 to the maximum on CIFAR-10 and IMAGENET. There are several interesting observations:
1) As k increases, the detection performance exhibits a tendency of slight improvement initially, followed by a sharp decline. 2) When the value of k is small, the gap in detection performance is not large. 3) The optimal k value is 2 on CIFAR-10 and 4 on IMAGENET.

TTA Strategy. Our method differs from KNN in that it searches for the nearest neighbors in the samples generated by TTA, rather than in the reference set. Therefore, an appropriate TTA strategy can effectively enhance the detection performance of our method. Table 7 illustrates the detection performance of different TTA strategies on CIFAR-10. The FiveCrop and FiveMask strategies involve cropping and masking the four corners and center of the image, while the TenCrop and TenMask strategies include a horizontally flipped version of the image. It can be observed that sequential

TT 11

7 D



Figure 8: Detection perfor-Figure 9: The Visualization of Different Mask Types. mance of different k.

Table /: Performance of Different	I IA Strategies on CIFAR-10.

C---- 10

Method	Cifar100	SVHN	OC Texture	D Datasets Places 365	iSUN	LSUN	Average
	Churro	5,11,	Itatuit	1 Iucessoo	ISCIN	Louit	meruge
Sequential Mask	90.79	95.17	93.50	91.29	96.95	97.45	94.19
Edge Mask	90.90	95.00	93.19	91.43	97.04	97.25	94.14
Central Mask	88.00	95.41	89.72	88.78	96.04	98.15	92.68
Five Mask	90.26	95.77	92.30	91.31	96.63	98.00	94.05
Ten Mask	90.26	95.94	90.96	91.63	96.77	98.41	94.00
FiveCrop	86.35	93.22	90.00	90.11	95.84	97.03	92.09
TenCrop	86.84	94.12	90.51	90.50	96.14	97.42	92.59
SimCLR	86.00	92.37	88.78	90.01	94.16	96.43	91.29

masking is the most effective TTA strategy. Furthermore, we conducted a study on the impact of 455 different masking methods on detection performance. Figure 9 presents visualizations of different 456 mask methods. We found that the performance of edge masking is the closest to that of sequential masking. We believe this is because edge masking is milder than center masking, and hence more 458 conducive to OOD detection, which is consistent with the observations in Sec. 2. 459

Architecture. Table 8 shows the detection performance of our method on different model architec-460 tures. From the table, we can see that our method shows good performance for any OOD dataset, 461 regardless of the model employed. As a plug-and-play approach, our method does not require modifi-462 cation of the model structure and parameters. Therefore, there is no additional cost in switching our 463 method between different model structures. Notably, a small decrease in the detection performance 464 of our method occurs when using swin transformer as the backbone. We further test the detection 465 performance of baselines when using the swin transformer as the backbone in Appendix F. The 466 results show that the performance of baselines all declined and our method remains optimal.

467 468 469

470

471

457

439

440

441

> 5 **RELATED WORK**

5.1 **OOD DETECTION METHODS**

472 **OOD Data Exposure Approach.** Some works collect a bunch of external OOD samples to help 473 OOD detectors better learn ID/OOD differences. Outlier Exposure (Hendrycks et al., 2018a) utilizes 474 an auxiliary OOD dataset to improve OOD detection. Lee et al. (2017) use GAN to generate OOD 475 samples that are located near ID samples. Several methods including MCD (Yu & Aizawa, 2019), 476 NGC (Wu et al., 2021), and UDG (Yang et al., 2021b) can leverage external unlabeled noisy data to enhance OOD detection performance. Although using external OOD data is a simple and effective 477 approach, how to effectively select additional data and how to prevent the model to overfit the given 478 OOD is still an open problem. 479

480 InD-Dependent Approach. Some InD-dependent methods require InD data as a reference 481 set. Lee et al. (2018) measures the minimum Mahalanobis distance of class centroids, KL-482 Matching (Hendrycks et al., 2019a) computes the minimum KL divergence between softmax and the mean class conditional distribution, and KNN (Sun et al., 2022) performs a K-nearest neighbor 483 search on the reference set. VIM (Wang et al., 2022) uses InD data to estimate the covariance of 484 features to analyze the main space of features. Another part of the InD-dependent methods requires 485 InD data for training. ConfBranch (DeVries & Taylor, 2018) builds an additional branch from the

487						
488	Anabitaaturaa		00	D Datas	ets	
489	Arcintectures	iNaturalist	Places	SUN	Texture	Average
490	ResNet50(He et al., 2016)	92.61	75.78	91.88	91.39	87.92
404	DenseNet121(Huang et al., 2017)	92.03	74.25	91.53	93.21	87.75
491	WideResNet101(Zagoruyko & Komodakis, 2016)	94.41	84.28	86.36	83.80	87.21
492	Vit-b-16(Dosovitskiy et al., 2020)	92.70	82.81	84.71	85.43	86.43
493	Swin-t(Liu et al., 2021)	88.95	81.54	82.17	81.70	83.36

Table 8: Performance of Our Method with Different Architectures on IMAGENET.

494 495

486

penultimate layer to estimate confidence scores. CSI (Tack et al., 2020) explores the effectiveness of
OOD detectors against learned objectives. MOS (Huang & Li, 2021) uses priors on supercategories
to perform hierarchical OOD detection. VOS (Du et al., 2022) produces better energy scores with the
support of synthetic virtual outliers. The high performance of InD-dependent methods depends on
the quantity and quality of InD data.

500 **InD-Independent Approach.** InD-independent methods attempt to perform OOD detection by 501 devising scoring functions. MSP (Hendrycks & Gimpel, 2016) and ML (Hendrycks et al., 2019a) 502 directly use the maximum SoftMax score and maximum logits score to detect OOD. ODIN (Liang 503 et al., 2017) uses temperature scaling and gradient-based input perturbation. Energy Liu et al. (2020) 504 uses energy-based functions. GRAM (Sastry & Oore, 2020) computes the gram matrix within hidden 505 layers. DICE (Sun & Li, 2022) performs weight sparsification in the last layer. GradNorm (Huang et al., 2021) focuses on gradient statistics. ReAct (Sun et al., 2021) uses rectified activations, and 506 ASH (Djurisic et al.) reshapes the activation by three shaping algorithms. 507

509 5.2 Augmentation for OOD Detection

510 Some works have observed that regularizing the model during the training phase using data augmen-511 tation will help to better estimate the uncertainty. Mixup Zhang et al. (2017) mixes samples by pair, 512 and AugMix Hendrycks et al. (2019b) mixes samples with their augmentations. CutMix Yun et al. 513 (2019) replaces cut regions in a sample with patches from another image, and PixMix Hendrycks et al. 514 (2022) combines images through additive or multiplicative fusion with additional mixing datasets. 515 YOCO Han et al. (2022) crops images both vertically and horizontally, then mix them in pairs. 516 Mohseni et al. (2021) search for the optimal combination of augmentations through reinforcement 517 learning. Geiping et al. (2022) systematically studied the effect of data enhancement in the training 518 phase on OOD generalization. They found that aggressive augmentations result in more diverse features, while mild augmentations lead to more consistent features. As a result, aggressive augmen-519 tations provide a higher but unstable gain, whereas mild augmentations yield a lower but more stable 520 gain. However, the research on the impact of TTA on OOD detection remains elusive. 521

522 523

524

508

6 CONCLUSION

This paper presents the first systematic study on the impact of TTA for OOD detection and demonstrates that IDA at test time is beneficial and data-efficient for OOD detection. Furthermore, we propose a new TTA-based OOD detection method, which conducts a K-nearest neighbor search on TTAs. Our method only requires a handful of TTAs and spares the need for InD data as a reference set and external OOD data. Extensive experiments show that our method outperforms the SOTA methods on several OOD detection benchmarks. We hope that our work can inspire future research on data-efficient OOD detection using TTAs. We also do not see any immediate ethical concerns or negative societal impacts from this study.

- 533
- 534
- 535
- 536
- 537
- 538
- 539

540 REFERENCES 541

542	Mohammad Azizmalayeri, Arshia Soltani Moakhar, Arman Zarei, Reihaneh Zohrabi, Mohammad
543	Manzuri, and Mohammad Hossein Rohban. Your out-of-distribution detection method is not
544	robust! Advances in Neural Information Processing Systems, 35:4887–4901, 2022.
545	Julian Bitterwolf, Maximilian Mueller, and Matthias Hein. In or out? fixing imagenet out-of-
546	distribution detection evaluation. In ICML, 2023. URL https://proceedings.mlr.
547	press/v202/bitterwolf23a.html.
548	
549 550	<i>ieee symposium on security and privacy (sp)</i> , pp. 39–57. Ieee, 2017.
551	
552	contrastive learning of visual representations. In <i>International conference on machine learning</i> , pp.
553 554	1597–1607. PMLR, 2020.
555 556	Terrance DeVries and Graham W Taylor. Learning confidence for out-of-distribution detection in neural networks. <i>arXiv preprint arXiv:1802.04865</i> , 2018.
557	Andrija Diuricic, Nebojca Bozanic, Ariun Ashok, and Bosanne Liu, Extremely simple activation
558 559	shaping for out-of-distribution detection. In <i>The Eleventh International Conference on Learning</i>
560	Representations.
561	Alexev Dosovitskiv, Lucas Bever, Alexander Kolesnikov, Dirk Weissenborn, Xiaohua Zhai, Thomas
562	Unterthiner, Mostafa Dehghani, Matthias Minderer, Georg Heigold, Sylvain Gelly, et al. An
563	image is worth 16x16 words: Transformers for image recognition at scale. arXiv preprint
564	arXiv:2010.11929, 2020.
565	Verfanz Der Zhanning Ware, Mar Coil and Viewen Li. Vers Lanning unbet von den it hanne bereitent
566	Autering Du, Zhaoning Wang, Mu Cai, and Yixuan Li. vos: Learning what you don't know by virtual outlier synthesis. arXiv preprint arXiv:2202.01107, 2022
567	outher synthesis. <i>urxiv preprint urxiv.2202.01197</i> , 2022.
568	Jonas Geiping, Micah Goldblum, Gowthami Somepalli, Ravid Shwartz-Ziv, Tom Goldstein, and
569 570	Andrew Gordon Wilson. How much data are augmentations worth? an investigation into scaling laws, invariance, and implicit regularization. <i>arXiv preprint arXiv:2210.06441</i> , 2022.
571	
572 573	Ian J Goodfellow, Jonathon Shlens, and Christian Szegedy. Explaining and harnessing adversarial examples. <i>arXiv preprint arXiv:1412.6572</i> , 2014.
574	Junlin Han Dangfai Fang Waihao Li Jia Hang Mahammad Ali Armin Jan Daid Larg Dataresan and
575	Hongdong Li, You only cut once: Boosting data augmentation with a single cut. In International
576 577	Conference on Machine Learning, pp. 8196–8212. PMLR, 2022.
578	Haowei He, Jiave Teng, and Yang Yuan. Anomaly detection with test time augmentation and
579	consistency evaluation. arXiv preprint arXiv:2206.02345, 2022.
580	Kaiming He. Xiangyu Zhang, Shaoqing Ren, and Iian Sun. Deen residual learning for image
581	recognition. In Proceedings of the IEEE conference on computer vision and pattern recognition.
582	pp. 770–778, 2016.
583	
584	Dan Hendrycks and Kevin Gimpel. A baseline for detecting misclassified and out-of-distribution
505	examples in neural networks. arxiv preprint arXiv:1010.02130, 2016.
500	Dan Hendrycks, Mantas Mazeika, and Thomas Dietterich. Deep anomaly detection with outlier
588	exposure. arXiv preprint arXiv:1812.04606, 2018a.
589	Den Handmales Mantes Marsiles and Theorem D'attacks D. 1. 1. 1. 1. 1. 1. 1. 1.
590	Dan Hendrycks, Mantas Mazeika, and Thomas Dietterich. Deep anomaly detection with outlier
591	спрозию. игли рисрии игли.1012.04000, 20100.
592	Dan Hendrycks, Steven Basart, Mantas Mazeika, Andy Zou, Joe Kwon, Mohammadreza Mostajabi,
593	Jacob Steinhardt, and Dawn Song. Scaling out-of-distribution detection for real-world settings. <i>arXiv preprint arXiv:1911.11132</i> , 2019a.

- 594 Dan Hendrycks, Norman Mu, Ekin D Cubuk, Barret Zoph, Justin Gilmer, and Balaji Lakshmi-595 narayanan. Augmix: A simple data processing method to improve robustness and uncertainty. 596 arXiv preprint arXiv:1912.02781, 2019b. 597 Dan Hendrycks, Andy Zou, Mantas Mazeika, Leonard Tang, Bo Li, Dawn Song, and Jacob Steinhardt. 598 Pixmix: Dreamlike pictures comprehensively improve safety measures. In Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition, pp. 16783–16792, 2022. 600 601 Gao Huang, Zhuang Liu, Laurens Van Der Maaten, and Kilian Q Weinberger. Densely connected 602 convolutional networks. In Proceedings of the IEEE conference on computer vision and pattern recognition, pp. 4700-4708, 2017. 603 604 Rui Huang and Yixuan Li. Mos: Towards scaling out-of-distribution detection for large semantic 605 space. In Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition, 606 pp. 8710-8719, 2021. 607 Rui Huang, Andrew Geng, and Yixuan Li. On the importance of gradients for detecting distributional 608 shifts in the wild. Advances in Neural Information Processing Systems, 34:677–689, 2021. 609 610 Bernd Kitt, Andreas Geiger, and Henning Lategahn. Visual odometry based on stereo image 611 sequences with ransac-based outlier rejection scheme. In 2010 ieee intelligent vehicles symposium, 612 pp. 486-492. IEEE, 2010. 613 Alex Krizhevsky, Geoffrey Hinton, et al. Learning multiple layers of features from tiny images. 2009. 614 615 Alex Krizhevsky, Ilya Sutskever, and Geoffrey E Hinton. Imagenet classification with deep convolu-616 tional neural networks. Communications of the ACM, 60(6):84-90, 2017. 617 Gustaf Kylberg. Kylberg texture dataset v. 1.0. Centre for Image Analysis, Swedish University of 618 Agricultural Sciences and ..., 2011. 619 620 Kimin Lee, Honglak Lee, Kibok Lee, and Jinwoo Shin. Training confidence-calibrated classifiers for 621 detecting out-of-distribution samples. arXiv preprint arXiv:1711.09325, 2017. 622 Kimin Lee, Kibok Lee, Honglak Lee, and Jinwoo Shin. A simple unified framework for detecting 623 out-of-distribution samples and adversarial attacks. Advances in neural information processing 624 systems, 31, 2018. 625 Shiyu Liang, Yixuan Li, and Rayadurgam Srikant. Enhancing the reliability of out-of-distribution 626 image detection in neural networks. arXiv preprint arXiv:1706.02690, 2017. 627 628 Weitang Liu, Xiaoyun Wang, John Owens, and Yixuan Li. Energy-based out-of-distribution detection. 629 Advances in neural information processing systems, 33:21464–21475, 2020. 630 Ze Liu, Yutong Lin, Yue Cao, Han Hu, Yixuan Wei, Zheng Zhang, Stephen Lin, and Baining Guo. 631 Swin transformer: Hierarchical vision transformer using shifted windows. In *Proceedings of the* 632 *IEEE/CVF international conference on computer vision*, pp. 10012–10022, 2021. 633 634 I Loshchilov and F Hutter. Stochastic gradient descent with warm restarts. In Proceedings of the 5th 635 Int. Conf. Learning Representations, pp. 1–16. 636 Aleksander Madry, Aleksandar Makelov, Ludwig Schmidt, Dimitris Tsipras, and Adrian Vladu. 637 Towards deep learning models resistant to adversarial attacks. arXiv preprint arXiv:1706.06083, 638 2017. 639 640 TorchVision maintainers and contributors. Torchvision: Pytorch's computer vision library. https: 641 //github.com/pytorch/vision, 2016. 642 Inderjeet Mani and I Zhang. knn approach to unbalanced data distributions: a case study involving 643 information extraction. In Proceedings of workshop on learning from imbalanced datasets, volume 644 126, pp. 1–7. ICML, 2003. 645 Yifei Ming, Yiyou Sun, Ousmane Dia, and Yixuan Li. How to exploit hyperspherical embed-646
- 646 Ther Ming, Tryou Sun, Ousmane Dia, and Tixuan Li. How to exploit hyperspherical embed 647 dings for out-of-distribution detection? In *The Eleventh International Conference on Learning Representations*, 2023.

648 Sina Mohseni, Arash Vahdat, and Jay Yadawa. Shifting transformation learning for out-of-distribution 649 detection. arXiv preprint arXiv:2106.03899, 2021. 650 Yuval Netzer, Tao Wang, Adam Coates, Alessandro Bissacco, Bo Wu, and Andrew Y Ng. Reading 651 digits in natural images with unsupervised feature learning. 2011. 652 653 Chandramouli Shama Sastry and Sageev Oore. Detecting out-of-distribution examples with gram 654 matrices. In International Conference on Machine Learning, pp. 8491–8501. PMLR, 2020. 655 656 Thomas Schlegl, Philipp Seeböck, Sebastian M Waldstein, Ursula Schmidt-Erfurth, and Georg Langs. 657 Unsupervised anomaly detection with generative adversarial networks to guide marker discovery. In Information Processing in Medical Imaging: 25th International Conference, IPMI 2017, Boone, 658 NC, USA, June 25-30, 2017, Proceedings, pp. 146–157. Springer, 2017. 659 660 Yiyou Sun and Yixuan Li. Dice: Leveraging sparsification for out-of-distribution detection. In 661 Computer Vision–ECCV 2022: 17th European Conference, Tel Aviv, Israel, October 23–27, 2022, 662 Proceedings, Part XXIV, pp. 691–708. Springer, 2022. 663 664 Yiyou Sun, Chuan Guo, and Yixuan Li. React: Out-of-distribution detection with rectified activations. 665 Advances in Neural Information Processing Systems, 34:144–157, 2021. 666 Yiyou Sun, Yifei Ming, Xiaojin Zhu, and Yixuan Li. Out-of-distribution detection with deep nearest 667 neighbors. In International Conference on Machine Learning, pp. 20827–20840. PMLR, 2022. 668 669 Jihoon Tack, Sangwoo Mo, Jongheon Jeong, and Jinwoo Shin. Csi: Novelty detection via contrastive 670 learning on distributionally shifted instances. Advances in neural information processing systems, 671 33:11839–11852, 2020. 672 Grant Van Horn, Oisin Mac Aodha, Yang Song, Yin Cui, Chen Sun, Alex Shepard, Hartwig Adam, 673 Pietro Perona, and Serge Belongie. The inaturalist species classification and detection dataset. In 674 Proceedings of the IEEE conference on computer vision and pattern recognition, pp. 8769–8778, 675 2018. 676 677 Sagar Vaze, Kai Han, Andrea Vedaldi, and Andrew Zisserman. Open-set recognition: A good 678 closed-set classifier is all you need. In ICLR, 2022. 679 Haoqi Wang, Zhizhong Li, Litong Feng, and Wayne Zhang. Vim: Out-of-distribution with virtual-680 logit matching. In Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern 681 Recognition, pp. 4921–4930, 2022. 682 683 Zhi-Fan Wu, Tong Wei, Jianwen Jiang, Chaojie Mao, Mingqian Tang, and Yu-Feng Li. Ngc: A 684 unified framework for learning with open-world noisy data. In Proceedings of the IEEE/CVF 685 International Conference on Computer Vision, pp. 62–71, 2021. 686 Jianxiong Xiao, James Hays, Krista A Ehinger, Aude Oliva, and Antonio Torralba. Sun database: 687 Large-scale scene recognition from abbey to zoo. In 2010 IEEE computer society conference on 688 computer vision and pattern recognition, pp. 3485–3492. IEEE, 2010. 689 690 Pingmei Xu, Krista A Ehinger, Yinda Zhang, Adam Finkelstein, Sanjeev R Kulkarni, and Jianxiong 691 Xiao. Turkergaze: Crowdsourcing saliency with webcam based eye tracking. arXiv preprint 692 arXiv:1504.06755, 2015. 693 Jingkang Yang, Haoqi Wang, Litong Feng, Xiaopeng Yan, Huabin Zheng, Wayne Zhang, and 694 Ziwei Liu. Semantically coherent out-of-distribution detection. In Proceedings of the IEEE/CVF 695 International Conference on Computer Vision, pp. 8301–8309, 2021a. 696 697 Jingkang Yang, Haoqi Wang, Litong Feng, Xiaopeng Yan, Huabin Zheng, Wayne Zhang, and Ziwei Liu. Semantically coherent out-of-distribution detection. In Proceedings of the IEEE/CVF 699 International Conference on Computer Vision, pp. 8301–8309, 2021b. 700 Jingkang Yang, Kaiyang Zhou, Yixuan Li, and Ziwei Liu. Generalized out-of-distribution detection: 701 A survey. arXiv preprint arXiv:2110.11334, 2021c.

- 702 Jingkang Yang, Pengyun Wang, Dejian Zou, Zitang Zhou, Kunyuan Ding, Wenxuan Peng, Haoqi 703 Wang, Guangyao Chen, Bo Li, Yiyou Sun, et al. Openood: Benchmarking generalized out-of-704 distribution detection. arXiv preprint arXiv:2210.07242, 2022. 705 Fisher Yu, Ari Seff, Yinda Zhang, Shuran Song, Thomas Funkhouser, and Jianxiong Xiao. Lsun: 706 Construction of a large-scale image dataset using deep learning with humans in the loop. arXiv 707 preprint arXiv:1506.03365, 2015. 708 709 Qing Yu and Kiyoharu Aizawa. Unsupervised out-of-distribution detection by maximum classifier 710 discrepancy. In Proceedings of the IEEE/CVF international conference on computer vision, pp. 711 9518-9526, 2019. 712 713 Sangdoo Yun, Dongyoon Han, Seong Joon Oh, Sanghyuk Chun, Junsuk Choe, and Youngjoon Yoo. 714 Cutmix: Regularization strategy to train strong classifiers with localizable features. In Proceedings 715 of the IEEE/CVF international conference on computer vision, pp. 6023–6032, 2019. 716 Sergey Zagoruyko and Nikos Komodakis. Wide residual networks. arXiv preprint arXiv:1605.07146, 717 2016. 718 719 Hongyi Zhang, Moustapha Cisse, Yann N Dauphin, and David Lopez-Paz. mixup: Beyond empirical 720 risk minimization. arXiv preprint arXiv:1710.09412, 2017. 721 722 Bolei Zhou, Agata Lapedriza, Aditya Khosla, Aude Oliva, and Antonio Torralba. Places: A 10 723 million image database for scene recognition. IEEE transactions on pattern analysis and machine intelligence, 40(6):1452-1464, 2017. 724 725 726 APPENDIX 727 Α 728 729 **EXPERIMENTS DETAILS** Α 730 731 Software and Hardware. All methods are implemented in PyTorch 1.13. We run all the experiments 732 on NVIDIA GeForce RTX-3090 GPU. 733 Detains of augmentations. In Table 1, the mask size of CenterMask is 4x4, and the size of 734 CenterCrop cropped image is 30x30 and then resize to 32x32. Both Fourier high-pass filtering and 735 low-pass filtering preserve 90% of the high-pass or low-pass signals. The angle of rotation is 90. In 736 ColorJitter, brightness is 0.4, contrast is 0.4, saturation is 0.4, hue is 0.1. 737 **Hyperparameters for Baselines.** For VIM, when feature spaces of dimension N > 1500, we set the 738 dimension of the main space to D = 1000, otherwise set D = 512. For KNN, the dimension of the 739 penultimate feature where we perform the nearest neighbor search is 512 and 2048 on CIFAR-10 and 740 IMAGENET respectively, and we choose k = 50 following Yang et al. (2022) for detection. 741 Hyperparameters for Adversarial Attacks. We compare the robustness of our method to adversarial 742 attacks with existing OOD detection methods in Table 5. The attack methods we use are FGSM, 743 PGD, and C&W. Among them, the perturbation budget of FGSM is 0.05 ($\epsilon = 0.05$), and that of PGD 744 and C&W is 8/255 ($\epsilon = 8/255$). The number of PGD attack steps is 50, and the step size is 0.002. 745 The maximum number of iterations for C&W is 1000. 746 747 748 В HYPER-PARAMETERS IN AUGMENTATIONS 749 750 Table 10 investigates the detection performance of rotation and ColorJitter with large disturbance 751 degree. It can be seen that the detection performance of these two augmentations is poor i.e., both 752 are OODA. Moreover, we investigate the detection performance for different rotation angles in the
- Table 12. Results show that when the angle is small, the detection performance is higher than when
 the angle is slightly larger. This matches the intuition. When the rotation angle is small, it does not
 change the image features and can be regarded as IDA; when the rotation angle reaches a certain
 number of degrees such that it changes the image features, it becomes OODA.

	ТТА		OOD	Dataset	s	
	IIA	iNaturalist	Places365	SUN	Texture	Average
	Hflip	80.67	73.46	73.22	70.46	74.45
	Gray	85.89	69.18	75.03	66.67	74.19
	CenterMask	81.58	68.68	76.11	73.25	74.91
	CenterCrop	80.11	74.24	75.49	74.22	76.02
	Fourier Low Pass	82.36	71.58	73.46	71.92	74.83
	Hflip + Gray	82.75	74.44	74.93	71.22	75.83
IDA	Hflip + Gray + CenterMask	82.30	73.37	76.47	72.41	76.13
IDA	Hflip + Gray + CenterMask + CenterCrop	83.63	73.97	76.76	73.33	76.92
	Hflip + CenterMask	80.97	71.81	76.96	72.88	75.66
	Hflip + CenterCrop	83.13	74.46	75.23	72.53	76.34
	Gray + CenterMask	80.19	70.75	77.99	73.18	75.53
	Gray + CenterCrop	82.28	72.97	76.70	73.36	76.33
	CenterMask + CenterCrop	81.27	71.75	77.75	73.95	76.18
	Gray + CenterMask + CenterCrop	81.81	72.12	78.16	73.98	76.52
	Vflip	43.42	63.61	75.30	55.72	59.51
	Rotate	43.38	63.61	75.26	55.46	59.43
OODA	ColorJitter	70.28	59.21	71.80	57.91	64.80
	Invert	76.55	58.89	82.01	62.40	69.96
	Fourier High Pass	84.37	66.37	72.08	56.41	69.81

756 Table 9: OOD Detection Performance of TTAs on IMAGENET. The detection performance of IDA is much higher than that of OODA, and using multiple augmentations leads to the optimal performance.

Table 10: Detection performance of OODA under different parameters. For ColorJitter, the 4 numbers represent brightness, contrast, saturation and hue.

-	InD Datasat		Rotate			ColorJitter				
	IID Dataset	00	100	270	0.1,0.1	0.2,0.2	0.3,0.3	0.4,0.4		
		90	180) 270 0.1,0		0.2,0.1	0.3,0.1	0.4,0.1		
	Cifar10	54.79	54.83	54.64	68.81	68.32	67.55	66.55		
	ImageNet	59.43	63.28	63.49	64.79	64.80	64.81	64.80		

784 785 786

787

791

776

777

778 779

781 782 783

AUGMENTATION USED IN THE TRAINING PHASE С

788 To test the effect of adding augmentation during the training phase on the detection of IDA and 789 OODA, we design three sets of experiments in Table 11 to compare the detection performance of 790 using horizontal flip and vertical flip as TTA on models trained with horizontal flip, vertical flip and no augmentation. It can be observed that the detection performance of horizontal flip is much better 792 than that of vertical flip on the model trained without augmentation. In addition, the performance of 793 vertical flipping is improved on the model trained with vertical flipping. However, it is still weaker 794 than the performance of horizontal flip.

795 Therefore, since our approach is to compare the output similarity of samples and augmentations, 796 adding some kind of augmentation during the training phase will make this augmentation more like 797 IDA, but it will still not perform as well as a deterministic IDA (e.g., horizontal flipping). Furthermore, 798 since we are using multiple augmentations with K-nearest neighbor search, adding some OODAs 799 will only slightly decrease the overall performance.

- 800 801
- 802 803

D OOD DETECTION PERFORMANCE OF TTAS ON IMAGENET

804 We compare the OOD detection performance of different augmentations when CIFAR-10 is the InD 805 dataset in Sec. 2. Table 9 shows the OOD detection performance of different augmentations on the 806 large-scale dataset (IMAGENET). Consistent with the results in Sec. 2, the detection performance of 807 IDA is much higher than that of OODA, which proves that the division of IDA and OODA is based on whether to destroy common features, and does not depend on the target dataset. Moreover, the 808 detection performance is further improved when a k-nearest neighbor search is conducted on multiple 809 augmentations.

Training Augmentation	Hflip	Vflip	-	InD Detect	Ro	tate Deg	ree	
Hflip	92.76	54.70		IID Dataset	5	15	30	
No Aug	90.09	56.18	-	Cifar10	92.05	85.26	46.03	
Vflip	89.58	78.23		ImageNet	75.85	68.40	54.09	

Table 11: Augmentation used in the training Table 12: Detection Performance of Rotation

with different degrees.

E VISUALIZATION

phase

Sec. 2 shows that horizontal flipping can cause a difference between the heatmaps of InD and OOD data. To further demonstrate the impact of IDA and OODA on image features, we show the heat maps of common IDAs and OODAs on large-scale datasets in Figure 10. The visualization results of CIFAR-10 are not shown because its resolution is too low. It can be observed that OODA has a great influence on the features of both InD and OOD data. IDA will not change the high thermal area of InD, while OOD will be affected by IDA. Based on the observation of a large number of visualization results, we have obtained the following empirical conclusions:

- OOD data has a larger proportion of high thermal regions than InD data, that is, the useful features of OOD are more dispersed.
- IDAs do not change the high thermal region of InD, but they will change the high thermal region of OOD. And OODAs have an impact on the features of both InD and OOD. Therefore, IDA can be used for OOD detection, and OODA cannot be used for OOD detection.
 - No single IDA was able to cause changes in the high thermal regions of all OOD data. Horizontal flip is an effective TTA for OOD Detection, but the third row of Figure 10 (Places365) shows that horizontal flip does not have as much impact on the heatmap as other TTAs.

Based on the above conclusions, we designed Sequential Mask for OOD detection. First, masking is
an IDA that can effectively detect OOD. Then, since the useful features of OOD are more dispersed
than InD, the features of OOD are more likely to be changed in the masked samples produced by
sequential mask. Finally, The sequential mask can generate multiple Masked samples to make up for
the inability of a single IDA to maintain high detection performance for all OODs.

Moreover, we visualise the samples with their masked augmentations in Fig. 11 (a), and it can be seen that there may be some kind of "non-ideal" mask that causes the InD and OOD and their enhancements to be far apart. However, the use of multiple IDAs makes the distance between the InD and its nearest neighbour significantly smaller than that of the OOD.

We also show the distribution of embedding similarity between images from different datasets and
their 16 IDAs in Fig. 11 (b). It also shows that multiple IDAs will lead to a significant difference in
the distribution of embedding similarity between InD and OOD.

F DETECTION PERFORMANCE OF BASELINES ON SWIN TRANSFORMER

In Table 8, Our method has significant performance degradation only on the Swin Transformer. To
further verify whether our method is architecture-sensitive, we tested the detection performance of
common OOD detection methods on Swin Transformer in Table 13. It can be observed that all the
detection methods show performance degradation on Swin Transformer. In particular, ODIN shows
an average performance degradation of 59.37%. While the average performance of our method is
83.36%, which still outperforms all baselines. Therefore, we conclude that it is not that our method
is architecture-sensitive, but that there are some architectures (e.g., Swin Transformer) that are not
suitable for OOD detection.

G ALGORITHM

The Algorithm 1 details the three main components of our method: sequential mask generation, embedding similarity computation, and KNN-based OOD scoring. Sequential Mask Generation:



Figure 10: Heatmaps of IDAs and OODAs for InD and OOD. The visualization technology we use is the improved Grad-CAM, which uses a global average of the gradients backpropagted from the Energy score to compute the weights of the feature maps.



Figure 11: (a) Visualization of embeddings of InD and OOD, as well as their IDAs, It can be observed that the distance between InD and its nearest neighbor is much smaller than OOD. (b) The distribution of embedding similarity between images and their 16 IDAs. It shows that InD (Cifar10) has a higher embedding similarity to its IDAs than OOD.

Given an input image $x \in \mathbb{R}^{H \times W \times C}$, we generate K masked versions using a sequential strategy. Unlike random masking, our approach ensures uniform coverage of the image space.

Similarity Computation: For the original image x and its masked versions $\{x_1, ..., x_K\}$, we calculate the cosine similarity on the embedding space of a pre-trained model $f(\cdot)$.

KNN-based OOD Detection: Our method uses the *k*-th highest similarity as the OOD score.

Table 13: Detection Performance of Different OOD Detection Methods on Swin Transformer.

-	AUC (%)	NINCO	SSB-hard	iNaturalist	Places365	SUN	Texture	Avg
-	MSP	80.22	71.14	89.94	77.93	79.65	80.57	79.91
	ML	81.15	68.20	89.07	73.06	75.58	79.08	77.69
	ODIN	62.65	63.14	70.57	46.30	55.13	65.47	60.54
	Energy	77.14	68.47	84.99	67.47	70.88	76.44	74.23
	VIM	81.03	69.08	91.34	76.44	77.52	87.54	80.49
	KNN	79.44	64.17	87.59	77.18	76.49	88.28	78.86
	GradNorm	45.52	49.98	38.70	26.41	32.78	35.46	38.14
	DICE	41.20	57.20	32.60	32.53	35.55	70.80	44.98
	GEN	80.66	68.04	90.68	80.50	81.64	82.32	80.64
	NAC	76.58	67.29	91.48	75.53	80.87	83.14	79.15
	ASH-B	82.26	70.13	94.32	85.14	88.10	89.75	84.95
	ASH-S	80.24	68.24	92.61	81.64	85.56	87.65	82.66
	ASH-P	82.35	67.73	93.19	83.42	87.48	89.05	83.87
	Ours	81.37	67.71	90.79	78.58	81.89	84.04	80.73

⊳ Set of masked images ⊳ Stride
⊳ Set of masked images ⊳ Stride
▷ Set of masked images ▷ Stride
▷ Set of masked images ▷ Stride
▷ Set of masked images ▷ Stride
▷ Set of masked images ▷ Stride
⊳ Set of masked images ⊳ Stride
▷ Set of masked images ▷ Stride
▷ Set of masked images ▷ Stride
▷ Set of masked images ▷ Stride
⊳ Stride
⊳ Stride
\triangleright Cosine similarity
▷ Original embedding
⊳ I IA enibedunigs ⊳ Similarities
▷ KNN similarity
·