

ReweightOOD: Loss Reweighting for Distance-based OOD Detection

Sudarshan Regmi^{1,2*}, Bibek Panthi², Yifei Ming³,
Prashna K Gyawali⁴, Danail Stoyanov¹, Binod Bhattarai^{1,5}

¹ University College London, UK

² NepAI Applied Mathematics and Informatics Institute for research, Nepal

³ University of Wisconsin-Madison, USA

⁴ West Virginia University, USA

⁵ University of Aberdeen, UK

Abstract

*Out-of-Distribution (OOD) detection is crucial for ensuring safety and reliability of neural networks in critical applications. Distance-based OOD detection is based on the assumption that OOD samples are mapped far from In-Distribution (ID) clusters in embedding space. A recent approach for obtaining OOD-detection-friendly embedding space has been contrastive optimization of pulling similar pairs and pushing apart dissimilar pairs. It assigns equal significance to all similarity instances with the implicit objective of maximizing the mean proximity between samples with their corresponding hypothetical class centroids. However, the emphasis should be directed towards reducing the Minimum Enclosing Sphere (MES) for each class and achieving higher inter-class dispersion to effectively mitigate the potential for ID-OOD overlap. Optimizing low-signal dissimilar pairs might potentially act against achieving maximal inter-class dispersion while less-optimized similar pairs prevent achieving smaller MES. Based on this, we propose a reweighting scheme **ReweightOOD**, that adopts the similarity optimization which prioritizes the optimization of less-optimized contrasting pairs while assigning lower importance to already well-optimized contrasting pairs. Such a reweighting scheme serves to minimize the MES for each class while achieving maximal inter-class dispersion. Experimental results on a challenging CIFAR100 benchmark using ResNet-18 network demonstrate that ReweightOOD outperforms supervised contrastive loss by a whopping 38% in the average FPR metric. In various classification datasets, our method provides a promising solution for enhancing OOD detection capabilities in neural networks.*

*Correspondence: {sudarshan.regmi}@ucl.ac.uk

1. Introduction

OOD detection refers to detecting the samples lying beyond the scope of training distribution. During the inference phase, it is indeed imperative to prevent the prediction of unknown samples, referred to as OOD samples, as the model lacks familiarity with such instances, and consequently, they should be accurately flagged. This issue becomes even more critical in domains like autonomous driving and medical imaging, where entrusting neural networks to handling unforeseen scenarios is detrimental. In these contexts, either relinquishing appropriate control to human discretion or flagging the instance becomes essential. The incorporation of OOD detection mechanisms holds paramount importance in ensuring safety and reliability. Rather than solely excelling at the primary task, models are now expected to possess the capability of identifying OOD samples effectively too.

OOD samples inherently possess distinct characteristics that set them apart from in-distribution (ID) data. These differentiating characteristics can be observed in softmax probability [15], embedding space [24, 42], or in some scoring functions [27, 49]. Distance-based methods exploit the embedding space to quantify the OOD-ness of the samples. Two popular postprocessing approaches in distance-based OOD methods are Mahalanobis distance [24] and K-nearest neighbor [42]. A key assumption of these approaches is that OOD samples lie far away from ID clusters. Hence, the focus should be on obtaining such desirable embedding space for superior OOD detection performance.

Training-time regularization techniques can be employed to regularize neural networks to enhance OOD detection. Some approaches [33, 50] utilize the hyperspherical constraint during cross-entropy-based training to reduce overconfidence. Contrastive learning, a recent alternative, which also deals with hyperspherical embeddings to promote

class-separable representations, as demonstrated by self-supervised contrastive learning [37], supervised contrastive learning (SupCon) [19], and CIDER [31]. While these contrastive-based methods, when coupled with distance-based postprocessing, show promise, they lack consideration for the current proximity of the contrasting pairs during training. In essence, they consistently optimize the cosine similarity without considering whether the pairs have been adequately optimized. Our proposition suggests reweighting contrastive pairs based on cosine similarity in the embedding space better OOD performance. Specifically, we propose prioritizing pair instances where their corresponding embeddings are not aligned, and deprioritizing pair instances that are sufficiently aligned. By dynamically adjusting loss weights based on embedding space proximity, contrastive learning can focus more on challenging or unoptimized pairs, thereby reducing the Minimum Enclosing Sphere (MES) for each class and maximizing inter-class dispersion.

Hence, we present an effective OOD detection framework **ReweightOOD** based on loss reweighting. Our reweighting mechanism consists of a linear transformation of the cosine similarity followed by the application of the reweighting function. We employ scaling and shifting operations to achieve the desired range, and we employ the sigmoid function as reweighting function. This approach improves the OOD detection by a significant 38% improvement in FPR metric in a challenging CIFAR100 benchmark using ResNet-18 network. Our approach outperforms the current approaches making it a promising approach for detecting OOD samples. We summarize our contributions in the following points:

- We propose a similarity reweighting framework ReweightOOD in contrastive optimization for superior distance-based OOD detection. We show a simple reweighting mechanism can outperform supervised contrastive loss by 38% in the average FPR metric in challenging the CIFAR100 benchmark.
- We provide the design of the reweighting mechanism for the first time in OOD detection by coupling linear transformation and sigmoid weighting function. We illustrate that our domain for the reweighting mechanism can be flexibly adjusted by scaling and shifting using hyperparameters.
- We reveal the implication of the reweighting in achieving an MES of a smaller radius for all classes and higher class-centroid dispersion in the embedding space. Specifically, in a challenging CIFAR100 benchmark, the reweighting mechanism reduces mean MES radius by 14.28% and increases mean inter-class dispersion by a factor of ~ 2 .

2. Preliminaries

2.1. Out-of-Distribution Detection

We consider multi-class classification scenario, wherein $\mathcal{P}_{in} = (x_i, y_i)_{i=1}^N$ represents the training distribution, commonly referred to as the In-Distribution. In this context, the tuple (x_i, y_i) signifies an image-label pair, where y_i is an element of the set $\{1, 2, \dots, C\}$, with C representing total number of classes. During the testing phase, samples from a distribution \mathcal{P}_{out} , differing from the training distribution \mathcal{P}_{in} , are encountered. Out-of-distribution (OOD) detection is framed as a binary classification task, where a scoring function $SC(\mathbf{x})$ and a threshold λ guide the decision process with those exceeding λ labeled as ID and the rest as OOD. The threshold λ is often set for a 95% true positive rate on training data.

2.2. Hyperspherical Embeddings

The embeddings lying on the surface of the hypersphere of radius r_h are known as hyperspherical embeddings. An embedding can be transformed into a hyperspherical one by employing L_2 normalization. We employ our reweighting mechanism in contrastive training after transforming the raw embedding into the hyperspherical one.

3. Method

3.1. Contrastive optimization

Contrastive learning aims to learn useful representations by maximizing within-class cosine similarity s_w and minimizing between-class cosine similarity s_b . If $(x_{anchor}^j, x_{pos}^j)$ and $(x_{anchor}^i, x_{neg}^i)$ are pairs of images of the same class and different classes respectively, any given instance of within-class cosine similarity s_w^j and between-class cosine similarity s_b^i can be expressed as $s_w^j = h_{anchor}^j \cdot \hat{h}_{pos}^j$ and $s_b^i = h_{anchor}^i \cdot \hat{h}_{neg}^i$ where h denotes latent representation of respective inputs. Considering the availability of n between-class similarity s_b and o within-class similarity s_w , loss formulation for a sample k in a batch of size $(n + o + 1)$ with temperature τ can be expressed as:

$$\mathcal{L}_k = \log \left(\sum_{i=1}^n \exp(s_b^i / \tau) \right) - \log \left(\sum_{j=1}^o \exp(s_w^j / \tau) \right) \quad (1)$$

Assumption of Equation 1 : This (unweighted) optimization assumes an equal role of each between-class similarity s_b and within-class similarity s_w in obtaining optimal embedding space for distance-based OOD detection. In the subsequent section, we delve into the implication of this assumption.

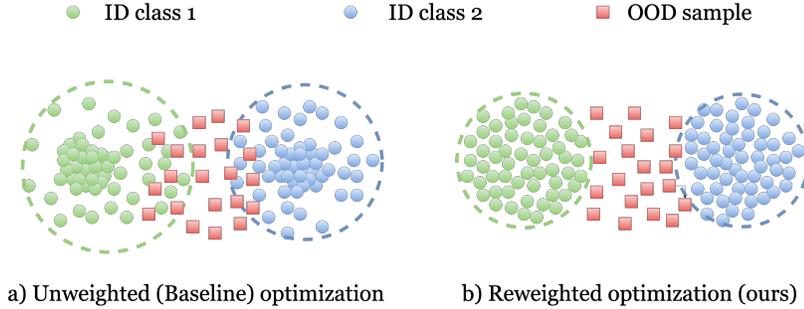


Figure 1. Comparison of (a) Unweighted optimization and (b) Reweighted optimization leading to different extents of overlapping with OOD samples in the embedding space.

3.2. Implication of unweighted optimization

Contrastive learning attempts to map all the instances of a category to its ideal centroid. However, as shown schematically in Figure 1 (a), the complexities inherent in real-world images make the idealistic goal of mapping all instances of a class very close to its ideal centroid in contrastive learning impractical. We define samples that are easy to pull near the centroid as *easy positives* and those samples that are difficult to pull near the centroid as *hard positives*. The compact clustering of *easy positives* around the centroid, as shown in Figure 1 (a), adds practically no value in OOD separation. However, as shown in Figure 1 (b), trading off the easy compact clustering with more weightage given on optimizing (pulling) hard positives around the centroid has a potentially beneficial effect on obtaining the Minimum Enclosing Sphere of smaller radius for all classes. Obtaining a smaller MES radius has a direct advantage linked with a smaller possibility of ID-OOD overlapping, as shown in Figure 1 (b).

Furthermore, given an anchor sample, samples that are easily distinguishable from the anchor can be referred to as *easy-negatives*. Conversely, samples that are similar and not easily distinguishable from the anchor sample can be referred to as *hard negatives*. In a multi-class setup, there is a greater presence of *easy-negatives* that don't provide useful learning signals. Optimizing these *easy negatives* can rather be a noisy process that potentially hinders the maximal inter-class dispersion. Furthermore, *hard negatives* are more informative for maximizing inter-class dispersion. From a separate perspective, *hard negatives* have a greater likelihood of getting overlapped with OOD instances. Hence, suppressing the effect of *easy negatives* and prioritizing *hard negatives* seem to be of utmost importance for maximizing the inter-class dispersion.

3.3. ReweightOOD

An overview of the proposed OOD detection framework ReweightOOD is shown in Figure 2. ReweightOOD con-

sists of backbone (encoder) network f_θ and projection head g_θ . The hyperspherical representation $\hat{h}_i = g_\theta(f_\theta(x_i))$ is obtained from ReweightOOD framework for each image x_i . Hyperspherical representations $\{\hat{h}_i\}_{i=1}^N$ form contrastive pairs that are weighted on the basis of their respective cosine similarities prior to contrastive optimization.

3.4. Reweighting mechanism for similarity scores

A requirement for the optimum embedding learning for OOD detection is: to give more importance to samples that are difficult to align (*hard negatives* and *hard positives*). Since similarity during optimization can convey the difficulty of the sample, the requirement for designing the reweighting mechanism is to make it the function of the similarity score. We use the linear transformation of the score and apply the sigmoid function to obtain the reweighting factor. Linear transformation basically consists of two operations:

Scaling The original range of cosine similarity is $[-1, 1]$. The scaling operation is utilized to rescale the similarity scores prior to the weighting function. Specifically, the scaling enables adjustment of the slope of the weighting function, thereby controlling the rate of increase in the reweighting factors based on the similarity scores. Scaling similarity scores s with scalar m resulting in the domain $[-m, m]$ from $[-1, 1]$, the weighting factor can be given as: $S \rightarrow s \cdot m$

Shifting Shifting allows shifting of the domain of rescaled similarity S by given scalar c to determine the desirable part of the weighting function depending on the nature of similarity score s . $\mathcal{T} \rightarrow S + c, \mathcal{T} \rightarrow s \cdot m + c$

Final Linear Transformation Hence, the final linear transformation can be expressed as $\mathcal{T} = s \cdot m + c$. As the two similarity scores might have different optimal hyperparameters, we allow defining different sets of linear transformation. So, we denote two such linear transformations as $\mathcal{T}_B = s_b \cdot m_b + c_b$ and $\mathcal{T}_W = s_w \cdot m_w + c_w$ for between-class and within-class similarities.

Reweighting function The scaled similarity scores are then

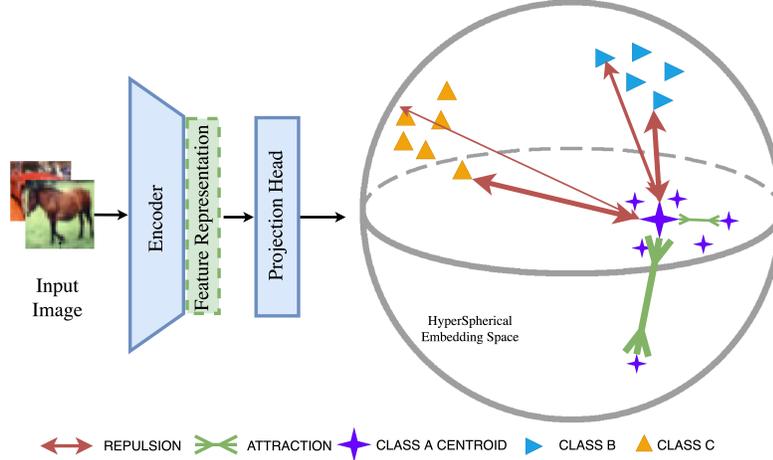


Figure 2. The figure shows an overview of the optimization process in ReweightOOD. ReweightOOD uses encoder (backbone) and the projection head to generate raw embeddings, which are subsequently converted into hyperspherical embeddings. The thickness of the depicted lines in the hypersphere visually represents the strength of the reweighting factor during pair optimization.

passed through the weighting function, which maps them to values in a predefined range to obtain reweighting factors. Since we already established in the previous section regarding the unequal role of various similarity scores in obtaining optimal embedding for OOD detection, we need to impose the increasing importance of between-class similarity s_b as it progresses towards positive value from negative value. Since the range of similarity scores due to linear transformation can be both negative as well as non-negative, we propose sigmoid function for obtaining its reweighting factor as shown in Figure 3. The sigmoid function can be expressed as : $\sigma(\mathcal{T}_B) = \frac{1}{1+e^{-\mathcal{T}_B}} = \frac{1}{1+e^{-s_b \cdot m_b - c_b}}$. Similarly, we have already established the decreasing importance of within-class s_w similarity scores as it progress towards positive value from negative value, we need the reweighting function for s_w to possess such characteristics. Hence, we propose *reverse-sigmoid* function for s_w reweighting as shown in Figure 4. It is basically the modified version of the sigmoid function which can be expressed as : $\sigma'(\mathcal{T}_W) = \frac{1}{1+e^{\mathcal{T}_W}} = \frac{1}{1+e^{s_w \cdot m_w + c_w}}$. So, accommodating the reweighting mechanism in Equation 1, the optimization then can be reformulated as:

$$\begin{aligned} \mathcal{L}_k &= \log \left(\sum_{i=1}^n \exp(\sigma(\mathcal{T}_B^i) \cdot s_b^i / \tau) \right) \\ &- \log \left(\sum_{j=1}^o \exp(\sigma'(\mathcal{T}_W^j) \cdot s_w^j / \tau) \right) \\ \mathcal{L}_k &= \log \left(\sum_{i=1}^n \exp \left(\frac{1}{1+e^{-s_b \cdot m_b - c_b}} \cdot \frac{s_b^i}{\tau} \right) \right) \\ &- \log \left(\sum_{j=1}^o \exp \left(\frac{1}{1+e^{s_w \cdot m_w + c_w}} \cdot \frac{s_w^j}{\tau} \right) \right) \end{aligned}$$

Reweighting flexibility and bounded range The transformation consisting of scaling and shifting allows flexible control over reweighting specific to the nature of similarity

(between-class and within-class). This allows a better bet in obtaining optimal embedding for OOD detection. Furthermore, the sigmoid function exhibits a bounded range that lies within the interval $[0, 1]$. The bounded range makes the weighting mechanism controlled and stable.

4. Experiments

Datasets The ID datasets CIFAR10 and CIFAR100 [21] are used for the training models from scratch while ImageNet100 is used for fine-tuning pretrained models. The OOD detection performance of CIFAR datasets is evaluated in the following datasets: MNIST [8], iSUN [52], LSUN-r [53], LSUN-c [53], SVHN [32], Textures [22], and Places365 [54]. For ImageNet100, the OOD datasets used are iNaturalist [45], SUN [51], Places365 [54], and Textures [22], NINCO [2], OpenImage-O [49], and Semantic Shift Benchmark (SSB) [46].

Metrics We mainly use two OOD metrics (AUROC and FPR@95) to quantify the OOD detection performance. AUROC stands for the Area Under Receiver-Operator Characteristics, and FPR@95 stands for False Positive Rate @ 95. A higher AUROC score quantifies a higher probability of correct OOD/ID classification, and a lower FPR suggests a lower probability of ID samples getting misclassified as OOD.

Training pipelines Similar to previous approaches KNN+ [42] and CIDER [31], we perform experiments with non-contrastive approaches for 100 epochs and contrastive approaches for 500 epochs. For posthoc methods, we train a standard model using vanilla cross-entropy loss. We train

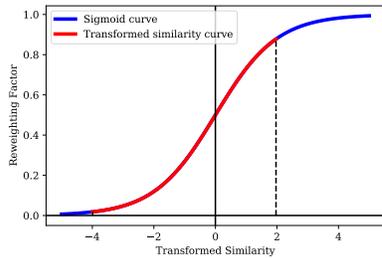


Figure 3. Reweighting mechanism for s_b

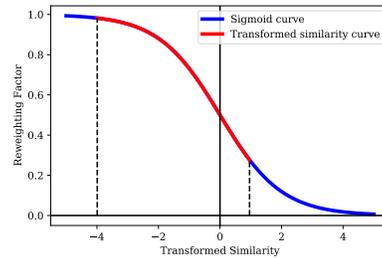


Figure 4. Reweighting mechanism for s_w

our model with a learning rate of 0.5 using a cosine annealing decay schedule with a batch size of 512 and 0.0001 weight decay. The temperature parameter τ is set to 0.1. The hyperparameters are optimized with respect to the validation set (Gaussian noise). For a fair comparison, we train all the methods in the same setting. We use ResNet-18 architecture for CIFAR-10/100 experiments. The linear transformation hyperparameters (m_b, c_b, m_w, c_w) for CIFAR100 and CIFAR10 experiments using ResNet18 network are set to $(5, -2, 2, 1)$ and $(5, -4, 2, 1)$ respectively. We also use WideResNet and DenseNet architecture to test architectural compatibility. The ablation regarding the linear transformation of the reweighting mechanism is provided in the appendix.

OOD detection scores Since we focus on learning a suitable embedding for OOD detection, we use two distance-based OOD scores in the embedding space: KNN and Mahalanobis distance. We use the KNN postprocessor by default and also investigate the performance with Mahalanobis distance (MDS). Like the previous approach CIDER, we use $K=100$ for CIFAR-10 experiments and $K=300$ for CIFAR-100 experiments for KNN postprocessor.

4.1. Quantification of embedding quality for OOD detection

Minimum Enclosing Sphere The concept of radius of the Minimum Enclosing Sphere (MES) serves to characterize the overall radius of a class while downplaying the significance of achieving a compact representation for easily distinguishable positive instances. This emphasis on class radius r_{cl} is motivated by the observation that embeddings associated with samples far from its ideal centroid tend to intersect with OOD samples, thereby compromising the performance of OOD detection. In essence, from the lens of ideal perspective, the ID samples residing at the periphery of a class should ideally be closer to the empirical centroid to avoid compromise in OOD detection performance. This notion can be effectively encapsulated through the concept of MES radius. Thus, from the perspective of ID-OOD sep-

arability, the MES radius emerges as a suitable metric for quantifying the effective compactness of class embeddings. It follows that the smaller the MES radius, the greater the effective compactness of class cl for OOD detection purposes. The empirical centroid, denoted as μ_{cl} , is a straightforward computation involving the summation of all embeddings corresponding to category cl over the entire set of samples, given by $\mu_{cl} = \frac{\sum_{\mathbf{h}_i \in \mathcal{H}_{cl}} \mathbf{h}_i}{N_{cl}}$ where \mathcal{H}_{cl} denotes normalized embedding representation of all samples in category cl and N_{cl} is the total number of samples in category cl .

$$r_{cl} = \max_{\mathbf{h}_i \in \mathcal{H}_{cl}} \|\mathbf{h}_i - \mu_{cl}\|_2 (\downarrow) \quad (2)$$

Centroid Dispersion To enhance OOD detection performance, it is essential to ensure that centroids are distributed sufficiently far apart, allowing for the effective delineation of OOD samples within the unoccupied space between these centroids. This notion of centroid dispersion can be precisely quantified by measuring the angular distance between the empirical centroids of two distinct categories. Mathematically, we represent the centroid dispersion between two categories, denoted as cl_a and cl_b , as follows:

$$d_{ab} = \frac{\mu_a \cdot \mu_b}{\|\mu_a\|_2 \cdot \|\mu_b\|_2}, \quad a \neq b (\uparrow) \quad (3)$$

Overall embedding quality can be assessed by computing the mean dispersion value across all category pairs and the mean MES radius across all categories.

Embedding observations: Table 1 and Table 2 present statistics on MES radius and centroid dispersion. ReweightOOD objective optimizes for a smaller overall radius across all CIFAR100 categories, as evidenced in Table 1 which reduces ID-OOD overlapping. Additionally, higher dispersion due to ReweightOOD indicates that ID classes are sufficiently spread apart, facilitating meaningful distance mapping for OOD samples. Consequently, reweighted optimization yields improved embedding quality. Furthermore, the qualitative UMAP visualization comparing the embedding space obtained with the CE objective and ReweightOOD objective is shown in Figure

Table 1. MES radius for first 10 classes and mean over 100 classes of CIFAR100 datasets in unweighted and weighted optimization.

Method	Apples	Aquarium Fish	Baby	Bear	Beaver	Bed	Bee	Beetle	Bicycle	Bottles	...	Mean
Baseline	1.09	1.11	1.07	0.93	0.97	1.07	1.03	1.07	1.10	1.07	...	1.05
SupCon	0.97	1.01	0.97	1.00	1.00	0.98	0.99	0.97	1.04	1.03	...	1.01
CIDER	0.96	0.94	0.89	0.91	0.86	0.88	0.87	0.88	1.04	0.99	...	0.92
(ReweightOOD) Ours	0.95	0.90	0.90	0.89	0.84	0.90	0.89	0.91	0.99	0.96	...	0.90

Table 2. Average centroid dispersion over 100 classes in CIFAR100 datasets.

Method	Mean dispersion (\uparrow)
Baseline	0.29
SupCon	0.42
CIDER	0.64
(ReweightOOD) Ours	0.63

5. It shows uniformly dispersed and highly separable embeddings without class-overlapping.

4.2. Empirical Analysis

Quantitative results Quantitative results including the extensive comparisons of current approaches along with our approach are presented in Table 3. For all experiments in Table 3, ResNet-18 is trained with CIFAR-100 as the ID dataset. The OOD performance is shown in two metrics (FPR and AUROC) only. We compare our results with current contrastive approaches as well as non-contrastive approaches. Posthoc methods are applied to the classification model trained with vanilla cross-entropy. All the experiments assume the unavailability of OOD / outliers during the training time. Posthoc methods include MSP [15], ODIN [25], Mahalanobis [23], DICE [40], Activation Shaping (ASH) [10], React [41], GradNorm [18], RankFeat [39] and Energy [27]. Two non-contrastive training-time regularization approaches are GODIN [17] and LogitNorm [50]. We use default hyperparameters provided in the original work whenever required. In contrastive approaches, we compare our method with ProxyAnchor [20], CSI [43], SSD+ [37], KNN+ [42], and CIDER [31]. Our approach leads to the best performance in both metrics. Furthermore, we present the OOD detection performance in CIFAR-10 experiments in the appendix which also shows our approach being highly performant in comparison to both contrastive as well as non-contrastive approaches. We present the sensitivity study of the linear transformation hyperparameters in terms of average FPR in Table 5.

Comparison with *hard negative mining* We compare our approach with vanilla *hard negative mining* to verify the superiority of the reweighting mechanism. Specifically,

we ignore the optimization for between-class cosine similarity scores s_b lying in the range $[-1, \alpha]$ to perform *hard negative mining*. The comparison of OOD detection performance of our approach with *hard negative mining* strategy for the CIFAR-100(ID) dataset in terms of FPR/AUROC using ResNet18 is given in Table 4. Though *hard negative mining* benefits OOD detection performance to some extent in comparison to the baseline, the results in Table 4 establish the superiority of the reweighting mechanism.

Compatibility with Mahalanobis distance (MDS) In addition to the non-parametric method KNN, we also analyze the empirical quality of the embedding produced by various contrastive approaches by the use of Mahalanobis distance. As can be observed from Table 6, the superiority of the embedding quality produced by our method is evident from FPR/AUROC scores.

Accuracy While improving OOD detection performance, neural network-based OOD detectors ideally should not compromise in accuracy. Training linear classifier on frozen features obtained from WRN-40-2, pretrained on ReweightOOD objective, we obtained a 75.54% accuracy on CIFAR100, similar to the 74.96% accuracy from the cross-entropy objective, demonstrating the effectiveness of ReweightOOD in both OOD detection and category classification.

Compatibility with various backbones In addition to ResNet-18, we experiment with diverse backbones, including WideResNet (WRN-40-2) and DenseNet architectures, to assess the adaptability of our method. As depicted in Table 8, in comparison to the baseline (unweighted formulation) and SupCon, our approach consistently leads to superior performance across various architectures in terms of all OOD metrics. Specifically, compared to the baseline, our approach leads to 10% and 20% performance improvement in WRN-40-2 and DenseNet architectures.

Evaluation on large-scale ImageNet-100 dataset In addition to conducting experiments on the CIFAR datasets, we assess the efficacy of our approach on the large-scale ImageNet-100 dataset within the context of fine-tuning pretrained models. We use the ImageNet-100 dataset, a sub-

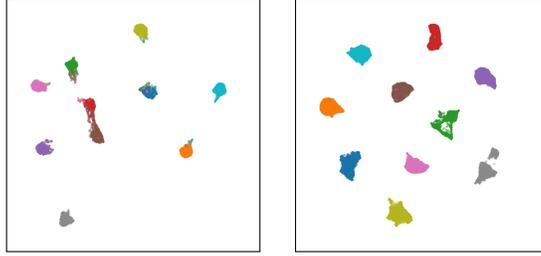


Figure 5. UMAP [28] visualization of embedding space (CIFAR10) obtained from (left) CE objective and (right) ReweightOOD objective. The ReweightOOD objective allows the embeddings to be uniformly distributed and highly separable without class overlapping.

Table 3. Mean OOD detection performance for CIFAR-100 (ID) with ResNet-18.

Method	MNIST		iSUN		LSUN		OOD Dataset LSUN-r		SVHN		Texture		Places365		Average	
	FPR↓	AUROC↑	FPR↓	AUROC↑	FPR↓	AUROC↑	FPR↓	AUROC↑	FPR↓	AUROC↑	FPR↓	AUROC↑	FPR↓	AUROC↑	FPR↓	AUROC↑
Without Contrastive Learning																
MSP	86.05	78.75	66.97	84.91	78.21	80.84	68.19	84.36	63.87	86.42	79.88	79.12	80.98	78.92	74.88	81.92
ODIN	73.64	84.61	40.07	92.54	72.70	85.75	42.38	92.23	74.80	84.45	72.22	81.63	81.05	79.06	65.27	85.75
Mahalanobis	81.91	77.22	95.23	59.99	95.45	56.16	95.14	61.16	92.47	64.96	75.55	73.95	92.84	62.89	89.90	65.19
Energy	88.57	79.05	63.27	88.05	78.04	84.63	63.95	87.56	59.09	89.84	78.94	80.68	83.58	79.02	73.63	84.12
DICE	81.96	79.46	67.60	87.04	67.11	86.97	70.25	86.00	60.45	89.78	76.01	80.17	83.76	78.76	72.45	84.03
React	88.29	78.55	63.22	87.85	77.73	84.89	63.89	87.23	58.06	90.16	78.35	81.75	83.47	79.17	73.29	84.23
ASH	78.75	81.14	70.04	81.92	77.26	83.31	70.72	80.54	57.94	88.22	76.10	81.14	82.55	77.53	73.34	81.97
GradNorm	86.54	63.98	68.82	78.28	71.14	84.48	70.75	75.27	60.92	83.80	77.96	69.68	84.79	69.29	74.42	74.97
RankFeat	95.62	61.39	87.99	74.29	95.73	67.85	88.66	73.81	79.82	80.68	91.63	66.11	91.17	66.41	90.09	70.08
GODIN	48.88	92.09	22.14	96.00	63.91	85.55	19.05	96.72	70.66	86.74	56.49	89.37	78.95	78.12	51.44	89.23
LogitNorm	51.65	90.28	92.84	69.00	15.52	97.23	92.68	70.77	73.71	84.15	86.85	71.27	77.98	80.77	70.18	80.50
With Contrastive Learning																
ProxyAnchor	65.96	78.93	88.90	77.71	57.29	88.28	86.30	77.60	31.16	93.47	57.54	88.30	77.25	79.69	66.34	83.43
CSI	75.27	82.20	68.37	81.91	49.43	89.11	66.19	83.17	65.83	81.21	77.53	75.13	79.11	79.80	67.74	81.22
SSD+	82.52	76.80	79.71	83.85	49.86	89.91	78.00	85.19	23.03	95.70	59.72	88.22	77.80	80.86	64.38	85.79
KNN+	76.21	83.06	67.44	85.12	55.09	86.30	67.59	85.59	44.03	91.85	47.91	90.08	78.63	78.19	62.42	85.74
CIDER	63.24	85.64	73.78	77.96	26.51	93.37	75.98	78.03	17.58	96.33	34.15	92.34	78.56	73.04	52.83	85.24
Baseline	78.91	69.01	85.09	84.28	41.09	91.93	79.90	85.07	25.25	94.63	46.38	90.33	74.44	80.50	61.58	85.11
(ReweightOOD) Ours	19.24	96.86	57.56	87.54	19.59	96.86	56.31	88.23	8.39	98.31	28.72	94.11	78.70	76.01	38.36	90.91

Table 4. Comparison of our approach with *hard negative* mining strategy for CIFAR-100(ID) dataset in terms of FPR/AUROC using ResNet18.

Ignored range for s_b	FPR (↓)	AUROC (↑)
$[-1, -0.3]$	61.18	86.33
$[-1, -0.1]$	54.20	85.84
$[-1, 0.1]$	58.03	85.76
$[-1, 0.3]$	54.44	86.51
Baseline	61.58	85.11
(ReweightOOD) ours	38.36	90.91

m_b	FPR ↓	c_b	FPR ↓	m_w	FPR ↓	c_w	FPR ↓
4	51.01	1	44.96	1	69.10	1	38.36
5	38.36	2	38.36	2	38.36	2	67.63
6	39.14	3	52.66	3	43.44	3	70.84

Table 5. Sensitivity of linear transformation hyperparameters with CIFAR-100 as ID in terms of average FPR.

set of ImageNet, as the ID dataset for finetuning the pre-trained ResNet-50 model. ImageNet-100 consists of images

from 100 randomly sampled categories from the ImageNet dataset. The projection head is a non-linear MLP with a projection dimension of 128. The first three layers of ResNet50 are frozen and only the last layer along with the projection head is fine-tuned for 10 epochs with a learning rate of 0.01 and weight decay of 0.0001 using cosine annealing. The linear transformation hyperparameters (m_b, c_b, m_w, c_w) are set to (5, -4, 2, 1). The performance is evaluated with KNN postprocessing (K=300). We compare the OOD detection performance of our method with baseline and SupCon loss in terms of FPR and AUROC metrics as shown in Table 7. It depicts the superior performance of our approach in comparison to compared losses. It provides further empirical justification for producing superior embeddings for OOD detection.

5. Related Works

OOD detection Posthoc approaches of OOD detection derive scores from pretrained models without any retraining. Some of these approaches deal directly with output space [10, 15, 27, 30, 40] while recently more approaches have attempted to exploit the information from embedding

Table 6. Compatibility with MDS using CIFAR-100 (ID) dataset in terms of FPR using ResNet18.

Method	MNIST	iSUN	LSUN	LSUN-r	SVHN	Texture	Places365	Average FPR ↓
ProxyAnchor	75.48	88.94	52.78	87.62	7.69	58.21	74.85	63.65
SSD+	82.52	79.71	49.86	78.00	23.03	59.72	77.80	64.38
CIDER	76.82	74.10	21.40	75.40	9.78	45.27	74.37	53.88
Baseline	80.68	88.95	21.31	85.63	5.83	40.51	66.83	55.68
(ReweightOOD) Ours	51.58	62.91	17.00	62.00	5.89	44.29	74.83	45.50

Table 7. OOD detection performance in large-scale experiments (ImageNet-100) in terms of FPR by fine-tuning pretrained ResNet50.

Method	iNaturalist	SUN	Textures	Places	SSB Hard	Ninco	Openimage	Average FPR ↓
Baseline	3.07	2.39	4.57	5.47	35.39	29.15	7.05	12.44
SupCon	2.43	1.98	2.59	5.43	34.25	25.58	5.28	11.08
CIDER	5.07	1.85	1.77	5.70	37.35	27.93	5.73	12.20
(ReweightOOD) Ours	2.18	1.97	2.73	5.29	32.00	24.63	5.06	10.55

Table 8. Architecture compatibility of various methods with CIFAR100 (ID) datasets.

Method	Architectures			
	WRN-40-2		DenseNet	
	FPR↓	AUROC↑	FPR↓	AUROC↑
Baseline	53.55	87.07	39.03	91.11
SupCon	49.95	87.75	44.28	90.10
(ReweightOOD) Ours	47.94	88.45	31.36	92.21

space [11, 24, 29, 31, 35, 37, 42, 43, 55] for OOD detection. OOD detection has also been explored by dealing with both feature and output spaces [49]. Furthermore, some works [39, 41, 56] deal with feature activations. The gradient information [18] has also been used for OOD detection. LogitNorm [50] and T2FNorm [33] make use of normalization in logit and feature space respectively to mitigate the overconfidence issue in neural networks. Few works [9, 16, 17] propose various ways of regularizing neural networks during training to enhance the OOD detection performance. Furthermore, temperature scaling [13] has been widely used as a simple postprocessing technique to improve neural network calibration.

Deep Metric Learning A fundamental focus of deep metric learning is to learn highly discriminative features. Research areas such as face recognition and face verification have seen the introduction of many useful loss functions on hyperspherical embeddings [7, 26, 47, 48] to satiate this objective. Techapanurak, et. al. [44] deals with cosine loss to achieve hyperparameter-free OOD detection.

Contrastive Learning Chopra et al. [6], Schroff et al. [36], and Sohn et al. [38] were the earliest works that explored the concept of contrastive loss. In recent years, contrastive learning has garnered significant attention in the domain of vision representational learning, en-

compassing both unsupervised and supervised paradigms [3, 5, 14, 19, 34]. While the majority of these approaches explicitly formulate positive and negative pairs, some recent works [1, 4, 12] exclusively concentrate on positive pairs only. Few works [19, 31, 37, 43] have explored the use of off-the-shelf contrastive learning in the context of OOD detection. However, it should be noted that contrastive learning in OOD detection has remained relatively understudied. Our work deals with the contrastive approach in OOD detection.

6. Conclusions

In summary, this study introduces **ReweightOOD**, a reweighting mechanism, aimed at enhancing embedding quality to improve OOD detection performance. Our approach focuses on optimizing the cosine similarity of contrasting pairs by considering their current proximity, assigning higher priority to less-optimized pairs and lower priority to well-optimized ones. Experimental results across various classification datasets demonstrate non-trivial performance enhancement in OOD detection resulting from our approach. Furthermore, we reveal that our reweighting method reduces radius of the Minimum Enclosing Sphere for each class and increases inter-class dispersion, thereby enhancing the separation between ID and OOD samples in the embedding space.

7. Acknowledgement

This work was supported by the Wellcome/EPSCRC Centre for Interventional and Surgical Sciences (WEISS) [203145Z/16/Z]; Engineering and Physical Sciences Research Council (EPSRC) [EP/P027938/1, EP/R004080/1, EP/P012841/1]; The Royal Academy of Engineering Chair in Emerging Technologies scheme; and the EndoMapper project by Horizon 2020 FET (GA 863146).

References

- [1] Adrien Bardes, Jean Ponce, and Yann LeCun. VI-CReg: Variance-invariance-covariance regularization for self-supervised learning. In *International Conference on Learning Representations*, 2022. 8
- [2] Julian Bitterwolf, Maximilian Müller, and Matthias Hein. In or out? fixing imagenet out-of-distribution detection evaluation. *arXiv preprint arXiv:2306.00826*, 2023. 4
- [3] Ting Chen, Simon Kornblith, Mohammad Norouzi, and Geoffrey Hinton. A simple framework for contrastive learning of visual representations. *arXiv preprint arXiv:2002.05709*, 2020. 8
- [4] Xinlei Chen and Kaiming He. Exploring simple siamese representation learning. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition*, pages 15750–15758, 2021. 8
- [5] Xinlei Chen, Haoqi Fan, Ross Girshick, and Kaiming He. Improved baselines with momentum contrastive learning. *arXiv preprint arXiv:2003.04297*, 2020. 8
- [6] Sumit Chopra, Raia Hadsell, and Yann LeCun. Learning a similarity metric discriminatively, with application to face verification. In *2005 IEEE Computer Society Conference on Computer Vision and Pattern Recognition (CVPR'05)*, pages 539–546. IEEE, 2005. 8
- [7] Jiankang Deng, Jia Guo, Niannan Xue, and Stefanos Zafeiriou. Arcface: Additive angular margin loss for deep face recognition. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition*, pages 4690–4699, 2019. 8
- [8] Li Deng. The mnist database of handwritten digit images for machine learning research. *IEEE Signal Processing Magazine*, 2012. 4
- [9] Terrance DeVries and Graham W Taylor. Learning confidence for out-of-distribution detection in neural networks. *arXiv preprint arXiv:1802.04865*, 2018. 8
- [10] Andrija Djuric, Nebojsa Bozanic, Arjun Ashok, and Rosanne Liu. Extremely simple activation shaping for out-of-distribution detection. In *The Eleventh International Conference on Learning Representations*, 2023. 6, 7
- [11] Xuefeng Du, Gabriel Gozum, Yifei Ming, and Yixuan Li. Siren: Shaping representations for detecting out-of-distribution objects. In *Advances in Neural Information Processing Systems*, 2022. 8
- [12] Jean-Bastien Grill, Florian Strub, Florent Althé, Corentin Tallec, Pierre Richemond, Elena Buchatskaya, Carl Doersch, Bernardo Avila Pires, Zhaohan Guo, Mohammad Gheshlaghi Azar, et al. Bootstrap your own latent—a new approach to self-supervised learning. *Advances in neural information processing systems*, 33:21271–21284, 2020. 8
- [13] Chuan Guo, Geoff Pleiss, Yu Sun, and Kilian Q Weinberger. On calibration of modern neural networks. In *International conference on Machine Learning*, pages 1321–1330. PMLR, 2017. 8
- [14] Kaiming He, Haoqi Fan, Yuxin Wu, Saining Xie, and Ross Girshick. Momentum contrast for unsupervised visual representation learning. In *2020 IEEE/CVF Conference on Computer Vision and Pattern Recognition (CVPR)*, pages 9726–9735, 2020. 8
- [15] Dan Hendrycks and Kevin Gimpel. A baseline for detecting misclassified and out-of-distribution examples in neural networks. In *5th International Conference on Learning Representations, ICLR 2017*, 2017. 1, 6, 7
- [16] Dan Hendrycks, Mantas Mazeika, Saurav Kadavath, and Dawn Song. Using self-supervised learning can improve model robustness and uncertainty. In *NeurIPS*, 2019. 8
- [17] Yen-Chang Hsu, Yilin Shen, Hongxia Jin, and Zsolt Kira. Generalized odin: Detecting out-of-distribution image without learning from out-of-distribution data. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 10951–10960, 2020. 6, 8, 1
- [18] Rui Huang, Andrew Geng, and Yixuan Li. On the importance of gradients for detecting distributional shifts in the wild. *Advances in Neural Information Processing Systems*, 34:677–689, 2021. 6, 8
- [19] Prannay Khosla, Piotr Teterwak, Chen Wang, Aaron Sarna, Yonglong Tian, Phillip Isola, Aaron Maschiot, Ce Liu, and Dilip Krishnan. Supervised contrastive learning. In *Advances in Neural Information Processing Systems*, pages 18661–18673, 2020. 2, 8
- [20] Sungyeon Kim, Dongwon Kim, Minsu Cho, and Suha Kwak. Proxy anchor loss for deep metric learning. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition*, pages 3238–3247, 2020. 6, 1
- [21] Alex Krizhevsky, Vinod Nair, and Geoffrey Hinton. Cifar-10 and cifar-100 datasets. URL: <https://www.cs.toronto.edu/kriz/cifar.html>, 6(1):1, 2009. 4
- [22] Gustaf Kylberg. Kylberg texture dataset v. 1.0. Centre for Image Analysis, Swedish University of Agricultural Sciences and . . . , 2011. 4
- [23] Kimin Lee, Honglak Lee, Kibok Lee, and Jinwoo Shin. Training confidence-calibrated classifiers for detecting out-of-distribution samples. *arXiv preprint arXiv:1711.09325*, 2017. 6, 1
- [24] Kimin Lee, Kibok Lee, Honglak Lee, and Jinwoo Shin. A simple unified framework for detecting out-of-distribution samples and adversarial attacks. In *Advances in Neural Information Processing Systems*. Curran Associates, Inc., 2018. 1, 8
- [25] Shiyu Liang, Yixuan Li, and Rayadurgam Srikant. Enhancing the reliability of out-of-distribution image detection in neural networks. *arXiv preprint arXiv:1706.02690*, 2017. 6, 1
- [26] Weiyang Liu, Yandong Wen, Zhiding Yu, Ming Li, Bhiksha Raj, and Le Song. Sphereface: Deep hypersphere embedding for face recognition. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 212–220, 2017. 8
- [27] Weitang Liu, Xiaoyun Wang, John Owens, and Yixuan Li. Energy-based out-of-distribution detection. *Advances in neural information processing systems*, 33:21464–21475, 2020. 1, 6, 7
- [28] Leland McInnes, John Healy, Nathaniel Saul, and Lukas Grossberger. Umap: Uniform manifold approximation and

- projection. *The Journal of Open Source Software*, 3(29):861, 2018. 7
- [29] Yifei Ming, Ziyang Cai, Jiuxiang Gu, Yiyu Sun, Wei Li, and Yixuan Li. Delving into out-of-distribution detection with vision-language representations. In *Advances in Neural Information Processing Systems*, 2022. 8
- [30] Yifei Ming, Ying Fan, and Yixuan Li. Poem: Out-of-distribution detection with posterior sampling. In *International Conference on Machine Learning*, pages 15650–15665. PMLR, 2022. 7
- [31] Yifei Ming, Yiyu Sun, Ousmane Dia, and Yixuan Li. How to exploit hyperspherical embeddings for out-of-distribution detection? In *The Eleventh International Conference on Learning Representations*, 2023. 2, 4, 6, 8, 1
- [32] Yuval Netzer, Tao Wang, Adam Coates, Alessandro Bisacco, Bo Wu, and Andrew Y. Ng. Reading digits in natural images with unsupervised feature learning. 2011. 4
- [33] Sudarshan Regmi, Bibek Panthi, Sakar Dotel, Prashna K Gyawali, Danail Stoyanov, and Binod Bhattarai. T2fnorm: Extremely simple scaled train-time feature normalization for ood detection. *arXiv preprint arXiv:2305.17797*, 2023. 1, 8
- [34] Joshua David Robinson, Ching-Yao Chuang, Suvrit Sra, and Stefanie Jegelka. Contrastive learning with hard negative samples. In *International Conference on Learning Representations*, 2021. 8
- [35] Chandramouli Shama Sastry and Sageev Oore. Detecting out-of-distribution examples with Gram matrices. In *Proceedings of the 37th International Conference on Machine Learning*. PMLR, 2020. 8
- [36] Florian Schroff, Dmitry Kalenichenko, and James Philbin. Facenet: A unified embedding for face recognition and clustering. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 815–823, 2015. 8
- [37] Vikash Sehwal, Mung Chiang, and Prateek Mittal. Ssd: A unified framework for self-supervised outlier detection. In *International Conference on Learning Representations*, 2021. 2, 6, 8, 1
- [38] Kihyuk Sohn. Improved deep metric learning with multi-class n-pair loss objective. *Advances in neural information processing systems*, 29, 2016. 8
- [39] Yue Song, Nicu Sebe, and Wei Wang. Rankfeat: Rank-1 feature removal for out-of-distribution detection. *Advances in Neural Information Processing Systems*, 35:17885–17898, 2022. 6, 8
- [40] Yiyu Sun and Yixuan Li. Dice: Leveraging sparsification for out-of-distribution detection. In *European Conference on Computer Vision*, 2022. 6, 7, 1
- [41] Yiyu Sun, Chuan Guo, and Yixuan Li. React: Out-of-distribution detection with rectified activations. *Advances in Neural Information Processing Systems*, 34:144–157, 2021. 6, 8
- [42] Yiyu Sun, Yifei Ming, Xiaojin Zhu, and Yixuan Li. Out-of-distribution detection with deep nearest neighbors. *International Conference on Machine Learning*, 2022. 1, 4, 6, 8
- [43] Jihoon Tack, Sangwoo Mo, Jongheon Jeong, and Jinwoo Shin. Csi: Novelty detection via contrastive learning on distributionally shifted instances. In *Advances in Neural Information Processing Systems*, 2020. 6, 8, 1
- [44] Engkarat Techapanurak, Masanori Suganuma, and Takayuki Okatani. Hyperparameter-free out-of-distribution detection using cosine similarity. In *Proceedings of the Asian conference on computer vision*, 2020. 8
- [45] Grant Van Horn, Oisín Mac Aodha, Yang Song, Yin Cui, Chen Sun, Alex Shepard, Hartwig Adam, Pietro Perona, and Serge Belongie. The inaturalist species classification and detection dataset. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 8769–8778, 2018. 4
- [46] Sagar Vaze, Kai Han, Andrea Vedaldi, and Andrew Zisserman. Open-set recognition: A good closed-set classifier is all you need. In *International Conference on Learning Representations*, 2021. 4
- [47] Feng Wang, Xiang Xiang, Jian Cheng, and Alan Loddon Yuille. Normface: L2 hypersphere embedding for face verification. In *Proceedings of the 25th ACM international conference on Multimedia*, pages 1041–1049, 2017. 8
- [48] Hao Wang, Yitong Wang, Zheng Zhou, Xing Ji, Dihong Gong, Jingchao Zhou, Zhifeng Li, and Wei Liu. Cosface: Large margin cosine loss for deep face recognition. In *Proceedings of the IEEE conference on computer vision and pattern recognition*, pages 5265–5274, 2018. 8
- [49] Haoqi Wang, Zhizhong Li, Litong Feng, and Wayne Zhang. Vim: Out-of-distribution with virtual-logit matching. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition*, pages 4921–4930, 2022. 1, 4, 8
- [50] Hongxin Wei, Renchunzi Xie, Hao Cheng, Lei Feng, Bo An, and Yixuan Li. Mitigating neural network overconfidence with logit normalization. In *International Conference on Machine Learning*, pages 23631–23644. PMLR, 2022. 1, 6, 8
- [51] Jianxiong Xiao, James Hays, Krista A Ehinger, Aude Oliva, and Antonio Torralba. Sun database: Large-scale scene recognition from abbey to zoo. In *2010 IEEE computer society conference on computer vision and pattern recognition (CVPR)*, pages 3485–3492. IEEE, 2010. 4
- [52] Pingmei Xu, Krista A Ehinger, Yinda Zhang, Adam Finkelstein, Sanjeev R Kulkarni, and Jianxiong Xiao. Turkergaze: Crowdsourcing saliency with webcam based eye tracking. *arXiv preprint arXiv:1504.06755*, 2015. 4
- [53] Fisher Yu, Ari Seff, Yinda Zhang, Shuran Song, Thomas Funkhouser, and Jianxiong Xiao. Lsun: Construction of a large-scale image dataset using deep learning with humans in the loop. *arXiv preprint arXiv:1506.03365*, 2015. 4
- [54] Bolei Zhou, Agata Lapedriza, Aditya Khosla, Aude Oliva, and Antonio Torralba. Places: A 10 million image database for scene recognition. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 2017. 4
- [55] Zhi Zhou, Lan-Zhe Guo, Zhanzhan Cheng, Yu-Feng Li, and Shiliang Pu. Step: Out-of-distribution detection in the presence of limited in-distribution labeled data. In *Advances in Neural Information Processing Systems*, 2021. 8
- [56] Yao Zhu, YueFeng Chen, Chuanlong Xie, Xiaodan Li, Rong Zhang, Hui Xue, Xiang Tian, Yaowu Chen, et al. Boosting

out-of-distribution detection with typical features. *Advances in Neural Information Processing Systems*, 35:20758–20769, 2022. 8