The Effect of Covariate Shift and Network Training on Out-of-Distribution Detection

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The field of Out-of-Distribution (OOD) detection aims to separate OOD data from in-distribution (ID) data in Abstract: order to make safe predictions. With the increasing application of Convolutional Neural Networks (CNNs) in sensitive environments such as autonomous driving and security, this field is bound to become indispensable in the future. Although the OOD detection field has made some progress in recent years, a fundamental understanding of the underlying phenomena enabling the separation of datasets remains lacking. We find that the OOD detection relies heavily on the covariate shift of the data and not so much on the semantic shift, i.e. a CNN does not carry explicit semantic information and relies solely on differences in features. Although these features can be affected by the underlying semantics, this relation does not seem strong enough to rely on. Conversely, we found that since the CNN training setup determines what features are learned, that it is an important factor for the OOD performance. We found that variations in the model training can lead to an increase or decrease in the OOD detection performance. Through this insight, we obtain an increase in OOD detection performance on the common OOD detection benchmarks by changing the training procedure and using the simple Maximum Softmax Probability (MSP) model introduced by (Hendrycks and Gimpel, 2016). We hope to inspire others to look more closely into the fundamental principles underlying the separation of two datasets. The code for reproducing our results can be found at https://github.com/SimonMariani/OODdetection.

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1 INTRODUCTION

Although Convolutional Neural Networks (CNNs) achieve good performance on many different tasks, their deployment in sensitive environments does not come without problems. In order to use CNNs safely in tasks for self driving cars (Vojir et al., 2021; Boone et al., 2022), medical image analysis (Mehrtash et al., 2020; Raghu et al., 2019) or face recognition (Chang et al., 2020; Betta et al., 2011), some degree of certainty must be given to the predictions of such a network, as a misclassification can be problematic. This is often referred to as misclassification detection and is generally done on samples that can be seen as drawn from the same distribution as the training data, i.e. the In-Distribution (ID). Besides such samples that are drawn from the ID, it can also be the case that a sample was drawn from a different distribution. Such a sample can then be referred to as an Outof-Distribution (OOD) sample and is likely to affect the output of the CNN. Therefore, the field of OOD detection is concerned with separating OOD samples from ID samples, as to increase the reliability of CNNs. Although access to OOD data is generally not available, some *ID-OOD dataset pairs* have emerged and are being extensively used as the general benchmark (Hendrycks and Gimpel, 2016; Lee et al., 2018; Lee et al., 2017). Succeeding work has been concerned with the scalability of OOD detection methods and propose larger benchmark datasets (Hendrycks et al., 2019a; Huang and Li, 2021; Roady et al., 2019). These benchmarks are currently the primary way of comparing OOD detection methods and are vital for the development of new OOD detection methods.

For this reason, we will also use the existing benchmarks to measure performance and show that detecting OOD samples relies heavily on the covariate shift of the data and largely ignores actual class differences. We do so by looking at the OOD samples that share and do not share classes with the ID data, as some of the commonly used benchmark dataset pairs have some class overlap. For this purpose, we use

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the ID labels for OOD samples provided by (Yang et al., 2021b), who proposed the *Semantically Coherent OOD detection* framework where the OOD samples that share a class with the ID data are treated as if they were from the ID data. We merely use their class labels to link OOD detection to the *covariate* and *semantic* shift encompassed by the *Generalized OOD Detection* framework (Yang et al., 2021a), which makes a clear distinction between a shift in the feature space of the data (covariate), versus a shift in the class space of the data (semantic).

Consequently, as the CNN training forms the feature space, it can thus improve or worsen the OOD detection performance. We argue that the effect of the model training on the OOD detection performance is important to highlight. For this reason, we investigate several training approaches and their relation to the OOD detection performance on several ID-OOD dataset pairs. We show that the CNN training has a non-negligible impact on the OOD performance and should be taken into account as it can drastically diminish performance. We also show that the model training can be used to improve not only the classification accuracy, but also the OOD detection performance without the use of additional OOD data.

In summary, we list our contributions as follows:

- We show that OOD detection methods rely on the covariate shift of the data and mainly neglect the semantic shift. We do so by looking at the relation between the OOD performance for separating OOD samples that do and do not share a class with the ID data. Additionally, we explain the theoretical implications of this result.
- We show that by focusing on the covariate shift during training, the OOD detection performance can be improved even when using the simple MSP model (Hendrycks and Gimpel, 2016). We also show that model training can harm the OOD detection performance and explain why.

2 RELATED WORK

Output Based Methods. The most fundamental group of OOD detection approaches uses the final model output or an enhanced version of the model output as OOD score. One of the first and most widely used baseline methods uses the unmodified *Maximum Softmax Probability* (MSP) as OOD score (Hendrycks and Gimpel, 2016). Following this work, the *True Class Probability* (Corbière et al., 2019) and *Max Logit* (Hendrycks et al., 2019b) provide alternative output values to use as OOD scores.

Another well known approach is called *ODIN* (Liang et al., 2017) and enhances the model output by applying image perturbations to the input image and applying temperature scaling to the output. The output layer can also be modified by adding a *rectified activation* (ReAct) after the penultimate layer of the model (Sun et al., 2021) or the entire model can be cast as an *energy based model* (EBM) by only changing the output layer (Liu et al., 2020).

Feature Space Methods. An different group of OOD detection methods uses the induced feature space of a CNN to formulate OOD scores. The features in the feature space can be modelled with a Multivariate Gaussian distribution, for which then the Mahalanobis distance can be used to obtain the distance of a sample to the different class distributions. Because the feature distribution does not necessarily follow a Gaussian distribution, (Zisselman and Tamar, 2020) propose to use a residual flow model to map the feature space to a Gaussian distribution rather than using the Feature space directly. The feature representations can also be enhanced by calculating higher order gram matrix of the feature representations and calculating the deviation from the min-max range (Sastry and Oore, 2020).

Similarly, the feature space can be enhanced by changing the model in order to obtain more distinct and better separable representations. One such way uses *contrastive training* (Winkens et al., 2020) by adding an additional head to the model and feeding it different augmentations of the original images in order to map different representations of the same image closer together. Alternatively, the representations of pretrained transformer models already provide a more discriminative representations and can also be used for OOD detection (Fort et al., 2021).

3 METHODOLOGY

This section explains the two OOD detection methods that we use in our study, as well as the training variations that we use to compare the effect of the model training on the OOD detection performance.

Maximum Softmax Probability. One of the first and simplest OOD detection methods for CNN was proposed by (Hendrycks and Gimpel, 2016) and uses the maximum softmax probability as OOD score. The idea is that if the probability of the predicted class is high, that the model is certain and the sample is likely to be of the same distribution as the training data, i.e.

	Training variation	Explanation		
Data Augmentations	MixUp	MixUp (Zhang et al., 2018) uses linear interpolations of images to learn linear		
		interpolations of labels.		
	Blur	Adding Gaussian blur to images makes the images smoother, thus more uniform.		
	Equalize	The equalize operation equalizes the intensity histogram of an image, creating more uniformly distributed data.		
	Colorjitter	This data augmentation randomly changes the brightness, saturation and hue.		
	Erase	The random erasing data transform (Zhong et al., 2020) randomly chooses a rect-		
		angular region and randomizes its pixel values.		
	Perspective	The perspective data transform randomly changes the perspective of the image,		
		making it seem like the image is viewed from a different angle.		
	Augment policy	Instead of manually searching for data augmentation policies, (Cubuk et al., 2019)		
		propose to automatically search for the best data augmentation policy.		
otimizer	Momentum	We change the default Stochastic Gradient Descent momentum with Nesterov mo-		
		mentum (Nesterov, 1983).		
	Scheduler	We vary the cosine annealing learning rate scheduler with the multi step learning		
Ō		rate scheduler, which multiplies the learning rate by a factor γ at pre-set intervals.		
Loss	Weight decay	As a training variation, we remove weight decay from our default setup, thereby		
		implicitly allowing large weights in the model.		
	Gradient penalty	Gradient penalties (Drucker and Cun, 1992) ensure smaller gradients and therefore		
		make the training more sensitive.		
Other	Pretrained model	The authors of the Mahalanobis distance paper (Lee et al., 2018) have open		
		sourced a RESNET34 model. Since this model has since been re-used in other		
		works (Sastry and Oore, 2020; Zisselman and Tamar, 2020), we also include it as		
		a training variation for the sake of completeness.		

Table 1: All the training variations including a short explanation. The training variations can be categorized in data augmentations, optimizer, loss and other variations.

it is ID. Vice versa, when the output probability of the predicted class is low, the sample is likely to be of some other distribution i.e it is OOD. This approach is often used as a baseline method as it is easy to implement and obtains reasonable OOD detection performance.

Mahalanobis Distance. The second method that we use to investigate the OOD benchmarks, uses the intermediate features of a CNN to obtain a Gaussian distribution and uses the Mahalanobis distance as the OOD score (Lee et al., 2018). The class mean μ_c and tied covariance σ can be calculated from the training data by representing every image as a vector in this feature space. The distance from any sample to a class distribution can then be determined with the Mahalanobis distance, which is defined as the probability density function of the unnormalized multivariate Gaussian distribution.

The authors of the original Mahalanobis distance based approach (Lee et al., 2018) also introduce a perturbation hyperparameter which is said to make the ID and OOD data more separable. Because setting the hyperparameters for the perturbation strength requires the use of validation OOD data, we have chosen to omit this parameter altogether. Furthermore, in order to obtain the best average over the layers, the authors also train a regression model using validation samples in order to find the best layer weights. As this also requires OOD validation data, we have chosen to omit this as well and use a regular average over the layers of the Mahalanobis distances.

Training Variations. For our standard model training we use the training parameters provided by (Kuangliu, 2021) and change one parameter at a time in order to isolate the effect of the parameter choice. All changed parameters are shown in Table 1.

4 EXPERIMENTS

4.1 Experimental Setup

This section describes the employed ID and OOD datasets, as well as the CNNs and OOD detection metrics.

Datasets. As training/ID dataset we use CIFAR10, CIFAR100 and SVHN. As OOD datasets we use CIFAR10, SVHN, Tiny ImageNet, LSUN, Places,



(c) Pytorch nearest resize.

(d) Open sourced resized data by ODIN (Liang et al., 2017).

Figure 1: Resized samples of the Tiny ImageNet dataset for different resizing methods. Different resizes produce different images as noise can be introduced which can affect the OOD detection performance.



Figure 2: The AUROC scores for separating tiny ImageNet (2a) and LSUN (2b) with different resizes for both the baseline model as well as the Mahalanobis distance based model. Different resizes lead to large differences in scores, indicating the importance of the resize method and therefore the feature space.

CIFAR100 and Textures. This follows the standard OOD data setup followed by many such as (Hendrycks and Gimpel, 2016; Lee et al., 2018; Lee et al., 2017), but also the higher dimensional OOD datasets used by (Huang and Li, 2021; Hendrycks et al., 2019a; Roady et al., 2019). For a correct OOD detection setting, we always use the exact same test transform for the OOD data as for the ID data. The resizing operation used for every OOD dataset is the PyTorch default bilinear resizing operation.

Models. We first train the RESNET34 model (He et al., 2015) on the CIFAR10, CIFAR100 and SVHN datasets from scratch, by using the training parameters provided by (Kuangliu, 2021) and obtain the same performance. We then vary the training as described in Section 3 and use the resulting model for the MSP and Mahalanobis methods. The models are then indicated as {model}-{variety} s.t. {model} either indicates the MSP or Mahalanobis model, and {variety} one of the training variations.

Metrics. The OOD detection on an ID-OOD dataset pair can be viewed as a binary classification problem, where samples from the ID are labeled as positive samples and samples from the OOD data as negative samples. We then look at the Area Under the Receiver Operator Curve (AUROC), the Detection Accuracy (Detection Acc.) and the True Negative Rate at 95% True Positive Rate (TNR at TPR 95). These are the generally included metrics for OOD detection. Finally, in order to look at the relation between performances, the Pearson correlation coefficient is used.

4.2 Impact of Covariate Shift

This section describes two experiments that show how the data is generally separated with an emphasis on the covariate shift of the ID-OOD dataset pairs.

Resizing and Noise. For the preparation of ID-OOD dataset pairs images might need to be resized. For example, the images from CIFAR10 have a size of 32×32 while the images from Tiny ImageNet have a size of 64×64 pixels. This means that in order to use Tiny ImageNet as the OOD dataset, the images will have to be resized to match the CIFAR10 data. Although not a lot of attention has been brought to this matter, from Figure 1 we can see that different resizes produce different images. Especially in Figure 1c, the resizing introduces a lot of noise into the images. These images are very similar to the samples shown in Figure 1d which come from the already resized dataset that was open sourced by the authors of the paper that introduced ODIN (Liang et al., 2017). Although many have since used this data, to our knowledge there has been no mention of the noise that is present in the images and its effects.

In Figure 2, the Area Under the Receiver Operator Curve (AUROC) is plotted for the MSP model and the Mahalanobis model for separating different resizes of Tiny ImageNet and LSUN from CIFAR10. The model has been trained using the default setup explained in Section 3. We can see that especially the Mahalanobis model performs a lot better depending on the resizing operation that is used, indicating that it is detecting the noise in the images of the data and using it to separate the OOD data from the ID data. This makes sense, as the Mahalanobis distance is the distance calculated in the feature space where the noise in the images has a large impact. On the other hand, the performance of the MSP model does not increase as drastically for different resizing methods. This is likely because the class of the noisy images is still prominent despite the noise and that the goal of the output layer is to find that class, therefore mainly ignoring the noise. To conclude, noise in the OOD images can lead to an artificial increase in OOD performance, especially for methods that utilize the feature space. Since noise can be introduced because of the resizing method, the resizing method must be chosen carefully.

Covariate and Semantic Data Shift. Some samples from the OOD datasets can share classes with the ID data. This can pose issues, as there is still some controversy around if semantically similar samples should be viewed as OOD for the sake of generalization (Yang et al., 2021a; Yang et al., 2021b; Huang and Li, 2021). For this reason, it is important to investigate the relation between OOD performance on samples that share a class and samples that do not share a class with the ID data. This allows us to determine how the model separates the OOD from the ID data and if it relies on semantics or not. More specifically, we want to know if OOD detection methods can actually make a distinction between the semantic and covariate shift between the ID and OOD data. We do so, by looking at the relation between the separation of semantically similar and semantically dissimilar samples from the ID dataset.

Figure 3 shows the AUROC for separating samples that do not share a class (disjoint), against the AUROC for separating samples that do share a class (joint) with the CIFAR10 dataset. In this figure, a



Figure 3: The AUROC for separating OOD samples that share a class, against the AUROC for separating OOD samples that do not share a class with the CIFAR10 dataset. The Tiny ImageNet and Places datasets are used as OOD dataset. A fairly strong correlation between the two is visible.

fairly strong correlation between the two is shown. This correlation indicates that if a model becomes better at separating samples that share a class, it also become better at separating samples that do not share a class and vice versa.

Because samples with semantically dissimilar classes can only be separated based on non-semantic features, an increase in OOD performance can only be explained by an increase in more discriminative non-semantic features. Because there is a correlation between the OOD performance for separating the samples with disjoint classes and separating the samples with joint classes, it must be the case that the samples with joint classes are also being separated based on these non-semantic features. This means that the methods at hand mostly separate the samples based on their covariate shift and not on their semantic shift. However, it can be argued that semantic features do not exist and that the semantic properties of a model/image merely emerge from a set of nonsemantic features. Nevertheless, this would mean the same thing, since the model would still be unable to make a distinction between class dependent and independent features. From this, we can conclude that the OOD detection depends on the covariate shift between the ID and OOD datasets.

However, as long as there are semantic differences, there must also be covariate differences. This follows from the fact that a difference in class must also lead to difference in images. If these differences are not captured by the model, it can be viewed as a shortcoming of the model. Theoretically, as long as the feature space is descriptive and highlevel enough, separating any two semantically nonoverlapping datasets should be possible. The same can however not be said for semantically overlapping datasets, since semantically similar samples are not bound to have different features given a more descriptive feature space. This is only true if the features are also on a high-enough level. For example, when two sets of semantically non-overlapping images contain the same low-level features, it becomes impossible to separate them based on the low-level feature space.

4.3 CNN Training and OOD Detection

As the separation of ID and OOD data strongly depends on the image features, looking at the effect of the model training is important, because the model training determines what features are learned. This section provides insight about the effect of the training setup on the OOD detection performance.

CNN Accuracy and OOD Detection. When a CNN is trained, the network learns different features that aid to the minimization of the learning objective (Ilyas et al., 2019), and as we have shown in the previous sections, the discriminativeness of the feature space is crucial for OOD detection. Therefore, by training a model to have a more discriminative or less discriminative feature space, the OOD detection performance can be improved or diminished respectively. This is in line with many other methods that use some form of OOD data during training in order to obtain more distinguishable features (Hendrycks et al., 2018; DeVries and Taylor, 2018; Lee et al., 2017).

In order to investigate the effect of different training approaches on the OOD detection performance, we trained several models on CIFAR10 with a single difference in the setup in order to isolate its effect. In Figure 4, we plotted the classification accuracy of the trained model, against the average AUROC and average TNR at 95% TPR of the OOD performance across all datasets for all of the training variations. This figure shows a fairly strong correlation between the classification accuracy and the OOD performance, although not very consistent.

For example, even though MixUp improves the model accuracy, it reduces the OOD performance with the MSP model compared to the basic MSP model. Similarly, we see that when not using weight decay or when using a multi step scheduler, that the OOD performance is low compared to other training variations with a similar accuracy. This shows that although there is some correlation between the accuracy and OOD performance, that the individual train-



Figure 4: The accuracy against the average AUROC and the average TNR at 95% TPR for all training variations. A fairly strong correlation between the OOD performance and the Accuracy is visible, but not very consistent.

ing methods have a bigger latent impact on the OOD detection performance and are not necessarily related to the accuracy of the model.

Benchmarking. By changing the training setup, the classification accuracy as well as the OOD detection performance can be improved. Table 2 shows that by changing the training approach, the OOD detection performance can be increased relative to the same model with a different training setup. This table also shows that when using the erase method, the performance increases quite steadily with the exception of the CIFAR100 dataset as ID dataset. Because random patches are being set to random values, thereby obscuring the images during training, the model is forced to learn different and less typical features in order to minimize the loss. Because these features are more typical of the ID data and thus more distinguishable from the OOD data, they aid the OOD detection performance.

When using the SVHN and Textures datasets as OOD, the Mahalanobis method with erase consistently performs the best. Conversely, when using the SVHN dataset as the ID dataset, the Mahalanobis method with erase performs the best for all OOD datasets. This shows that the features learned by using the erase data augmentation are generally more discriminative than without the erase data augmentation.

Although for the CIFAR10 and SVHN datasets the erase method performs the best, both with the MSP or the Mahalanobis model, the CIFAR100 dataset deviates from this trend. From the table it

Table 2: The OOD detection results for the commonly used ID-OOD dataset pairs and several metrics. The MSP and Mahalanobis distance on the default setup as well as the MSP and Mahalanobis distance with the erase data augmentation setup variations are shown. The highest scores are printed in bold.

		MSP / Mahalanobis / MSP + erase / Mahalanobis + erase		
ID	OOD	AUROC	Detection acc.	TNR at TPR 95%
CIFAR10	SVHN	.947 / .966 / .971 / .987	.920 / .941 / .950 / .958	.662 / .786 / .830 / .938
	TinyImageNet	.877 / .895 / .897 / .891	.827 / .829 / .845 / .824	.461 / .498 / .533 / .456
	LSUN	.911 / .913 / .930 / .911	.857 / .850 / .878 / .848	.511 / .514 / .595 / .475
	Places	.893 / .899 / .912 / .899	.872 / .878 / .889 / .884	.494 / .500 / .563 / .470
	CIFAR100	.881 / .896 / .905 / .895	.827 / .830 / .852 / .826	.446 / .492 / .525 / .457
	Textures	.914 / .968 / .928 / .983	.855 / .905 / .873 / .933	.544 / .799 / .594 / .903
CIFAR100	SVHN	.723 / .840 / .785 / .894	.777 / .817 / .811 / .869	.142 / .363 / .197 / .412
	TinyImageNet	.801 / .806 / .790 / .737	.737 / .745 / .728 / .687	.246 / .236 / .227 / .119
	LSUN	.749 / .726 / .748 / .645	.700 / .685 / .697 / .624	.152 / .122 / .141 / .054
	Places	.775 / .766 / .773 / .699	.818 / .805 / .826 / .802	.207 / .201 / .195 / .094
	CIFAR10	.783 / .753 / .775 / .628	.719 / .708 / .713 / .612	.216 / .157 / .197 / .042
	Textures	.787 / .931 / .805 / .951	.718 / .852 / .727 / .882	.204 / .658 / .248 / .745
SVHN	CIFAR10	.913 / .983 / .930 / .994	.893 / .942 / .891 / .967	.715/.922/.721/ .982
	TinyImageNet	.915 / .984 / .923 / .995	.895 / .944 / .889 / .970	.725 / .927 / .714 / .983
	LSUN	.899 / .981 / .906 / .994	.885 / .939 / .879 / .968	.680 / .906 / .674 / .985
	Places	.909 / .984 / .920 / .995	.869 / .950 / .867 / .973	.704 / .921 / .703 / .988
	CIFAR100	.913 / .983 / .923 / .993	.892 / .941 / .888 / .965	.713 / .917 / .711 / .980
	Textures	.893 / .991 / .890 / .997	.904 / .963 / .898 / .980	.684 / .963 / .651 / .991

is evident that with the exception of the SVHN and Textures datasets, the standard MSP and Mahalanobis models perform the best when using CIFAR100 as ID data. This is likely the case because when training on the CIFAR100 data, the model learns more different features than when training on CIFAR10 or SVHN. This means that the features from the OOD datasets are more likely to be present in the known features of the model due to its inclusiveness. This also explains why Mixup obtains high accuracy but a low OOD performance. Due to the more inclusive features, the features of the OOD data are more likely to fall within the same range as the features of the ID data.

5 CONCLUSION

We have shown that current OOD detection methods rely heavily on the difference in features between datasets and are therefore only able to detect the covariate shift. This reliance on covariate shift poses some future problems since detecting the semantic shift between images is debatably just as crucial.

The model training can then be altered in order to obtain better OOD detection methods. In this work we have highlighted the erase data augmentation, which obtains the best performance with only a single adaption to the training procedure for most ID-OOD dataset pairs. When using the erase method in combination with the Mahalanobis distance, it also consistently obtains the best results when using the SVHN and Textures datasets as OOD.

Although model training seems to be a useful tool for improving OOD detection performance, it does come with problems. As seen in Table 2, when using CIFAR100 as ID dataset, the OOD performance drops as opposed to the other ID datasets. This likely happens because of the more inclusive feature space learned by the model. A similar phenomenon is also seen when using Mixup to train the CNN, although the accuracy improves, the OOD performance is relatively low. This also makes it difficult to state that a richer feature space would lead to better OOD performance, as it can go both ways. It is therefore more fair to state that a more discriminative feature space leads to better OOD performance and that a more discriminative feature space is often the result of a richer feature space.

As a future work, it should be investigated what it means to have a more discriminative feature space as opposed to a rich feature space. When does a model become more inclusive and when does it become more discriminative? Conversely, how can we define discriminative and inclusiveness in OOD detection? These research questions pair well with the investigation of Mixup, which obtains better classification performance but does not increase OOD detection performance, as well as the investigation of why the OOD performance when training on CIFAR100 is so different from the OOD performance when training on CIFAR10. We believe that these future research questions combined with the results from this paper pave the way for safer use of neural networks.

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