Out-of-Distribution Detection without Class Labels

Niv Cohen Ron Abutbul Yedid Hoshen
School of Computer Science and Engineering
The Hebrew University of Jerusalem, Israel

Abstract

Anomaly detection methods identify samples that deviate from the normal behavior of the dataset. It is typically tackled either for training sets containing normal data from multiple labeled classes or a single unlabeled class. Current methods struggle when faced with training data consisting of multiple classes but no labels. In this work, we first discover that classifiers learned by self-supervised image clustering methods provide a strong baseline for anomaly detection on unlabeled multi-class datasets. Perhaps surprisingly, we find that initializing clustering methods with pre-trained features does not improve over their self-supervised counterparts. This is due to the phenomenon of catastrophic forgetting. Instead, we suggest a two stage approach. We first cluster images using self-supervised methods and obtain a cluster label for every image. We use the cluster labels as “pseudo supervision” for out-of-distribution (OOD) methods. Specifically, we fine-tune pretrained features on the task of classifying images by their cluster labels. We provide extensive analyses of our method and demonstrate the necessity of our two-stage approach. We evaluate it against the state-of-the-art self-supervised and pretrained methods and demonstrate superior performance.

1. Introduction

Detecting anomalies, images that are semantically different from normal ones, is a key ability required by many intelligent systems. Some applications include: detecting new, unknown scientific phenomena (e.g. supernovae) or detecting safety-critical events (e.g. alerting an autonomous car when an unexpected object is encountered). Due to the generality of the task, it has been studied in multiple settings. Here, we deal with the case where the training set consists of normal images only. A trained model is used at test time to classify new samples as normal (similar to previously seen examples) or anomalous (different from previously seen examples). In general, the normal data may consist of a single semantic class (e.g. dog images) or multiple classes (e.g. various species of animals).

Most recent works that address the setting where the normal data are multi-class ("multi-modal anomaly detection") have relied on supervised class labels for each class of normal samples. Multi-modal anomaly detection using supervised class labels is called out-of-distribution detection (OOD). Methods that do not assume such labels have focused on single-class data ("uni-modal anomaly detection"), and are called One-Class Classification (OCC). Here, we address the multi-modal anomaly detection setting, but do not assume class labels for the normal data.

In Sec. 3, we propose a new method based on the core idea of leveraging self-supervised clustering for learning representations better suited for multi-modal anomaly detection. In accordance with many recent works on out-of-distribution detection [11, 15], anomaly segmentation [31], and video anomaly detection [39], our main results utilize off-the-shelf, general purpose, pretrained feature extractors. Note that although we share the setting of using auxiliary data with the Outlier Exposure (OE) setting, we do not require the external data to be particularly related to the normal or anomalous data. As discussed by previous works [31], pretrained features can often be transferred even for data domains which are relatively far from the pretraining data (whereas such data could not be used for OE).

In our evaluation in Sec. 4, we find that our method outperforms state-of-the-art self-supervised [40] and pretrained [1, 32] anomaly detection methods. We provide a careful analysis of our method in Sec. 5. We conclude with a discussion of the advantages and limitations of our methods in Sec. 6.

Our main contributions are:

1. A few OCC anomaly detection methods do evaluate on multi-modal data without labels, and we compare to them in this work.
1. Demonstrating that deep self-supervised image clustering methods can obtain comparable to state-of-the-art results in multi-modal anomaly detection.

2. Presenting a framework that uses image cluster labels to improve feature representations for multi-modal anomaly detection.

3. Strong results on commonly used, unlabelled, multi-modal anomaly detection datasets.

1.1. Related Works

**Anomaly detection settings.** Anomaly detection is a challenging task, as models are trained based only on normal data and no anomalies. At test time, they are expected to discriminate between normal data and anomalies that come from an unknown distribution. This makes the optimal choice of a decision boundary highly ambiguous. To make progress on this task, anomaly detection methods must rely on inductive biases or simplifying assumptions to learn the decision boundary. One very strong assumption is that a (potentially small) number of anomalies is available for training, which reduces the task to classification with highly imbalanced datasets. This setting is often called supervised anomaly detection or low-shot anomaly detection [28, 38]. Another related setting is outlier exposure (OE) [7, 14, 15, 31], where true anomalies are unavailable but another distribution that is more similar to anomalies than to normal data is provided. We do not consider such approaches here as they require knowledge of the anomalies, which is unavailable in many cases.

**One Class Classification.** In the absence of positive or pseudo-positive anomaly examples, anomaly detection methods design inductive biases allowing models to detect anomalies without seeing any. The common thread behind these methods is learning a strong representation of the data with which separating between normal and anomalous data is easily done. This approach is shared with other self-supervised learning problems e.g. image clustering [41] or disentanglement [17]. Learning representations cannot be performed by using actual labels of the normal training data. Therefore, anomaly detection algorithms, as other self-supervised method, use a variety of techniques to design the inductive bias of the model toward having desired properties. Such techniques include self-supervised training to increase the model sensitivity to the properties essential for the task at hand [12, 15], simulating samples which may resemble expected anomalies [21], and data augmentation used to guide the model to ignore nuisance variation modes [40].

**Clustering-based Anomaly Detection.** Most anomaly detection methods perform some form of density estimation of the normal data. When the normal training data is multimodal i.e. consists of multiple clusters, it is natural that the density model would include this inductive bias. Indeed, multiple clustering-based approaches have been used for anomaly detection including: K-means [24] and GMMs [22]. As clustering the raw data directly is unlikely to achieve strong results for images, deep learning methods have been applied to learn better representations, notably DAGMM [45]. In the past few years, clustering methods have not dominated anomaly detection benchmarks, even for multi-modal data. In this paper, we revisit clustering-based anomaly detection and show that it achieves very strong performance for multi-modal anomaly detection with and without pre-trained features. We note that SSD, a recently published work, uses k-means clustering for anomaly scoring in the setting of OOD without labels [36]. We show that k-means clustering is less successful than our method on this task.

**Adaptation of Pre-trained Representations.** When pre-trained representations are available, they can be used to significantly improve anomaly detection accuracy. The top performing methods adapt pre-trained representations to the normal training data. Early attempts include [35] which suggested a compactness loss to map the normal training data closer together, relying on auto-encoder pretraining. Similar techniques were adopted by [30] and improved by [31, 34]. Adaptation of pre-trained representations using contrastive learning was recently suggested by [32]. Pre-trained representations were lately adapted for the OE setting as well [7, 31].

**Out-of-Distribution Detection (OOD).** In some settings, the normal data are provided with their semantic class ground truth labels. Using these labels for supervised training highly increases the model’s ability to detect OOD samples [13]. A model trained to classify labelled semantic classes, may have less confidence in predicting the class label of a sample coming from a new distribution. Moreover, training a model to distinguish between semantic classes of the normal data enhances the sensitivity of the learnt features for desired attribute. For example, a model trained to distinguish between animal species may learn a representation sensitive to their attributes (such as skin color and texture, head shape, etc.) and less sensitive to nuisance attributes (angle of view, lighting conditions, etc.). Such representation can be leveraged into an even stronger out-of-distribution detection capabilities, where anomalous sample can be detected according to a large Mahalanobis distance in representation space [11, 20].

**Self-Supervised Image Clustering.** The task of clustering images without labels with pretrained had been extensively studied. Most recent method learn deep features simultaneously with optimizing the images cluster assignments [3]. Methods free to optimize their own features are prone to cluster according to nuisance properties, which the self-learnt feature might pick up. A large variety of techniques
have been used to mitigate this problem, including augmentations [16] and contrastive feature learning [27, 41].

2. Preliminaries

Our method proposes to use deep image clustering as “pseudo supervision” for OOD methods. In this section, we present details of the main methods that we extend.

2.1. Deep Image Clustering

In recent years, deep image clustering has made significant progress. This is mostly thanks to improvements in self-supervised representation learning, which relies on image augmentation. In this paper we take advantage of SCAN [41], a state-of-the-art unsupervised image clustering method. SCAN operates in three steps:

(i) Representation learning. SimCLR [4], a contrastive self-supervised representation learning method, is used to learn a strong feature extractor $\phi_{\text{SimCLR}}$.

(ii) Classifier training. The feature extractor $\phi_{\text{SimCLR}}$ is used to compute the nearest neighbors for every training image. A classifier $C$ is trained (initialized with the features of $\phi_{\text{SimCLR}}$) to classify each training image $x$ into one of $K$ clusters. The classifier $C$ is trained under two constraints: i) equal number of images are assigned to each cluster, or the entropy of $E_{x \in X_{\text{train}}} C(x)$ is optimized to be as high as possible ii) an image is confidently assigned to a similar cluster as its nearest neighbours, or formally, we minimize $\sum_{x \in kNN(x)} \log(C(x) \cdot C(\tilde{x}))$. By the end of training the classifier produces a clustering of the training set.

(iii) Self-training. In the final stage, the clustering is improved using a self-training approach [23].

In Sec. 3.2, we will adapt recent deep image clustering methods for anomaly detection of multi-modal data without labels.

2.2. Feature-Adaptation for Out-of-Distribution Detection

In the OOD task, each normal training image $x$ is labeled with its class label $y$. Standard OOD methods, train a classifier $C$ to predict the class probability vector $C(x)$ given $x$. The standard confidence-based score, measures for a test image $x_{\text{test}}$ the maximum prediction probability (probability of the most confident class).

$$\text{Confidence} = \max \left(C(x_{\text{test}})\right) \quad (1)$$

Images with low maximal confidence, are denoted as anomalous. Many techniques have been proposed to improve the OOD detection accuracy of this technique. Here, we extend the work of Hendrycks et al. [15] and Fort et al. [11] which suggested initializing the classifier $C$ with weights that are pretrained on a large-scale datasets (such as ImageNet or CLIP). This significantly increases the OOD detection accuracy. Differently from the OOD methods, we do not assume that training data is provided with class labels. We will propose a clustering-based technique for adapting these methods to unlabeled datasets.

3. Deep Clustering for Multi-Modal Anomaly Detection

In this work, we deal with anomaly detection when the normal training data is composed of many different semantic classes but no labels. We suggest taking advantage of the multi-modal nature of the normal data as an inductive bias. The knowledge that the normal data comes from different, relatively distinct classes, rather than a single unimodal class, or other possible distributions, serves us to learn better representations. As illustrated in Fig.1, adapting features for better inter-cluster separation can provide better discrimination of anomalies, even when the cluster labels are imperfect. After learning features based on this inductive bias, they are used to provide anomaly scores for new images. Recent methods suggested a per-class Mahalanobis approach [11] deeming a sample normal if it lies within a small Mahalanobis distance to any of the cluster centers (Fig.1). However, when the provided labels are not accurate this approach might fail. False cluster assignment may distort the Mahalanobis distance which relies on the empirical covariance matrix of each cluster. Our method therefore relies as kNN scoring (Fig.1) which is less sensitive to the clustering accuracy and can identify anomalous samples by their distance to the closest normal sample provided in the training set.

3.1. Self-Supervised Clustering for Anomaly Detection

Recent self-supervised clustering methods have demonstrated promising results in grouping large unlabelled datasets of images by their ground truth semantic classes. We present a simple approach: First, we run the SCAN algorithm on the normal training images. We use the features from the penultimate layer from the SCAN-trained classifier to represent each image. These features are then combined with a kNN criterion for anomaly detection. We show in Sec.4.2 that this simple method already achieves competitive results with the state-of-the-art in the setting of fully self-supervised anomaly detection with no auxiliary data. This motivates revisiting unsupervised clustering methods for anomaly detection.

3.2. Finetuning with Imperfect Labels

While fully self-supervised methods without auxiliary data often achieve strong anomaly detection results, in many cases pretrained features can significantly boost performance. Features pretrained on very large datasets, that
my or may not be supervised, often have inductive biases towards representations that are more semantic to humans. For example, ImageNet pretraining learns visual features transferable for almost all images taken by an optical camera, and even other imaging modalities [31]. The knowledge gained by the model on the visual attributes present in the ImageNet dataset is useful in describing the semantics not only of normal training data, but also of unseen images; even without ever seeing samples of the target anomalous classes.

Here, our goal is to combine multi-modal distributional priors with pretrained features. A naive approach one may try would be to initialize a clustering method, such as SCAN, with pretrained features. While such a modification may allow SCAN to enjoy the knowledge represented in the pretrained features for clustering, we find that we end up with weaker feature representation than the original pretrained features. This constitutes a case of catastrophic forgetting, where a network extensively trained for a new task loses capabilities and knowledge that it had during pretraining.

To overcome this limitation, we suggest a two stage approach (Fig. 2). In the first stage, we simply train a self-supervised clustering method on the training data $X_{train}$ achieving approximate “pseudo-labels” as the output of the clustering algorithm. In the second stage, we transfer the knowledge obtained from the self-supervised clustering into the pretrained network. To do this, we follow [11] and fine-tune our pretrained network to classify training images into their pseudo-labels $\tilde{y}_{train}$. Note this is similar to standard OOD methods with pretrained features, the difference is that our data are unlabeled, and therefore the labeled are obtained in an unsupervised manner. We train a classifier models $C_{OOD}$, using standard cross entropy loss $L_{CE}$:

$$L_{CE} = -\sum_i (\tilde{y}_{train})_i \cdot \log \left( (C_{OOD}(X_{train})_i) \right)$$ (2)

Utilizing pseudo-labels knowledge: Although our two stage approach allow us to enjoy the multi-modal distributional assumption together with pretrained features, training the network with imperfect labels indefinitely may still results in catastrophic forgetting. During finetuning, the network gains knowledge from the clusters we found, but forgets its pretrained knowledge, which is crucial for our density estimation-based kNN anomaly detection. Although the model on one particular epochs may achieve the best performance, it is non-trivial to select the correct training epoch a-priori. Therefore, we choose to score our anomalies with an average model, taken as the moving average of the weights of the model during training epochs.

4. Results

Datasets: We evaluate our method on two commonly used OOD detection datasets. We use a variety of other datasets as our “anomalies”:

CIFAR-10 [19]: Contains images from 10 different classes, with a 32x32 resolution. We evaluate it against a variety of dataset supplied in a similar resolution, namely: CIFAR-100 [19], SVHN [25], LSUN [43]. The hardest benchmark here is the CIFAR-100 which contain the most similar classes to CIFAR-10. For LSUN we report both a version with some artifacts used by previous works, and a
version where the downsampling was done more carefully to avoid these artifacts suggested by CSI [40]. We do not compare on ImageNet [8], as this is the exact dataset used for pretraining.

ImageNet-30: Contain images from 30 classes of high resolution images chosen from the ImageNet [8] dataset. Accordingly, we evaluate it against a variety of datasets that have similar resolution, namely: CUB-200 [42], Dogs [8], Pets [29], Flowers [26], Food [2], Places [44], Caltech [10], DTD [6].

4.1. OOD Detection With Pretrained Features

In this section we provide results for the case where pretrained features are available.

Methods: We perform a comparison of anomaly detection methods that rely pretrained features, and can deal with the setting of unlabeled normal data. We show a comparison to a naive combination of pretrained features and clustering in Sec.5.

DN2 [31]: A kNN density estimation method based on pretrained features. Test samples are scored according to the distance to their nearest normal training images. A larger distance indicates a low density of normal samples, and therefore a high probability of abnormality. We follow MeanShifted [32] with normalizing features to lie on the unit sphere before scoring anomalies.

MeanShifted [32]: A state-of-the-art method for adapting pretrained features for anomaly detection using contrastive learning. It suggests using the contrastive loss computed around the mean of the normal training data features to mitigate catastrophic forgetting.

Ours: We use our method for clustering-based adaptation of pretrained features as described in Sec.3.1. The hyperparameters and implementation details are described in Sec.4.3.

Comparison: As can be seen in Tab. 2 and Tab. 3, our method significantly outperforms other feature adaptation methods that use on pretrained features. MeanShifted, designed to utilize the uni-modal nature of standard OCC data, show some positive adaptation results on multi-modal anomaly detection. Yet, our method outperforms using a multi-modal distribution assumption.

Our method can also be easily adapted to using stronger pretraining networks, which significantly improve the results. Similarly to [11], we find that ViT [9] pretrained on ImageNet-21 [18] achieves better results than ResNet152 pretrained on ImageNet. For the ImageNet-30 dataset, we used a CLIP pretrained ViT architecture for all pretrained methods (including ours), as ImageNet pretraining include the exact ImageNet class labels we wish to avoid in our setting.

4.2. OOD Detection Without Pretraining

Although strong pretrained features are often available, sometimes we cannot always assume their availability. In this case, we find that self-supervised clustering on its own can often learn a good enough representation to outperform previous state-of-the-art on unlabelled OOD detection without pretraining.

Methods: We compare the following methods:

Density based methods: Classical methods use direct density estimation techniques to estimate the likelihood of the data. Different methods suggested modification to this score to account for the dataset statistics (Likelihood Ratio [33]) or its complexity (Input Complexity [37]).

ROT / ROT+Trans [15]: A classification based method utilizing an auxiliary task of rotation prediction for self-supervised detection of anomalies.

GOAD [1]: Another rotation-prediction method, that proposed to learn a feature space where inter-class separation of the normal data is relatively small.

CSI [40]: A contrastive learning method which contrasts distribution-shifted augmentations of the data samples along with other samples.

SCAN [41]: Features taken from the last stage of the SCAN clustering methods, used to score anomalies as in DN2 (see Sec.3.2).

SSD [36]: A self-supervised method with similar features to CSI [40]. It scores anomalies using the Mahalanobis distance with respect to k-means clusters. Although this method is somewhat similar to ours, it relies on Mahalanobis distance and kMeans clustering, which are not optimal for feature adaptation without labels (see Sec.5). We note that SSD [36] also reports higher results for the ResNet-34 architecture, which is non-standard for AD without pretraining methods.

Comparison: As can be seen in Tab.2, simple utilization of SCAN features often performs on par with the best competing method that does not use pretraining. We note that the last stage of the SCAN method, namely, self-labeling, is somewhat similar to adapting on pseudo-label performed by our method. Therefore, we do not expect our method to provide further gains over adapting SCAN’s final representation according to its own labels. We also report the OOD detection accuracy with the representation achieved in the different stages of the SCAN algorithm in Tab.4.

Although clustering methods such as k-means and GMM have classically been very popular, most recent deep learning methods typically do not use clustering. The results reported here provide strong motivation for revisiting self-supervised clustering methods for anomaly detection. We conclude that relying on the multi-modal distribution prior often allows us to outperform other methods even in the setting where no pretraining is allowed.
Table 2. OOD Without Ground Truth Labels On CIFAR-10 ROCAUC(%)

| Network | CIFAR-100 | SVHN | LSUN | LSUN (FIX) |
|---------|-----------|------|------|------------|
| Likelihood Glow | 58.2 | 8.3 | - | - |
| Likelihood Ratio PixelCNN++ | - | 91.2 | - | - |
| Input Complexity Glow | 73.6 | 95.0 | - | - |
| ROT ResNet-18 | 79.0 | 97.6 | 89.2 | 77.7 |
| ROT+Trans ResNet-18 | 82.3 | 97.8 | 92.8 | 81.6 |
| GOAD ResNet-18 | 77.2 | 96.3 | 89.3 | 78.8 |
| CSI ResNet-18 | 89.2 | 99.8 | 97.5 | 90.3 |
| SSD ResNet-18 | 89.6 | - | - | - |
| SCAN Features ResNet-18 | 90.2 | 94.3 | 92.4 | 92.1 |

Table 3. OOD Without Ground Truth Labels On ImageNet-30 ROCAUC(%)

| Network | CUB-200 | Dogs | Pets | Flowers-102 | Food-101 | Places-365 | Caltech-256 | DTD |
|---------|---------|------|------|-------------|----------|------------|-------------|-----|
| ROT+Trans ResNet-18 | 74.5 | 77.8 | 70.0 | 86.3 | 71.6 | 53.1 | 70.0 | 89.4 |
| GOAD ResNet-18 | 71.5 | 74.3 | 65.5 | 82.8 | 68.7 | 51.0 | 67.4 | 87.5 |
| CSI ResNet-18 | 90.5 | 97.1 | 89.7 | 93.2 | 95.7 | 96.7 | 90.3 | 98.6 |

| Pretrained | CLIP ViT |
|-----------|---------|
| DN2 | 93.8 | 94.2 | 89.7 | 93.2 | 95.7 | 96.7 | 90.3 | 98.6 |
| Ours | 99.4 | 95.9 | 94.9 | 98.3 | 96.4 | 96.1 | 94.4 | 98.6 |

Table 4. Comparison between OOD with the representations obtained by different stages of the SCAN clustering method (CIFAR-10 vs. CIFAR-100) ROCAUC (%)

| Network | CUB-200 | Dogs | Pets | Flowers-102 | Food-101 | Places-365 | Caltech-256 | DTD |
|---------|---------|------|------|-------------|----------|------------|-------------|-----|
| SIMCLR | SCAN | Self-Labelling |
| 87.3 | 83.4 | 89.3 |

4.3. Implementation Details

Clustering: We use SCAN’s official implementation[^1] for all clustering tasks unless mentioned otherwise. We ran all of our clustering algorithms with the same number of clusters $K = 10$ (for further discussion see Sec.5). We use the SCAN algorithm’s default parameters for each dataset. For ImageNet-30 dataset we use the configuration originally provided by the authors for the ImageNet-50 dataset. We note that SCAN unsupervised image clustering use a MoCo [5] pretraining on the entire ImageNet dataset (without labels). We therefore do not compare it to self-supervised methods that do not use pretraining.

Pretraining: For all models using ResNet152, we use ImageNet [8] pretraining. For ViT, we used ImageNet-21 [18] pretraining for all models. For our pretraining with ImageNet-30 we used the CLIP ViT visual head for to avoid using a model pretrained on ImageNet dataset with labels in Tab.3.

Optimization: We run the adaptation for 5 epochs and Adam optimizer. We used Cosine Annealing learning rate scheduler with an initial learning rate of $1e^{-5}$ and final learning rate of $1e^{-6}$.

Scoring: we used $k = 1$ for all our kNN evaluations.

Comparison to MeanShifted: For the MeanShifted comparison we experimented with 5, 10 and 100 training epochs, and chose the best performing number of epochs. The rest of the parameters were left unchanged. We do not report MeanShifted for any ViT architecture, as such architectures are not currently supported by the official implementation.

[^1]: https://github.com/wvangansbeke/Unsupervised-Classification
5. Discussion

**Comparison between our two-stage method and naive one-stage adaptation:** We compare pretrained feature adaptation using our two stage method to direct adaptation by using the pretrained features as the initialization of SCAN clustering. To do so, we replace the features learned by SimCLR used to initialize the kNN and the second and third stages of scan by ResNet152 ImageNet pretrained features (which our method uses). We can see in Tab.5 that the results are far worse than the results achieved by our two-stage approach. During the clustering stage, the pretrained features are used to improve clustering performance but at the same time, the features deteriorate further away from their pretrained initialization.

The initial pretrained features representation may include both attributes that are useful for splitting our normal data to its clusters; and additional attributes which may help a density estimation algorithm to isolate anomalies. Finetuning our pretrained representation for clustering of the normal data may result in catastrophic forgetting of the network ability to semantically represent attributes not needed for that task (a similar phenomena can be seen also Tab.4). This justifies our two stage approach, which better conserves the expressivity of the initial pretrained features.

Table 5. Comparison between naive and two-stage clustering based adaptation of pretrained features (CIFAR-10 vs. CIFAR-100) ROCAUC (%)

| Ours  | Naive |
|-------|-------|
| 93.8  | 88.1  |

Is kNN density estimation preferable to other anomaly scoring methods? Yes. Previous works used a variety of scoring criterion for OOD detection. Although the Mahalanobis distance was shown to give stronger results in a previous work, it is sensitive to the inaccurate labels that are typically generated self-supervised clustering (see Fig.1 for an illustration). A comparison between the different scoring methods can be shown in Tab.6.

Table 6. Comparison between scoring methods using our obtained features (CIFAR-10 vs. CIFAR-100, epoch = 1) ROCAUC (%)

| kNN        | Confidence | Mahalanobis |
|------------|------------|-------------|
| 93.7       | 89.6       | 92.8        |

Can simple K-means clustering be used to recursively fine-tune features? To some extent. One may expect that a simple clustering method (e.g. K-means) could not yield a significant adaptation of the very same features used to find the clusters. While the K-means algorithm does rely on multi-modal distributional priors, the expressivity of the clustering choices allowed to the K-means algorithm is limited. Therefore, the additional knowledge our representation can gain from pseudo-labels is expected to be limited as well. We indeed find that to be the case: although a minor improvement by adaptation is still possible, the OOD detection results do not improve much (Tab.7).

Table 7. Comparison between raw pretrained features and pretrained features adapted on the labels of K-means clustering (CIFAR-10 vs. CIFAR-100) ROCAUC (%)

| Raw | kMeans |
|-----|--------|
| 86.5| 87.3   |

Can our labels be utilized by other labelled OOD methods in the no-pretraining setting? To some extent. To answer this question we feed the labels we obtained from clustering to support the CSI labelled OOD detection method. While supervising CSI with the labels from SCAN does not outperform the unlabelled CSI version, the pseudo-labels from SPICE can significantly improve performance.

Table 8. Comparison of self-supervised features with different pseudo labels sources (CIFAR-10 vs. CIFAR-100) ROCAUC (%)

| Unlabelled | SCAN | SPICE |
|------------|------|-------|
| CSI        | 89.1 | 89.0  | 92.6  |

Can we expect better clustering methods to yield even further result improvements? Yes. The cluster labels obtained by SPICE [27] yield stronger results on CIFAR-10 using the checkpoints provided in their GitHub repository. For example, SPICE-based adaptation achieved 97.6% on CIFAR-10 vs. CIFAR-100 (compared to 96.7% using the SCAN-based adaptation). We conclude that further improvement in self-supervised clustering can be utilized in the future to improve our method in a very similar manner. By the time of writing this paper, there were still technical issues with the official implementation of SPICE, preventing us from reporting full results with it and using it as our main clustering method.

Can using a larger model with ImageNet pretraining assist the SCAN clustering performance? Not significantly. We tried to initialize the SCAN algorithm with a ResNet152 pretrained on ImageNet, but achieved only a minor improvement in the clustering accuracy. Although an adaptation of pretrained network using scan results in catastrophic forgetting (Tab.5) it is very likely that image cluster-
ing accuracy can be substantially improved with a method designed to take advantage of such representations. Such future improvements in image clustering are likely to directly enhance the results of our approach as well.

Does our model averaging give a good representation with respect to individual epochs? Yes. Model weight averaging can yield a similar or better OOD detection to that of the optimal epoch along the training process. For example, on CIFAR-10 vs. CIFAR-100 with pretrained ResNet152, the initial pretrained features scored anomalies with 86.5% ROCAUC. The 5 individual training epochs scored 92.9%, 93.4%, 92.9%, 92.6%, 92.3%. The averaged model scored 94.5% ROCAUC. While we do not claim the averaging method always outperforms all individual checkpoints, we find it alternative for have to elect the optimal training epoch.

What is sensitivity of our method to the chosen number of clusters $K$? While changing $K$ may somewhat vary the results, our method can perform useful adaptation without knowing the exact ground truth number of classes (Tab.9). If available, the groundtruth number of clusters $K$ should be used.

How does adaptation with the pseudo-labels obtained by clustering compare truth labels? Although there is still a significant gap between the pseudo-labels provided by our clustering algorithm and the ground truth class labels (88.3%, SCAN accuracy on CIFAR-10), the gap in the OOD detection results seems to be smaller. For example, on CIFAR-10 vs. CIFAR-100 OOD task, our method achieves 96.2% ROCAUC, while a similar method by Fort et al. [11] using the ground truth labels achieves 98.4% ROCAUC. Even though this a significant difference, we find it is relatively small given the still significant inaccuracy of self-supervised clustering used.

Relation to auxiliary-task based anomaly detection: An alternative view is that our work can be seen as an extension of a line of methods utilizing auxiliary tasks to address a one-class-classification setting. Such methods were previously suggested for image anomaly detection [12] [15] and also for other data modalities [1]. These methods rely on predefined augmentations to create an auxiliary task in order to guide the model learning toward meaningful properties of our data. Predicting pseudo-labels from a clustering algorithm may be seen as another kind of such auxiliary task. Future works may suggest new kinds of data-adaptive auxiliary tasks for similar settings.

New data modalities: Multi-modal anomaly detection may be encountered in other modalities beyond images. Data modalities where transfer learning and self-supervised learning show promising results include natural language, video and audio. Therefore, we believe similar methods may provide similar improvement on multi-modal anomaly detection on these modalities.

Guided anomaly detection: Another interesting application of clustering based out-of-distribution detection is using the pseudo labels to guide our anomaly detection algorithm on the type of samples that we wish to consider as anomalies. For example, if one wishes to define anomalies according to colors, they may use augmentations to guide the clustering procedure toward finding color-based clusters.

### 6. Limitations

Highly unbalanced multi-modal datasets: Most state of the art clustering algorithms rely on the assumption of an approximately even split of the data among the clusters at least on one stage of their training. As our method and results rely on such algorithms, we are currently prone to lower performance when this assumption does not hold. Yet, future self-supervised algorithm may overcome this limitation, removing this limitation from our method as well.

Fine-grained and non-standard classes: Many state of the art self-supervised learning algorithms, including self-supervised clustering, heavily rely on augmentations and other sources of inductive bias, such as architecture. Mostly, the inductive bias in these methods guides the model to be sensitive to a single salient object in the center of the image. In cases when the anomalies or the semantic classes in the normal data are fine-grained, currents may not perform as well. While this is limitation of our method, it is similarly a limitation of many other anomaly detection techniques reliant on self-supervised learning, including nearly all competing baseline methods. We therefore consider this as a limitation of the field in general, rather than a limitation specific to our method.

Pretrained features: The main results of our paper are reliant on pretrained features, although we also suggest an approach reliant only on self-supervised learning. As discussed, pretrained features achieve strong results on most datasets, but may not be a good choice in some settings. To overcome this limitation in practical settings where the preferred method cannot be determined in advance, we propose to use an ensemble of pretrained and fully self-supervised methods.

### Table 9. Comparison of different numbers of clusters $K$ (ImageNet-30 vs. CUB-200) ROCAUC (%)

| $K$  | 10  | 20  | 30  | No Adaptation |
|------|-----|-----|-----|---------------|
| ROCAUC | 99.1 | 98.3 | 98.9 | 93.8          |

Data modalities where transfer learning and self-supervised learning show promising results include natural language, video and audio. Therefore, we believe similar methods may provide similar improvement on multi-modal anomaly detection on these modalities.

Guided anomaly detection: Another interesting application of clustering based out-of-distribution detection is using the pseudo labels to guide our anomaly detection algorithm on the type of samples that we wish to consider as anomalies. For example, if one wishes to define anomalies according to colors, they may use augmentations to guide the clustering procedure toward finding color-based clusters.
7. Conclusion

We address the problem of OOD detection without labels. Taking a well known assumption of the multi-modal distribution of the normal data together with modern image clustering methods gives a significant boost to multi-modal anomaly detection performance. We propose a conceptually simple but effective method to leverage improvements in OOD detection with pretrained features, outperforming state-of-the-art feature adaptation methods. Future work may utilize the evolving methods of self-supervised clustering of image datasets to further improve anomaly detection results. We also expect similar improvements in other data modalities such as natural language, video, audio and time-series.

8. Acknowledgements

This work was partly supported by the Varadi foundation.
References

[1] Liron Bergman and Yedid Hoshen. Classification-based anomaly detection for general data. In ICLR, 2020. 1, 5, 8

[2] Lukas Bossard, Matthieu Guillaumin, and Luc Van Gool. Food-101 – mining discriminative components with random forests. In European Conference on Computer Vision, 2014. 5

[3] Mathilde Caron, Piotr Bojanowski, Armand Joulin, and Matthijs Douze. Deep clustering for unsupervised learning of visual features. In Proceedings of the European Conference on Computer Vision (ECCV), pages 132–149, 2018. 2

[4] Ting Chen, Simon Kornblith, Mohammad Norouzi, and Geoffrey Hinton. A simple framework for contrastive learning of visual representations. In International conference on machine learning, pages 1597–1607. PMLR, 2020. 3

[5] Xinlei Chen, Haoqi Fan, Ross Girshick, and Kaiming He. Improved baselines with momentum contrastive learning. arXiv preprint arXiv:2003.04297, 2020. 6

[6] M. Cimpoi, S. Maji, I. Kokkinos, S. Mohamed, , and A. Vedaldi. Describing textures in the wild. In Proceedings of the IEEE Conf. on Computer Vision and Pattern Recognition (CVPR), 2014. 5

[7] Lucas Deecke, Lukas Ruff, Robert A Vandermeulen, and Hakan Bilen. Transfer-based semantic anomaly detection. In International Conference on Machine Learning, pages 2546–2555. PMLR, 2021. 2

[8] Jia Deng, Wei Dong, Richard Socher, Li-Jia Li, Kai Li, and Li Fei-Fei. Imagenet: A large-scale hierarchical image database. In 2009 IEEE conference on computer vision and pattern recognition, pages 248–255. Ieee, 2009. 5, 6

[9] Alexey Dosovitskiy, Lucas Beyer, Alexander Kolesnikov, Dirk Weissenborn, Xiaohua Zhai, Thomas Unterthiner, Mostafa Dehghani, Matthias Minderer, Georg Heigold, Sylvain Gelly, et al. An image is worth 16x16 words: Transformers for image representation at scale. arXiv preprint arXiv:2010.11929, 2020. 5

[10] Li Fei-Fei, Rob Fergus, and Pietro Perona. Learning generative visual models from few training examples: An incremental bayesian approach tested on 101 object categories. In 2004 conference on computer vision and pattern recognition workshop, pages 178–178. IEEE, 2004. 5

[11] Stanislav Fort, Jie Ren, and Balaji Lakshminarayanan. Exploring the limits of out-of-distribution detection. arXiv preprint arXiv:2106.03004, 2021. 1, 2, 3, 4, 5, 8

[12] Izhak Golan and Ran El-Yaniv. Deep anomaly detection using geometric transformations. arXiv preprint arXiv:1805.10917, 2018. 2, 8

[13] Dan Hendrycks and Kevin Gimpel. A baseline for detecting misclassified and out-of-distribution examples in neural networks. arXiv preprint arXiv:1610.02136, 2016. 2

[14] Dan Hendrycks, Mantas Mazeika, and Thomas Dietterich. Deep anomaly detection with outlier exposure. In International Conference on Learning Representations, 2019. 2

[15] Dan Hendrycks, Mantas Mazeika, Saurav Kadavath, and Dawn Song. Using self-supervised learning can improve model robustness and uncertainty. arXiv preprint arXiv:1906.12340, 2019. 1, 2, 3, 5, 8

[16] Xu Ji, Joao F Henriques, and Andrea Vedaldi. Invariant information clustering for unsupervised image classification and segmentation. In Proceedings of the IEEE/CVF International Conference on Computer Vision, pages 9865–9874, 2019. 3

[17] Diederik P Kingma and Max Welling. Auto-encoding variational bayes. arXiv preprint arXiv:1312.6114, 2013. 2

[18] Alexander Kolesnikov, Lucas Beyer, Xiaohua Zhai, Joan Puigcerver, Jessica Yung, Sylvain Gelly, and Neil Houlsby. Big transfer (bit): General visual representation learning. In Computer Vision–ECCV 2020: 16th European Conference, Glasgow, UK, August 23–28, 2020. Proceedings, Part V 16, pages 491–507. Springer, 2020. 5, 6

[19] Alex Krizhevsky, Geoffrey Hinton, et al. Learning multiple layers of features from tiny images. 2009. 4

[20] Kimin Lee, Kibok Lee, Honglak Lee, and Jinwoo Shin. A simple unified framework for detecting out-of-distribution samples and adversarial attacks. Advances in neural information processing systems, 31, 2018. 2

[21] Chun-Liang Li, Kihyuk Sohn, Jinsung Yoon, and Tomas Pfister. Cutpaste: Self-supervised learning for anomaly detection and localization. In Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition, pages 9664–9674, 2021. 2

[22] Lishuai Li, R John Hansman, Rafael Palacios, and Roy Welsch. Anomaly detection via a gaussian mixture model for flight operation and safety monitoring. Transportation Research Part C: Emerging Technologies, 64:45–57, 2016. 2

[23] Geoffrey J McLachlan. Iterative reclassification procedure for constructing an asymptotically optimal rule of allocation in discriminant analysis. Journal of the American Statistical Association, 70(350):365–369, 1975. 3

[24] Gerhard Münz, Sa Li, and Georg Carle. Traffic anomaly detection using k-means clustering. In GIITG Workshop MMBnet, pages 13–14, 2007. 2

[25] Yuval Netzer, Tao Wang, Adam Coates, Alessandro Bissacco, Bo Wu, and Andrew Y Ng. Reading digits in natural images with unsupervised feature learning. 2011. 4

[26] Maria-Elena Nilsback and Andrew Zisserman. Automated flower classification over a large number of classes. In Indian Conference on Computer Vision, Graphics and Image Processing, Dec 2008. 5

[27] Chuang Niu, Hongming Shan, and Ge Wang. Spice: Semantic pseudo-labeling for image clustering. arXiv preprint arXiv:2103.09382, 2021. 3, 7

[28] Guansong Pang, Longbing Cao, Ling Chen, and Huan Liu. Learning representations of ultrahigh-dimensional data for random distance-based outlier detection. In Proceedings of the 24th ACM SIGKDD international conference on knowledge discovery & data mining, 2018. 2

[29] Omkar M. Parkhi, Andrea Vedaldi, Andrew Zisserman, and C. V. Jawahar. Cats and dogs. In IEEE Conference on Computer Vision and Pattern Recognition, 2012. 5
[30] Pramuditha Perera and Vishal M Patel. Learning deep features for one-class classification. *IEEE Transactions on Image Processing*, 28(11):5450–5463, 2019. 2

[31] Tal Reiss, Niv Cohen, Liron Bergman, and Yedid Hoshen. Panda: Adapting pretrained features for anomaly detection and segmentation. In *Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, pages 2806–2814, 2021. 1, 2, 4, 5

[32] Tal Reiss and Yedid Hoshen. Mean-shifted contrastive loss for anomaly detection. *arXiv preprint arXiv:2106.03844*, 2021. 1, 2, 5

[33] Jie Ren, Peter J Liu, Emily Fertig, Jasper Snoek, Ryan Poplin, Mark A DePristo, Joshua V Dillon, and Balaji Lakshminarayanan. Likelihood ratios for out-of-distribution detection. *arXiv preprint arXiv:1906.02845*, 2019. 5

[34] Oliver Rippel, Arnav Chavan, Chucai Lei, and Dorit Merhof. Transfer learning gaussian anomaly detection by fine-tuning representations. *arXiv preprint arXiv:2108.04116*, 2021. 2

[35] Lukas Ruff, Robert Vandermeylen, Nico Goernitz, Lucas Deecke, Shoaih Ahmed Siddiqui, Alexander Binder, Emmanuel Müller, and Marius Kloft. Deep one-class classification. In *International conference on machine learning*, pages 4393–4402. PMLR, 2018. 2

[36] Vikash Sehwag, Mung Chiang, and Prateek Mittal. Ssd: A unified framework for self-supervised outlier detection. *arXiv preprint arXiv:2103.12051*, 2021. 2, 5

[37] Joan Serrà, David Álvarez, Vicenç Gómez, Olga Slizovskaia, José F Núñez, and Jordi Luque. Input complexity and out-of-distribution detection with likelihood-based generative models. *arXiv preprint arXiv:1909.11480*, 2019. 5

[38] Shelly Sheynin, Sagie Benaim, and Lior Wolf. A hierarchical transformation-discriminating generative model for few shot anomaly detection. In *ICCV*, 2021. 2

[39] Sorina Smeureanu, Radu Tudor Ionescu, Marius Popescu, and Bogdan Alexe. Deep appearance features for abnormal behavior detection in video. In *International Conference on Image Analysis and Processing*, pages 779–789. Springer, 2017. 1

[40] Jihoon Tack, Sangwoo Mo, Jongheon Jeong, and Jinwoo Shin. Csi: Novelty detection via contrastive learning on distributionally shifted instances. In *NeurIPS*, 2020. 1, 2, 5

[41] Wouter Van Gansbeke, Simon Vandenhende, Stamatios Georgoulis, Marc Proesmans, and Luc Van Gool. Scan: Learning to classify images without labels. In *European Conference on Computer Vision*, pages 268–285. Springer, 2020. 2, 3, 5

[42] P. Welinder, S. Branson, T. Mita, C. Wah, F. Schroff, S. Belongie, and P. Perona. Caltech-UCSD Birds 200. Technical Report CNS-TR-2010-001, California Institute of Technology, 2010. 5

[43] 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

[44] Bolei Zhou, Agata Lapedriza, Jianxiong Xiao, Antonio Torralba, and Aude Oliva. Learning deep features for scene recognition using places database. 2014. 5

[45] Bo Zong, Qi Song, Martin Renqiang Min, Wei Cheng, Cristian Lumezanu, Daeki Cho, and Haifeng Chen. Deep autoencoding gaussian mixture model for unsupervised anomaly detection. In *International conference on learning representations*, 2018. 2