

Anomaly Clustering: Grouping Images into Coherent Clusters of Anomaly Types

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Abstract

We study anomaly clustering, grouping data into coherent clusters of anomaly types. This is different from anomaly detection that aims to divide anomalies from normal data. Unlike object-centered image clustering, anomaly clustering is particularly challenging as anomalous patterns are subtle and local. We present a simple yet effective clustering framework using a patch-based pretrained deep embeddings and off-the-shelf clustering methods. We define a distance function between images, each of which is represented as a bag of embeddings, by the Euclidean distance between weighted averaged embeddings. The weight defines the importance of instances (i.e., patch embeddings) in the bag, which may highlight defective regions. We compute weights in an unsupervised way or in a semi-supervised way when labeled normal data is available. Extensive experimental studies show the effectiveness of the proposed clustering framework along with a novel distance function upon existing multiple instance or deep clustering frameworks. Overall, our framework achieves 0.451 and 0.674 normalized mutual information scores on MVTec object and texture categories and further improve with a few labeled normal data (0.577, 0.669), far exceeding the baselines (0.244, 0.273) or state-of-the-art deep clustering methods (0.176, 0.277).

1. Introduction

Anomaly detection aims to detect anomalous data when majority of the data is normal. To deal with the scarcity of the labeled anomalous data at train time, anomaly detection problems are often formulated as a one-class classification problem [53, 59, 52], where one builds a classifier that could separate anomalous data from normal ones at test time using only normal data at train time. As a result of anomaly detection, one would get a binary label of normalcy or anomaly.

However, a binary label has limited expression as there could be many sources of anomalous behaviors as in Figure 1a. On the other hand, grouping data into multiple, semantically coherent clusters, as in Figure 1b, would be valuable for some reasons. For example, cluster assignments could be used to generate the query data for active learning,

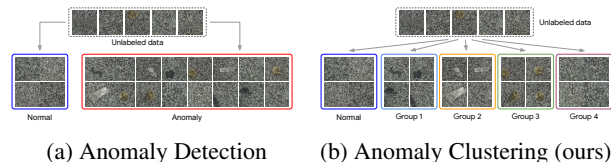


Figure 1: Different from existing works on (1a) anomaly detection [3, 4, 36, 51], (1b) we study anomaly clustering that groups unlabeled data automatically into multiple clusters, each of which may represent different types of anomaly.

where diversity is important [43, 40, 23, 55], to improve the performance of anomaly detector. Moreover, it would help data scientists analyze the root causes of various anomaly types, hoping to fix their manufacturing pipeline to reduce anomalous behaviors. This paper deals with the problem of clustering images with anomalous patterns.

Clustering could be used for our problem. Classic methods like KMeans [41], spectral clustering [42], or hierarchical agglomerative clustering [62], focus on grouping data given representations, while recent deep clustering methods [65, 6, 28, 60, 44] aim to learn high-level representations and their grouping jointly. They have shown impressive clustering accuracy on several vision datasets such as CIFAR-10 [31] or ImageNet [14].

In this paper, we introduce anomaly clustering, a problem of grouping images into different anomalous patterns. While there has been a substantial progress in image clustering research [63, 60], anomaly clustering poses unique challenges. Firstly, unlike typical image clustering datasets, images for anomaly clustering may not be object-centered. Rather, images are mostly similar to each other but differs at local regions. To our knowledge, grouping images by capturing fine-grained details, as opposed to the coarse-grained object semantics, has not been studied in existing works. Secondly, it is common that the data is limited in industrial applications, making state-of-the-art deep clustering methods, which are usually trained on large datasets, less applicable. We highlight challenges of anomaly clustering via empirical comparisons to deep clustering in Section 4.2.

We present an anomaly clustering framework to tackle this important real-world problem. To resolve the limited-data issue, we employ the pretrained deep representation,

similar to solutions for anomaly detection [50, 13, 51], followed by similarity-based clustering methods. To tackle the non-object-centric issue, we represent an image as a bag of patch embeddings, as in Figure 2, instead of a holistic representation. This casts the problem naturally into a multiple instance clustering [70]. The question boils down to defining a distance function between bags of instances (i.e., patch embeddings), and we propose a weighted average distance, which aggregates patch embeddings with weights followed by the Euclidean distance. The weight indicates which instances to attend to, and could be derived in an unsupervised way or in a semi-supervised way using extra labeled normal images. The proposed framework is described in Figure 2.

We conduct comprehensive experiments on two anomaly detection datasets, MVTec anomaly detection [3] and magnetic tile defect [26]. We present a new experimental protocol for anomaly clustering, whose performance is evaluated using ground-truth defect type annotations. We test the proposed clustering framework using various distance functions, including variants of Hausdorff distances [27, 17, 70] and our weighted average distance. We also compare with state-of-the-art deep clustering methods [28, 60, 44] for anomaly clustering. While being conceptually and computationally simple, our results show that the proposed framework solves the anomaly clustering problem significantly better than existing deep clustering methods. Our weighted average distance also demonstrates the efficacy over existing distance functions for multiple instance clustering.

Finally, we summarize our contributions as follows:

1. We introduce an anomaly clustering problem and cast it as a multiple instance clustering using patch-based deep embeddings for an image representation.
2. We propose a weighted average distance that computes the distance by focusing on important instances in unsupervised or semi-supervised ways.
3. We conduct experiments on industrial anomaly detection datasets, showing solid improvements over multiple instance and deep clustering baselines.

2. Related Work

Anomaly detection has been extensively studied under various settings [7], such as supervised with both labeled normal and anomalous data, semi-supervised with labeled normal data [53, 59], or unsupervised with unlabeled data [5, 38, 68], to train classifiers. While anomaly detection divides data into two classes of normalcy and anomaly, our goal is to group them into many clusters, each of which represents various anomalous behaviors.

Thanks to deep learning there has been a solid progress in visual anomaly detection. Self-supervised representation learning methods [21, 9] have been adopted to build deep one-class classifiers [22, 25, 2, 57, 56], showing improvement in anomaly detection [4, 67, 36]. In addition, the deep

image representations trained on large-scale object recognition datasets [15] have shown to be a good feature for visual anomaly detection [4, 50, 49, 13, 51]. While we follow the similar intuition as we represent an image as a bag of patch embeddings with pretrained networks, we propose a method for grouping images into multiple clusters instead of building one-class classifier for binary classification.

Image clustering is an active research area, whose main concern is at image representation. Typical approaches [35, 12] include bag-of-keypoints [12], where one builds a histogram of local descriptors (e.g., SIFT [39] or Texton [30]), and spatial pooling [34], aggregating local descriptors by averaging, to obtain a holistic representation of an image. Some applications relevant to our work include texture and material classification [35, 61, 33] and description [19, 11]. While their goal is to classify images of different texture or material properties with supervision, our goal is to cluster images with subtle differences due to defects without or with a minimal supervision. Moreover, we use patch representations and cast the problem as multiple instance clustering by automatically identifying important instances.

On the other hand, deep clustering [65, 6, 28, 60, 44] jointly learns image representations and group assignments using deep neural networks. While there has been a huge progress in clustering natural and object-centered images, such as those from CIFAR-10 [31] or ImageNet [14], state-of-the-art deep clustering algorithms do not work well for anomaly clustering, which requires to capture subtle differences of various anomaly types, as in Section 4.2.

3. Anomaly Clustering

We introduce the proposed anomaly clustering, where in Section 3.1 we formulate it as a multiple instance clustering problem [70]. In Section 3.2, we define a distance measure under unsupervised setting in Section 3.2.1 and under semi-supervised setting with a few normal data in Section 3.2.2.

3.1. Framework Overview

Let $\mathcal{X} = \{\mathbf{x}_i \in \mathbb{R}^{W \times H \times 3}\}$ be a set of images to cluster into K groups. Following deep clustering literature [6, 60], for a given deep feature extractor, a straightforward way to formulate a framework is to extract a holistic deep representation of an image and apply off-the-shelf clustering methods on unlabeled images. While plausible, this approach does not take into account that anomalous behaviors may happen happening locally (e.g., Figure 3). As a result, it shows suboptimal clustering performance (see Section 5.1).

To account for the local nature of anomalous patterns in images, we propose to represent images with a bag of patch embeddings, similar to recent works on visual anomaly detection [67, 50, 13, 51]. Let $Z_i \triangleq Z(\mathbf{x}_i) = \{\mathbf{z}_1^i, \dots, \mathbf{z}_M^i\}$, where $\mathbf{z}_m^i \in \mathbb{R}^D$ is a patch embedding from an image using pretrained deep neural networks. As we have bags of patch

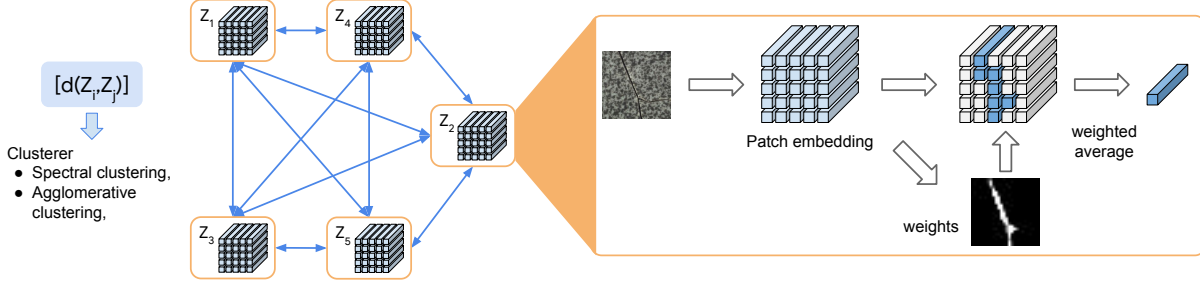


Figure 2: The proposed anomaly clustering framework uses similarity-based clustering methods, such as spectral clustering or hierarchical clustering. We compute the distance between images, each of which is represented as a bag of patch embeddings from a pretrained deep neural network, by the Euclidean distance of weighted averaged embeddings, whose weight represents the “importance” (e.g., defectiveness) of patch embeddings.

embeddings, each of which is from a single image, while wanting to assign a cluster membership to each bag, we can formulate it as a multiple instance clustering (MIC) [70] problem. In particular, we propose an anomaly clustering framework that follows steps below:

1. Extract patch embeddings and define embeddings from an image as a *bag*.
2. Compute the distance between bags.
3. Apply similarity-based clustering methods.

Figure 2 visualizes the proposed framework. We note that it is crucial to define a proper distance measure for clustering. In what follows, we discuss distance measures between bags computed in unsupervised (Section 3.2.1) or semi-supervised (Section 3.2.2) ways.

3.2. Weighted Average Distance between Bags

For the unsupervised setting, we are given a data $\{\mathbf{x}_i\}$, or equivalently, bags of instances $\{Z_i\}$, to cluster without any label information. We are interested in grouping these data using off-the-shelf similarity-based clustering methods, and we need to define the distance between bags $d(Z_i, Z_j)$.

There are at least two ways to compute the distance between bags. First, we compute distances between pairs of instances from two bags then aggregate. On the other hand, we aggregate instances to have a single representation for each bag and compute the distance. We take the second approach as it reduces the distance computation significantly.

We note that not all instances should contribute equal to the distance between bags. For example, we do not expect a patch embedding corresponding to the background that are common across both normal and abnormal data to represent an anomaly. Instead, we may want instances for anomalous patterns to contribute more to the distance. To this end, we propose a distance between weighted average embeddings

of two bags as follows:

$$d_{WA}(Z_i, Z_j) = \left\| \left(\sum_{m=1}^M \alpha_m^i \mathbf{z}_m^i \right) - \left(\sum_{n=1}^M \alpha_n^j \mathbf{z}_n^j \right) \right\| \quad (1)$$

where $\alpha \in \Delta^M$ is a weight vector specifying which instance to attend to.

3.2.1 Defining α Without Supervision.

The remaining question is how to define the weight α . Intuitively speaking, we expect α to attend to discriminative instances, e.g., patch embeddings of defective regions, rather than those of normal regions. In MIC literature [70, 10], the maximum Hausdorff distance [27, 17, 18] has been a popular choice, whose distance metric is written as follows:

$$d_{\max H}(Z_i, Z_j) = \max \{d(Z_i, Z_j), d(Z_j, Z_i)\}, \quad (2)$$

$$d(Z_i, Z_j) = \max_{m=1, \dots, M} \min_{n=1, \dots, M} \{\|\mathbf{z}_m^i - \mathbf{z}_n^j\|\} \quad (3)$$

Eq. (3) returns the maximum over instances in Z_i of minimum distances to instances in Z_j , and is likely the distance between inhomogeneous instances of two bags, as shown in Figure 3. Moreover, when α_m^i and α_n^j are determined as below (with a bit abuse of notation), Eq. (1) recovers Eq. (3).

$$\begin{aligned} \alpha_{m^*}^i &= 1, \quad m^* = \arg \max_m \min_n \{\|\mathbf{z}_m^i - \mathbf{z}_n^j\|\} \\ \alpha_{n^*}^j &= 1, \quad n^* = \arg \min_n \{\|\mathbf{z}_{m^*}^i - \mathbf{z}_n^j\|\} \end{aligned} \quad (4)$$

One downside of maximum Hausdorff distance is that, as is clear from Eq. (4), it only focuses on the distance between a single instance from two bags. [70] has proposed an average Hausdorff distance to account for such cases by taking an average instead of maximum of minimum distances, but we find them less suitable for anomaly clustering problem, as shown empirically in Section 4.1.

Alternatively, we propose the soft weight as follows:

$$\alpha_m^i \propto \exp \left(\frac{1}{\tau} \mathbb{E}_{j \neq i} \left\{ \min_n \|\mathbf{z}_m^i - \mathbf{z}_n^j\| \right\} \right) \quad (5)$$

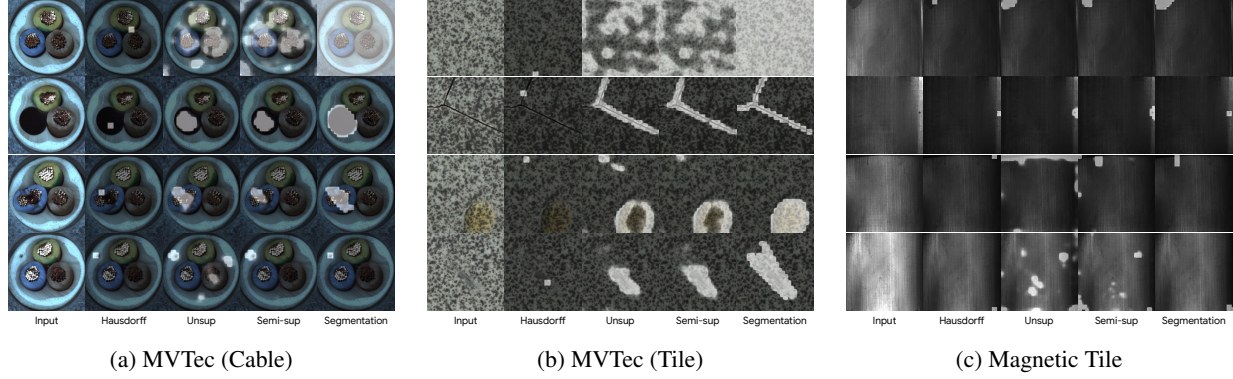


Figure 3: Visualization of weights (α) overlaid on images. From the second column, we show instances (e.g., patches) chosen to compute maximum Hausdorff distances in Equation (4), unsupervised in Equation (5), semi-supervised in Equation (6), and ground-truth segmentation label-based weights.

where τ controls the smoothness of α . For example, when $\tau \rightarrow 0$, we tend to focus on a single instance of m with the maximum average minimum distance, while $\tau \rightarrow \infty$ evenly distributes weights across instances. The inner min operator finds the most similar instance of other bags, and it allows instances that commonly occur across images in the dataset, e.g., patches relevant to non-defective regions, to be down-weighted when computing α . While we choose to aggregate minimum distances with expectation ($\mathbb{E}_{j \neq i}$), there are alternatives, such as $\max(\max_{j \neq i})$ or $\min(\min_{j \neq i})$. However, \max operator would suffer for aligned objects as some normal instances may not be found from an anomalous images. \min operator would suffer if there are duplicates. More explanations on these insights are in Appendix B. Finally, we ablate with combinations of operators in Section 5.3.

We show α chosen by maximum Hausdorff distance criteria of Eq. (4) in the second column, and those based on Eq. (5) in the third column of Figure 3. We observe that defective areas are highlighted for most cases, with an extra granularity for soft weights.

3.2.2 Defining α with Labeled Normal Data.

As in Figure 3, the highlighted regions from unsupervised distance measures are around defective areas. This motivates us to directly derive weight vectors that are designed to attend the defective areas. Motivated by the recent success in semi-supervised defect localization [4, 67, 36, 51], we propose a semi-supervised anomaly clustering, where a few normal data are given to help compute weight vectors. Specifically, we extend Eq. (5) as follows:

$$\alpha_m^i \propto \exp\left(\frac{1}{\tau} \min_{\mathbf{z} \in Z_{\text{tr}}} \|\mathbf{z}_m^i - \mathbf{z}\|\right) \quad (6)$$

where $Z_{\text{tr}} = \bigcup_{\mathbf{x} \in \mathcal{X}_{\text{tr}}} Z(\mathbf{x})$ is a union of bags of normal data $\mathbf{x} \in \mathcal{X}_{\text{tr}}$. Since we put all instances from bags of normal data we do not need expectation. We visualize weight vectors by

Eq. (6) in the fourth column of Figure 3, followed by the ground-truth segmentation mask based weights.

3.3. Comparison to BAMIC [70]

BAMIC [70] is a multiple-instance clustering framework that requires a pairwise distance measure and the similarity-based clustering methods. An instance in [70] uses variants of Hausdorff measure to compute distances and k-medoids for clustering. However, the method following [70] (maxH and k-medoids) performs poorly on anomaly clustering as in Table 2. Besides improved clustering accuracy, our proposal has a few other advantages as we discuss below.

Time complexity. Let N be the number of data. The time complexity of distance measures are written as follows:

$$\begin{aligned} \text{Maximum Hausdorff :} & \quad O(N^2 M^2 D) \\ \text{Weighted Average :} & \quad O\left(\underbrace{N^2 M^2 D}_{\text{Weights in Eq. (5)}} + \underbrace{N^2 D}_{\text{Distance in Eq. (1)}}\right) \end{aligned}$$

While WA appears to be slightly more expensive due to the second term, it is negligible for large bag sizes (M). Importantly, it can be substantially reduced by subsampling the data when computing weights in Eq. (5):

$$\alpha_m^i \propto \exp\left(\frac{1}{\tau} \mathbb{E}_{Z_{\text{sub}} \setminus \{i\}} \left\{ \min_n \|\mathbf{z}_m^i - \mathbf{z}_n^j\| \right\}\right), \quad (7)$$

resulting in $O(N|Z_{\text{sub}}|M^2 D + N^2 D)$, which would be beneficial when $N \gg |Z_{\text{sub}}|$.

Use of labeled normal data. In Section 4.3 we show that the semi-supervised WA distance measure could drastically lift the clustering performance using a small amount of labeled normal data (see Section A.2 for an ablation study). This is a unique feature of WA measure and such an extension has not been discussed in [70]. Notably, the time complexity of semi-supervised WA measure is $O(N|Z_{\text{tr}}|B^2 D + N^2 D)$, making our method scalable with large N .

4. Experiments

We test the anomaly clustering using anomaly detection benchmarks, including MVTec dataset [3] and magnetic tile defect (MTD) dataset [26]. MVTec dataset has 10 object and 5 texture categories. The training set of each category includes normal (non-defective) images, whose number varies from 60 to 391. The test set contains both normal and anomalous (defective) images and anomalous images are grouped into 2~9 sub-categories by defect types. See Figure 1b for an example of anomaly sub-categories. Magnetic Tile Defect dataset has 952 non-defective and 392 defective images. Defective images are grouped into 5 sub-categories, such as blowhole, break, crack, fray or uneven.

Protocol. We test unsupervised and semi-supervised clustering. For unsupervised case, no labeled data is provided for clustering, whereas for semi-supervised case, labeled normal data in the anomaly detection train set is given to compute α in Eq. (6). We emphasize that *no labeled defective images are provided* until we compute evaluation metrics to report. All clustering experiments are under a transductive setting [20, 8] and no training is involved other than deep clustering experiments.

Note that we exclude `combined` sub-categories from evaluation metric computation as images of `combined` category may contain multiple defect types in a single image or their ground-truth labels may not be accurate [3].

Methods. We evaluate combinations of distance measures and clustering methods. For distance measure, we consider (uniform) average, variants of Hausdorff (Table 5) [70], and the proposed weighted average in unsupervised and semi-supervised ways. For clustering, k-means, GMM, spectral clustering, and hierarchical clustering with various linkage options are tested (Table 2). BAMIC [70] is a special case, which combines variants of Hausdorff distance and k-medoids [45] for clustering. Lastly, we make a comparison with state-of-the-art deep clustering methods, including IIC [28], GATCluster [44], and SCAN [60]. A comprehensive comparison to existing methods is in Section 4.2.

Metric. Normalized Mutual Information (NMI) [54] and Adjusted Rand Index (ARI) [48] are two popular metrics for clustering quality analysis when ground-truth cluster assignments are given for test set. We also report the F1 score to account for the label imbalance. The optimal matching between ground-truth and predicted cluster assignments are computed efficiently using Hungarian algorithm [32]. The maximum values of these metrics are 1.0 and higher values indicate a better clustering quality.

Implementation. We use PyTorch [46] for neural network implementations and vision models [64] and scikit-learn [47] for clustering methods.

ImageNet pretrained WideResNet-50 (WRN-50) is used by default to extract patch embeddings, similarly to [51].

Specifically, we use the output of the second residual block followed by 3×3 average pooling. Each patch embedding is then normalized to have unit L2 norm before fed into clustering method. In addition, we conduct an extensive study with diverse pretrained networks (e.g., EfficientNet [58] and Vision Transformer (ViT) [16]) in Appendix A.4.

4.1. Unsupervised Clustering Experiments

In Table 1, we report NMI, ARI, and F1 scores of unsupervised clustering methods on MVTec object, texture and MTD datasets. We test with diverse distance measures, including average (i.e., $\alpha = \frac{1}{M}$ in Eq. (1)), maximum Hausdorff in Eq. (2), and the proposed weighted average in Eq. (5). Finally, hierarchical clustering with Ward linkage [62] is used for clustering. A study using different clustering methods is in Section 4.2.

We confirm that the distance measure using average embeddings performs poorly, whereas that based on discriminative instances chosen by max-min criteria of maximum Hausdorff distance significantly improves the performance. The proposed weighted average distance further improves the clustering NMI score by 0.041 on average. As shown in Figure 3, generated weights attend to multiple discriminative instances instead of a single pair of instances, resulting in improved clustering accuracy.

4.2. Comparison to Other Clustering Methods

In this section, we report the clustering performance with various clustering methods under unsupervised setting. We test spectral clustering and hierarchical clustering with single, complete, and average linkages. In addition, as the bag can be represented as a single aggregated embedding for weighted average distance, we test KMeans and Gaussian Mixture Model (GMM) with full covariance.

Moreover, we test state-of-the-art deep clustering methods that learn deep representations and cluster assignments jointly. It has been studied extensively in recent years [65, 66, 29, 28, 60, 44] and demonstrated a strong performance over shallow counterparts in clustering object-centered images. We study a few state-of-the-art methods, including IIC [28], GATCluster [44], and SCAN [60]. Since we only have a few images per category, methods like SCAN that require a self-supervised pretraining may be suboptimal. In that case, we use the ImageNet pretrained model. Implementation details are in the Appendix C.1.

The results are in Table 2. We find that hierarchical clustering with Ward linkage is particularly effective, followed by the complete linkage. Linkages such as single or average that take into account distances between nearest neighbors between clusters do not perform well for anomaly clustering. Spectral clustering appears to be moderately effective. As mentioned before, the weighted average distance is compatible with more scalable, center based clustering methods

Table 1: NMI, ARI and F1 scores of unsupervised and semi-supervised clustering methods on MVTec (object, texture) and MTD datasets. Compared to the baseline method (“average”) that uses a holistic representation via average pooling of patch embeddings, the multiple instance clustering framework with various distance measures, such as maximum Hausdorff or the proposed weighted average distances, show huge improvement. We also report the performance of weighted average distance whose weights are computed using labeled normal data (“Semi”). We provide per-category results in Table 7 of Appendix.

Supervision	Unsupervised									Semi		
Distance	Average			Maximum Hausdorff			Weighted Average			Weighted Average		
Metric	NMI	ARI	F1	NMI	ARI	F1	NMI	ARI	F1	NMI	ARI	F1
MVTec (object)	0.244	0.109	0.399	0.415	0.275	0.526	0.451	0.346	0.553	0.577	0.449	0.628
MVTec (texture)	0.273	0.123	0.402	0.625	0.534	0.708	0.674	0.601	0.707	0.669	0.570	0.698
MTD	0.065	0.024	0.289	0.193	0.112	0.381	0.179	0.120	0.346	0.390	0.314	0.490
Overall	0.251	0.112	0.394	0.532	0.427	0.631	0.573	0.491	0.636	0.623	0.516	0.663

Table 2: Comparison to other clustering methods, including KMeans, KMedoids, GMM, spectral, and hierarchical clustering with various linkages, using maximum Hausdorff (maxH) or weighted average (WA) distances, and deep clustering methods, such as IIC [28], GATCluster [44], or SCAN [60]. For deep clustering methods, we provide in the parenthesis the performance of the best training epoch chosen by test set accuracy. We report NMIs, and complete results are in the Table 8 of Appendix.

Dataset	MVTEC (object)		MVTEC (texture)		MTD	
Distance	maxH	WA	maxH	WA	maxH	WA
KMeans	–	0.429	–	0.642	–	0.204
GMM	–	0.395	–	0.578	–	0.204
KMedoids	0.140	0.235	0.274	0.430	0.050	0.076
Spectral	0.419	0.428	0.609	0.606	0.143	0.150
Single	0.108	0.133	0.078	0.108	0.087	0.065
Complete	0.316	0.294	0.360	0.452	0.128	0.116
Average	0.245	0.276	0.223	0.400	0.080	0.094
Ward	0.415	0.451	0.625	0.674	0.193	0.179
IIC	0.086 (0.170)		0.107 (0.188)		0.064 (0.034)	
GATCluster	0.119 (0.265)		0.171 (0.298)		0.028 (0.113)	
SCAN	0.176 (0.198)		0.277 (0.314)		0.071 (0.087)	

such as KMeans or GMM, though they perform a bit worse than hierarchical Ward clustering. Finally, we note that the proposed weighted average distance shows higher NMIs for most cases regardless of clustering methods.

We find that state-of-the-art deep clustering methods do not work well on anomaly clustering. Even if we report the best performance chosen via early stopping based on the test set performance (numbers in the parentheses of Table 2), the performance is not as good as our method. The suboptimal performance of deep clustering methods might be due to a lack of data, but requirement for a large amount of data could be their own limitation for industrial applications.

4.3. Semi-supervised Clustering Experiments

We test the semi-supervised clustering described in Section 3.2.2. In this setting we are given labeled normal data

from train set to compute instance weights of Eq. (6). Similarly, we use the hierarchical Ward clustering. The results are described in Table 1. We observe a significant boost in performance over unsupervised clustering methods. For example, we improve upon the best unsupervised clustering method by 0.050 in NMI on average.

Where is the improvement from? We hypothesize that weights derived in a semi-supervised way localize defective instances better than the unsupervised counterpart and make distance more meaningful, leading to an improved clustering accuracy. To answer this question, we visualize semi-supervised weights in Figure 3. While the proposed unsupervised weights are already good at localizing defective areas, we find that it also has a few false positives (e.g., third row of Figure 3b, fourth row of Figure 3a). Whereas, semi-supervised weights effectively remove those false positives. Moreover, we evaluate the pixel-level anomaly localization AUC, achieving 0.973 AUC with semi-supervised weights, improving upon 0.912 AUC of unsupervised weights. This suggests that the lift in clustering accuracy is from better localization of defective patches. We believe that more advanced defect localization and segmentation methods [37] could improve the performance of anomaly clustering.

From this finding, we test using weights derived from the ground-truth segmentation masks,¹ achieving 0.724, 0.685, and 0.467 NMIs for MVTEC object, texture and MTD, respectively, further improving upon unsupervised and semi-supervised clustering performance.

4.4. Cluster Purity

While we report clustering accuracy with known number of clusters in Section 4.1 and 4.3, the number of cluster may not be available in practice. What could be important is the purity of clusters when data is over-clustered. For example,

¹We compute weights by resizing the ground-truth binary segmentation masks with 1 for anomalous and 0 for normal pixels into the same spatial dimension of patch embeddings and normalize their values to sum up to 1.

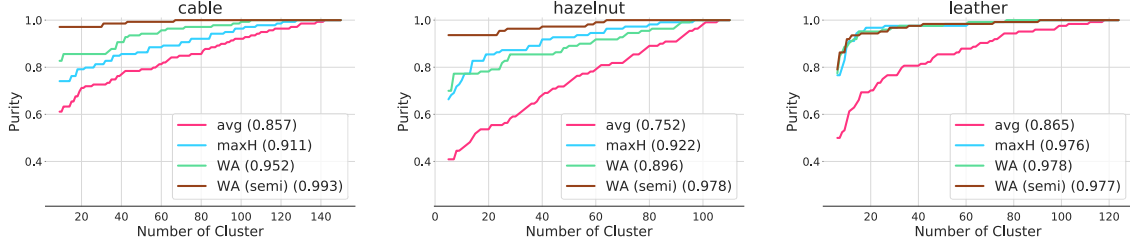


Figure 4: Purity of clusters on a few MVTec categories. Ward clustering is used for clustering method. Numbers in the bracket represent the area under the curve divided by the total number of examples (mAUC). Complete results are in Appendix A.5.

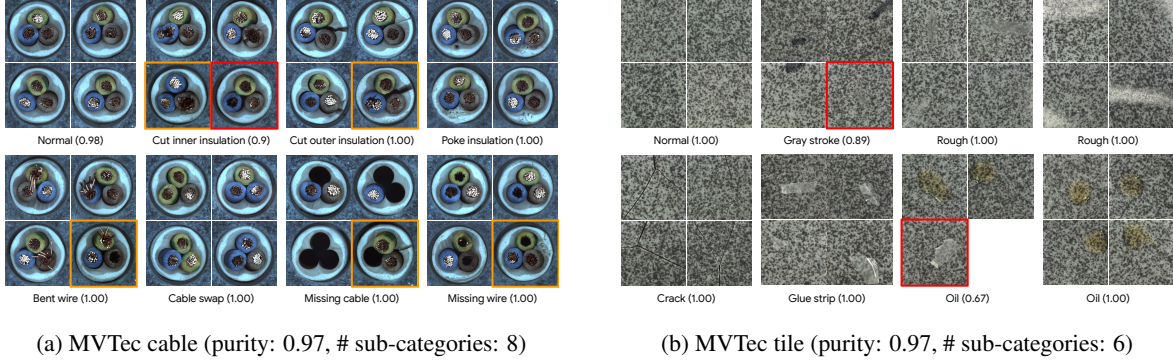


Figure 5: Visualization of images in each cluster using semi-supervised WA distance and Ward clustering with 16 target clusters. We annotate the name of the major sub-category and the purity in parenthesis to each cluster. We highlight images with red if they do not belong to the major sub-category, and with orange when they contain multiple defect types.

the labeling effort could be reduced from the number of data to the number of clusters if we can achieve a high purity.

Figure 4 shows the cluster purity with different number of target clusters for Ward clustering on a few MVTec categories. We see a clear gain in purity with the proposed clustering framework (brown, green, light blue) over the baseline (pink). Moreover, we report purity metrics in Table 3, including mAUC, the area under the curve divided by the total number of examples, and R@P, the reduction in the number of clusters at a given purity.² We confirm that the proposed framework improves the purity. For example, we improve R@0.95 on object categories from 0.231 to 0.527, meaning that we can reduce the number of clusters to label by 53% (compared to exhaustively labeling all images) while retaining 95% cluster purity.

4.5. Cluster Visualization

In Figure 5, we show images of discovered clusters. We over-cluster with 16 clusters using semi-supervised WA distance and hierarchical Ward clustering. We annotate the major defect types to each cluster and the purity in parenthesis.

We verify from Figure 5 that clusters are fairly pure and images with the same or similar type of defects are grouped together. This is because our proposed distance measure is able to attend to discriminative defective areas to compute

Dataset and Metric		average	maxH	WA	WA (semi)
object	mAUC (↑)	0.819	0.868	0.860	0.915
	R@0.9 (↑)	0.380	0.533	0.474	0.671
	R@0.95 (↑)	0.231	0.373	0.346	0.527
	R@0.99 (↑)	0.094	0.204	0.192	0.327
texture	mAUC (↑)	0.807	0.926	0.907	0.940
	R@0.9 (↑)	0.378	0.769	0.760	0.824
	R@0.95 (↑)	0.243	0.702	0.629	0.666
	R@0.99 (↑)	0.083	0.346	0.393	0.366

Table 3: Cluster purity in mAUC, R@0.9, 0.95, 0.99 on MVTec object and texture categories with various distances.

the distance between images. While some images are clustered incorrectly (highlighted in red), they do not seem too different to other images in the same cluster. Another interesting observation is that two “rough” clusters in Figure 5b indeed show somewhat distinctive textures and our method is able to pick such a fine-grained difference to cluster them separately. Finally, there are some images that contain more than one defect type highlighted in orange. For example, in Figure 5a, the one in “bent wire” cluster not only has bent wires but also a missing wire. It is promising that our method at least groups it into one of two correct candidate clusters. We leave a multi-label anomaly clustering, which could assign multiple cluster labels to an image with multiple defect types, as a future work.

²R@P = 1 - (# clusters required to reach purity P)/(# data).

5. Ablation study

In this section we conduct in-depth study of the proposed anomaly clustering framework. Due to space constraint, we provide extra study, such as an impact of number of labeled normal data (Section A.2) or diverse feature extractors (Section A.4), in the Appendix.

5.1. Patch vs Holistic Representation

We highlight the importance of patch embeddings with multiple instance clustering over the holistic representation. For the holistic representation, we use the last hidden layer of WRN-50 after average pooling, resulting in 2048 dimensional vector, as is commonly used in deep clustering literature [60]. For fair comparison, we use the same hidden layer for patch embeddings but without average pooling. For example, we obtain 8×8 2048 dimensional patch embeddings for input of size 256×256 .

In Table 4, we find that holistic representations, though better than learning-based deep clustering methods in Section 4.2, perform worse than our proposed patch-based multiple instance clustering methods. We observe similar trends using various ResNet [24, 69] and EfficientNet [58] models, whose results are in Appendix A.3.

Datasets	Holistic	Hausdorff	WA	WA (semi)
Object	0.256	0.281	0.320	0.381
Texture	0.507	0.542	0.568	0.597
MTD	0.205	0.250	0.227	0.280

Table 4: NMI scores of holistic and patch representations.

5.2. Sensitivity Analysis on τ

Weights in Eq. (5) and (6) play an important role in anomaly clustering. Specifically, both formulations involve the hyperparameter τ that controls the smoothness of the distribution of α , which we ablate in this section. Moreover, we study the variant of weights, called hard weights, where we select k most discriminative instances (instead of softly weighing them) in Appendix A.1.

Figure 6 presents the sensitivity analysis of τ . It shows a trend that intermediate values of τ are preferred and the performance deteriorates as we increase their values as the model converges to uniform weights. Texture classes still shows outstanding performances even with small τ as they can focus on the smaller regions, which is consistent with our observation that some texture anomalies are tiny in size.

5.3. Variants of Distance Measure

Variants of Hausdorff distance metrics are proposed to compute similarities between bags. [10] present variants by replacing max or min operators of Eq. (2) and (3). For example, one can replace max operator in Eq. (2) into mean as suggested in [17]. Exact formulations are in Appendix C.

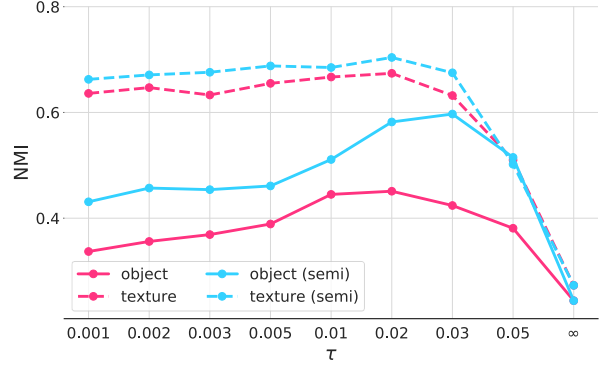


Figure 6: Sensitivity analysis of τ on MVTec dataset.

Variants	Eq. (3)	Eq. (2)	Object	Texture	MTD
Hausdorff distance	mean mean	—	0.196	0.232	0.071
	max min	max	0.415	0.625	0.193
	max min	mean	0.372	0.562	0.160
	min min	—	0.126	0.187	0.130
	mean min	max	0.220	0.400	0.141
	mean min	mean	0.235	0.348	0.134
Variants	Eq. (5)		Object	Texture	MTD
Unsup. weights	$\mathbb{E}_{j \neq i}$		0.451	0.674	0.179
	$\max_{j \neq i}$		0.252	0.614	0.138
	$\min_{j \neq i}$		0.472	0.625	0.052

Table 5: NMIs of anomaly clustering using variants of Hausdorff distance and unsupervised weights.

We report results using variants of Hausdorff distance in Table 5 (top). For asymmetric distance measure such as max min or mean min of Eq. (3), aggregating them by max for Eq. (2) shows better performance. Replacing the first max in Eq. (3) into min or mean degrades the performance, as it deludes the attention to non-discriminative instances, which is critical for clustering data based on anomaly types.

We study variants of unsupervised weight by replacing \mathbb{E} in Eq. (5) into max or min. The results are in Table 5 (bottom). We find that \mathbb{E} works the robustly across datasets. We provide more qualitative analysis in Appendix B.

6. Conclusion

We introduce anomaly clustering, a challenging problem that existing approaches like deep clustering do not work well on. We propose to frame it as a multiple instance clustering problem by taking into account certain characteristics of industrial defects and present a novel distance function that focuses on the defective regions when exist. Experimental results show our proposed framework is promising. Future directions include an extension to multiple instance deep clustering and active anomaly classification. We believe that the proposed framework is not only effective for anomaly clustering, but could also be useful for clustering images of fine-grained deformable objects.

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