

Clustering with Outlier Removal

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ABSTRACT

Cluster analysis and outlier detection are strongly coupled tasks in data mining area. Cluster structure can be easily destroyed by few outliers; on the contrary, the outliers are defined by the concept of cluster, which are recognized as the points belonging to none of the clusters. However, most existing studies handle them separately. In light of this, we consider the joint cluster analysis and outlier detection problem, and propose the Clustering with Outlier Removal (COR) algorithm. Generally speaking, the original space is transformed into the binary space via generating basic partitions in order to define clusters. Then an objective function based Holoentropy is designed to enhance the compactness of each cluster with a few outliers removed. With further analyses on the objective function, only partial of the problem can be handled by K-means optimization. To provide an integrated solution, an auxiliary binary matrix is nontrivially introduced so that COR completely and efficiently solves the challenging problem via a unified K-means--with theoretical supports. Extensive experimental results on numerous data sets in various domains demonstrate the effectiveness and efficiency of COR significantly over the rivals including K-means--and other state-of-the-art outlier detection methods in terms of cluster validity and outlier detection. Some key factors in COR are further analyzed for practical use. Finally, an application on flight trajectory is provided to demonstrate the effectiveness of COR in the real-world scenario.

CCS CONCEPTS

• Security and privacy → Intrusion/anomaly detection and malware mitigation; • Theory of computation → Unsupervised learning and clustering; • Computing methodologies → Cluster analysis;

KEYWORDS

Clustering, Outlier Detection, K-means--

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1 INTRODUCTION

Cluster analysis and outlier detection are two hot topics in data mining community, which have caught raising attention recently. For cluster analysis, a bunch of points are separated into different groups so that similar points are assigned into the same cluster; and for outlier detection, the points with deviating characters are identified as outliers. Tremendous efforts are made to thrive these two areas. To handle outliers or noisy data, some robust clustering methods have been proposed to recover the clean data. Metric learning aims to learn a robust distance function to resist the outliers [6]; L_1 norm is employed to alleviate the negative impact of outliers on the cluster structure [7]; low-rank representation separates the data as the clean part and outliers, and constrains the clean part with the lowest rank for a robust representation [16]. For outlier detection, various methods are put forward from different aspects, including density-based LOF[2], COF[26], distance-based LODF [33], angle-based FABOD [24], ensemble-based iForest [15], eigenvector-based OPCA [14], cluster-based TONMF [12], and so on.

Although cluster analysis and outlier detection are clearly distinct tasks, they are strongly coupled. Cluster structure can be easily destroyed by few outliers [10]; on the contrary, the outliers are defined by the concept of cluster, which are recognized as the points belonging to none of the clusters [2]. However, few of the existing works treat the cluster analysis and outlier detection in a unified framework. The most representative work is K-means--[4]. It aims to detect o outliers and partition the rest points into K clusters, where the instances far away from the nearest centroid are regarded as outliers during the clustering process. Since this problem is a discrete optimization problem in essence, naturally Lagrangian Relaxation (LP) [23] formulates the clustering with outliers as an integer programming problem with several constants, which requires the cluster creation costs as the input parameter. Although these two pioneering works provide new directions for joint clustering and outlier detection, the spherical structure assumption of K-means-- and the original feature space limit its capacity for complex data analysis, and the setup of input parameters and high time complexity in LP make it infeasible for large-scale data.

In this paper, we focus on the joint cluster analysis and outlier detection problem, and propose the Clustering with Outlier Removal (COR) algorithm. Since the outliers are relied on the concept of clusters, we transform the original space into the partition space via running some clustering algorithms (e.g. K-means) with different parameters to generate a set of different basic partitions. By this means, the continuous data are mapped into a binary space via one hot encoding of basic partitions. In the partition space, an objective function is designed based on Holoentropy [31] to increase the compactness of each cluster after some outliers are removed. With further analyses, we transform the partial problem of the objective function into a K-means optimization. To provide a complete and

neat solution, an auxiliary binary matrix derived from basic partitions is introduced. Then COR is conducted on the concatenated matrix, which completely and efficiently solves the challenging problem via a unified K-means-- with theoretical supports. To evaluate the performance of COR, we conduct extensive experimental results on numerous data sets in various domains. Compared with K-means-- and numerous outlier detection methods, COR outperforms rivals over in terms of cluster validity and outlier detection by four metrics. Moreover, we demonstrate the high efficiency of COR, which indicates it is suitable for large-scale and high-dimensional data analysis. Some key factors in COR are further analyzed for practical use. Finally, an application on flight trajectory is provided to demonstrate the effectiveness of COR in the real-world scenario. Here we summarize our major contributions as follows.

- To our best knowledge, we are the first to conduct the clustering with outlier removal in the partition space, which achieves simultaneous consensus clustering and outlier detection.
- Based on Holoentropy, we design the objective function from the aspect of outlier detection, which is partially solved by K-means clustering. By introducing an auxiliary binary matrix, we completely transform the non K-means clustering problem into a K-means-- optimization with theoretical supports.
- Extensive experimental results demonstrated the effectiveness and efficiency of our proposed COR significantly over the state-of-the-art rivals in terms of cluster validity and outlier detection.

2 RELATED WORK

In this section, we present the related work in terms of robust clustering, outlier detection, and highlight the difference between existing work and ours.

To alleviate the impact of outliers, robust clustering¹ has been proposed from different aspects. From the distance function, metric learning is used to learn a robust metric to measure the similarity between two points by taking the outliers into account [6, 32]; L_1 norm models the outliers as the sparse constraint for cluster analysis [7, 9]. From the data, the outliers are assigned few weights during the clustering process [8]; low-rank representation models the data as the clean part and outliers, and constrains the clean part with the lowest rank [16]. From the model fusion, ensemble clustering integrates different partitions into a consensus one to deliver a robust result [20, 25].

Outlier detection, also known as anomaly detection, seeks the points deviation from others and identifies these points as outliers, where most of the existing studies focus on unsupervised outlier detection. Some criteria are designed to assign a score to each point, and the points with large scores are regarded as the outlier candidates. Some representative methods include density-based LOF[2], COF[26], distance-based LODF [33], frequent pattern-based Fp-outlier [11], angle-based ABOD [13] and its fast version FABOD [24], ensemble-based iForest [15], BSOD [22], eigenvector-based OPCA [14], cluster-based TONMF [12].

¹The concept of robust clustering means that the partition is robust to outliers, rather than noisy features.

Cluster analysis and outlier detection are consistently hot topics in data mining area; however, they are usually considered as two independent tasks. Although robust clustering resists to the impact of outliers, each point including outliers is assigned the cluster label. Few of the existing works treat the cluster analysis and outlier detection in a unified framework. K-means-- [4] detects o outliers and partition partitions the rest points into K clusters, where the instances with large distance to the nearest centroid are regarded as outliers during the clustering process. Langrangian Relaxation (LP) [23] formulates the clustering with outliers as an integer programming problem, which requires the cluster creation costs as the input parameter. This problem has also been theoretically studied in facility location. Charikar *et al.* proposed a bi-criteria approximation algorithm for the facility location with outliers problem [3]. Chen proposed a constant factor approximation algorithm for the K-median with outliers problem [5].

In this paper, we consider the clustering with outlier removal problem. Although some pioneering works provide new directions for joint clustering and outlier detection, none of these algorithms expect K-means-- are amenable to a practical implementation on large data sets, while of theoretical interests. Moreover, the spherical structure assumption of K-means-- and the original feature space limit its capacity for complex data analysis. In light of this, we transform the original feature space into the partition space, where based on Holoentropy, the COR is designed to achieve simultaneous consensus clustering and outlier detection.

3 PROBLEM FORMULATION

Cluster analysis and outlier detection are closely coupled tasks. Cluster structure can be easily destroyed by few outlier points; on the contrary, the outliers are defined by the concept of cluster, which are recognized as the points belonging to none of the clusters. To cope with this challenge, we focus on the Clustering with Outlier Removal (COR). Specifically, the outlier detection and clustering tasks are jointly conducted, where o points are detected as the outliers and the rest instances are partitioned into K clusters. Table 1 shows the notations used in the following sections.

Since the definition of outliers relies on the clusters, we first transform the data from the original feature space into partition space via generating several basic partitions. This process is similar to generate basic partitions in consensus clustering [17, 18]. Let X denote the data matrix with n points and d features. A partition of X into K crisp clusters can be represented as a collection of K subsets of objects with a label vector $\pi = (L_\pi(x_1), \dots, L_\pi(x_n))$, $1 \leq l \leq n$, where $L_\pi(x_l)$ maps x_l to one of the K labels in $\{1, 2, \dots, K\}$. Some basic partition generation strategy, such as K-means clustering with different cluster numbers can be applied to obtain r basic partitions $\Pi = \{\pi_i\}$, $1 \leq i \leq r$. Let K_i denote the cluster number for π_i and $R = \sum_{i=1}^r K_i$. Then a binary matrix $B = \{b_l\}$, $1 \leq l \leq n$ can be derived from Π as follows.

$$\begin{aligned} b_l &= (b_{l,1}, \dots, b_{l,i}, \dots, b_{l,r}), \text{ with} \\ b_{l,i} &= (b_{l,i1}, \dots, b_{l,ij}, \dots, b_{l,iK_i}), \text{ and} \\ b_{l,ij} &= \begin{cases} 1, & \text{if } L_{\pi_i}(x_l) = j \\ 0, & \text{otherwise} \end{cases} \end{aligned} \quad (1)$$

Table 1: The Contingency Matrix

Notation	Domain	Description
n	\mathbb{Z}	Number of instances
d	\mathbb{Z}	Number of features
K	\mathbb{Z}	Number of clusters
o	\mathbb{Z}	Number of outliers
r	\mathbb{Z}	Number of basic partitions
X	$\mathcal{R}^{(n \times d)}$	Data set
O	$\mathcal{R}^{(o \times d)}$	Outlier set
Π	$\mathbb{Z}^{(n \times r)}$	Set of basic partitions
B	$\{0, 1\}^{n \times R}$	Binary matrix derived from Π

The benefits to transform the original space into the partition space lie in (1) the binary value indicates the cluster-belonging information, which is particularly designed according to the definition of outliers, and (2) compared with the continuous space, the binary space is more easier to identify the outliers due to the categorical features. For example, Holoentropy is a widely used outlier detection metric for categorical data [31], which is defined as follows.

Definition 3.1 (Holoentropy). The holoentropy $HL(\mathcal{Y})$ is defined as the sum of the entropy and the total correlation of the random vector \mathcal{Y} , and can be expressed by the sum of the entropies on all attributes.

In Ref [31], the authors aimed to minimize the Holoentropy of the data set with o outliers removed. Here we assume there exists the cluster structure within the whole data set. Therefore, it is more reasonable to minimize the Holoentropy of each cluster. In such a way, the clusters become compact after the outliers are removed, rather than the entire data set. Therefore, based on Holoentropy of each cluster, we give our objective function of COR as follows.

$$\min_{\pi} \sum_{k=1}^K p_k HL(C_k), \quad (2)$$

where π is the cluster indicator, including K clusters $C_1 \cup \dots \cup C_K = X \setminus O$, with $C_k \cap C_{k'} = \emptyset$ if $k \neq k'$ and $p_{k+} = |C_k|/(n - o)$. Actually, the objective function in Eq. (2) is the summation of weighted Holoentropy of each cluster, where the weight p_k is proportional to the cluster size. Here the number of cluster K and the number of outliers o are two parameters of our proposed algorithm, which is the same setting with K-means- [4], and we treat determining K and o as an orthogonal problem beyond this paper. In the next section, we provide an efficient solution for COR by introducing another auxiliary binary matrix.

4 CLUSTERING WITH OUTLIER REMOVAL

To solve the problem in Eq. (2), we provide a detailed objective function on the binary matrix B as follows.

$$\sum_{k=1}^K p_k HL(C_k) \propto \sum_{k=1}^K \sum_{b_l \in C_k} \sum_{i=1}^r \sum_{j=1}^{K_i} H(C_{k,ij}), \text{ and} \quad (3)$$

$$H(C_{k,ij}) = -(1-p) \log(1-p) - p \log p,$$

where H denotes the Shannon entropy and p denotes the probability of $b_{l,ij} = 1$ in the ij -th column of C_k .

To better understand the meaning of p in Eq. (3), we provide the following lemma.

LEMMA 4.1. For K -means clustering on the binary data set B , the k -th centroid satisfies

$$\begin{aligned} m_k &= (m_{k,1}, \dots, m_{k,i}, \dots, m_{k,r}), \text{ with} \\ m_{k,i} &= (m_{k,i1}, \dots, m_{k,ij}, \dots, m_{k,iK_i}), \text{ and} \\ m_{k,ij} &= \sum_{b_{l,ij} \in C_k} b_{l,ij} / |C_k| = p, \forall k, i, j. \end{aligned} \quad (4)$$

The proof of Lemma 4.1 is self-evident according to the arithmetic mean of the centroid in K-means clustering. Although Lemma 4.1 is very simple, it builds a bridge between the problem in Eq. (3) and K-means clustering on the binary matrix B .

THEOREM 4.2. If K -means is conducted on $n - o$ inliers of the binary matrix B , we have

$$\max \sum_{k=1}^K \sum_{b_l \in C_k} \sum_{i=1}^r \sum_{j=1}^{K_i} p \log p \Leftrightarrow \min \sum_{k=1}^K \sum_{b_l \in C_k} f(b_l, m_k), \quad (5)$$

where m_k is the k -th centroid by Eq. (4) and the distance function $f(b_l, m_k) = \sum_{i=1}^r \sum_{j=1}^{K_i} D_{KL}(b_{l,ij} || m_{k,ij})$, here $D_{KL}(\cdot || \cdot)$ is the KL-divergence.

PROOF. According to the Bregman divergence [1], we have $D_{KL}(s || t) = H(t) - H(s) + (s - t)^T \nabla H(t)$, where s and t are two vectors with the same length. Then we start on the right side of Eq. (5).

$$\begin{aligned} & \sum_{k=1}^K \sum_{b_l \in C_k} f(b_l, m_k) \\ &= \sum_{k=1}^K \sum_{b_l \in C_k} \sum_{i=1}^r \sum_{j=1}^{K_i} (H(m_{k,ij}) - H(b_{l,ij}) \\ & \quad + (b_{l,ij} - m_{k,ij})^T \nabla H(m_{k,ij})) \\ &= \sum_{k=1}^K |C_k| \sum_{i=1}^r \sum_{j=1}^{K_i} H(m_{k,ij}) - \sum_{k=1}^K \sum_{b_l \in C_k} \sum_{i=1}^r \sum_{j=1}^{K_i} H(b_{l,ij}). \end{aligned} \quad (6)$$

The above equation holds due to $\sum_{b_l \in C_k} (b_{l,ij} - m_{k,ij}) = 0$, and the second term is a constant given the binary matrix B . According to Lemma 4.1, we finish the proof. \square

REMARK 1. Theorem 4.2 uncovers the equivalent relationship between the second part in Eq. (3) and K-means on the binary matrix B . By this means, some part of this complex problem can be efficiently solved by the simple K-means clustering with KL-divergence on each dimension.

Although Theorem 4.2 formulates the second part in Eq. (3) into a K-means optimization problem on the binary matrix B , there still remains two challenges. (1) The first part in Eq. (3) is difficult to formulate into a K-means objective function, and (2) Lemma 4.1 and Theorem 4.2 are conducted on $n - o$ inliers, rather than the whole matrix B . In the following, we focus on these two challenges, respectively.

The second part in Eq. (3) can be solved by K-means clustering, which inspires us to make efforts in order to transform the complete problem into the K-means solution. Since $1 - p$ is difficult involved

into the K-means clustering by Theorem 4.2, which means $1 - p$ cannot be modeled by the binary matrix B , here we aim to model it by introducing another binary matrix $\tilde{B} = \{\tilde{b}_l\}, 1 \leq l \leq n$ as follows.

$$\begin{aligned} \tilde{b}_l &= (\tilde{b}_{l,1}, \dots, \tilde{b}_{l,i}, \dots, \tilde{b}_{l,r}), \text{ with} \\ \tilde{b}_{l,i} &= (\tilde{b}_{l,i,1}, \dots, \tilde{b}_{l,i,j}, \dots, \tilde{b}_{l,i,K_i}), \text{ and} \\ \tilde{b}_{l,i,j} &= \begin{cases} 0, & \text{if } L_{\pi_i}(x_l) = j \\ 1, & \text{otherwise} \end{cases}. \end{aligned} \quad (7)$$

From Eq. (7), \tilde{B} is also derived from Π . Compared with the binary matrix B in Eq. (1), \tilde{B} can be regarded as the flip of B . In fact, B and \tilde{B} are the 1-of- K_i and (K_i-1) -of- K_i codings of the original data, respectively. Based on \tilde{B} , we can define $\tilde{m}_k^{(b)}$ according to Eq. (4), then we have $\tilde{m}_{k,i,j} = 1 - m_{k,i,j} = 1 - p$.

Based on the binary matrices B and \tilde{B} , we transform the problem in Eq. (3) into a unified K-means optimization by the following theorem.

THEOREM 4.3. *If K-means is conducted on $n - o$ inliers of the binary matrix $[B \tilde{B}]$, we have*

$$\min_{\pi} \sum_{k=1}^K p_k HL(C_k) \Leftrightarrow \min \sum_{k=1}^K \sum_{b_l \in C_k} (f(b_l, m_k) + f(\tilde{b}_l, \tilde{m}_k)),$$

where m_k, \tilde{m}_k are the k -th centroid by Eq. (4), and the distance function $f(b_l, m_k) = \sum_{i=1}^r \sum_{j=1}^{K_i} D_{KL}(b_{l,i,j} || m_{k,i,j})$, $f(\tilde{b}_l, \tilde{m}_k) = \sum_{i=1}^r \sum_{j=1}^{K_i} D_{KL}(\tilde{b}_{l,i,j} || \tilde{m}_{k,i,j})$, and $D_{KL}(\cdot || \cdot)$ is the KL-divergence.

REMARK 2. *The problem in Eq. (3) cannot be solved via K-means on the binary matrix B . Nontrivially, we introduce the auxiliary binary matrix \tilde{B} , a flip of B , in order to model $1 - p$. By this means, the complete problem can be formulated by K-means clustering on the concatenated binary matrix $[B \tilde{B}]$ in Theorem 4.3. The benefits not only lie in simplifying the problem with a neat mathematical formulation, but also inherit the efficiency from K-means, which is suitable for large-scale data clustering with outlier removal.*

The proof of Theorem 4.3 is similar to the one of Theorem 4.2, which is omitted here. Theorem 4.3 completely solves the first challenge that the problem in Eq. (2) with inliers with the auxiliary matrix \tilde{B} . This makes a partial K-means solution into a complete K-means solution. In the following, we handle the second challenge, which conducts on the entire data points, rather than $n - o$ inliers.

In this paper, we consider the clustering with outlier removal, which simultaneously partitions the data and discovers outliers. That means the outlier detection and clustering are conducted in a unified framework. Since the centroids in K-means clustering are vulnerable to outliers, these outliers should not contribute to the centroids. Inspired by K-means-- [4], the outliers are identified as the points with large distance to the nearest centroid.

Thanks to Theorem 4.3, we formulate the problem in Eq. (2) with inliers into K-means framework so that the second challenge can fortunately be solved by K-means-- on $[B \tilde{B}]$, where we calculate the distance between each point and its corresponding nearest centroid, and label o points as outliers with the largest distance. In light of this, we propose our clustering with outlier removal in Algorithm 1. The complex clustering with outlier removal problem in Eq. (2) can

Algorithm 1 Clustering with Outlier Removal

Input: X : data matrix;

K, o, r : number of clusters, outliers, basic partitions.

Output: K clusters C_1, \dots, C_K and outlier set O ;

- 1: Generate r basic partitions from X ;
 - 2: Build the binary matrices B and \tilde{B} by Eq. (1)&(7);
 - 3: Initialize K centroids from $[B \tilde{B}]$;
 - 4: **repeat**
 - 5: Calculate the distance between each point in $[B \tilde{B}]$ and its nearest centroid;
 - 6: Identify o points with largest distance as outliers;
 - 7: Assign the rest $n - o$ points to their nearest centroids;
 - 8: Update the centroids by arithmetic mean;
 - 9: **until** the objective value in Eq. (2) remains unchanged.
-

be exactly solved by the existing K-means-- algorithm on the binary concatenated matrix $[B \tilde{B}]$. The major difference is that K-means-- is proposed on the original feature space, while our problem starts from the Holoentropy on the partition space, and we formulate the problem into a K-means optimization with the auxiliary matrix \tilde{B} . After delicate transformation and derivation, K-means-- is used as a tool to solve the problem in Eq. (2), which returns K clusters C_1, \dots, C_K and outlier set O .

Next, we analyze the property of Algorithm 1 in terms of time complexity and convergence. In Line-1, we first generate r basic partitions, which are usually finished by K-means clustering with different cluster numbers. This step takes $O(rt'\bar{K}nd)$, where t' and \bar{K} are the average iteration number and cluster number, respectively. Line 5-8 denotes the standard K-means-- algorithm, which has the similar time complexity $O(tKnR)$, where $R = \sum_{i=1}^r K_i$ is the dimension of the binary matrix B and \tilde{B} . It is worthy to note that only R elements are non-zero in $[B \tilde{B}]$. In Line 6, we find o points with largest distances, rather than sorting n points so that it can be achieved with $O(n)$. It is worthy to note that r basic partitions can be generated via parallel computing, which dramatically decreases the execution time. Moreover, t', t, r and R are relatively small compared with the number of points n . Therefore, the time complexity of our algorithm is roughly linear to the number of points, which easily scales up for big data clustering with outliers.

Moreover, Algorithm 1 is also guaranteed to converge to a local optimum by the following theorem.

THEOREM 4.4. *Algorithm 1 converges to a local optimum.*

PROOF. The classical K-means consists of two iterative steps, assigning data points to their nearest centroids and updating the centroids, which is guaranteed to converge to a local optimum with Bregman divergence [1]. The distance function f in our algorithm is the summation of KL-divergence on each dimension, which can be generalized by Bregman divergence. That means if we conduct K-means clustering on n data points with f , the algorithm converges.

Here K-means-- is utilized for the solution, which has the similar iterative steps. In the following, we analyze the objective function value change of these two steps. $n - o$ points are assigned labels during K-means--, which means that o outliers do not contribute to the objective function. Since the objective function value decreases

in K-means with n points assigned labels, the objective function value with $n - o$ points in Eq. (2) decreases during the assignment phase in K-means-. For the phase of updating the centroids, arithmetic mean is optimal for the labeled $n - o$ points due to the fact that the derivation of the objective function to the centroids is zero. We finish the proof. \square

5 DISCUSSIONS

In this section, we launch several discussions on clustering with outlier removal. Generally speaking, we elaborate it in terms of the traditional clustering, outlier detection and consensus clustering.

Traditional cluster analysis aims to separate a bunch of points into different groups that the points in the same cluster are similar to each other. Each point is assigned with a hard or soft label. Although robust clustering is put forward to alleviate the impact of outliers, each point including outliers are assigned the cluster label. Differently, the problem we address here, clustering with outlier removal only assigns the labels for inliers and discovers the outlier set. Technically speaking, our COR belongs to the non-exhaustive clustering, where not all data points are assigned labels and some data points might belong to multiple clusters. NEO-K-Means [27] is one of the representative methods in this category. In fact, if we set the overlapping parameter to be zero in NEO-K-Means, it just degrades into K-means-. Our COR is different from K-means- in the feature space. The partition space not only naturally caters to the definition of outliers and Holoentropy, but also alleviates the spherical structure assumption of K-means optimization.

Outlier Detection is a hot research area, where tremendous efforts have been made to thrive this area from different aspects. Few of them simultaneously conduct cluster analysis and outlier detection. Except K-means-, Langrangian Relaxation (LP) [23] formulates the clustering with outliers as an integer programming problem, which requires the cluster creation costs as the input parameter. LP not only suffers from huge algorithmic complexity, but also struggles to set this parameter in practical scenarios, which leads LP to return the infeasible solutions. That is the reason that we fail to report the performance of LP in the experimental part. To our best knowledge, we are the first to solve the outlier detection in the partition space, and simultaneously achieve clustering and outlier removal. Our algorithm COR starts from the objective function in terms of outlier detection, and solves the problem via clustering tool, where demonstrates the deep connection between outlier detection domain and cluster analysis area.

Consensus Clustering aims to fuse several basic partitions into an intergrade one. In our previous work, we proposed K-means-based Consensus Clustering (KCC) [28, 29], which transforms the complex consensus clustering problem into a K-means solution with flexible KCC utility functions. Similarly, the input of our COR is also a set of basic partitions, and it delivers the partition with outliers via K-means-. The partition space derived from basic partitions enables COR not only to identify outliers, but also to fuse basic partition to achieve consensus clustering. From this view, Holoentropy can be regarded as the utility function to measure the similarity between the basic partition in B or \bar{B} and the final one. For the centroid updating, the missing values in basic partitions within KCC framework provide no utility, further do not contribute

the centroids. For COR, we can automatically identify the outliers, which do not participate into the centroid updating either.

6 EXPERIMENTAL RESULTS

In this section, we first introduce the experimental settings and data sets, then showcase the effectiveness of our proposed method compared with K-means and K-means-. Moreover, a variety of outlier detection methods are involved as the competitive methods. Some key factors in COR are further analyzed for practical use. Finally, an application on flight trajectory is provided to demonstrate the effectiveness of COR in the real-world scenario.

6.1 Experimental Settings

Data sets. To fully evaluate our COR algorithm, numerous data sets in different domains are employed. They include the gene expression data, image data, high-dimensional text data and other multivariate data. These data sets can be found from [19, 21] and UCI². For each data set, we treat the small clusters with few data points as outliers. Table 3 shows the numbers of instances, features, clusters and outliers of these data sets.

Competitive Methods. K-means and K-means- are used for comparisons. For our COR algorithm, 100 basic partitions are generated via K-means by different cluster numbers from 2 to $2K$ [29], then K-means- is employed with the distance function in Eq. (4.2) for the partition and outliers. Note that K-means- and COR are fed with K and o for fair comparisons, which are true numbers of clusters and outliers, respectively. For K-means, we set the cluster number as the true number plus one, the cluster found by K-means with the smallest size is regarded as the outlier set. Codes of K-means, K-means- and COR are implemented by MATLAB. Each algorithm runs 20 times, and returns the average result and standard deviation. Moreover, several classical outlier detection methods including density-based LOF[2], COF[26], distance-based LODF [33], angle-based FABOD [24], ensemble-based iForest [15], eigenvector-based OPCA [14], cluster-based TONMF [12] are also involved as the competitive methods to evaluate the outlier detection performance³. o points with the largest scores by these methods are regarded as outliers. For the outlier detection methods, some default settings in the original papers are used for stable results. The number of nearest neighbors in LOF, COF, LODF and FABOD is set to 50; the sub-sampling size and the number of trees in iForest are 200 and 100; the forgetting number is set to 0.1 in OPCA; the rank and two parameters in TONMF are 10, 10 and 0.1, respectively.

Validation metric. Although the clustering with outlier removal is an unsupervised task, we can still apply the ground truth to evaluate the performance with label information. Since we focus on the jointly clustering and outlier detection, four metrics are employed to evaluate the performance in terms of cluster validity and outlier detection. The outlier set is regarded as a special cluster in the ground truth.

Normalized Mutual Information (*NMI*) and Normalized Rand Index (R_n) are two widely used external measurements for cluster validity [30]. *NMI* measures the mutual information between

²<https://archive.ics.uci.edu/ml/datasets.html>

³The codes of outlier detection methods can be found at <https://github.com/dsmi-lab-ntust/AnomalyDetectionToolbox> and <https://github.com/ramkikannan/outliernmf>.

Table 2: Performance of clustering with outlier removal via different algorithms (%)

Data set	NMI			Rn			Jaccard			F-measure		
	K-means	K-means--	COR	K-means	K-means--	COR	K-means	K-means--	COR	K-means	K-means--	COR
ecoli	62.27±2.78	61.81±2.37	63.16±1.76	56.6±11.23	52.62±10.33	61.68±8.74	2.34±2.02	45.76±12.78	47.37±3.75	4.50±3.71	61.58±14.6	64.21±3.24
yeast	19.91±0.77	15.81±1.52	20.41±1.08	14.40±0.72	11.85±1.93	18.07±2.04	4.92±1.33	14.38±6.14	50.47±1.45	9.34±2.45	24.69±8.92	67.07±1.29
caltech	69.13±9.92	65.34±11.76	82.69±7.04	47.65±15.48	53.26±24.94	71.25±18.18	8.27±11.41	30.36±15.45	97.19±1.39	13.59±17.88	44.37±19.84	98.57±0.72
sun09	19.67±0.21	10.76±1.41	21.50±1.17	18.61±0.21	9.11±1.69	20.29±1.91	1.84±0.09	3.27±0.44	2.27±0.22	3.62±0.16	6.34±0.81	4.44±0.42
fbis	9.77±2.41	30.27±3.43	54.13±0.85	-0.90±0.23	9.00±3.65	38.36±2.32	0.02±0.07	5.21±0.15	23.77±2.24	0.03±0.14	9.91±0.27	38.35±2.95
k1b	34.4±18.55	33.11±17.06	50.00±5.15	25.12±18.87	21.74±22.48	32.19±9.82	0.00±0.00	0.00±0.00	20.53±0.82	0.00±0.00	0.00±0.00	34.06±1.12
re0	17.14±3.06	15.28±2.78	32.12±2.76	8.86±2.80	8.74±4.54	21.76±3.83	3.18±2.38	8.82±0.68	28.50±1.20	6.07±4.45	16.20±1.15	44.34±1.44
re1	16.19±3.47	11.57±3.92	35.46±2.69	2.79±1.36	3.59±1.81	20.79±2.51	0.29±0.25	16.75±0.34	27.64±1.88	0.59±0.50	28.70±0.51	43.28±2.30
tr11	9.61±0.68	14.89±6.95	58.69±3.94	0.40±0.12	3.92±4.71	50.95±8.55	0.00±0.00	9.93±0.42	34.06±3.03	0.00±0.00	18.06±0.70	50.74±3.44
tr23	7.08±0.81	9.82±2.86	19.43±6.60	-3.67±0.47	1.31±3.02	14.01±8.04	0.00±0.00	5.87±1.02	12.35±2.66	0.00±0.00	11.08±1.84	21.88±4.31
wap	40.51±2.85	22.75±10.42	48.31±2.47	12.03±2.31	6.33±6.33	29.24±7.40	0.60±0.51	10.98±0.31	22.01±1.30	1.18±0.99	19.78±0.50	36.06±1.74
glass	31.35±5.90	33.48±3.78	35.88±3.94	20.03±3.50	23.47±2.09	24.86±1.72	8.23±5.41	24.00±8.28	32.67±2.87	14.8±8.84	37.97±11.59	49.18±3.24
shuttle	11.06±12.49	22.95±3.21	30.74±5.41	18.18±22.67	27.73±5.71	47.40±12.89	0.00±0.00	5.39±0.00	5.58±0.93	0.00±0.00	10.22±0.00	10.56±1.73
kddcup	1.41±0.05	67.04±5.18	86.12±0.60	0.04±0.00	71.40±9.81	93.91±0.85	0.01±0.00	15.06±3.26	15.98±0.63	0.02±0.00	26.03±5.55	27.55±0.96
Average	24.96	29.63	45.62	15.72	21.72	38.91	2.12	12.98	30.03	3.84	22.49	42.16
Score	58.48	62.54	100	42.47	49.05	100	8.56	54.34	97.82	10.03	58.28	97.87

Table 3: Characteristics of data sets

Data set	Type	#instance	#feature	#cluster	#outlier
ecoli	Gene	336	7	5	9
yeast	Gene	1484	8	4	185
caltech	Image	1415	4096	4	67
sun09	Image	3282	4096	3	50
fbis	Text	2463	2000	10	332
k1b	Text	2340	21839	5	60
re0	Text	1504	2886	5	218
re1	Text	1657	3758	6	527
tr11	Text	414	6129	4	87
tr23	Text	204	5832	3	32
wap	Text	1560	8460	10	251
glass	UCI	214	9	3	39
shuttle	UCI	58000	9	3	244
kddcup	UCI	494021	38	3	54499

resulted cluster labels and ground truth labels, followed by a normalization operation, while R_n measures the similarity between two partitions in a statistical way. They can be computed as follows.

$$NMI = \frac{\sum_{i,j} n_{ij} \log \frac{n \cdot n_{ij}}{n_{i+} \cdot n_{+j}}}{\sqrt{(\sum_i n_{i+} \log \frac{n_{i+}}{n})(\sum_j n_{+j} \log \frac{n_{+j}}{n})}},$$

$$R_n = \frac{\sum_{i,j} \binom{n_{ij}}{2} - \sum_i \binom{n_{i+}}{2} \cdot \sum_j \binom{n_{+j}}{2} / \binom{n}{2}}{\sum_i \binom{n_{i+}}{2} / 2 + \sum_j \binom{n_{+j}}{2} / 2 - \sum_i \binom{n_{i+}}{2} \cdot \sum_j \binom{n_{+j}}{2} / \binom{n}{2}},$$

where n_{ij} , n_{i+} , n_{+j} are the co-occurrence number and cluster size of i -th and j -th cluster in the obtained partition and ground truth, respectively.

Jaccard index and F-measure are designed for the binary classification, which are employed to evaluate the outlier detection. They can be computed as follows.

$$Jaccard = \frac{|O \cap O^*|}{|O \cup O^*|},$$

$$F\text{-measure} = 2 * \frac{\text{precision} \cdot \text{recall}}{\text{precision} + \text{recall}},$$

where O and O^* are the outlier sets by the algorithm and ground truth, respectively, and F-measure is the harmonic average of the precision and recall for outlier class.

To evaluate the overall performance on all used data sets, we propose a score as follows.

$$score(A_i) = \sum_j \frac{P(A_i, D_j)}{\max_j P(A_i, D_j)},$$

where $P(A_i, D_j)$ denotes the performance of algorithm A_i on data set D_j in terms of some metric.

Note that these four metrics and the score are positive measurements, i.e., a larger value means better performance. Although R_n is normalized, it can still be negative, which means that the partition is even worse than random label assignment.

Environment. All experiments were run on a PC with an Intel Core i7-5930K@3.50 GHz and a 64 GB DDR3 RAM.

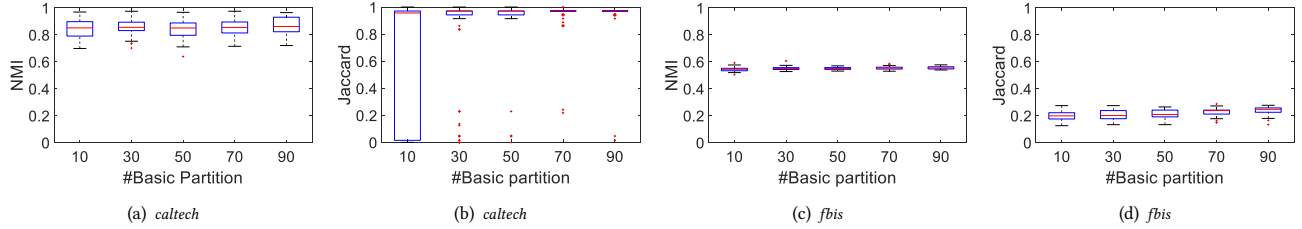
6.2 Algorithmic Performance

Here we evaluate the performance of COR by comparing with K-means-- and outlier detection methods. Table 2 shows the performance of clustering with outlier removal via K-means, K-means-- and COR. There are three obvious observations. (1) few outliers can easily destroy the whole cluster structure. This point can be verified from the fact that K-means delivers poor clustering results on *fbis*, *tr23* and *kddcup* in terms of NMI and Rn. Moreover, K-means fails to capture the outliers by simply increasing the cluster number. (2) K-means-- jointly learns the cluster structure and detects the outliers, which alleviates the negative impact of outliers on the clusters and achieves better performance over K-means on the average level. Although K-means-- slightly outperforms COR on *sun09* in terms of outlier detection, the cluster structure provided by K-means-- is much worse than COR, even K-means clustering. (3) COR exceeds K-means and K-means-- by a large margin in both cluster analysis and outlier detection. For example, COR gains more than 10%, 20% and 40% improvements by cluster validity over rivals on *caltech*, *fbis* and *tr11*, respectively. Moreover, COR also provides better outlier detection results. On *yeast* and *caltech*, there exists more than 30%, 50% gains over K-means--; especially, on *k1b*, COR achieves 25.53 and 34.06 in terms of Jaccard and F-measure; however, K-means-- fails to detect any outliers. Recall that COR is in essence K-means-- on the binary matrix $[B \ \bar{B}]$. The huge improvements result from the partition space, where defines the concept of clusters and achieves the joint consensus clustering and outlier removal. From the score, COR significantly outperforms K-means and K-means-- in terms of all four metrics. Since COR is conducted in the partition space, we also compare with K-means-based Consensus Clustering (KCC) [29] with the same basic partitions by adding one more cluster to capture the outliers. Due to the limited page, we report that on the average level, KCC delivers the competitive cluster results, where COR slightly outperforms KCC by 1.21% and 3.95% in terms of NMI and Rn. Unfortunately, KCC fails to detect any outliers on all the data sets due to different tasks.

Table 4: Performance of outlier detection via different algorithms (%)

Data set	Jaccard										F-measure									
	LOF	COF	LDOF	FABOD	iForest	OPCA	TONMF	K-means--	COR	LOF	COF	LDOF	FABOD	iForest	OPCA	TONMF	K-means--	COR		
ecoli	20.00	38.46	5.88	20.00	38.28	5.88	0.00	45.76	47.37	33.33	55.56	11.11	33.33	55.56	11.11	0.00	61.58	64.21		
yeast	11.45	11.45	5.11	13.85	23.75	26.71	8.66	14.38	50.47	20.54	20.54	9.73	24.32	38.38	42.16	8.11	24.69	67.07		
caltech	2.29	0.75	1.52	8.06	27.62	0.00	0.00	30.36	97.19	4.48	1.49	2.99	14.93	43.28	0.00	1.49	44.37	98.57		
sun09	1.01	2.04	0.00	2.04	2.04	0.00	0.00	3.27	2.27	2.00	4.00	0.00	4.00	4.00	0.00	6.00	6.34	4.44		
fbis	8.32	5.56	4.90	6.41	5.40	4.40	8.32	5.21	23.77	15.36	10.54	9.34	12.05	10.24	8.43	15.36	9.91	38.35		
k1b	0.00	0.00	0.00	0.84	0.00	0.00	1.69	0.00	20.53	0.00	0.00	0.00	1.67	0.00	0.00	3.33	0.00	34.06		
re0	2.59	5.31	3.07	6.34	2.83	11.79	7.13	8.82	28.50	5.05	10.09	5.96	11.93	5.50	21.10	13.30	16.20	44.34		
re1	21.85	15.44	15.19	18.83	16.85	17.77	16.98	16.75	27.64	35.86	26.76	26.38	31.69	28.84	30.17	29.03	28.70	43.28		
tr11	10.13	8.75	19.18	10.83	8.75	8.75	12.99	9.93	34.06	18.39	16.09	32.18	19.54	16.09	16.09	22.99	18.06	50.74		
tr23	4.92	4.92	6.67	10.34	6.67	1.59	10.34	5.87	12.35	9.37	9.37	12.50	18.75	12.50	3.12	18.75	11.08	21.88		
wap	10.82	12.30	6.36	12.81	11.31	6.58	7.49	10.98	22.01	19.52	21.91	11.95	22.71	23.75	12.35	13.94	19.78	36.06		
glass	16.42	36.84	4.00	25.81	13.04	14.71	0.00	24.00	32.67	28.21	53.85	76.90	41.03	23.08	25.64	0.00	37.97	49.18		
shuttle	12.44	12.96	0.21	7.25	1.46	3.61	0.00	5.39	5.58	22.13	22.95	0.41	13.52	2.87	6.97	0.00	10.22	10.56		
kddcup	N/A	N/A	N/A	N/A	21.22	15.66	8.66	15.06	15.98	N/A	N/A	N/A	N/A	35.01	27.08	15.94	26.03	27.55		
Average	9.40	11.91	5.55	11.03	12.80	8.39	5.83	12.98	30.03	16.48	19.47	15.34	19.19	21.36	14.59	10.59	22.49	42.16		
Score	34.33	41.88	18.73	40.10	42.14	28.54	30.72	48.15	91.17	37.09	42.80	27.79	43.02	46.70	31.48	33.60	51.13	89.91		

Note: We omit the standard deviations due to the determinacy of most outlier detection methods. N/A means failure to deliver results due to out-of-memory on a PC machine with 64G RAM.

**Figure 1: Performance of COR with different numbers of basic partitions on *caltech* and *fbis*.**

Beyond K-means and K-means--, we also compare COR with several outlier detection methods. Table 4 shows the performance of outlier detection in terms of Jaccard and F-measure. These algorithms are based on different assumptions including density, distance, angle, ensemble, eigenvector and clusters, and sometimes effective on certain data set. For example, COF and iForest get the best performance on *shuttle* and *kddcup*, respectively. However, in the most cases, these competitors show the obvious disadvantages in terms of performance. The reasons are complicated, but the original space and unsupervised parameter setting might be two of them. For TONMF, there are three parameters as the inputs, which are difficult to set without any knowledge from domain experts. Differently, COR requires two straightforward parameters, and benefits from the partition space and joint clustering with outlier removal, which brings the extra gains on several data sets. On *shuttle* and *kddcup*, COR does not deliver the results as good as the outlier detection methods. In the next subsection, we further improve the performance of COR via different basic partition generation strategy.

Next we continue to evaluate these algorithms in terms of efficiency. Table 5 shows the execution time of these methods on five large-scale or high-dimensional data sets. Generally speaking, the density-based, distance-based and angle-based methods become struggled on high-dimensional data sets, especially FABOD is the most time consuming method, while the cluster-based methods including TONMF, K-means-- are relatively fast. It is worthy to note that the density-based, distance-based and angle-based methods require to calculate the nearest neighbor matrix, which takes huge space complexity and fails to deliver results on large-scale data sets due to out-of-memory on a PC machine with 64G RAM. For COR, the time complexity is roughly linear to the number of instances; moreover, COR is conducted on the binary matrix, rather

Table 5: Execution time by second

Method	sun09	k1b	wap	shuttle	kddcup
K-means	1.12	4.55	1.25	0.22	0.62
LOF	65.16	150.38	26.81	11.93	N/A
COF	79.50	154.02	30.18	181.45	N/A
LDOF	277.25	2638.97	903.43	246.87	N/A
FABOD	567.47	5373.76	1811.28	495.43	N/A
iForest	12.55	12.88	8.53	165.42	1455.41
OPCA	0.40	6.18	1.75	0.30	2.51
TONMF	7.87	31.76	7.67	1.18	18.17
K-means--	3.56	65.28	12.73	0.33	5.98
BP	52.86	121.95	36.58	5.09	5.55
COR	2.31	0.15	0.19	0.57	2.89

Note: BP shows the time for generating 100 basic partitions.

than the original feature space. Thus, COR is also suitable for high-dimensional data. On *k1b*, COR only takes 0.15 seconds, over 400 times faster than K-means-- . Admittedly, COR requires a set of basic partitions as the input, which takes the extra execution time. In Table 5, we report the execution time of generating 100 basic partitions as well. This process can be further accelerated by parallel computing. Even taking the time of generating basic partition, COR is still much faster than the density-based, distance-based and angle-based outlier detection methods.

6.3 Factor Exploration

In this subsection, we provide further analyses on the factors inside COR, the number of basic partitions and the basic partition generation strategy.

In consensus clustering, the performance of clustering goes up with the increase of basic partitions [18, 19, 29]. Similarly, we test COR with different numbers of basic partitions. Figure 1 shows the boxplot of the performance of COR with 10, 30, 50, 70 and 90 basic partitions on *caltech* and *fbis* in terms of NMI and Jaccard. For a certain number of basic partitions, we generate 100 sets of basic partitions and run COR for the boxplot. From Figure 1, we have that COR delivers high quality partitions even with 10 basic partitions,

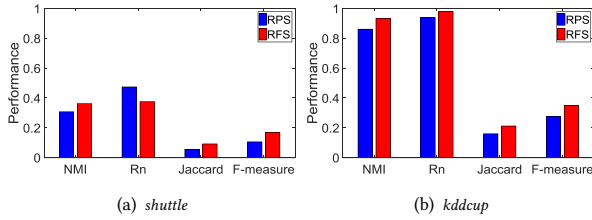


Figure 2: Performance of COR with different basic partition generation strategies.

and that for outlier detection, the performance slightly increases with more basic partitions and stabilizes in a small region. Generally speaking, 30 basic partitions are enough for COR to deliver a good result.

So far, we employ the Random Parameter Selection (RPS) strategy to generate basic partitions, which employs K-means clustering with different cluster numbers. In fact, Random Feature Selection (RFS) is another widely strategy to generation basic partitions, which randomly selects partial features for K-means clustering. In the following, we evaluate the performance of COR with RFS. Here we set the random feature selection ratio to be 50% for 100 basic partitions. Figure 2 shows the performance of COR with different basic partition generation strategies on *shuttle* and *kddcup*. RFS achieves some improvements over RPS on these two data sets with different metrics, except on *shuttle* in terms of Rn. This indicates that RFS is helpful to alleviate the negative impact of noisy features, and further produces high quality basic partitions for COR. It is worthy to note that COR with RFS on *kddcup* achieves 21.18 and 34.95 in terms of Jaccard and F-measure, which exceeds the one with RPS over 5% and 7%, and competes with iForest. This means that COR with RFS gets the competitive performance with the best rival on *kddcup*, and it is over 170 times faster than iForest.

6.4 Application on Trajectory Detection

Finally, we evaluate our COR in the real-world application on outlier trajectory detection. The data come from Flight Tracker⁴, including flightID, flightNum, timestamp, latitude, longitude, height, departure airport, arrival airport and other information. We employ the API to request the flight trajectory every 5 minutes, and collect one-year data from October, 2016 to September, 2017 all over the world. After the data processing, we organize the data with each row representing one flight with evolutionary latitude and longitude. Since these flights have different lengths of records, we uniformly sample 10 records for each flight, where only the latitude and longitude are used as features. Therefore, each flight is processed in a 20-length vector for further analysis. Here we select the Chinese flights between Beijing (PEK), Shanghai (PVG), Chengdu (CTU) and Guangzhou (CAN), and US flights between Seattle (SEA), San Francisco (SFO) and Atlanta (ATL) for further analysis. Figure 3(a) & 3(c) show the trajectories of these Chinese and US flights. By this means, we have the Chinese and US flight trajectory data sets with 85,990 and 33,648 flights, respectively.

Then COR is applied on these two data sets for outlier trajectory detection. Here we set the cluster numbers to be 6 and 3 for these

two data sets, and the outlier numbers are both 200. Figure 3(b) & 3(d) show the outlier trajectories in these two data sets. There are two kinds of outliers. The first category includes the outliers with extra ranges. Although we focus on 7 airports in China and US, there are some trajectories out of the scope of these airport locations in terms of latitude and longitude. The transmission error and loss lead to that the trajectories of different flights are mixed together. In such cases, the system stores a non-existence trajectory. The second category has the partial trajectories. The flight location is not captured due to the failure of the sensors. These two kinds of outliers detected by COR are advantageous to further analyze the problems in trajectory system, which demonstrates the effectiveness of COR in the real-world application.

7 CONCLUSION

In this paper, we considered the joint clustering and outlier detection problem and proposed the algorithm COR. Different from the existing K-means--, we first transformed the original feature space into the partition space according to the relationship between outliers and clusters. Then we provided the objective function based on the Holoentropy, which was partially solved by K-means optimization. Nontrivially, an auxiliary binary matrix was designed so that COR completely solved the challenging problem via K-means-- on the concatenated binary matrices. Extensive experimental results demonstrated the effectiveness and efficiency of COR significantly over the rivals including K-means-- and other state-of-the-art outlier detection methods in terms of cluster validity and outlier detection.

8 ACKNOWLEDGEMENT

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⁴<https://www.flightradar24.com>.

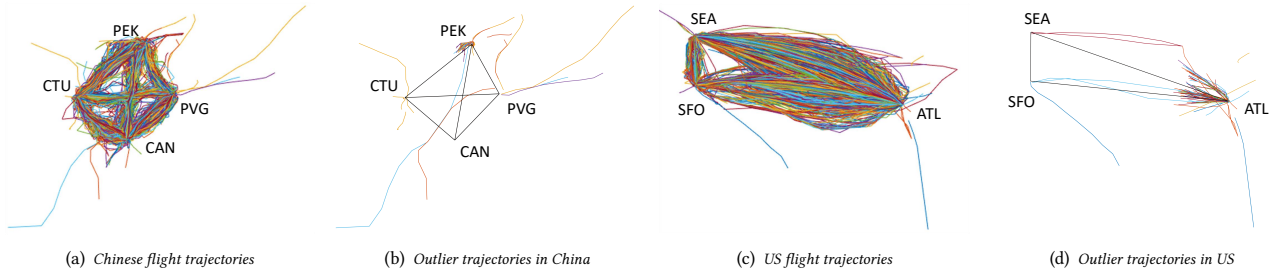


Figure 3: Chinese and US flight trajectories. (a) & (c) show the flight trajectories and (b) & (d) demonstrate the outlier trajectories detected by COR.

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