A Critical Note on the Evaluation of Clustering Algorithms

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ABSTRACT
Experimental evaluation is a major research methodology for investigating clustering algorithms. For this purpose, a number of benchmark datasets have been widely used in the literature and their quality plays an important role on the value of the research work. However, in most of the existing studies, little attention has been paid to the specific properties of the datasets and they are often regarded as black-box problems. In our work, with the help of advanced visualization and dimension reduction techniques, we show that there are potential issues with some of the popular benchmark datasets used to evaluate clustering algorithms that may seriously compromise the research quality and even may produce completely misleading results. We suggest that significant efforts need to be devoted to improving the current practice of experimental evaluation of clustering algorithms by having a principled analysis of each benchmark dataset of interest.

CCS CONCEPTS
• Analytics and machine learning → data mining.

KEYWORDS
Clustering, Experimental Evaluation, Benchmark Datasets

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1 INTRODUCTION
Clustering is one of the fundamental research areas in data science and has found numerous applications in a wide range of domains such as e-commerce, custom relationship management, image processing, and bioinformatics [1, 3, 8]. As an unsupervised learning paradigm, clustering does not require manually assigning labels to the original data, which may be very expensive in real-world scenarios. Instead, clustering aims at automatically exploring the inherent structure of the datasets to help people acquire an in-depth appreciation of the key properties of the data.

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Similar to the research work on classification, the common practice for investigating clustering techniques is by empirical studies where a set of benchmark datasets are used to quantitatively evaluate the performance of specific algorithms. As a result, it is clear that the quality of benchmark datasets plays a key role on the validness or effectiveness of the research outcomes.

To comprehend the current standard of clustering research, we reviewed a number of representative literatures, including survey papers [6, 12, 13] and some recent publications in leading journals and conferences [14, 15]. There are mainly two categories of datasets in use: i) synthetic datasets, which are often of low dimensions for illustration purpose; ii) real-world datasets, which can be flexible in terms of dimensionality. Normally, one or two synthetic 2D or 3D datasets are used to demonstrate the procedure and mechanism of the clustering algorithms, as they are relatively easy to be visualized. After that, real-world datasets come into play to provide further evidence on the practical performance of the clustering algorithms, as it is often assumed that as long as real-world datasets are in use, it is reasonably plausible to make conclusive claims.

Due to their unsupervised nature, clustering algorithms do not require the datasets to be labeled. However, they do need cluster labels as the ground truth against which to judge the quality of clustering. For instance, for a 2D or 3D dataset, it is possible for a researcher to visually identify its clustering pattern (i.e., the number of clusters and the membership of each data point) and use it as the ground truth. However, for higher dimensional datasets, it would be very challenging for a researcher to make the same judgement due to apparent difficulties in visualization. Consequently, people often choose to use standard benchmark datasets such as those in the UCI repository [10] that come with existing labels.

Unfortunately, as this paper will point out, it is a serious flaw in clustering research that has been prevalent for many years without any sign of decease. We claim that this defective research methodology has significantly compromised the quality of clustering research, resulting in inaccurate or completely misleading results. The key issue is that those labels are defined for classification purpose, not clustering, and mixing the two scenarios without any clear justification can produce unpredictable consequences. For example, a dataset may be created by collecting some data from male subjects and female subjects, respectively, and assigning the label $\text{â‘jmaleâ‘A}$ or $\text{â‘jfemaleâ‘A}$ to each corresponding data record. In such case, the label itself can be only used to indicate the property of a certain data record (i.e., its class property), instead of the distribution of the entire dataset, which is the main concern of clustering analysis.

The major contribution of our paper is to highlight the importance of benchmark datasets and raise the alarm about the current practice of evaluating clustering algorithms. In the next section, we...
briefly introduce the performance metrics of clustering algorithms and visualization techniques to be used in our work. In Section 3 and Section 4, we present two insightful case studies to show why it is not technically sound to use class labels as the ground truth for cluster labels. This paper is concluded in Section 5 with further discussions on the better practice of clustering research.

2 PRELIMINARIES

2.1 Performance Metrics

Generally, the performance metrics for clustering can be divided into the following two categories:

1. Internal Criteria: focus on the similarities of clusters, such as the compactness of each cluster and the separation between clusters, which do not require cluster labels.

2. External Criteria: focus on the distribution differences between clustering results and ground truth, which require the true cluster labels.

2.1.1 Davies-Bouldin Index (DBI). DBI [2] is an internal criterion defined as:

$$DBI = \frac{1}{k} \sum_{i=1}^{k} \max_{j \neq i} \frac{\text{avg}(C_i) + \text{avg}(C_j)}{d_{cen}(\mu_i, \mu_j)} \tag{1}$$

where $d_{cen}(\mu_i, \mu_j)$ is the distance between vectors chosen as the representatives of clusters $i$ and $j$, and $\text{avg}(C_i)$ and $\text{avg}(C_j)$ are the dispersions of clusters $i$ and $j$, respectively, and $k$ is the number of clusters. The minimization of its value (ranged from $[0, +\infty)$) indicates natural partitions of datasets.

2.1.2 Silhouette Coefficient (SC). SC [9] is also an internal criterion where each cluster is represented by a silhouette and the entire clustering result is presented by combining the silhouettes into a single plot. The average silhouette width provides an estimation of clustering validity, which is defined as:

$$SC = \frac{1}{n} \sum_{i=1}^{n} SC(i) = \frac{1}{n} \sum_{i=1}^{n} \frac{b(i) - a(i)}{\max\{a(i), b(i)\}} \tag{2}$$

where $a(i)$ is the average dissimilarity of $i$ to all other objects of the same cluster and $b(i)$ is the minimum of the average dissimilarities of $i$ to all other clusters and $n$ is the number of objects in the dataset. The maximization of its value (ranged from $[0, 1]$) indicates the most reasonable clustering of datasets.

2.1.3 Adjusted Rand Index (ARI). ARI [5] is an external criterion used to measure the difference between two clustering results:

$$ARI = \frac{RI - E[RI]}{\max(RI) - E[RI]}, \quad RI = \frac{a + b}{C_n^2} \tag{3}$$

where $a$ is the number of paired objects that are placed in the same cluster in both partitions; $b$ is the number of paired objects that are placed in different clusters in both partitions; $n$ is the number of objects in the data; $C_n^2$ is the number of pairs that can be formed in the dataset. The maximization of its value (ranged from $[-1, 1]$) indicates the largest goodness of fit between the clustering result and the desired partition of data.

2.1.4 Normalized Mutual Information (NMI). The Mutual Information (MI) [11] is a measure that quantifies the mutual dependence between two random variables, or the information that two random variables share. In data mining, it can be used to determine the similarity of two clustering results $U$ and $V$ of a dataset, which is defined as:

$$\text{NMI}(U, V) = \frac{\text{MI}(U, V)}{\sqrt{H(U)H(V)}} \tag{4}$$

where $\text{MI}(U, V)$ is the MI between two partitions and $H(U)$ and $H(V)$ are the entropy values. The maximization of its value (ranged from $[0, 1]$) indicates the largest goodness of fit between two partitions.

2.2 Dimension Reduction

For clustering research, it is an essential yet challenging task to explore the structure of high-dimensional datasets. With the help of dimension reduction techniques, it is possible to have some intuitive clue about the key features of data distribution in the original space. For example, although two separate groups of data may overlap with each other once projected to a 2D space, two separate groups of data in a projected 2D space can imply that these two groups of data are also separate in the higher dimensional space.

The t-SNE algorithm [7] is a powerful tool for dimension reduction, which converts the distance between two points in space into probability. The distance in the original space is represented by a Gaussian distribution, and the probability in the embedded space is represented by a t-distribution. The Kullback-Leibler (KL) divergence of the joint probability density of the original space and the embedded space is used as the loss function, and the gradient descent rule is used to minimize the loss function to obtain the optimal solution. The KL divergence of the probability distributions $P$ and $Q$ is defined as:

$$D_{KL}(P||Q) = -\sum_{i} P(i) \ln \frac{Q(i)}{P(i)} \tag{5}$$

3 CASE STUDY 1: OVERLAPPING DATA

In this case study, we focus on the situation where groups of data with different class labels may overlap with each other. From clustering point of view, it means that some groups may be better regarded as a single cluster. Consequently, using class labels as the ground truth for clustering is not appropriate.

For example, Figure 1 (a) shows the data distribution of a 2D dataset Engytime\(^1\), where objects in different colors belong to different classes. It is clear that there is some overlapping region between the two classes, resulting in a single clustering structure instead of two clusters. Since it is a 2-class dataset, it may be assumed to consist of two clusters. The result of K-means ($k = 2$) is shown in Figure 1 (b) where all objects in the dataset were grouped into two non-overlapping clusters. We also run the density-based clustering algorithm DBSCAN [4], which does not require the number of clusters as input. As expected, all objects were grouped into a single cluster by DBSCAN, as shown in Figure 1 (c).

To further elucidate the issue, the clustering results of K-means, DBSCAN on Engytime were evaluated using the four metrics DBI, 

\(^1\)The download link of Engytime: https://github.com/deric/clustering-benchmark/blob/master/src/main/resources/datasets/artificial/engytime.arff
Figure 1: *Engytime* dataset (a), the clustering result of K-means (b) and the clustering result of DBSCAN (c).

Table 1: The comparison of clustering results on *Engytime*

| Class Label | DBI   | SC    | ARI   | NMI   |
|-------------|-------|-------|-------|-------|
| K-means (k = 2) | 0.999 | 0.406 | -     | -     |
| DBSCAN      | -     | -     | 0.002 | 0.002 |

SC, ARI and NMI. As shown in Table 1, in terms of internal criteria (DBI and SC), K-means was slightly better than directly using class labels to partition the dataset. Meanwhile, in terms of external criteria (ARI and NMI), the performance of DBSCAN, which only identified a single cluster, was extremely poor. However, since the two groups of data overlap with each other, it is more reasonable to regard the entire dataset as a single cluster instead of two clusters. Note that DBI and SC only make sense when there are at least two clusters.

In addition, we analyzed the 4D *Iris* dataset (3 classes) that often appears in clustering research. By visualizing the first three dimensions (sepal length, petal length, and petal width) as shown in Figure 2 (a), we found that the versicolor and virginica classes may be overlapped. However, since the two groups of data overlap with each other, it is more reasonable to regard the entire dataset as a single cluster instead of two clusters. Note that DBI and SC only make sense when there are at least two clusters.

Similarly, the clustering results of K-means (k = 3) and DBSCAN on *Iris* were evaluated, in comparison to using class labels as the cluster labels. In Table 2, in terms of internal criteria (DBI and SC), K-means was slightly better than directly regarding the class labels as the cluster labels. Meanwhile, DBSCAN correctly identified two clusters and achieved the best scores in terms of DBI and SC. However, when using class labels as the ground truth for clustering, it was inferior than K-means.

In summary, when using class labels as the ground truth, we have found significant inconsistences among the performance metrics regarding the same clustering algorithm as well as between its indicated performance and true performance.

### 4 CASE STUDY 2: SPLIT DATA

Another possibility is that objects with the same class label may correspond to multiple clusters. For example, Figure 3 (a) is the 3D plot of selected objects belonging to the two classes named *Climb_stairs* (green) and *Descend_stairs* (red) in *Accelerometer*.

It is clear that objects in the red class are split into roughly two parts and one of them overlaps with the green class. With k = 2, K-means created two clusters with one cluster containing objects from both classes, as shown in Figure 3 (b). Meanwhile, DBSCAN produced very similar results as K-means, as shown in Figure 3 (c).

In Table 3, the results of K-means and DBSCAN were much better than directly using class labels as cluster labels in terms of DBI and SC. However, given class labels as the ground truth, both K-means and DBSCAN produced very inferior ARI and NMI values, which was not consistent with the good clustering results as shown in Figure 3. This example demonstrates again that using class labels as the ground truth for clustering research can be problematic as objects with the same class label can be split into separate clusters.

For high-dimensional datasets, objects with the same class label are more likely to correspond to different clusters due to the sparsity of data in high-dimensional spaces. Figure 4 shows the 2D plot of *Vertebral* (6D, 2 classes) after dimension reduction using t-SNE.

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3The download link of *Accelerometer*: https://archive.ics.uci.edu/ml/datasets/Dataset+for+ADL+Recognition+with+Wrist-worn+Accelerometer

4The download link of *Vertebral*: https://archive.ics.uci.edu/ml/datasets/Vertebral+Column
Figure 3: Accelerometer dataset (a), the clustering result of K-means (b) and the clustering result of DBSCAN (c).

Table 3: The comparison of clustering results on Accelerometer

| Class Label | DBI  | SC   | ARI   | NMI  |
|-------------|------|------|-------|------|
| Class Label | 2.256| -0.044| -     | -    |
| K-means ($k = 2$) | 0.421| 0.722| -0.070| 0.107|
| DBSCAN      | 0.345| 0.719| -0.069| 0.095|

It shows that objects with class label 1 (green) were split into two clusters. Although we cannot tell whether some of them overlap with the objects with class label 0 (red) in the original space, it is sure that objects with class label 1 are not distributed in the form of a single cluster.

Figure 4: The 2D projection of Vertebral using t-SNE

In Table 4, both K-means ($k = 2$) and DBSCAN produced better results than directly using class labels as cluster labels. However, if the class label information is used as the ground truth for evaluating clustering algorithms, both two algorithms produced low ARI and NMI values.

5 CONCLUSION

This paper calls for the close attention from the clustering research community on the current standard of empirical studies. In particular, we show that it is problematic to directly use classification datasets in clustering research without any a priori justification. As shown in the two case studies, using class information as the ground truth for clustering may produce contradicting and misleading results.

Instead of arbitrarily choosing a few black-box datasets from public repositories, it is highly recommended to have a clear understanding about the structure of datasets to provide at least the basic level of assurance about their applicability. Furthermore, due to the challenge of accurately determining the true cluster labels for a non-trivial real-world dataset, advanced synthetic datasets with controlled structure may need to be purposefully generated to better support the principled evaluation of clustering algorithms.

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