A categorical data clustering framework on graph representation

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ABSTRACT

Clustering categorical data is an important task of machine learning, since the type of data widely exists in real world. However, the lack of an inherent order on the domains of categorical features prevents most of classical clustering algorithms from being directly applied for the type of data. Therefore, it is very key issue to learn an appropriate representation of categorical data for the clustering task. In order to address this issue, we develop a categorical data clustering framework based on graph representation. In this framework, a graph-based representation method for categorical data is proposed, which learns the representation of categorical values from their similar graph to provide similar representations for similar categorical values. We compared the proposed framework with other representation methods for categorical data clustering on benchmark data sets. The experiment results illustrate the proposed framework is very effective, compared to other methods.

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1. Introduction

Data clustering is an unsupervised classification technique that aims at grouping a set of unlabeled objects into meaningful clusters, with the requirement that the objects in the same cluster have high similarity but are very dissimilar with objects in other clusters. Clustering techniques have been extensively studied in several communities (e.g., [1] and references therein). Many high-quality clustering algorithms, such as k-means [2], density clustering [3], graph clustering [4–6] have been designed for numerical data. Unfortunately, these algorithms cannot be directly applied for clustering of categorical data, where domain values are discrete and have no ordering defined. Since categorical data is ubiquitous in real-world applications [78], increasing attentions have been paid to clustering the type of data [9,10].

Currently, the wide-used methods for clustering categorical data can be categorized into the following two types.

(1) Direct-clustering method that designs a clustering algorithm which is suitable for categorical data. Currently, there are three types of categorical data clustering algorithms, seen in [11]. The first type is extension of the numerical data clustering algorithms, such as ROCK [12], k-modes [13] and its variants [14–17], which define the distance measure and the cluster centroids for categorical data. Currently, a number of dissimilarity measures for categorical data have been developed, whose related works can be found in [18]. The second type [19–21] is to employ category utility function [22] as a clustering objective function to maximize the probability that two data objects in the same cluster obtain the same attribute values. The third type [23–25] is to use the information entropy to find out groups of similar objects that have lower entropy than those of dissimilar ones. The advantage of direct-clustering methods is that their interpretability is strong. They can sufficiently reflect the characteristics of categorical data. Their disadvantage is that their adaptability is weak. For different types of categorical data, we need to design the corresponding algorithms. Besides, most of state-of-the-art clustering algorithm for numerical data can not be directly applied for categorical data.

(2) Converting-based method that transform categorical data into numerical data and then cluster it by one of the existing clustering algorithms. The two most popular methods are ordinal encoding and one-hot encoding. In ordinal encoding, each categorical value is converted into an integer value. However, the converted numerical data does not necessarily produce meaningful results in the case where categorical domains are not ordered. In one-hot encoding, each category is mapped with a binary variable containing either 0 or 1. Here, 0 represents the absence, and 1 represents the presence of that category. People treat the binary features as numeric in the clustering algorithms [26]. In [27,28], the researchers proposed a link-based representation method which improves the binary features and used the similarity between categorical values, instead of 0. Furthermore, Jiao et al. [29,30], Zhu et al. [31] developed the coupled data embedding (CDE) technique to represent categorical data which can capture the couplings between categor-
ical values and clusters. Zheng et al. [32] make use of similarity between objects to define space structure and representation of categorical data. Besides, people make use of a similarity measure to convert the categorical data into a pairwise-similarity matrix which can be used for spectral clustering. For example, the metric learning methods for categorical data have been proposed in [33–35]. Compared to direct-clustering methods, the converting-based methods can reduce the costs of designing algorithms. However, its disadvantage is that the converted numerical data often has weak interpretability and may lead to information loss of the original categorical data.

In this paper, we focus on converting-based clustering. The effectiveness of categorical data clustering mainly depends on whether they sufficiently make use of the intrinsic similarity of categorical values. However, using numerical vectors to describe the similarity is a challenge for most of converting-based clustering algorithms. In order to solve this problem, we propose a new categorical data clustering framework based on graph representation. This framework divides a categorical data clustering problem into three subproblems: representation of categorical values, representation of objects, and numerical data clustering. Different from existing categorical data representation methods, our main work is to learn and integrate the representation of categorical values from their graph structure, which can sufficiently capture the potential similarity between categorical values and provide the similar numerical representations for similar values.

The outline of the rest of this paper is as follows. Section 2 presents a new categorical data clustering framework. Section 3 demonstrates the performance of the proposed framework. Section 4 concludes the paper with some remarks.

2. Categorical data clustering

2.1. Problem formulation

Let X be a n×m data matrix, where n is the number of objects and m is the number of m categorical features, , where is the jth feature, is the ith row of X which represents the ith objects with m feature values. is the jth feature value of . Each feature describes a domain of values, denoted by , associated with a defined semantic and a data type. Here, only consider two general data types, numerical and categorical, and assume other types used in database systems can be mapped to one of the two types. The domains of features associated with the two types are called numerical and categorical, respectively. A numerical domain consists of real numbers. A domain is defined as categorical if it is finite and unordered, i.e., where nj is the number of categories of feature ai for 1 ≤ j ≤ m. For any 1 ≤ p ≤ q ≤ nj, either or if each feature in A is categorical, X is called a categorical data set.

The aim of clustering categorical data X is to find out a partition of X into k clusters. Let U be a n×k partition matrix of X, where is membership degree of object xi to the ith cluster. Compared to numerical data, the difficulty of clustering categorical data is that we can not visually observe the similarity between categorical values. In order to solve this problem, we study categorical data clustering based on data representation, which transforms the categorical data into numerical data and cluster it.

2.2. Clustering framework

In this paper, we propose a new categorical data clustering framework based on graph representation, seen in Fig. 1. Its main idea is to learn a vector for each categorical value and integrate these vectors of the categorical values which an object includes to represent it. Based on this idea, the clustering problem with categorical data representation can be seen to learn three mappings which are defined as follows.

- f(aij) maps categorical value aij to a vector with p elements to represent it, for 1 ≤ j ≤ m and 1 ≤ h ≤ nj;
- g(xij) = ∪m j=1 f(xij) maps xij to a vector with q elements to represent it, where ∪ is an operation of integrating the vectors of the categorical values of the object;
- π(g(xij)) = [u1j, ··· , uqj] is a clustering function used to map g(xij) to the membership vector of xij.

f(·) and g(·) are used to transform objects into numerical representation. π(·) is to cluster the transformed data and get its membership matrix U. Therefore, we mainly need to discuss how to define f(·) and g(·).

2.3. Representation of categorical value

The one-hot encoding is the most commonly used method to define f(aij), i.e., f(aij) is a binary vector with ni elements, where the jth element is equal to 1 and others are 0. However, the one-hot encoding does not easily reflect the similarity between different categorical values. It can only determine whether two categorical values are the same. In order to solve this problem, we propose a graph-based representation method to get f(·). The main idea of this method is to construct a similarity-relational graph G of all the categorical values and use one of graph embedding methods to learn the representation of nodes in G, which is shown in Fig. 2.

For a graph embedding method, we can easily capture the inherent similarity between categorical values and find similar representations for similar categorical values.

We first construct the graph G. Let G = < V, W > be an undirected and weighted graph, where is an |V| × |V| weight matrix and W(aij, akl) is a weight of the edge between nodes aij and akl, which is computed by measuring the similarity between two objects = {xij = aij, xkl = akl} and = {xij = aij, xkl ∈ X}. We hope W(aij, akl) is proportional to the number of common objects with the categorical values aij and akl, i.e.,

W(aij, akl) ∝ |S(aij) ∩ S(alk)|.

Based on the assumption, we can employ one of set-similarity measures [36] to define W. The representatives of set-similarity measure are shown in Table 1.

Given the graph G of categorical values, the graph embedding is employed to find embedding of nodes to p-dimensions so that “similar” nodes in the graph have embeddings that are close together. Let be a graph embedding function which can transform W into a |V| × p representation matrix Z = φ(W). In this case, we get the representation vector of each categorical value as follows.

f(aij) = zr,

where r = ∑nj=1 ni + h and zr is the rth row of Z. We can employ one of graph embedding methods to get φ(W). Currently, a num-

<table>
<thead>
<tr>
<th>Table 1 Set-similarity measures.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Description</td>
</tr>
<tr>
<td>----------------------------------</td>
</tr>
<tr>
<td>Jaccard coefficient</td>
</tr>
<tr>
<td>Ochiai coefficient</td>
</tr>
<tr>
<td>Overlap coefficient</td>
</tr>
<tr>
<td>Dice coefficient</td>
</tr>
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</table>
Table 2

<table>
<thead>
<tr>
<th>Description</th>
<th>Equation</th>
</tr>
</thead>
<tbody>
<tr>
<td>NE</td>
<td>$Z = W$</td>
</tr>
<tr>
<td>SE</td>
<td>$\min_d tr[Z^T (D - W) Z]$</td>
</tr>
<tr>
<td>NMF</td>
<td>$\min_W</td>
</tr>
<tr>
<td>AE</td>
<td>$\min_{\phi, \psi}</td>
</tr>
</tbody>
</table>

3.5. Graph embedding methods

2.4. Representation of categorical data

Given $f(a_{jh})$ for each categorical value, in order to get $g(x_i)$ to represent objects, we need to define the integration operations $\odot$ which uses the numerical vectors of categorical values of an object to represent it. In this paper, we provide two methods which is shown in Fig. 3 to define $\odot$ as follows.

In the first method, $\odot$ is seen as a joint operation and $g(x_i)$ is defined as

$$g(x_i) = [f(x_{i1}), \ldots, f(x_{im})]$$

which is a mp-dimensional vector. If $f(a_{jh})$ is computed by non embedding, i.e., $Z = W$, the squared Euclidean distance between objects is described as

$$d^2(g(x_i), g(x_j)) = \sum_{h=1}^{m} \sum_{a_{r1} \in V} [W(x_{ih}, a_{r1}) - W(x_{jh}, a_{r1})]^2.$$
The distance does not directly measure the dissimilarity of between corresponding categorical values of two objects but evaluate the difference between the similarity of them with all the categorical values. This indicates that the inherent similarity between categorical values is sufficiently considered in the data representation.

In the second method, ⊙ is defined as a mean operation and then $g(x_i)$ becomes

$$g(x_i) = \frac{1}{m} \sum_{j=1}^{m} f(x_{ij})$$

which is a p-dimensional vector. Compared to the joint operation, this representation has low dimensions and smooth feature values.

2.5. Clustering categorical data

Given $g(x_i)$ for $1 \leq i \leq n$, we can employ one of classical clustering algorithms for numerical data to define the clustering function $\pi(\cdot)$. The clustering algorithm includes k-means, linkage, spectral clustering and so on. Therefore, the overall clustering process in the proposed framework is described in Algorithm 1, which is called “CDC_DR”. According to the description of the algorithm, the computational cost of the proposed framework is made up of constructing graph $O(|V|^2n)$, graph embedding, integration operation $O(nmp)$ and numerical data clustering $O(nk)$ if k-means is selected. For the graph embedding, different methods need different computational costs. The time complexities of NE, SE, NMF and AE (is set as the three-level network) are $O(1)$, $O(|V|^2p)$, $O(|V|^2p + |V|^3p)$ and $O(|V|^3p)$, respectively. We can see that the computational cost of NE is the lowest, since it does not represent graph. The time complexity of NMF is squared with $|V|$ and p. AE needs high training costs, compared to other methods. For spectral embedding (SE), its cost is mainly from eigen decomposition. If the number of nodes in a graph is not large, the computational cost can be acceptable.

3. Experiment analysis

3.1. Experiment environment

In order to examine the performance of the proposed framework, we select Ochiai coefficient as set-similarity measure and k-
means as clustering algorithm. Furthermore, we test four graph-embedding methods including NE, SE, NMF and AE, and two integration operations including Joint and Mean in this framework. While using NE, we know $p$ equal to the sum of the numbers of categorical values of all the features. For SE, NMF and AE, we set $p$ to their average number. We compare the proposed framework with categorical data clustering methods based on five different categorical data encodings: $k$-modes [13], $k$-means with ordinal encoding, one-hot encoding, link-graph encoding [28], and coupled data embedding [29]. Besides, we set the number of clusters on each tested data set to its “true” number of classes. The experiments are conducted on an Intel i9-7940X @ 3.10GHz personal computer with 128G RAM and Matlab 2016b.

In the experiments, we consider two scenarios of comparisons. The one is clustering categorical data sets. The second is clustering ensemble, where multiple clustering results of a data set are seen as its categorical features. A clustering ensemble problem can be seen as a categorical data clustering problem [39,40]. Therefore, in this paper, we also show the performance of the proposed framework on clustering ensemble. The comparisons are carried out on 13 benchmark data sets including (8 categorical data and 5 numerical data), which can be downloaded from https://archive.ics.uci.edu/ml and https://cs.nyu.edu/roweis/data.html. They are described in Table 3.

In these comparisons, we evaluate the clustering accuracy and computational cost of each method on each data set. In order to
measure the clustering accuracy, we employ two widely-used indices, i.e., the normalized mutual information (NMI) and the adjusted rand index (ARI) [36] which measure the similarity between a clustering result and the true partition on a data set. If a clustering result is close to the true partition, then its NMI and ARI values are high. We record the mean and standard deviation of ARI and NMI of each method on each data set. Besides, we count the running time (seconds) of each compared algorithm in the task of converting categorical data.

3.2. Clustering accuracy

Table 4 shows the clustering performance of different graph embedding and integration methods in the proposed framework on given eight categorical data sets. In this table, we also calculate their average and maximum values on each data set. According to the table, we can see that the performance of the proposed framework based on the mean operation is similar to the joint operation. However, the computation cost of the mean operation is obviously less than the joint operation. The main reason is the Matlab environment is more suitable for the mean operation. Thus, we need to further optimize the code of the joint operation. Besides, the joint operation easily makes each of converted data become a high-dimensional data, which further adds the computation costs. In Table 4, we also can observe that the effect of the different graph embedding methods on the clustering performance. We found that the quality of the converted categorical data based on non graph embedding is not worse than that
based on graph embedding. However, the non-graph embedding method needs high computational costs, due to the high dimensionality of the converted categorical data.

Furthermore, we compare the proposed framework based on spectral embedding (CDC_DR+SE) with other algorithms. We first show the visual results of categorical data encoding methods on different data sets, which can be seen in Figs. 4–11. These visual results were produced by using t-SNE [41] to map the encoded categorical data into 2-dimensional spaces. According to these figures, we can see that the visual results of CDC_DR+SE are better than other algorithms on most of data sets. We also can observe that the visual results of CDC_DR+SE with the joint operation are superior to the mean operation. However, since the information loss is caused by reducing dimensions, the performance of an algorithm can not be effectively evaluated in some cases. For example, on data set mushroom, we can not judge which algorithm is effective. Therefore, we need to further compare the clustering accuracy of different algorithms, which can be seen in Table 5. According to Table 5, we can observe that the clustering accuracy of the proposed framework is better than other algorithms on most of the tested data sets. The comparison results show that the proposed framework can obtain an appropriate representation for clustering categorical data in most cases. According to Tables 4 and 5, we also can observe that the maximum ARI and NMI values of the proposed framework with different graph embeddings in Table 4 are obviously superior to other algorithms in Table 5 on all the tested data sets.
data sets. This indicates that if we can select an appropriate graph embedding or integration method, a good representation of categorical data can be obtained.

Besides, in the experiment, we test the clustering performance of the proposed framework on clustering ensemble. We run $k$-means 60 times on each of given numerical data sets to get its categorical data. In order to make the categorical features as different as possible, we set different initial parameters in each time. We randomly select the number of clusters from the interval $[k/2, 2k]$ and the corresponding initial seeds from a data set. We test the proposed framework with different graph embedding and integration methods on the clustering ensemble tasks of given five data sets. The testing results are shown in Table 6. Furthermore, we select the proposed algorithm with spectral embedding to compare it with other algorithms, which is shown in Table 7. In the tables, the bold ARI and NMI values are higher than the best values of other compared algorithms. According to Tables 6 and 7, we can see that the categorical data converted by the proposed framework can further enhance the performance of clustering ensemble.

### 3.3. Clustering efficiency

Table 8 shows the time costs (seconds) for converting categorical data of each algorithm. We can see that the converting costs of $k$-modes, ordinal encoding and one-hot encoding are very low, since they need not learn the representation of categorical data. For some algorithms, e.g., Link, CDE and the proposed framework with NMF, their converting costs are very high on the tasks of clus-
### Table 5
Different methods for clustering categorical data.

<table>
<thead>
<tr>
<th>Dataset</th>
<th>Index</th>
<th>K-Modes</th>
<th>Ordinal</th>
<th>One-Hot</th>
<th>Link</th>
<th>CDE</th>
<th>CDC_DR+-SE</th>
</tr>
</thead>
<tbody>
<tr>
<td>Soybean</td>
<td>ARI</td>
<td>0.6340±0.17</td>
<td>0.6756±0.16</td>
<td>0.7263±0.2</td>
<td>0.6892±0.19</td>
<td>0.7297±0.19</td>
<td>0.7498±0.2</td>
</tr>
<tr>
<td>Zoo</td>
<td>ARI</td>
<td>0.6447±0.14</td>
<td>0.6461±0.16</td>
<td>0.6393±0.14</td>
<td>0.654±0.13</td>
<td>0.6285±0.16</td>
<td>0.6414±0.14</td>
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<tr>
<td>Heart</td>
<td>NMI</td>
<td>0.7552±0.06</td>
<td>0.7602±0.07</td>
<td>0.7603±0.06</td>
<td>0.7554±0.07</td>
<td>0.7625±0.07</td>
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<tr>
<td>Disease</td>
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<td>Derm-</td>
<td>ARI</td>
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<td>0.652±0.17</td>
<td>0.5955±0.18</td>
<td>0.6207±0.16</td>
<td>0.6887±0.16</td>
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<td>Atology</td>
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<td>0.7814±0.08</td>
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<td>Cancer</td>
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<td>0.8038±0.00</td>
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<td>DNA</td>
<td>ARI</td>
<td>0.0183±0.01</td>
<td>0.0395±0.02</td>
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<td>Letters</td>
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<td>Mush.</td>
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<td>Room</td>
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### Table 6
The proposed framework for clustering ensemble.

<table>
<thead>
<tr>
<th>Dataset</th>
<th>Index</th>
<th>NE</th>
<th>SE</th>
<th>NMF</th>
<th>AE</th>
<th>Average</th>
<th>Max</th>
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<tr>
<td>Iris</td>
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<td>0.5638±0.15</td>
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<tr>
<td>Isolet</td>
<td>NMI</td>
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<td>0.7029±0.09</td>
<td>0.7401±0.06</td>
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<td>0.7399±0.08</td>
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<tr>
<td>COIL20</td>
<td>ARI</td>
<td>0.5918±0.05</td>
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<tr>
<td>Optical-</td>
<td>NMI</td>
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### Table 7
Different methods for clustering ensemble.

<table>
<thead>
<tr>
<th>Dataset</th>
<th>Index</th>
<th><em>K</em>Modes</th>
<th>Ordinal</th>
<th>One-Hot</th>
<th>Link</th>
<th>CDE</th>
<th>CDC_DR+-SE</th>
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<tr>
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<td>ARI</td>
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<td>0.5991±0.14</td>
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<td>Isolet</td>
<td>NMI</td>
<td>0.6799±0.12</td>
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</tr>
<tr>
<td>COIL20</td>
<td>ARI</td>
<td>0.5323±0.03</td>
<td>0.5034±0.03</td>
<td>0.5277±0.04</td>
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<tr>
<td>Optical-</td>
<td>NMI</td>
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<td>0.5862±0.05</td>
<td>0.6080±0.05</td>
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### 4. Conclusions

In this paper, we have proposed a simple categorical data clustering framework based on data representation. In this framework,
we learn the representation of each categorical value by graph embedding and integrate the represented categorical values of a data object to convert it into numerical data. Since the proposed framework fully considers the relation between categorical values, it can help existing numerical clustering algorithms to cluster categorical data and find out its potential and meaningful cluster structure. In the experimental analysis, we have compared the proposed framework with other five representation methods of categorical data on 13 benchmark data sets. The comparison results have illustrated that the proposed framework has very good performance.

In the future work, we will consider more complex or advanced similarity measures to construct the graph of categorical values. Besides, we will try more graph embedding methods to represent the categorical values. We will further analyze the effect of the similarity measures and graph embeddings on the effectiveness of the proposed framework.

Declaration of Competing Interest

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References


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