CURE: Flexible Categorical Data Representation by Hierarchical Coupling Learning

Songlei Jian, Guansong Pang, Longbing Cao, *Senior Member, IEEE,* Kai Lu , Hang Gao

Abstract—The representation of categorical data with hierarchical value coupling relationships (i.e., various value-to-value cluster interactions) is very critical yet challenging for capturing complex data characteristics in learning tasks. This paper proposes a novel and flexible coupled unsupervised categorical data representation (CURE) framework, which not only captures the hierarchical couplings but is also flexible enough to be instantiated for contrastive learning tasks. CURE first learns the value clusters of different granularities based on multiple value coupling functions and then learns the value representation from the couplings between the obtained value clusters. With two complementary value coupling functions, CURE is instantiated into two models: coupled data embedding (CDE) for clustering and coupled outlier scoring of high-dimensional data (COSH) for outlier detection. These show that CURE is flexible for value clustering and coupling learning between value clusters for different learning tasks. CDE embeds categorical data into a new space in which features are independent and semantics are rich. COSH represents data w.r.t. an outlying vector to capture complex outlying behaviors of objects in high-dimensional data. Substantial experiments show that CDE significantly outperforms three popular unsupervised encoding methods and three state-of-the-art similarity measures, and COSH performs significantly better than five state-of-the-art outlier detection methods on high-dimensional data. CDE and COSH are scalable and stable, linear to data size and quadratic to the number of features, and are insensitive to their parameters.

Index Terms—Categorical Data Representation, Unsupervised Learning, Coupling Learning, Non-IID Learning, Clustering, Outlier Detection.

1 Introduction

Categorical non-IID data [1] with finite unordered feature values is ubiquitous in real-world applications and has received increasing recent attention for representation and learning [2], [3], [4]. Unlike numerical data, categorical data cannot be directly manipulated per algebraic operations; hence many popular numerical learning algorithms are not directly applicable. Further, learning non-IID data involves the learning of sophisticated coupling relationships (referring to various types and levels of explicit and implicit interactions, *couplings* for short) [5], [6], highly challenging in categorical data. In this work, we focus on learning an expressive numerical representation of categorical data with hierarchical value couplings.

1.1 Motivation

In general, a good representation should effectively capture the intrinsic data characteristics [7]. However, this is challenging for non-IID categorical data [1], in which a key data characteristic is the following hierarchical couplings embedded in feature values. (1) On the low level, there exist strong couplings between feature values, demonstrating the natural clustering of values. Taking census data as an example, it may be clear that the value *PhD* of feature *Education* is highly coupled with the values *Scientist* and *Professor* of feature *Occupation*; and these values form a semantic value cluster that characterizes one type of strong relations between education and occupation. In addition, different value clusters exist on different granularities and with different semantics [8]; e.g., all values belong to one super cluster at the coarsest granularity while each value is a cluster at the finest granularity. (2) On the high level, the clusters of feature values are further coupled with each other. Couplings exist between clusters of the same granularity and between clusters of different granularities.

Representing the above couplings in categorical data has been rarely studied, since couplings in complex data could be presented o different entities and in sophisticated forms and granularities [5], [6], forming an important feature and challenge of non-IID learning [1]. It is even more difficult for unsupervised learning of such coupled data, while existing representation learning mainly focuses on supervised learning of typically IID or partially related data. This work thus addresses this issue, and develops a flexible representation to handle two contrastive unsupervised learning tasks: clustering and outlier detection. Clustering assigns objects to different clusters and its clustering performance is mainly affected by the majority of data objects; while outlier detector identifies abnormal objects which are rare or inconsistent with the majority of objects, hence its performance is mainly affected by the minority of objects.

For clustering, the more relevant the information the representation captures, the more reliable the clustering is, especially for complex data where there are hierarchical couplings. However, existing embedding and similarity-based representation methods for clustering can capture only a part or none of these feature value couplings. Typical embedding-based representation methods transform cate-

- *Songlei Jian, Kai Lu and Hang Gao are with the Laboratory of Science and Technology on Parallel and Distributed Processing and the College of Computer, National University of Defense Technology, China. Songlei Jian is also visiting the Advanced Analytics Institute, University of Technology Sydney, Australia.*
- *Guansong Pang and Longbing Cao are with the Advanced Analytics Institute, University of Technology Sydney, Australia.*

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gorical data to numerical data by encoding schemes, e.g., one-hot encoding and Inverse Document Frequency (IDF) encoding [9]. These methods do not capture the couplings between feature values since they usually treat features independently. Some recent similarity-based representation methods, e.g., in [2], [10], [11], [12], incorporate feature relations into similarity or kernel matrices. However, they do not capture the couplings from value-to-value clusters or the couplings between value clusters, leading to insufficient representation power in handling data with such hierarchical value couplings.

For outlier detection, the representation capturing more relevant information, however, does not guarantee better performance. The captured information also needs to be outlier-discriminative. Most encoding or similarity-based methods [2], [10], [11] are majority objects-based representation, which does not capture the abnormal aspects of data. Different from these methods, most existing outlier detection methods for categorical data [13], [14], [15], [16] use pattern-based representation (i.e., the data is represented by a set of outlying/normal patterns) to disclose the characteristics of outliers. However, patterns are normally a subset of compactly predefined value combinations and can only capture partial couplings between values. This may result in less expressive representation power in data with sophisticated value couplings, in particular high-dimensional data, in which there exists a complex mixture of relevant and irrelevant features. A very recent method called CBRW [17] models the full value couplings to generate value-based representation for categorical outlier detection, which shows value-based representation is more fine-grained and flexible than pattern-based methods. However, CBRW captures only pairwise value couplings but not the high-order couplings between values.

1.2 Contributions

This work captures the hierarchical value-to-value cluster couplings, which reflect some intrinsic data characteristics and complexities. Such value cluster couplings need to be properly captured in data representations for different learning tasks and application scenarios. However, this is not trivial, and to our best knowledge, no work reported properly handles this. Accordingly, this paper proposes a flexible framework which captures the hierarchical value couplings and can be instantiated to solve two contrastive learning problems. The main contributions are as follows.

- A framework for Coupled Unsupervised categorical data REpresentation (CURE for short) is proposed, which has a hierarchical learning structure and is flexible enough to be instantiated. CURE defines multiple value coupling functions for clustering values with different granularities to capture the low-level complex couplings between values. CURE further learns the couplings between the multi-granularity value clusters to incorporate high-order couplings between values into our value-based data representation. This enables CURE to capture the intrinsic data characteristics and produce an effective numerical representation for categorical data with sophisticated couplings.
- CURE can handle contrastive unsupervised learning tasks: clustering and outlier detection. For clustering, we instantiate CURE into a Coupled Data Embedding (CDE for short) model to capture hierarchical value couplings between values of majority frequencies. CDE utilizes the couplings to embed categorical data into a new space with independent dimensions and rich semantics. This creates a meaningful Euclidean space for the subsequent object clustering.
- For outlier detection, CURE is instantiated into a model for the Coupled Outlier Scoring of High-dimensional data (COSH for short) to capture minority-based hierarchical value couplings. COSH uses the multi-granularity value clusters to compute the most outlying aspect of values, which enables it to obtain reliable outlier scores in data sets with many irrelevant and noisy features.

Substantial experiments show that (1) CDE significantly outperforms three popular encoding methods: one-hot encoding (noted as 0-1), one-hot encoding with PCA (0-1P), and inverse document frequency embedding (IDF), with a maximum F-score improvement of 19%. It also gains a maximum 8% F-score improvement over three state-of-the-art similarity measures for clustering: COS [2], DILCA [11] and ALGO [10] on 10 real-world data sets with different value coupling complexities; (2) COSH significantly outperforms (by a maximum 67% AUC improvement) five state-of-the-art outlier detection methods: CBRW [17], ZERO [18], iForest [19], ABOD [20] and LOF [21] on 10 high-dimensional data sets; (3) CDE and COSH obtain good scalability: they are linear to data size and quadratic to the number of features; and (4) CDE and COSH perform stably and are insensitive to their parameters.

The rest of this paper is organized as follows. We discuss the related work in Section 2. The CURE framework is detailed in Section 3. Two complementary value coupling functions are presented in Section 4. Two instances of CURE, CDE and COSH, are introduced in Section 5. Experimental results for clustering and outlier detection are provided in Section 6 and Section 7, respectively. A discussion of instantiating CURE is given in Section 8. The conclusion is drawn in Section 9.

2 Related Work

2.1 Representation for Clustering

Encoding methods are most widely used for categorical data representation [22]. One popular method is one-hot encoding which encodes each feature with a zero-one matrix. Feature f_i is encoded with $|\mathcal{V}_i|$-dimensional vectors, where each vector has a value '1' corresponding to one value, and all the rest of the entries are 0s. Although one-hot coding is reversible to its original data, it assumes that all values are independent and equal which often does not conform to data characteristics. Also, one-hot encoding results in very high dimensions if the original data has a large number of values, and consequently, it may lead to the curse of the dimensionality issue [23]. Dimension reduction methods, like principal component analysis (PCA) [24], are often conducted on a one-hot encoding matrix to alleviate this issue. Another well-known method is IDF encoding [9] which represents each value as the logarithm of its inverse

frequency. IDF captures the value couplings from the occurrence perspective. Although these encoding methods are easy to implement and have good efficiency, they cannot capture the complex value couplings in data.

Several effective embedding methods are available for textual data, such as latent semantic indexing (LSI) [25], latent Dirichlet allocation (LDA) [26], skip-gram [27] and their variants [28], [29], [30]. However, categorical data has an explicit feature structure, which is very different from unstructured textual data. These methods cannot be directly applied to categorical data which is the focus of this work.

Similarity learning represents categorical data with an object-object similarity matrix. Various similarity measures have been designed to capture value couplings in data: ALGO [10] uses the conditional probability of two feature values to describe the value couplings; DILCA [11] and DM [12] incorporate feature selection and feature weighting into capturing feature couplings respectively; and COS [2] takes inter- and intra-feature couplings into object similarity. These similarity measures focus on capturing the pairwise value couplings. They therefore fail to capture the couplings among multiple values and higher order couplings, which instead can be captured by CDE w.r.t. the couplings between value clusters.

In addition, there are some embedding methods, e.g., in [31], [32], which optimize the embedding on the similarity matrix, but their results heavily rely on the underlying similarity measures. Other embedding methods (e.g., [33], [34]) require class labels to learn distance, and thus they are inapplicable for unsupervised tasks.

2.2 Representation for Outlier Detection

Most existing outlier detection methods [13], [14], [15], [16] for categorical data unify the two successive tasks - data representation and outlier identification. These methods often aim to identify a set of outlying/normal patterns to represent data objects. Such outlier detection-oriented methods use scoring-based representation, which is very different from embedding or similarity measures. They separate model learning from data representation learning and focus on how to effectively transform the original data into a meaningful space to well enable outlier detection. However, these methods involve costly pattern discovery. As a result, their computational time is prohibitive in high-dimensional data. Also, these methods become ineffective in handling data with many irrelevant/noisy features [17].

There have been some methods (e.g., in [17], [18], [35]) which are scalable for high-dimensional data. The method CBRW [17] models the intra- and inter-feature value couplings to estimate the outlierness of values and uses value outlierness to represent the objects. CBRW is closely related to COSH as it also attempts to use value outlierness to represent data. CBRW avoids a costly pattern search and has good scalability w.r.t. data dimensionality. However, CBRW only captures pairwise value couplings and may fail to work in data with higher-order value couplings, e.g., high-dimensional data. The method ZERO++ [18] can efficiently handle high-dimensional data by working on a random set of feature subspaces, but the random subspace generation may include many irrelevant features and downgrade its performance on those data. The method ITB [35] identifies a set of outliers so that the removal of these outliers from the data mostly reduces entropy-based data uncertainty. However, it uses the full feature set to compute uncertainty and is largely affected by irrelevant features, thus it becomes less effective in high-dimensional data where outliers are manifested in a small subset of features.

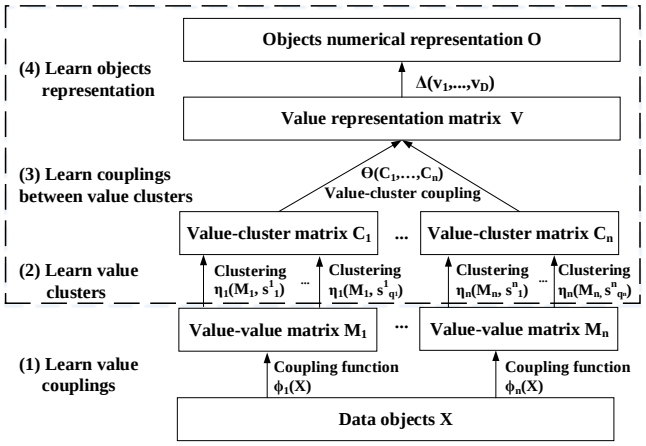

Fig. 1. The CURE framework: Φ, η, Θ and Δ can be customized according to different tasks. By changing the dashed line boxed part, we instantiate the framework into two instances: CDE and COSH.

Some methods like ABOD [20] and iForest [19] for high-dimensional numeric data may also be extended to handle categorical data by working on its embedding or similarity-based numeric representation, but their performance is heavily dependent on the effectiveness of the data representation methods.

More importantly, all the above methods estimate the outlier scores based on single-granularity outlierness representation, i.e., outlierness estimation operates with the same granularity. Our method COSH captures the outlierness with a wide range of granularities. Our outlierness estimation is therefore less likely to be biased by the overwhelming irrelevant features in high-dimensional data.

3 The CURE Framework for Categorical Data Representation

In this section, we introduce the CURE framework to model hierarchical couplings between values and value clusters so as to learn a numerical representation of categorical data. As shown in Fig. 1, CURE first learns the low-level couplings between values by several coupling functions. It then learns value clusters with different granularities by clustering on multiple value coupling matrices with different granularity settings. CURE further learns the couplings between value clusters to obtain the value representation and the object representation.

Let $\mathcal{X} = \{x_1, x_2, ..., x_N\}$ be a set of data objects with size N, described by a set of D categorical features $\mathcal{F} = \{f_1, ..., f_D\}$. Each feature f ($f \in \mathcal{F}$) has a value domain $\mathcal{V}_f = \{v_1, v_2, ...\}$ which consists of a finite set of possible feature values (at least two values). The value domains of different features are distinct, i.e., $\mathcal{V}_{f_i} \cap \mathcal{V}_{f_j} = \emptyset, \forall i \neq j$.

The whole value set of features is the union of all the value domains: $\mathcal{V} = \cup_{f \in \mathcal{F}} \mathcal{V}_f$, and the size of $\mathcal{V}$ is denoted as L.

The problem targeted in this work can then be stated as follows. Given a set of data objects $\mathcal{X}$, we aim to learn the object numerical representation $\mathbf{O}$ of $\mathcal{X}$. Following the CURE framework, we firstly construct the value coupling set $\Phi(\mathcal{X})$ by learning value couplings. Secondly, we learn the value clusters in the value clustering process Ω_η. Thirdly, the couplings between value clusters are learned in the coupling learning process Θ. Finally, the object representation are learned by Δ. The four components of CURE: Φ, Ω_η, Θ and Δ are introduced in detail in the following sections.

3.1 Learning Value Couplings

Value couplings refer to the explicit and implicit interactions between feature values which may include the interactions between values from the same feature and the interactions between values from different features. Such value couplings reflect the low-level interactions between values. The more value couplings are learned will be of more benefit to the following value clusters. The definition of the value coupling set is given as follows.

Definition 1 (Value Coupling Set)**.** *The value coupling set $\Phi(\mathcal{X})$ is defined as a set of multiple value coupling functions with size of n to capture the low level pairwise value couplings:*

$$\Phi(\mathcal{X}) = \{\phi_i(\mathcal{X}), i = 1, 2, .., n\}, \tag{1}$$

where $\phi_i(\cdot) : \mathcal{X} \mapsto \mathbf{M}_i \in \mathbb{R}^{L \times L}$ is one kind of value coupling functions to capture the value couplings from one specific perspective. The output of ϕ_i is a value coupling matrix $\mathbf{M}_i$ which consists of couplings between each value pair.

These value coupling matrices are decided by the value coupling functions and reflect the low-level data characteristics. The value coupling functions can be specified from several aspects [1], [6], e.g., occurrence-based and co-occurrence-based functions, set theory-based functions (such as intersection of value sets), value neighbourhood-based functions, and/or non co-occurrence-based functions. Good value coupling functions should capture different kinds of couplings.

3.2 Learning Value Clusters

A *value cluster* refers to the value set which consists of multiple similar values. The value clusters reflect the couplings among multiple values instead of pairwise value coupling, e.g., all values belong to one super value cluster at the coarsest granularity while each value is a cluster at the finest granularity. The definition of the value clustering process is given as follows.

Definition 2 (Value Clustering Process)**.** *The value clustering process w.r.t. value coupling matrix $\mathbf{M}$ consists of multiple clustering on value coupling matrices at different granularities, which is defined as follows:*

$$\Omega_\eta = \{\eta_i(\mathbf{M}_i, s_j^i), j = 1, 2, ..., q^i\}, \tag{2}$$

where η_i is the one clustering process on the value coupling matrix $\mathbf{M}_i$, and s_j^i is the clustering parameter which decides the granularity of clusters. The output of η_i is a value cluster matrix $\mathbf{C}_i \in \mathbb{R}^{L \times q^i}$.

The value clustering process can be done by various clustering methods, e.g., centroid-based clustering algorithm, hierarchical clustering algorithms, distribution-based clustering, and density-based clustering algorithms. The granularities of value clusters can be decided by the predefined algorithm parameters, e.g., the cluster number, and the density range parameter. Different clustering algorithms prefer different kinds of clusters. For example, centroid-based clustering algorithms capture the convex shape of clusters, while density-based clustering algorithms are able to capture the manifold shape of clusters. We can conduct different clustering algorithms on different value coupling matrices or apply only one clustering algorithm on all coupling matrices with different parameters. The choice of clustering process is decided by the cluster characteristics captured by the clustering algorithm and its efficiency.

3.3 Learning Couplings between Value Clusters

The value clusters learned by clustering may contain couplings and redundancy. By learning the complex couplings between value clusters, CURE learns the meaningful value representation. The definition of coupling learning between value clusters is defined as follows.

Definition 3 (Coupling Learning Between Value Clusters)**.** *The coupling learning process Θ between value clusters is defined as follows:*

$$\mathbf{V} = \Theta\{\mathbf{C}_1, ..., \mathbf{C}_n\}, \tag{3}$$

where $\mathbf{C}_i$ is one value cluster matrix and $\mathbf{V} \in \mathbb{R}^{L \times \sum_{i=1}^{n} q^i}$ is the value representation matrix.

The coupling learning process between value clusters aims to learn the couplings between different value clusters and tries to eliminate the redundancy information among value clusters. Accordingly, Θ can be implemented by a dimensionality reduction process, a relation learning process, or an embedding model, e.g., PCA, LDA, matrix factorization, or a neural network. The choice of Θ depends on the data characteristics and the subsequent learning tasks.

3.4 Learning Object Representation

With the value representation, we further model the object representation.

Definition 4 (Object Representation Learning Function)**.** *The representation of an object x ($x \in \mathcal{X}$) is modelled by an object representation function w.r.t. value representations $\mathbf{V}$:*

$$\mathbf{O}^x = \Delta(\mathbf{V}_1^x, ..., \mathbf{V}_D^x), \tag{4}$$

where $\mathbf{V}_i^x$ is the value representation of object x from feature f_i.

The function $\Delta(\cdot)$ utilizes value representations to assign each object a numerical vector for object representation. The function can be specified according to learning applications and purpose, e.g., by concatenation, weighted sum, or maximum.

4 COMPLEMENTARY VALUE COUPLINGS

In this paper, we instantiate the CURE framework into two models: CDE for clustering and COSH for outlier detection to address contrastive learning goals. Both CDE and COSH are based on the same value coupling functions, which is the base for further learning value clusters. In this section, we introduce the two value coupling functions and prove their complementary discriminative ability.

4.1 Two Value Coupling Functions

To learn value couplings, we construct two value influence matrices to capture the value couplings from two basic perspectives: occurrence and co-occurrence, whose complementary discriminative ability is proved in Section 4.2. Before introducing the value influence matrices, we introduce some preliminaries.

The value from feature f of object x is denoted by v_x^f and the feature to which the value v_i belongs is denoted as f_i. We assume that the probability $p(v)$ of a value can be computed by its frequency. The joint probability of two values v_i and v_j is $p(v_i, v_j) = \frac{|\{v_x^{f_i}=v_i \cap v_x^{f_j}=v_j, x\in\mathcal{X}\}|}{N}$.

We define the normalized mutual information [36] ψ to reflect the relation between two features as follows:

$$\psi(f_a, f_b) = \frac{2\sum\limits_{v_i\in\mathcal{V}_{f_a}}\sum\limits_{v_j\in\mathcal{V}_{f_b}} p(v_i,v_j)log\frac{p(v_i,v_j)}{p(v_i)p(v_j)}}{h(f_a)+h(f_b)}, \quad (5)$$

where $h(f_a) = -\sum_{v_i\in\mathcal{V}_{f_a}} p(v_i)log(p(v_i))$.

Definition 5 (Occurrence-based Value Influence Matrix)**.** *The occurrence-based value influence matrix $\mathbf{M}_o$ is defined as follows:*

$$\mathbf{M}_o = \begin{bmatrix} \phi_o(v_1,v_1) & \dots & \phi_o(v_1,v_L) \\ \vdots & \ddots & \vdots \\ \phi_o(v_L,v_1) & \dots & \phi_o(v_L,v_L) \end{bmatrix}, \quad (6)$$

where the coupling function $\phi_o(v_i, v_j) = \psi(f_i, f_j) \times \frac{p(v_j)}{p(v_i)}$, indicating the occurrence influence on value v_i from value v_j.

The occurrence (or marginal) probability is the basic univariate property of values, which can be used to differentiate values. Instead of using a symmetric distance measure between the marginal probabilities of two values, we use an asymmetric ratio to quantify the influence on one value from another so that $\mathbf{M}_o$ captures more information. Furthermore, we incorporate mutual information ψ as the weight of value couplings since marginal probabilities cannot differentiate features.

Definition 6 (Co-occurrence-based Value Influence Matrix)**.** *The co-occurrence-based value influence matrix $\mathbf{M}_c$ is defined as follows:*

$$\mathbf{M}_c = \begin{bmatrix} \phi_c(v_1,v_1) & \dots & \phi_c(v_1,v_L) \\ \vdots & \ddots & \vdots \\ \phi_c(v_L,v_1) & \dots & \phi_c(v_L,v_L) \end{bmatrix}, \quad (7)$$

where the coupling function $\phi_c(v_i, v_j) = \frac{p(v_i,v_j)}{p(v_i)}$ indicates the co-occurrence influence of value v_j on value v_i.

The co-occurrence (or joint) probability reflects the basic bivariate couplings between two values. We use asymmetric conditional probability to define the influence on one value from another value since the same joint probability may have a different influence on values with different marginal probabilities. The ϕ_c value of two values from the same feature always equals 0 since they never co-occur in the same object.

4.2 Complementary Discriminative Ability

The two coupling functions are complementary and discriminative for the values, which can be verified by the distance of $\mathbf{M}_o$ and $\mathbf{M}_c$. As we illustrate CDE and COSH to learn value clusters by *k*-means clustering, we thus take the Euclidean distance as an example to show the complementary discriminative ability of these two value coupling functions.

The distance matrix in *k*-means clustering determines the quality of value clusters. By proving the complementary discriminative ability of the two distance matrices, we can observe that the two value couplings have a complementary discriminative ability.

The occurrence distance between values v_i and v_j is defined as follows:

$$d_o(v_i, v_j) = \sqrt{\sum_{h=1}^{L}(\phi_o(v_i, v_h) - \phi_o(v_j, v_h))^2}, \quad (8)$$

where $\phi_o(v_i, v_h)$ is the occurrence coupling function defined in Definition 5, and L is the number of values.

The co-occurrence distance between values v_i and v_j is defined as follows:

$$d_c(v_i, v_j) = \sqrt{\sum_{h=1}^{L}(\phi_c(v_i, v_h) - \phi_c(v_j, v_h))^2}, \quad (9)$$

where $\phi_c(v_i, v_h)$ is the co-occurrence coupling function defined in Definition 6. If any two distinct values can be distinguished by d_o or d_c, then d_o and d_c are complementary.

Theorem 1 (Distance Complementarity)**.** *For any two values $v_i \neq v_j$, $d_o(v_i, v_j) \neq 0$ or $d_c(v_i, v_j) \neq 0$.*

Proof. To prove the above theorem, we prove that $v_i \neq v_j$ and $d_o(v_i, v_j) = 0$ satisfy $d_c(v_i, v_j) \neq 0$ for all cases and $v_i \neq v_j$ and $d_c(v_i, v_j) = 0$ satisfy $d_c(v_i, v_j) \neq 0$ for all cases.

We first prove that $v_i \neq v_j$ and $d_o(v_i, v_j) = 0$ satisfy $d_c(v_i, v_j) \neq 0$ for all cases. If $d_c(v_i, v_j) = 0$, then $\forall v_h \in \mathcal{V}, \phi_c(v_i, v_h) = \phi_c(v_j, v_h)$. To prove $d_c(v_i, v_j) \neq 0$, we only need to prove $\exists v_h \in \mathcal{V}, \phi_c(v_i, v_h) \neq \phi_c(v_j, v_h)$. We consider the proof for the following cases.

(1) If v_i and v_j belong to the same feature which means $\psi(f_i, f_h) = \psi(f_j, f_h)$, then $d_o(v_i, v_j) = 0$ if and only if $p(v_i) = p(v_j)$. Let $v_h = v_i$, then $\phi_c(v_i, v_h) = 1$ and $\phi_c(v_j, v_h) = 0$ since v_i, v_j belong to the same feature. Hence, $d_c(v_i, v_j) \neq 0$ when v_i and v_j belong to the same feature.

(2) If v_i and v_j belong to different features, and $d_o(v_i, v_j) = 0$ which means $\forall v_h \in \mathcal{V}, \psi(f_i, f_h)\frac{p(v_h)}{p(v_i)} = \psi(f_j, f_h)\frac{p(v_h)}{p(v_j)}$; When $\psi(f_i, f_h) \neq \psi(f_j, f_h)$ and $p(v_i) \neq p(v_j)$ (suppose $p(v_i) < p(v_j)$), then $p(v_i, v_j) < p(v_j)$. Let $v_h = v_i$, then $\phi_c(v_i, v_h) = 1$ and $\phi_c(v_j, v_h) > 0$.

Accordingly, $d_c(v_i, v_j) \neq 0$ when $p(v_i) \neq p(v_j)$. When $\psi(f_i, f_h) = \psi(f_j, f_h)$ and $p(v_i) = p(v_j)$, $\exists v_h$ in feature f_i and $p(v_j, v_h) > 0$, but $p(v_i, v_h) = 0$, then $\phi_c(v_j, v_h) \neq \phi_c(v_i, v_h)$. Therefore, $d_c(v_i, v_j) \neq 0$ when v_i and v_j belong to different features.

Further, we prove $v_i \neq v_j$ and $d_c(v_i, v_j) = 0$ satisfy $d_o(v_i, v_j) \neq 0$ for all cases. We consider the proof for the following cases.

(1) If v_i and v_j belong to the same feature, then we can let $v_h = v_i$ so that $\phi_c(v_i, v_h) = 1$ and $\phi_c(v_i, v_h) = 0$. Then we can prove that $d_o(v_i, v_j) \neq 0$.

(2) If v_i and v_j belong to different features, then we can consider $p(v_i) = p(v_j)$ or $p(v_i) \neq p(v_j)$. If $p(v_i) = p(v_j)$ and $d_c(v_i, v_j) = 0$, then $\psi(f_i, f_h) = 1$ which is impossible for different features. Otherwise, we let $v_h = v_i$ (suppose $p(v_i) < p(v_j)$) then $\phi_c(v_i, v_h) = 1$ and $\phi_c(v_j, v_h) < 0$, and $d_c(v_i, v_j)$ cannot be 0. So if $d_c(v_i, v_j) = 0$, then v_i and v_j must belong to the same feature. □

The above theorem shows that the two value couplings are able to distinguish any two different values. For clustering, the theorem says that at least one clustering process is able to differentiate any two values in an extreme case where each value belongs to one cluster. For outlier detection, the theorem states that the outlier detector could differentiate the outlying behaviors between any two values. For different applications, we can enhance the discriminative ability from a specific aspect by utilizing different information of value clusters. The following section demonstrates how to utilize the value couplings to learn the value clusters and the couplings between the value clusters for different goals.

5 Two Contrastive CURE Instances

In this section, we show two instances of CURE: CDE for clustering and COSH for outlier detection in high-dimensional data. CDE and COSH use the above value couplings, but they use different methods to learn the value clusters and the couplings between the value clusters.

5.1 CDE: A CURE Instance for Clustering

We instantiate CURE as CDE for clustering. CDE aims to capture the couplings among values with majority frequencies based on the above value couplings. CDE learns the value clusters with different granularities by multiple *k*-means clusterings with different cluster numbers k. By filtering the value clusters which have less discriminative information for majority values, CDE differentiates values according to the value-to-value cluster affiliation. Based on the information in the filtered value clusters, CDE learns the couplings between the value clusters with PCA. The object embedding is the concatenation of value representation.

5.1.1 Learning Value Clusters for Clustering

Based on the two value influence matrices, we can learn the value clusters with different granularities which represent different semantics and well reflect the data characteristics. To learn the value clusters with different granularities, here we conduct clustering on the value matrices with different cluster numbers.

We conduct *k*-means clustering on $\mathbf{M}_o$ with different k, i.e., $\{k_1, k_2, ..., k_{n_o}\}$, and on $\mathbf{M}_c$ with $\{k_1, k_2, ..., k_{n_c}\}$. The clustering results are represented by a cluster membership indicator matrix $\mathbf{C^I}$, which is defined as follows:

$$\mathbf{C^I}(i,j) = \begin{cases} 1 & \text{if } v_i \text{ is in cluster j,} \\ 0 & \text{if } v_i \text{ is not in cluster j.} \end{cases} \tag{10}$$

For the majority values, the value cluster with a small number of values has less discriminative information since CDE aims to generate the value clusters which can differentiate more values. Accordingly, we remove the small value clusters which only have one value. k is also decided by the removed small clusters which will be discussed in Section 5.1.3. We further concatenate the two indicator matrices derived from the two value influence matrices and get a large indicator matrix to represent each value whose dimensionality is no more than $(\sum_{i=1}^{n_o} k_i + \sum_{j=1}^{n_c} k_j)$.

k-means clustering is chosen for two major reasons: (1) The value influence matrices are numerical and the Euclidean distance fed to the *k*-means clustering captures the global relations between values. (2) *k*-means clustering is linear w.r.t. the size of the input matrix, which enables CDE to efficiently learn value clusters with different sizes.

5.1.2 Learning Linear Couplings between Value Clusters

The indicator matrix $\mathbf{C^I}$ conveys rich couplings between the value clusters with different granularities based on two value influence matrices. For simplicity, we here consider a simple type of couplings between value clusters – linear correlations and apply PCA on the indicator matrix to eliminate the linear correlations between value clusters to obtain a vector embedding for each value. PCA is chosen because (1) it reduces the data complexity with little loss of information by converting a matrix with linearly correlated variables to a new matrix with linearly uncorrelated components, and (2) it substantially reduces the dimensionality of the value embedding, which enables us to represent an object in a considerably lower-dimensional embedding space.

We first calculate the centralized matrix $\mathbf{Z}$ of the indicator matrix $\mathbf{C^I}$ by subtracting the mean of each column and further derive a covariance matrix $\mathbf{S}$ from $\mathbf{Z}$. The value embedding $\mathbf{V}$ is obtained by the following matrix decomposition:

$$\mathbf{V} = \mathbf{Z}\mathbf{Y}^T, \tag{11}$$

where $\mathbf{Y}$ is the principal component matrix derived from the singular value decomposition results of $\mathbf{S}$, i.e., $\mathbf{S} = \mathbf{U}\mathbf{\Sigma}\mathbf{Y}$.

After the PCA transformation, the dimensions of value embedding $\mathbf{V}$ are independent of each other so that the algebraic operations in the Euclidean space can be used on the embedded matrix.

5.1.3 The CDE Algorithm

Algorithm 1 presents the main procedures of CDE. The first step generates the value influence matrices $\mathbf{M}_o$ and $\mathbf{M}_c$ according to Definitions (5) and (6) by scanning the original data matrix. Specifically, we scan the data matrix by rows. For each row, we scan it by columns two times, and then we get the co-occurrences of any two values. After scanning all

Algorithm 1 *CDE ($\mathcal{D}$, α, β)*

Input: $\mathcal{D}$ - data set, α - proportion factor, β - dimension reducing factor
Output: $\mathbf{O}$ - the numerical representation of objects
1: Generate $\mathbf{M}_o$ and $\mathbf{M}_c$
2: Initialize $\mathbf{C^I} = \emptyset$
3: **for** $\mathbf{M} \in \{\mathbf{M}_o, \mathbf{M}_c\}$ **do**
4: Initialize $k = 2$
5: $\mathcal{C}_s = \emptyset$
6: **repeat**
7: $\mathbf{C^I} = [\mathbf{C^I}; kmeans(\mathbf{M}, k)]$
8: Store the clusters with one value in $\mathcal{C}_s$
9: Remove the clusters with one value from $\mathbf{C^I}$
10: $k+ = 1$
11: **until** $\frac{length(\mathcal{C}_s)}{k} \geq \alpha$
12: **end for**
13: $\mathbf{Z} = \mathbf{C^I} - mean(\mathbf{C^I})$
14: [$\mathbf{U}$, $\mathbf{\Sigma}$, $\mathbf{Y}$] = SVD ($\mathbf{S}$), $\mathbf{S}$ is the covariance matrix of $\mathbf{Z}$
15: $\mathbf{V} = \mathbf{ZY}^T$
16: Remove the columns whose range (maximum element minus minimum element) is less than β from $\mathbf{V}$.
17: Generate $\mathbf{O}$ by the concatenation of $\mathbf{V}$
18: **return** $\mathbf{O}$

the rows, we calculate the frequency of any value. Then we calculate the coupling functions.

k is the clustering parameter which decides the granularity of value clusters. Instead of setting k to a fixed value, we use another proportion factor α to decide the maximum cluster number, as shown in Steps (6-10) of Algorithm 1. The clusters that only have one value are meaningless to value cluster. Therefore, we remove these small clusters with only one value by controlling the proportion of small clusters through α. With the increasing of k more small clusters are generated. Until the proportion of small clusters, i.e., $\frac{length(\mathcal{C}_s)}{k}$, exceeds α, we stop increasing k whose initial value is 2. The final $\mathbf{C^I}$ is the concatenation of all clustering results with different k from $\mathbf{M}_o$ and $\mathbf{M}_c$.

After conducting PCA on the indicator matrix to learn the correlations between value clusters, we treat $\mathbf{V}$ as the original representation of values where each column represents a dimension. Since the distance between two values is the sum of the distance on each dimension, the columns with a small range make less contribution to the final distance. We remove those columns whose range (maximum element minus minimum element) is less than β from original representation $\mathbf{V}$. In this way, we control the dimension of the representation in a flexible data-dependent way. Finally, we calculate the object embedding $\mathbf{O}$ by concatenating the embedding vectors of its values from $\mathbf{V}$.

We generate $\mathbf{M}_o$ and $\mathbf{M}_c$ through the value frequency vector and co-occurrence matrix. Scanning the data set and counting the frequency of all values and co-occurrences of all value pairs incur the complexity of $O(ND^2)$. Generating $\mathbf{M}_o$ and $\mathbf{M}_c$ based on the frequency vector and co-occurrence matrix incurs the complexity of $O(L^2)$. The total number of clustering times is $(k_{max} - 1)$ due to that k_{max} increases from 2. Then clustering on the value matrix has complexity $O(k_{max}L)$ since k-means clustering has linear complexity w.r.t. the size of the input matrix. The number of value clusters is proportional to k_{max}^2 and then PCA has $O(k_{max}^6)$. With the numerical representation of values, generating the embedding matrix of objects has $O(ND)$. The computational complexity of CDE is $O(ND^2 + L^2 + k_{max}^6)$. Since k_{max} does not increase w.r.t. D and N and k_{max} is a relatively small constant, k_{max}^6 is much smaller than ND^2. And in real datasets, the average number of values per feature is often small, so L^2 is similar to D^2. Approximately, the time complexity of CDE is $O(ND^2)$.

5.2 COSH: A CURE Instance for Outlier Detection in High-dimensional Data

Here we further instantiate CURE to another instance COSH for outlier detection in high-dimensional data which contains complex value couplings and has been insufficiently explored. COSH uses the same clustering methods, i.e., *k*-means, to learn multi-granularity value clusters. Different from CDE that abandons small value clusters, COSH retains them as they may reflect the outlying behaviors of values. Unlike CDE which uses binary cluster membership to represent the value clusters, COSH represents them with continuous dissimilarity between values and cluster centers to better quantify the outlying behaviors of values. Based on the dissimilarity of value clusters, COSH learns couplings between value clusters. The object representation is the vector with outlying score of each value.

5.2.1 Learning Value Clusters for Outlier

In COSH, we also conduct *k*-means clustering on the two value coupling matrices. In addition to the reasons explained in Section 5.1.1, the sensitivity of *k*-means clustering is an important reason of using it to learn value clusters for outlier detection.

Instead of indicator matrix, we use the value-cluster dissimilarity matrix to represent the clustering result for each clustering process. The definition of value-cluster dissimilarity matrix $\mathbf{C}^k$ w.r.t. cluster number k is below:

$$\mathbf{C}^k = \begin{bmatrix} dis(\mathbf{v}_1, \mathbf{c}_1) & \dots & dis(\mathbf{v}_1, \mathbf{c}_k) \\ \vdots & \ddots & \vdots \\ dis(\mathbf{v}_L, \mathbf{c}_1) & \dots & dis(\mathbf{v}_L, \mathbf{c}_k) \end{bmatrix}, \tag{12}$$

where $\mathbf{v}$ is a row of a value coupling matrix $\mathbf{M}$, $\mathbf{c}$ is the centroid vector of one cluster. dis is defined as follows:

$$d(\mathbf{v}, \mathbf{c}) = \begin{cases} 0 \text{ , if } \mathbf{v} \text{ and } \mathbf{c} \text{ are in different clusters} \\ max(0, \sum_{i=1}^{L} \mathbf{c}(i) - \mathbf{v}(i)), \text{otherwise.} \end{cases} \tag{13}$$

The use of the above asymmetry dissimilarity measure instead of distance measures, e.g., Euclidean distance, is decided by the semantic meaning of $\mathbf{M}_o$ and $\mathbf{M}_c$. There is a basic assumption that outlying values are infrequent among all values. The value coupling matrices $\mathbf{M}_o$ and $\mathbf{M}_c$ are correlated with value frequency. Hence, a smaller value from $\mathbf{M}_o$ and $\mathbf{M}_c$ indicates the greater likelihood that it could be an outlying value. Further, a value smaller than the centroid has a larger chance of being an outlier than a value larger than the centroid.

Algorithm 2 *COSH ($\mathcal{D}$, α)*

Input: $\mathcal{D}$ - data set, α - proportion factor
Output: $\mathbf{O}$ - the outlier scores of all objects
1: Generate $\mathbf{M}_o$ and $\mathbf{M}_c$
2: Initialize $i = 0$
3: **for** $\mathbf{M} \in \{\mathbf{M}_o, \mathbf{M}_c\}$ **do**
4: Initialize $\mathbf{k} = \emptyset$ and $j = 2$
5: $\mathcal{C}_s = \emptyset$
6: **repeat**
7: $\mathbf{k}(i) = j$
8: $\mathbf{C}^i = kmeans(\mathbf{M}, \mathbf{k}(i))$
9: Calculate $\mathbf{D}_i$
10: Store the clusters with one value in $\mathcal{C}_s$
11: $j+ = 1$ and $i+ = 1$
12: **until** $\frac{length(\mathcal{C}_s)}{\mathbf{k}(i)} \geq \alpha$
13: **end for**
14: $\mathbf{V} = max_e\{\mathbf{C}^q\mathbf{D}_q\mathbf{1}_{\mathbf{k}(q)}, q = 1, 2, ..., i\}$,
15: **for** each $x \in \mathcal{X}$ **do**
16: $\mathbf{O}^x = [\mathbf{V}_1^x, ..., \mathbf{V}_D^x]$
17: **end for**
18: **return** $\mathbf{O}$

5.2.2 Learning Outlying Couplings between Value Clusters

We consider two properties of the outlying value and the outlying value cluster: (1) The outlying value is quite different from the centroid. (2) The outlier cluster is quite different from the other clusters. The value cluster matrix $\mathbf{C}^k$ defined in Section 5.2.1 has considered the difference between a value and the centroid. We use another cluster-cluster matrix to incorporate the outlying couplings of value clusters, which is defined as follows:

$$\mathbf{D}_k = \begin{bmatrix} dis(\mathbf{c}_1, \mathbf{c}_1) & \dots & dis(\mathbf{c}_1, \mathbf{c}_k) \\ \vdots & \ddots & \vdots \\ dis(\mathbf{c}_k, \mathbf{c}_1) & \dots & dis(\mathbf{c}_k, \mathbf{c}_k) \end{bmatrix}, \quad (14)$$

where $dis(\cdot)$ is the dissimilarity defined in Equation 13.

Based on these two properties, we learn the value outlier scores w.r.t. to the value cluster difference matrix $\mathbf{C}^k$ and cluster-cluster matrix $\mathbf{D}_k$ as follows:

$$\mathbf{V} = max_e\{\mathbf{C}^{k_1}\mathbf{D}_{k_1}\mathbf{1}_{k_1}, \mathbf{C}^{k_2}\mathbf{D}_{k_2}\mathbf{1}_{k_2}, ...\}, \quad (15)$$

where $\mathbf{1}_k$ is a vector with size k of ones, max_e chooses the element-wise maximum value across different vectors. Each entry in $\mathbf{V}$ is the outlier score for one value. Large entry values indicate higher outlierness.

The outlier object representation $\mathbf{O}$ for object $x \in \mathcal{X}$ is $[\mathbf{V}_1^x, ..., \mathbf{V}_D^x]$. The outlier score of object x is the summation of the value outlying scores, which is $outlier(x) = \sum_j^D \mathbf{V}_j^x$.

5.2.3 The COSH Method

Algorithm 2 presents the main procedures of COSH, which is similar to CDE. Different from CDE, COSH represents a value cluster with $\mathbf{C}^i$ and computes the dissimilarity between the value clusters in Steps (8-9); COSH uses different methods to represent values as shown in Steps (14-16).

As shown in Section 5.1.3, generating $\mathbf{M}_o$ and $\mathbf{M}_c$ takes the complexity of $O(ND^2 + L^2)$ and clustering on the matrices has complexity $O(k_{max}L)$. Computing the outlier scores of values has complexity $O(Lk_{max}^2)$, where k_{max} is the number of times for clustering on one value matrix which is much less than L. With the outlier scores of values, generating the outlier scores of objects has $O(ND)$. In real datasets, the average number of values per feature is often small, so L^2 is similar to D^2. Correspondingly, the time complexity of COSH is $O(ND^2)$.

5.3 Contrastive Analysis of CDE and COSH

CDE and COSH are both instantiated from CURE which is based on hierarchical value coupling learning. The shared base between CDE and COSH is the two value coupling functions which are shown to be complementary and discriminative in Section 4.2. However, the other parts, i.e., value cluster learning and coupling learning between value clusters, are customized according to the different goals of CDE and COSH. In this section, we compare these components and analyze the intrinsic motivation of these instances.

5.3.1 Contrastive Value Clustering

The value clusters contain abundant information so that value clusters can be customized flexibly according to different applications. In the following section, we analyze why CDE and COSH use different value cluster learning strategies to achieve different goals.

When generating value clusters, CDE removes the small value clusters because the small value clusters have less discriminative ability for majority values and contribute less to the final clustering process. Meanwhile, COSH keeps all the small value clusters or prefers small value clusters since small clusters have a higher discriminative ability for outlying values and contribute more to outlier detection.

When representing value clusters, CDE uses the cluster membership indicator matrix $\mathbf{C}^{\mathbf{I}}$ which keeps consensus information and differentiates values from different value clusters. Further, by multiple clustering with different cluster numbers, the value clusters group values from different granularities and keep different levels of consensus information which is helpful to distinguish similar values. Different from CDE, COSH uses the value-cluster dissimilarity matrix $\mathbf{C}^k$ to represent value clusters which is able to differentiate two values within or across value clusters. $\mathbf{C}^k$ keeps the most distinguishable information for each value, so that COSH can use it to give each value an outlying score and differentiate the outlier values from normal values.

5.3.2 Contrastive Value Cluster Coupling Learning

Since CDE and COSH use different learning strategies to learn the value clusters, the couplings between value clusters are different. In the following section, we analyze why CDE and COSH learn different couplings between value clusters and use different representations.

CDE uses the concatenation of multiple cluster membership matrices to represent values, and one dimension of value representation corresponds to one value cluster. Since value clusters are generated by the same clustering methods, there are redundancy and correlations in value representation. It is better for CDE to keep all the useful discriminative information in addition to redundancy since it is designed for clustering. Meanwhile, we expect that the dimensions of new representation are independent and

uncorrelated so that the algebraic operations can be applied for the further learning tasks. Therefore, we use PCA which does not cause any information loss to eliminate the redundancy and learn linear correlative couplings in $\mathbf{C^I}$.

COSH is designed for outlier detection which emphasizes the outlying behaviors of values and value clusters. Accordingly, COSH uses the dissimilarity matrix $\mathbf{D}_k$ to quantify the outlying couplings between value clusters. The value cluster which is far from the other value clusters could be regarded as the outlying value cluster in which the values have greater likelihood of being outlying values. Each value cluster produces one outlying score for each value which is concise and is enough to distinguish the normal values and outliers. Furthermore, the maximum operation across all the outlying scores from different value clusters ensure that COSH cannot miss any outlying value.

6 Experiments for Clustering

6.1 Experimental Settings

6.1.1 Data Representation Methods and Parameter Settings

To test the embedding performance, CDE is compared with three commonly-used encoding methods for categorical data: 0-1, 0-1P, and IDF. The 0-1 representation keeps the most complete information in the original data. The 0-1P incorporates feature correlations into the representation. IDF differentiates values w.r.t. frequency.

To the best of our knowledge, no existing embedding methods capture the value couplings in categorical data as in CDE. To test the CDE-based learning performance, we compute the Gaussian similarity based on CDE (denoted by CDE^G) and compare it with three typical and well-performing similarity measures which involve feature relations: COS [2], DILCA [11] and ALGO [10].

In Table 2, $|C|$ is the number of ground-truth classes in data, which is used for the clustering evaluation. We set parameter $\alpha = 10$ in CDE and parameter $\beta = 10^{-10}$ in PCA used by CDE and 0-1P. In COS, DILCA and ALGO, we use the default parameters in their original papers.

6.1.2 Data Representation Evaluation Methods

We apply CDE and other representation methods to *K*-means clustering to evaluate their performance. These representation methods transform categorical data into numerical data, hence *k*-means clustering can cluster objects without computing the pairwise object similarity matrix. Spectral clustering is used to evaluate the performance of this object similarity matrix against other object similarity matrices obtained by CDE^G, COS, DILCA and ALGO.

F-score and NMI [37] are two popular evaluation methods. Since we fix the cluster number to the number of classes in each data set for evaluation, NMI performs similarly to F-score. Here we only report the results of F-score. A higher F-score indicates better clustering accuracy driven by a better representation method. The p-value results are based on the paired two-tailed t-test using the null hypothesis as the clustering results of CDE and other methods come from distributions with equal means. For each data set, the F-score is the average over 50 validations of clustering with distinct starting points.

CDE and other comparison methods are implemented in MATLAB and clustering experiments are performed at 3.4GHz Titan Cluster with 96GB memory.

6.1.3 Data Indicators for Clustering

We use ten real-world UCI data sets from different domains for the experiments.[1] The basic data information consists of data size (denoted by $|\mathcal{X}|$), the number of features (denoted by $|\mathcal{F}|$), the number of feature values (denoted by $|\mathcal{V}|$), and the number of classes (denoted by $|C|$) for clustering, as demonstrated in Table 1 and Table 2.

Various *data indicators* are used to measure the underlying characteristics of data sets, which are associated with the learning performance of representation methods. Two key data indicators and their quantization are defined below, and the results are reported in Table 1 and Table 2.

- The *feature correlation index* (FCI) measures the average correlation strength between features:

$$FCI = \frac{2}{D(D-1)} \sum_{i=1}^{D-1} \sum_{j=i}^{D} SU(f_i, f_j) \qquad (16)$$

  SU measures the correlation between features f_i and f_j by the symmetric uncertainty [38]. A larger *FCI* indicates a stronger correlation between features.
- The *value cluster index* (VCI) is the average of the maximum non-overlapping ratio between value sets contained in different classes for each feature:

$$VCI = \frac{1}{D} \sum_{h=1}^{D} max_{i,j}\{1 - \frac{|\mathcal{V}^h_{C_i} \bigcap \mathcal{V}^h_{C_j}|}{|\mathcal{V}^h_{C_i} \bigcup \mathcal{V}^h_{C_j}|}\} \qquad (17)$$

  where $\mathcal{V}^h_{C_i}$ is the value set in class C_i for feature f_h. Larger *VCI* indicates the higher discriminative ability of the value sets.

6.2 Evaluation Results

CDE is firstly compared with three encoding methods, followed by a comparison with three similarity measures. We then conduct the scalability and sensitivity test of CDE.

6.2.1 Comparison with Three Encoding Methods

The F-scores of CDE, compared with 0-1, 0-1P and IDF, are shown in Table 1. CDE obtains the best F-score performance on seven data sets, which are significantly better than the other encoding methods. On average, it demonstrates an approximate 9%, 5% and 19% improvement over 0-1, 0-1P and IDF, respectively. The significance test results show that CDE significantly outperforms these three encoding methods at the 95% confidence level.

According to the data indicator FCI, the F-score performance of CDE, 0-1 and 0-1P has a downward trend with the decrease of FCI. CDE outperforms all the other encoding methods. This is because CDE is able to capture more sophisticated pairwise feature correlation than the other methods, which is illustrated by the performance on data sets with higher FCI, e.g., *Wisconsin, Soybeansmall, Mammographic, Zoo, Dermatology*. This also explains the improvement of 0-1P over 0-1. In addition to the couplings

1. https://archive.ics.uci.edu/ml/datasets.html

TABLE 1
F-score Results of CDE vs. Three Encoding Methods by *k*-means Clustering on 10 Data Sets. The best performance for each data set is boldfaced. The datasets are sorted in descending order of FCI.

Basic Data Info. & Data Indicator				F-score			
Data	$\|\mathcal{X}\|$	$\|\mathcal{V}\|$	FCI	CDE	0-1	0-1P	IDF
Wisconsin	683	89	0.212	**0.967**	0.946	0.946	0.943
Soybeansmall	47	58	0.180	**0.915**	0.829	0.854	0.763
Mushroom	5644	97	0.148	**0.731**	0.709	0.694	0.506
Mammographic	830	20	0.116	0.809	0.793	**0.815**	0.517
Zoo	101	30	0.110	**0.647**	0.596	0.607	0.537
Dermatology	366	129	0.089	**0.670**	0.598	0.606	0.616
Hepatitis	155	36	0.085	0.680	**0.681**	0.667	0.535
Adult	30162	98	0.060	**0.654**	0.585	0.588	0.479
Lymphography	148	59	0.057	0.418	0.381	0.379	**0.561**
Primarytumor	339	42	0.020	**0.240**	0.230	0.238	0.190
Average				**0.673**	0.635	0.640	0.565
				p-value	0.003	0.003	0.020

TABLE 2
F-score Results of CDE-G vs. Three Similarity Measures by Spectral Clustering on 10 Data Sets. COS, DILCA and ALGO run out of memory on *Adult*. The average values are computed according to the data sets except *Adult*.

Basic Data Info. & Data Indicator				F-score			
Data	$\|\mathcal{F}\|$	$\|C\|$	VCI	CDE^G	COS	DILCA	ALGO
Wisconsin	9	2	0.237	0.962	**0.973**	0.921	0.971
Soybeansmall	21	4	0.712	**1.000**	0.893	0.910	0.911
Mushroom	21	2	0.310	**0.828**	0.825	0.826	0.826
Mammographic	4	2	0.071	0.817	**0.828**	0.826	0.818
Zoo	15	7	0.733	**0.644**	0.538	0.583	0.547
Dermatology	33	6	0.664	0.784	0.730	**0.808**	0.710
Hepatitis	13	2	0.141	0.667	0.463	**0.679**	0.662
Adult	8	2	0.032	**0.676**	NA	NA	NA
Lymphography	18	4	0.699	**0.397**	0.395	0.353	0.366
Primarytumor	17	21	0.873	**0.242**	0.196	0.224	0.209
Average				**0.704**	0.649	0.681	0.669
				p-value	0.050	0.100	0.032

between features, CDE also captures the couplings across the values clusters, which means CDE performs well on data sets with high-order feature correlation, e.g., *Adult* and *Primarytumor* which have lower FCI but may have high-order feature correlation. IDF is only sensitive to value frequency couplings, i.e., ϕ_o, while CDE is based on ϕ_o and ϕ_c which capture two complementary discriminative couplings. This explains why IDF can only obtain good results on the data sets where objects are discriminative in terms of value frequency, e.g., *Lymphography*.

6.2.2 Comparison with Three Similarity Measures

CDE^G is compared with three well-performing feature relation-based similarity measures: COS, DILCA and ALGO. As shown in Table 2, although COS and DILCA obtain the best performance on two data sets, CDE^G remains the best performer on half of the data sets. CDE^G obtains about 8%, 3% and 5% improvement over COS, DILCA and ALGO respectively in terms of F-score. The significance test results show that CDE^G significantly outperforms the other similarity measures at the 90% confidence level. It is noted that tests on COS, DILCA and ALGO on data set *Adult* run out of memory since the computation of object similarity needs a large amount of memory.

CDE^G achieves better performance than the other similarity measures, especially on data sets with larger VCI and larger $|C|$, e.g., *Primarytumor, Zoo, Soybeansmall, and Lymphograph*. This is because CDE^G learns the value clusters with different granularities and considers the couplings between these value clusters, which enables CDE^G to obtain more faithful value similarities than the other similarity measures that do not consider such couplings. Also, compared to the performance of 0-1, 0-1P and IDF shown in Table 1, the performance of similarity measures is better on the data sets with higher FCI, e.g., *Wisconsin, Soybeansmall, Mushroom, and Mammographic* according to Table 2 . This is because CDE^G, COS, DILCA and ALGO are able to capture the pairwise relations between features.

6.2.3 Scalability Test

We use five subsets of the largest data set *Adult* to test the scalability w.r.t. data size. All these subsets contain eight features. The execution time excludes the running time of clustering. In terms of scalability w.r.t the number of features, we generate five synthetic data sets with the smallest dimension of 25 and the largest dimension of 400. Each feature has two values which are randomly distributed. All the synthetic data sets have 10,000 objects.

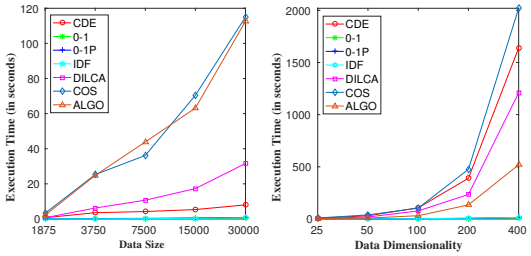

Fig. 2. Scalability Test Results.

The left panel of Fig. 2 shows that, CDE runs significantly faster than COS, DILCA and ALGO and one order magnitude slower than 0-1, 0-1P and IDF encoding. This is because CDE is linear to the data size (N), while DILCA has $O(N^2D^2logD)$, COS has $O(N^2D^3R^3)$, and ALGO has $O(N^2D^2 + D^2R^3)$, where R denotes the maximum number of distinct values for each feature. The right panel of Fig. 2 shows that CDE has a similar runtime with COS and DILCA, and they run considerably slower than ALGO because ALGO is quadratic to the number of features (D) according to the computational complexity. All coupled methods run much slower than the encoding methods, i.e., 0-1, 0-1P and IDF, since modeling complex value couplings and/or feature correlations is costly.

6.2.4 Sensitivity Test

There are two parameters in CDE: α controls the dimension of value embedding before PCA and β controls the dimension of value embedding after PCA. Since the results on all data sets have a similar trend, we demonstrate the results of four data sets: *Adult, Dermatology, Wisconsin, Primarytumor*, which have the largest $|O|$, largest $|V|$, largest FCI and largest VCI, respectively.

Fig. 3 shows the dimension of value embedding before PCA and the clustering performance with different α which directly influences the value of k in Algorithm 1. k deter-

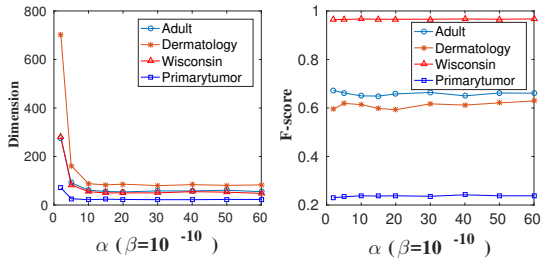

Fig. 3. Sensitivity Test of Parameter α on the Four Data Sets in Terms of Dimensionality and F-score.

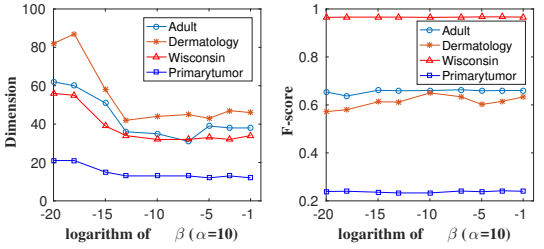

Fig. 4. Sensitivity Test of Parameter β on the Four Data Sets in Terms of Dimensionality and F-score.

mines the granularity of value clusters which constitutes the original value embedding. Since we only drop the clusters with only one value, the clustering performance is stable with parameter α. According to Fig. 3, the dimension is stable when $\alpha \geq 10$.

Fig. 4 shows the dimension of the final value embedding and the clustering performance w.r.t. β which influences the dimension of the embedding matrix during the PCA process. The smaller the β value, the higher the dimension of the value embedding vector. This shows that the performance of the clustering is stable w.r.t. β. When $\beta \geq 10^{-15}$, the dimension of the value embedding vectors decreases with the increase of β on all data sets.

As shown in Fig. 3 and Fig. 4, the clustering performance is not sensitive to parameters α and β. The dimension is stable when $\alpha \geq 10$ and $\beta \geq 10^{-15}$.

7 Experiments for Outlier Detection

7.1 Experimental Settings

7.1.1 Outlier Detectors and Their Parameter Settings

COSH represents a categorical data object with an outlying vector, so it can be applied to detecting outliers directly. To evaluate the effectiveness of COSH, we compare COSH with two scoring-based representations and three other outlier detectors on ten real-world high-dimensional data sets. Similar to COSH, CBRW [17] and ZERO++ [18] (denoted by ZERO) unify data representation and outlier detection as one learning task. CBRW is the state-of-the-art outlier detector for categorical data and is also a coupled method since it learns the low-level value couplings to estimate the outlier score of values. ZERO is a recently proposed subspace method for handling high-dimensional data.

The other three outlier detectors work on embedding-based representation (i.e., iForest [19]) or similarity-based representation (i.e., ABOD [39] and LOF [21]). iForest handles high-dimensional data by working on the feature subspace. ABOD is an angle-based method which is designed for high-dimensional data. LOF is one of the most popular methods which works on the full dimension. To keep the most complete information in the original data sets and to avoid introducing noisy information for outlier detectors, we transform the categorical data into numerical space with one-hot encoding to enable iForest, ABOD and LOF to work on categorical data. Another reason for using one-hot encoding instead of similarity measures is that there is no consistently effective similarity for different data sets [40] and one-hot encoding performs comparably well to other embedding- or similarity-based representation while it is much more efficient [18], [40].

COSH uses k-means, so its result is not deterministic. ZERO and iForest are also non-deterministic methods, so the results of these three methods are averaged from 10 runs. We set parameter $\alpha = 30$ in COSH and parameter $\alpha = 0.95$ as recommended in CBRW [17]. We use $t = 50, n = 256$ in iForest and $t = 50, n = 8$ in ZERO. LOF is parameter free. Since a small k is suggested in [21], we use $k = 5$ in LOF.

7.1.2 Evaluation Methods for Outlier Detection

COSH is implemented in MATLAB and the other five outlier detectors are implemented in JAVA. All the COSH related experiments were performed on a node 3.4GHz Titan Cluster with 96GB memory.

All the outlier detectors also produce a ranking based on the outlier scores. As shown in [41], the quality of ranking can be estimated by the area under the ROC curve (AUC) which is computed by the Mann-Whitney-Wilcoxon test. AUC is one of the most popular performance evaluation methods and it takes class imbalance into consideration. A higher AUC indicates better outlier detection accuracy.

7.1.3 Data Sets and Data Indicators for Outlier Detection

Ten publicly available real-world data sets [2] are used, which cover diverse domains, e.g., Internet advertising, image object recognition, web page classification, and text classification. The basic data information is shown in Table 3. Six of the data sets are directly transformed from highly imbalanced classification data, where the smallest class is treated as outliers and the largest class is regarded as a normal class. We transform the other four data sets (*PC*, *BASE*, *web*, *RELA*) by randomly sampling a small subset of the smallest class as outliers to ensure the data sets contain 2% outliers. The performance of these downsampled data sets is averaged over 10 times of sampling.

We use two data indicators to quantify the value separability and the couplings between outlier values. We define two data indicators *value separability index* (VSI) and *outlier coupling index* (OCI) below and the quantization results are shown in Table 3.

2. The used data sets are available at http://featureselection.asu.edu, https://www.csie.ntu.edu.tw/~cjlin/libsvmtools/, http://mmlab.ie.cuhk.edu.hk/projects/CelebA.html and http://tunedit.org/repo/Data

- *VSI* is quantified by the value overlapping in normal objects and outlier objects, defined as follows:

$$VSI = \min\{\frac{|\{x|x \in \mathcal{X}_n \cap v_j^x \in \mathcal{V}_j^{\mathcal{X}_o}\}|}{|\mathcal{X}_n|}, j \in \mathcal{F}\}, \quad (18)$$

where $\mathcal{X}_n$ is the set of normal objects and $\mathcal{X}_o$ is the set of outlier objects, and v_j^x denotes the value of object x in feature j. A larger *VSI* indicates a weaker separability of values.

- The OCI is quantified by the pointwise mutual information between outlier values and normal values, which is defined as follows:

$$OCI = \frac{pmi(v_o, v_o')}{pmi(v_o, v_o') + pmi(v_o, v_n)}, \quad (19)$$

where $pmi(v_o, v_o')$ is the averaged pointwise mutual information within outlier values, which is calculated by $pmi(v_o, v_o') = average\{\frac{p(v_o, v_o')}{p(v_o)p(v_o')}, v_o, v_o' \in \mathcal{V}_o\}$. $OCI > 0.5$ indicates that the couplings within outlier values are stronger than the couplings between outlier values and normal values.

7.2 Evaluation Results

7.2.1 Outlier Detection Effectiveness

The AUC performance of COSH and its five competitors: CBRW, ZERO, iForest, ABOD and LOF is reported in Table 3. COSH performs better than its five competitors on seven data sets, and significantly outperforms them at the 95% confidence level. On average, COSH obtains more than 17%, 27%, 39%, 29% and 44% improvement over CBRW, ZERO, iForest, ABOD and LOF, respectively. Of all the outlier detection methods, COSH, CBRW and ZERO are scoring-based representation since they integrate model learning and data representation into representation, while iForest, ABOD and LOF are outlier detectors based on embedding representation. From Table 3, the performance of scoring-based representation is much better than pure outlier detectors that rely on data conversion.

In Table 3, the data sets are sorted in the descending order of VSI. The data indicator VSI describes the separability of values from a single feature according to the overlapping values of outlier objects and normal objects. COSH obtains the best performance on all the data sets with higher VSI (e.g. $VSI > 60\%$), and it achieves, on average, substantial AUC improvement over its five competitors CBRW, ZERO, iForest, ABOD and LOF by more than 28%, 46%, 67%, 50% and 30%, respectively. VSI quantifies the separability of a single feature, while some outliers could be identified by multiple features. COSH captures high-order couplings through value-cluster couplings, which helps to detect outliers in data sets without strongly coupled features (i.e., low VSI).

OCI captures the couplings between outliers and normal values across two features. The larger OCI is, the stronger the couplings which exist within outliers and the weaker the couplings between outliers and normal objects. In the data sets with the highest OCI, i.e., *w7a*, COSH achieves much better performance than the others, whereas COSH does not show its superiority in the data sets with the lowest OCI, i.e., *Cal28*.

TABLE 3
AUC Results of COSH vs. Five Outlier Detectors on 10 Data Sets. Note: CBRW runs out of memory on high-dimensional data *WebKB* and *Reuters8*. ABOD runs out-of-memory on large data *w7a* and *CelebA*

Data Info.			Data Indicator		AUC Performance					
Data	$\|\mathcal{X}\|$	$\|\mathcal{F}\|$	VSI	OCI	COSH	CBRW	ZERO	iForest	ABOD	LOF
w7a	49749	300	0.950	0.589	**0.835**	0.646	0.538	0.404	NA	0.500
CelebA	202599	39	0.845	0.501	**0.716**	0.646	0.538	0.404	NA	0.500
WebKB	1658	6601	0.814	0.551	**0.753**	NA	0.698	0.678	0.670	0.825
RELATHE	794	4080	0.788	0.501	**0.896**	0.701	0.605	0.556	0.569	0.743
BASEHOCK	1019	4320	0.706	0.513	**0.909**	0.618	0.529	0.471	0.488	0.664
PCMAC	1002	3039	0.698	0.536	**0.890**	0.633	0.528	0.476	0.490	0.620
Reuters8	3974	9467	0.260	0.552	0.872	NA	0.883	0.839	0.786	**0.892**
Caltech-28	829	727	0.088	0.500	0.943	**0.960**	0.954	0.934	0.927	0.439
Caltech-16	829	253	0.054	0.510	**0.996**	0.993	0.988	0.972	0.977	0.388
wap.wc	346	4229	0.038	0.534	**0.975**	0.790	0.657	0.579	0.524	0.516
Average					**0.879**	0.748	0.692	0.631	0.679	0.609
					p-value	0.023	0.020	0.002	0.008	0.010

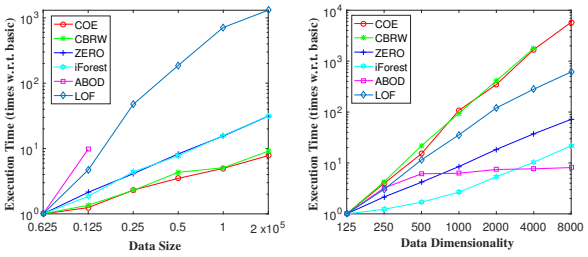

Fig. 5. Scalability Test Results. ABOD and CBRW run out of memory when the number of objects reaches 25,000 and the number of features reaches 8,000, respectively

7.2.2 Scalability Test

COSH is implemented in MATLAB while the other methods are implemented in JAVA, so the absolute time is not comparable. We demonstrate the ratio of the execution time to the base time which is from the smallest data set. We use six subsets of the largest data set *CelebA* to test the scalability w.r.t. data size. All these data sets contain the same number of features, i.e., 39. The execution time on the smallest data set is: 26.6s for COSH, 0.344s for CBRW, 3.416s for ZERO, 0.299s for iForest, 3685.467s for ABOD, and 2.439s for LOF.

In terms of scalability w.r.t. the number of features, seven subsets of the data sets with the largest number of features, *R8* are used. All these seven data sets contain the same number of objects, i.e., 3,974. The execution time on the smallest data set is: 88.21s for COSH, 1.657s for CBRW, 7.244s for ZERO, 0.182s for iForest, 84.345s for ABOD, and 0.581s for LOF.

The computational complexities of CBRW, ZERO, iForest, ABOD and LOF are $O(ND^2)$, $O(ND)$, $O(ND)$, $O(N^3D)$ and $O(N^2D)$ respectively. As shown in the right panel of Fig. 5, COSH is one of the most efficient methods compared with other state-of-the-art outlier detection methods w.r.t. the number of objects, since COSH is linear to the data size and quadratic to the number of features. In the left panel of Fig. 5, COSH and CBRW have similar runtime and they run considerably slower than the other four detectors, since both COSH and CBRW capture complex value couplings while the other methods ignore them. Although COSH and CBRW run slower, they obtain significantly better AUC performance than their competitors, as shown in Table 3.

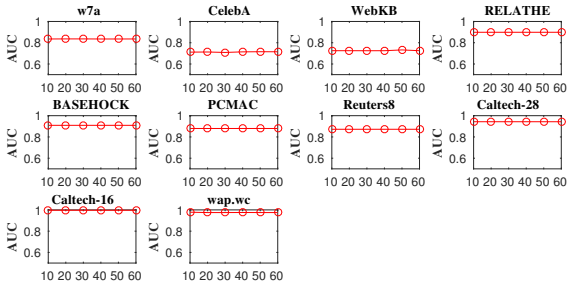

Fig. 6. Sensitivity Test Results w.r.t. α on Ten Data Sets.

7.2.3 Sensitivity Test

We investigate the sensitivity test of COSH w.r.t. its only parameter α on all the 10 data sets using a wide range of α, i.e., $\{10, 20, 30, 40, 50, 60\}$. The sensitivity test results of COSH are shown in Fig. 6. COSH performs stably w.r.t. α on all data sets. The larger α means the less number of clustering times and a smaller number of value clusters.

8 Discussions

CURE is a hierarchical framework which can be customized from multiple levels. We instantiate CURE by customizing the value cluster learning and coupling learning between value clusters according to different applications based on the same coupling functions. More instances may be derived by capturing other forms or levels of couplings [6] for specific applications.

The two complementary coupling functions used by CDE and COSH capture only pairwise couplings. Instantiating CURE by incorporating arbitrary length patterns and their couplings may improve the discriminative ability of the low-level value coupling functions, and further improve the representation quality.

One important CURE component is the value cluster learning, which is instantiated by *k*-means clustering in CDE and COSH. Although *k*-means has multiple advantages, it has some limitations for detecting the special shape of clusters and overlapping clusters. Learning arbitrary shapes of value clusters with different clustering methods may enrich the information of value clusters. However, various kinds of value clusters may induce more heterogeneous couplings or noises. Therefore, more advanced methods may be required to capture couplings between value clusters in this case.

Another important part of CURE is the coupling learning between value clusters, which is highly related to the properties of value clusters. There may be various forms of couplings between value clusters, which are also hard to capture and interpret. Incorporating more sophisticated methods to learn explicit and implicit complex value couplings, e.g., by deep models, may be explored to improve the utility of each value cluster.

9 Conclusions and Future Work

This paper proposes a novel unsupervised representation framework (CURE) for categorical data which models hierarchical value couplings in terms of feature value couplings and value cluster couplings. Instantiating CURE, CDE and COSH are respectively introduced for clustering and outlier detection, which are based on two complementary and discriminative value couplings. A contrastive analysis of CDE and COSH explains the contrasting instantiation capability of CURE.

Different from existing encoding-based embedding and feature correlation-based similarity measures, CDE learns the data embedding from value clusters w.r.t. couplings within and between value clusters. Extensive experiments show that (1) CDE significantly outperforms typical embedding methods and similarity measures for clustering; (2) two data indicators can facilitate the explanation of clustering performance on complex data sets; (3) CDE has good scalability and is more efficient than similarity-based representation; and (4) CDE performance is insensitive to the two parameters.

Different from existing single-granular outlier detection methods, COSH observes hierarchical outlying behaviors from value-to-value clusters with different granularities. Extensive experiments show that (1) COSH significantly outperforms five state-of-the-art outlier detection methods. (2) Two data indicators can facilitate the explanation of outlier detection on complex data sets. (3) COSH has a good scalability which suits high-dimensional data sets. (4) There is only one parameter in COSH and it has little influence on the outlier detection performance.

As discussed, there are great opportunities to further expand CURE for different learning tasks and scenarios with complex coupling relationships.

Acknowledgments

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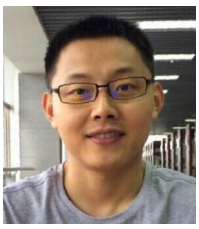
Songlei Jian Songlei Jian is currently working toward a Ph.D. degree, jointly supervised at the National University of Defense Technology, China and the University of Technology Sydney, Australia. Her research interests include data representation, unsupervised learning and complex network analysis.

Guansong Pang Guansong Pang is a PhD candidate in the Advanced Analytics Institute at the University of Technology Sydney. Before joining AAI, he received a Master of Philosophy in data mining from Monash University. His research interests include data mining and non-IID learning.

Longbing Cao Longbing Cao is a Professor at the University of Technology Sydney. He has a PhD in Pattern Recognition and Intelligent Systems and another in Computing Sciences. His research interests include data science, analytics and machine learning, and behavior informatics and their enterprise applications.

Kai Lu Kai Lu is a Professor and the Deputy Dean of the College of Computer Science, National University of Defense Technology, China. His research interests include parallel and distributed system software, operating systems, and big data analytics.



Hang Gao Hang Gao is a Ph.D. graduate of National University of Defense Technology, China. His research interests include machine learning, data analytics and mining.