# Unsupervised Coupled Metric Similarity for Non-IID Categorical Data

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

**Abstract**—Appropriate similarity measures always play a critical role in data analytics, learning and processing. Measuring the intrinsic similarity of categorical data for unsupervised learning has not been substantially addressed, and even less effort has been made for the similarity analysis of categorical data that is not independent and identically distributed (non-IID). In this work, a Coupled Metric Similarity (CMS) is defined for unsupervised learning which flexibly captures the value-to-attribute-to-object heterogeneous coupling relationships. CMS learns the similarities in terms of intrinsic heterogeneous intra- and inter-attribute couplings and attribute-to-object couplings in categorical data. The CMS validity is guaranteed by satisfying metric properties and conditions, and CMS can flexibly adapt to IID to non-IID data. CMS is incorporated into spectral clustering and k-modes clustering and compared with relevant state-of-the-art similarity measures that are not necessarily metrics. The experimental results and theoretical analysis show the CMS effectiveness of capturing independent and coupled data characteristics, which significantly outperforms other similarity measures on most datasets.

**Index Terms**—Similarity learning, metric learning, non-IID data, coupling learning, categorical data, unsupervised learning, clustering.

## 1 Introduction

Appropriately measuring similarity or distance between objects is fundamental for effective data analytics, including tasks in data mining [1], machine learning [2], [3], image processing [4], computer vision [5], and information retrieval tasks [6], and in particular for complex data. It determines whether the learned outcomes of data analytics and learning are reliable and the underlying models genuinely capture intrinsic data characteristics.

Similarity measures for categorical (nominal) and numerical data are usually distinct. Most existing work on similarity learning focuses on numerical data, such as the commonly used Euclidean and Manhattan distances. The similarity (or distance) of categorical data is not as straightforward as it is for numerical data, since the different values of a categorical attribute may not be inherently ordered or comparable. Although there may be no inherent order in categorical data, other factors like matching statistics and frequency distribution exist and thus indicate similarity. Among existing work, the most straightforward and widely used distance metric is the Hamming distance [7]. It corresponds to matching-based similarity measures, which use 0 and 1 to distinguish the similarity between distinct and identical categorical values. Other similarity measures take the frequency distribution of different attribute values into account, such as the *Inverse Occurrence Frequency (IOF)* and *Occurrence Frequency (OF)* [8]. These similarity measures only capture the characteristics within an attribute but ignore the relationships between attributes.

### 1.1 Motivating toy example

We illustrate the problem with the existing work and the inherent challenges in analyzing the similarity of categorical data by taking the staff data of a lab in Table 1 as an example. The staff data consists of four categorical attributes: *Sex*, *Education*, *Occupation* and *Marriage*. From the *matching* perspective, the similarity between *Staff 1* and *Staff 2* is the same as that between *Staff 1* and *Staff 3*, because they are both 0.5. However, from both education and occupation perspectives, professors and assistant professors should be more similar than professors and students in the lab.

Further, the frequency distribution of an attribute value and the co-occurrences between attributes have shown to be valuable for categorical similarity learning. From the OF perspective, two values of an attribute are similar if they present analogous frequency distributions [8]. For example, the similarity between Professor and Assistance Professor is greater than that between Professor and Student, because the occurrence frequency of Professor and Assistant Professor in this staff data is the same. Although the attribute values can disclose more information than simple matching, the value frequency-based similarity is not sufficient. For example, the similarity between the education levels Doctor and Master is the same as that between Doctor and Bachelor. This is because the frequency distribution only captures the count statistics of attribute values, but ignores the coupling relationships within and between attributes. The co-occurrences of attribute values induced on other attributes is more comparable [9], [10], and complements the accuracy of frequency-based value similarity. By incorporating the co-occurrence-based attribute similarity, the pair Doctor and Master is more similar than Doctor and Bachelor, because

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*Manuscript received April 19, 2015; revised August 26, 2015.*

TABLE 1
An Example: The Staff Data

| Staff | Sex | Education | Occupation | Marriage |
|---|---|---|---|---|
| Staff 1 | F | Doctor | Professor | Married |
| Staff 2 | M | Doctor | Assistant Professor | Married |
| Staff 3 | F | Master | Student | Married |
| Staff 4 | M | Master | Student | Single |
| Staff 5 | F | Bachelor | Student | Single |
| Staff 6 | M | Bachelor | Student | Single |

the former pair co-occurs with the same occupation and marriage, while the latter does not.

### 1.2 Major issues and contributions

The above example shows that it is often much more complicated in defining the similarity of categorical data, especially when data is embedded with complex relationships [11], [12]. Complex data applications become increasingly important and popular, heterogeneous and hierarchical coupling relationships [11], [13] are embedded in categorical attributes, values and objects, which make it even more difficult to measure similarity or dissimilarity. For example, the market dynamics in a stock market may be related to many factors, such as psychological, economic, social, organizational, political, cultural or even military aspects. Data presenting explicit and/or implicit couplings and heterogeneity is not independent and identically distributed (i.e., non-IID) [14], [15], [16]. Such data does not fit the IID assumption widely taken by classic analytics and learning and their similarity measures.

Non-IID learning has attracted increasing attention in the relevant communities, which usually only consider the non-IIDness [14] at the sample level [15], [16]. Model-based approaches are typically used to address non-IID samples, such as analyzing non-IID textual data by higher order Naive Bayes [17], classification with non-IID samples [18], developing chromatic PAC-Bayes bounds for non-IID data [19], and learning from dependent observations [20].

The real-life data may be often embodied with various non-IIDness [14] in terms of diverse couplings and heterogeneities between values, between attributes, and between objects, forming the value-to-object hierarchical non-IIDness [13], [14]. Learning such non-IID data has been recognized as a foundational issue in complex data analytics, with fundamental tasks including learning the hierarchical non-IIDness and ensuring the robustness and generalization [21] of learning metrics and models. For this, the *Hamming* and *OF*-based measures cannot fully capture the genuine similarity of non-IID categorical data as they only capture particular aspects.

In recent years, increasing efforts have been made to address the above type of non-IID categorical data, with a typical focus on learning the value-to-object hierarchical couplings. Coupled Object Similarity (COS) [10], [22] involves the couplings within and between attributes before object similarity is defined. Other related work incorporates couplings into various types of learning tasks, including coupled clustering [10], coupled KNN for classification [23], term coupling-based document analysis [24], coupled keyword queries [25], coupled matrix factorization by item and user couplings into recommender systems [26], understanding relationships between patterns for pattern relation analysis [27], [28], and analyzing image couplings [29], [30].

Many of the existing similarity measures for categorical data face two issues. One is that few methods are metric-based and provide a sound theoretical foundation to satisfy the metric properties: positivity, reflexivity, commutativity and triangle inequality (details in Section 3). A *metric* is a function that defines a distance between each pair of elements in a set. A set with a metric is called a *metric space* which induces a topology on this set. A metric-based similarity is derived from a metric by a bijection function. In fact, a lot of properties and theorems have been derived in the metric spaces and the corresponding algorithms only work for sound reasons when built on similarity metrics. For example, the most classic clustering algorithm k-means was defined with metrics like the Euclidean or Hamming distance, whose clustering outcomes are explainable. The other issue is that few of existing methods capture the value-to-object hierarchical couplings. COS is the only one catering for both intra- and inter-attribute similarities, but it is not a metric. Therefore, it is important to develop appropriate metric-based similarity measures for non-IID categorical data.

In this paper, building on the idea of incorporating heterogeneous and hierarchical value-to-object coupling relationships [13] into learning systems, we propose a *coupled metric similarity* (CMS) metric for non-IID categorical data. CMS integrates the frequency-based intra-attribute similarity with the co-occurrence-based inter-attribute similarity before object similarity is measured. The intra-attribute similarity captures the frequency distribution and the couplings between values in an attribute. The inter-attribute similarity aggregates the attribute dependency between values of different attributes by considering the intersection of their co-occurrence conditional probability. CMS integrates intra-attribute similarity with inter-attribute similarity by catering for their contributions. Further, we prove that CMS is a valid similarity metric that satisfies the metric properties.

Our main contributions are detailed below:

- A coupled metric similarity (CMS) measure is proposed for the unsupervised learning of non-IID categorical data. CMS captures both the intra- and inter-attribute couplings and further learns heterogeneous and hierarchical value-to-object couplings to measure the object similarity.
- By introducing a control parameter, CMS combines intra- and inter-attribute similarities based on the data characteristics of given data, adapting to both IID and non-IID data. This shows the flexibility of CMS.
- Four theorems are proposed and proved to ensure the validity of CMS as a metric.
- CMS is compared with the state-of-the-art similarity measures by incorporating them into both distance-based clustering and similarity-based clustering algorithms on nineteen UCI benchmark datasets. Evaluation and empirical analysis of the resultant statis-

tically significant outcomes are provided to understand why CMS works well from the perspectives of both similarity constituents and capturing various couplings.

The remainder of the paper is organized as follows. In Section 2, we discuss the related work. The problem is specified in Section 3. Section 4 introduces the CMS measure. The proof of CMS validity and theoretical analyses of metric properties are given in Section 5. We demonstrate the CMS effectiveness and efficiency by experiments and analysis in Section 6, and discuss the underlying working mechanisms of CMS in Section 7. Lastly, conclusions and future work are discussed in Section 8.

## 2 Related work

The similarity learning of categorical data has attracted increasing attention in recent years [8], [31], [32]. Compared to numeric data similarity learning, learning categorical data similarity is more complicated, and limited research outcomes have been reported. The matching-based measures are typical for categorical data. A matching-based measure simply assigns the similarity as 1 if the values of an attribute for two objects are identical; otherwise it assigns 0. However, such simple matching-based measures often result in misleading learning outcomes as discussed in the above, and they disregard the hidden similarity between categorical values [33]. Further, the Inverse Occurrence Frequency (IOF) and Occurrence Frequency (OF) based measures take the occurrence frequency distribution into account. IOF is related to the concept of inverse document frequency, which was designed for text mining [34] and assigns lower similarity to mismatches on more frequent values, and vice versa. An OF measure gives the opposite weight of the IOF measure for mismatches.

Intensive studies have been conducted on learning the similarity between two categorical values in supervised learning [35], [36], [37]. A classic similarity measure in supervised learning is the Value Distance Matrix (VDM) and the Modified Value Distance Matrix (MVDM) [38] based on class labels. Both methods measure the distance between two numeric attribute values in a multi-dimensional attribute space for supervised learning and modify the distance with a weighting scheme. Wilson and Martineza designed a Heterogeneous Value Difference Metric (HVDM) [39] to cater for categorical attributes.

An increasing number of researchers have also paid attention to similarity analysis for unsupervised learning [40], [41]. A key point is that the attribute value similarity is also dependent on other attributes [8], [11]. Typical efforts in this area applied the Pearson and Jaccard coefficients between values [22], [31]. The Pearson correlation coefficient only reflects the strength of linear dependence [42] within numeric data. The Jaccard similarity coefficient statistically compares the similarity and diversity of sample sets and is widely used in data mining tasks [43].

A variety of techniques for learning the similarity of categorical data have been explored. Believing that the attribute and object similarities are interdependent, Das and Mannila [44] presented the Iterated Contextual Distances (ICD) algorithm. ICD considers and iterates attribute similarity, sub-relation similarity, and row similarity; however, it faces a number of issues including the selection of starting points, database scan times, iterations, and convergence. Ahmad and Dey [9] proposed a distance-based measure in terms of value co-occurrences. Their work considers the overall distribution of two attribute values in a dataset along with their co-occurrences with the values of other attributes. Their similarity only considers value co-occurrences, and does not cater for value-to-object hierarchical similarity; in addition, computation is costly. No theoretical foundation and analysis about metric properties were provided.

Built on the concepts of intra- and inter-behavior coupling relationships [13] and coupled behavior similarity for coupled behavior analysis [11], the coupled object similarity (COS) [10], [22] was proposed to learn categorical data similarity. COS is based on the belief that object similarity, attribute similarity and value similarity form an interactive and inter-dependent hierarchical system which cannot be ignored in the similarity definition for complex data. Accordingly, COS captures the Intra-coupled Attribute Value Similarity (IaAVS), the Inter-coupled Attribute Value Similarity (IeAVS) and their integration to learn object similarity. Experiments show that COS achieves significant improvement over existing similarity measures in clustering categorical data. The CBA and COS methods have been applied in classification [23], recommender systems [26], text mining [24], keyword query [25], and video processing [30]. However, COS is not a metric-based similarity, and no theoretical foundation and analysis have been provided to verify its metric properties and determine why it works for sound reasons.

To address the above relevant issues, this work takes a step forward by proposing the concept and similarity learning system Coupled Metric Similarity (CMS). CMS learns object similarity by proposing hierarchical similarity measures that capture both horizontal and vertical coupling relationships between the values of an attribute, between attributes, and between objects. CMS ensures that these value-to-attribute-to-object similarity measures satisfy metric properties with sound theoretical design and proof and this foundation makes CMS applicable to distance-based algorithms.

## 3 Problem formulation

In this section, we first discuss the necessary conditions for a valid distance-based function and a metric similarity measure. Further, preliminaries are provided to establish the foundation for proposing new similarity metrics. These will form the theoretical foundation for the concept of CMS, which will be discussed in Section 5.

### 3.1 Metric properties

A metric space is an ordered pair $(M, \delta)$ where $M$ is a set and $\delta$ is a metric on $M$, i.e., a function: $d : M \times M \to \mathbb{R}$ so that, for any $u_x, u_y, u_z \in M$, the following properties hold [45]:

1) non-negativity: $\delta(u_x, u_y) \geq 0$
2) reflexivity: $\delta(u_x, u_y) = 0 \Leftrightarrow u_x = u_y$

3) commutativity: $\delta(u_x, u_y) = \delta(u_y, u_x)$
4) triangle inequality: $\delta(u_x, u_z) \leq \delta(u_x, u_y) + \delta(u_y, u_z)$

The function $\delta()$ is called a *distance function* (here simply called *distance*).

A valid metric needs to satisfy the above properties. Given the above metric function $\delta()$, the following bijection function [8] is applied to convert a metric distance to a metric-based similarity:

$$s(u_x, u_y) = \frac{1}{1 + \delta(u_x, u_y)}, \tag{1}$$

where $s(u_x, u_y)$ is the similarity between two data points $u_x$ and $u_y$, and $\delta(u_x, u_y)$ is the distance between $u_x$ and $u_y$.

With the above mapping function, we can deduce the following conditions that a metric-based similarity measure should hold:

1) positivity: $0 < s(u_x, u_y) \leq 1$
2) reflexivity: $s(u_x, u_y) = 1 \Leftrightarrow$ then $u_x$ is exactly the same as $u_y$
3) commutativity: $s(u_x, u_y) = s(u_y, u_x)$
4) triangle inequality: $\frac{1}{s(u_x,u_y)} + \frac{1}{s(u_y,u_z)} \geq 1 + \frac{1}{s(u_x,u_z)}$

### 3.2 Problem statement

Assume a dataset $DB$ consists of a number of data objects $U$ that are described by a set of attributes $A$. $DB$ can be organized as an information table $S =< U, A, V >$, where $U = \{u_1, ..., u_n\}$ is composed of a non-empty finite set of data objects; $A = \{a_1, ..., a_m\}$ is a finite set of attributes; $V = \cup_{j=1}^{m} V_j$ consists of sets of values of all attributes, in which $V_j$ is the set of values of attribute $a_j$.

For the better readability by illustrating CMS-based similarity calculations in the following sections, the information table shown in Table 2 is used as an example. Symbols $A_1$ and $A_2$ represent two distinct values of attribute $a_1$; $B_1$ and $B_2$ represent two distinct values of attribute $a_2$; and $C_1$ and $C_2$ represent two distinct values of attribute $a_3$. Table 2 thus consists of six objects $\{u_1, ..., u_6\}$ and four attributes $\{a_1, a_2, a_3, a_4\}$, and the value set of attribute $a_2$ is $V_2 = \{B_1, B_2\}$.

We assume that the similarity between two objects $u_x$ and $u_y$ ($u_x, u_y \in U$) is the summation of the similarities between attribute values $v_j^x$, $v_j^y$ ($v_j^x$, $v_j^y \in V_j$) for any attribute $a_j$, where $j \in [1, m]$), and $v_j^x$ and $v_j^y$ indicate the respective attribute values of objects $u_x$ and $u_y$ on the attribute $a_j$. For instance, $v_1^2 = A_2$ and $v_2^1 = B_1$. Several basic concepts are defined below to form the foundation of introducing the CMS measure, a new object similarity metric for categorical data in Section 4.

***Definition 1 (Conditional Probability of Attribute Values).*** Given the value $v_k$ of attribute $a_k$ ($a_k \in A$), and the value $v_j^x$ ($v_j^x \in V_j$) of object $u_x$ on attribute $a_j$, then the conditional probability of $v_k$ with respect to $v_j^x$ is $p(v_k|v_j^x)$, defined as:

$$p(v_k|v_j^x) = \frac{|I(v_j^x, v_k)|}{|I(v_j^x)|}, \tag{2}$$

where $I(v_j^x, v_k)$ denotes the set of the objects $u_x$ whose attribute value of $a_j$ is $v_j^x$ and attribute value of $a_k$ is $v_k$, $I(v_j^x)$ denotes the set of the objects whose attribute value of $a_j$ is $v_j^x$, $|\cdot|$ denotes the number of elements in the contained set.

TABLE 2
Toy Example: A Car Data Set

| A<br>U | $a_1$ | $a_2$ | $a_3$ |
|---|---|---|---|
| $u_1$ | $A_1$ | $B_1$ | $C_1$ |
| $u_2$ | $A_2$ | $B_1$ | $C_2$ |
| $u_3$ | $A_1$ | $B_2$ | $C_1$ |
| $u_4$ | $A_1$ | $B_2$ | $C_2$ |
| $u_5$ | $A_2$ | $B_2$ | $C_1$ |
| $u_6$ | $A_1$ | $B_1$ | $C_2$ |

TABLE 3
List of Main Notations

| Notation | Explanation |
|---|---|
| $\{u_1, ..., u_n\}$ | The set of $n$ objects |
| $\{a_1, ..., a_m\}$ | The set of $m$ attributes |
| $v_j^x, v_j^y$ | Specific values of attribute $a_j$ for objects $u_x, u_y$ |
| $v_k$ | Any value of attribute $a_k$ |
| $I(v_j^x)$ | The set of the objects whose value of attribute $a_j$ is $v_j^x$ |
| $I(v_j^x, v_k)$ | The set of the objects whose value of attribute $a_j$ is $v_j^x$ and value of attribute $a_k$ is $v_k$ |
| $V_j^I$ | The set of values of attribute $a_j$ for all objects in the object set $I$ |
| $\|I\|$ | The size of set $I$, i.e., the number of objects in $I$ |
| $\delta(u_i, u_j)$ | The similarity between objects $u_i$ and $u_j$ |
| $p(v_k\|v_j^x)$ | The conditional probability of $v_k$ w.r.t. $v_j^x$ |

For example, the values for two objects $u_1$ and $u_2$ on attribute $a_1$ are $v_1^1 = A_1$ and $v_1^2 = A_2$, hence $I(v_1^1) = I(A_1) = \{u_1, u_3, u_6\}$, for the value $B_1$ of attribute $a_2$, $I(A_1, B_1) = \{u_1, u_6\}$, $p(B_1|A_1) = |I(A_1, B_1)|/|I(A_1)| = 2/3$.

The above notations and definitions form the CMS foundation, which will be presented in the following section. The main notations in this paper are listed in Table 3.

## 4 Coupled Metric Similarity Measures

In this section, we discuss the learning framework, working mechanism, and key components that form the Coupled Metric Similarity (CMS) measures.

### 4.1 The learning framework

We propose the coupled metric similarity to capture the object similarity by considering and integrating both intra- and inter-attribute similarities as well as object similarities. Fig. 1 illustrates its learning framework, working mechanism, and corresponding key similarity measures. The coupled metric similarity is built on an information table for categorical data as discussed in Session 3.2. It first captures the value couplings in terms of intra-attribute similarities ($s_{Ia}^{j}(v_j^x, v_j^y)$), followed by the feature couplings in terms of inter-attribute similarities ($s_{Ie}^{k|j}(v_j^x, v_j^y)$). The intra- and inter-attribute similarities are then integrated into the coupled metric attribute value similarity $s^j(v^x_j, v^y_j)$, which are further aggregated into the coupled metric similarity to measure object similarities.

The intra-attribute similarity captures the value co-occurrence distribution within an attribute. For example, in Table 2, the intra-attribute similarity between attribute values $A_1$ and $A_2$ is related to the frequency of the values $A_1$ and $A_2$, which are both 3. The inter-attribute similarity between values $A_1$ and $A_2$ of attribute $a_1$ depends on the attribute values of other two attributes ($a_2$ and $a_3$). The coupled metric similarity further adaptively combines the intra-attribute similarity and the inter-attribute similarity to measure the object similarity. We ensure the metric validity of the proposed intra-attribute similarity, the inter-attribute similarity, and the CMS.

### 4.2 Intra-attribute similarity

According to [31], the discrepancy in attribute value occurrence times reflects the value similarity in terms of frequency distribution. The similarity between two objects is related to their commonality. Accordingly, the intra-attribute similarity considers the relationship between the frequency of the attribute values of an attribute, defined as follows.

***Definition 2 (Intra-attribute Similarity).*** The intra-attribute similarity between two attribute values $v^x_j, v^y_j$ of objects $u_x$ and $u_y$ on attribute $a_j$ is $s^j_{Ia}(v^x_j, v^y_j)$, defined as follows:

$$s^j_{Ia}(v^x_j, v^y_j) = \begin{cases} 1 & \text{if } v^x_j = v^y_j, \\ \dfrac{\log p \cdot \log q}{\log(p \cdot q) + \log p \cdot \log q} & \text{otherwise} \end{cases} \quad (3)$$

where $log$ represents the natural logarithm, $p$ denotes $|I(v^x_j)| + 1$, and $q$ denotes $|I(v^y_j)| + 1$. $I(v^x_j)$ is the set of objects whose values of attribute $a_j$ are $v^x_j$. Similarly, $I(v^y_j)$ is the set of objects whose values of attribute $a_j$ is $v^y_j$.

According to metric similarity conditions defined in Section 3, if the attribute values are identical, the similarity between them should be 1. When the attribute values are not identical, their occurrence frequencies indicate their similarity. Equation (3) is designed to satisfy the following three principles.

- The maximum similarity between two attribute values is reached when the values are identical.
- The greater similarity is assigned to the attribute value pair which shares approximately equal frequencies.
- The higher the frequency of two values, the closer two values are.

Equation (3) reflects that different occurrence frequencies indicate distinct levels of attribute value significance. When the size of the data increases sharply, the log function can control the growth of similarity. To prevent the denominator from being zero, we add 1 to each term. Since $1 \leq |I(v^x_j)|, |I(v^y_j)| \leq m$, then $s^j_{Ia}(v^x_j, v^y_j) \in (0, 1]$. If $v^x_j \neq v^y_j$, $s^j_{Ia}(v^x_j, v^y_j)$ achieves the maximum value when $|I(v^x_j)| = |I(v^y_j)| = m/2$. For example, in Table 2, $|I(A_1)| = 3$ and $|I(A_2)| = 3$, $s^1_{Ia}(A_1, A_2) = 0.41$.

### 4.3 Inter-attribute similarity

The above intra-attribute similarity reflects the coupling relationships between the attribute values of one attribute $a_j$, which does not involve the couplings between other attributes $a_k$ ($k \neq j$) and attribute $a_j$. Accordingly, we discuss the inter-attribute similarity, which involves the couplings between attributes and is much more complicated than intra-attribute couplings.

We note that the Modified Value Distance Matrix (MVDM) [38] measures the dissimilarity between categorical values w.r.t. class labels. It shows that attribute values are similar if they occur with similar relative frequency for all classifiers. Based on MVDM, Wang et. al. [10], [22] replaced the class labels with other attributes to enable unsupervised learning and proposed the *Inter-coupled Relative Similarity based on Power Set* (IRSP). They also proposed the *Inter-coupled Relative Similarity based on Join Set* (IRSJ), and the *Inter-coupled Relative Similarity based on Intersection Set* (IRSI), and proved that these measures are equivalent to each other in achieving the same accuracy in calculating value similarity [10], [22]. They prove that IRSI is the most efficient of the above measures; however, IRSI cannot retain the conditions of a metric similarity which are discussed in Section 3. Below, we propose a new inter-attribute similarity measure to satisfy metric properties.

Before calculating the inter-attribute similarity, we define the intersection set of co-occurrence conditional probability $W_k$.

***Definition 3 (Intersection Set of Co-occurrence Conditional Probability of Attribute Values).*** The intersection set of co-occurrence conditional probability of values $v^x_j$, $v^y_j$ of attribute $a_j$ with the co-occurrence values of attribute $a_k$ ($j \neq k$) is:

$$W_k = V_k^{I(v^x_j)} \cap V_k^{I(v^y_j)}, \quad (4)$$

$V_k^{I(v^x_j)}$ is the set of values of attribute $a_k$ for all objects in $I(v^x_j)$. $W_k$ consists of those attribute values of attribute $a_k$ which co-occur with both $v^x_j$ and $v^y_j$.

The Jaccard similarity coefficient is widely used in clustering and classification. The Jaccard similarity coefficient is defined as:

$$J(\mathbf{f}, \mathbf{g}) = \frac{\sum_i \min(f_i, g_j)}{\sum_i \max(f_i, g_j)}, \quad (5)$$

where $\mathbf{f} = (f_1, f_2, ..., f_n)$ and $\mathbf{g} = (g_1, g_2, ..., g_n)$ are two vectors with all real numbers.

The Jaccard distance is a distance metric [46] as follows:

$$\delta_J(u_x, u_y) = 1 - J(x, y). \quad (6)$$

According to the Jaccard distance and Equation (1) discussed in the previous section, we define the inter-attribute similarity with the Jaccard similarity based on IRSI [10] and $W_k$ as follows.

***Definition 4 (Inter-attribute Similarity of Attribute Values w.r.t. Another Attribute).*** The *inter-attribute similarity*

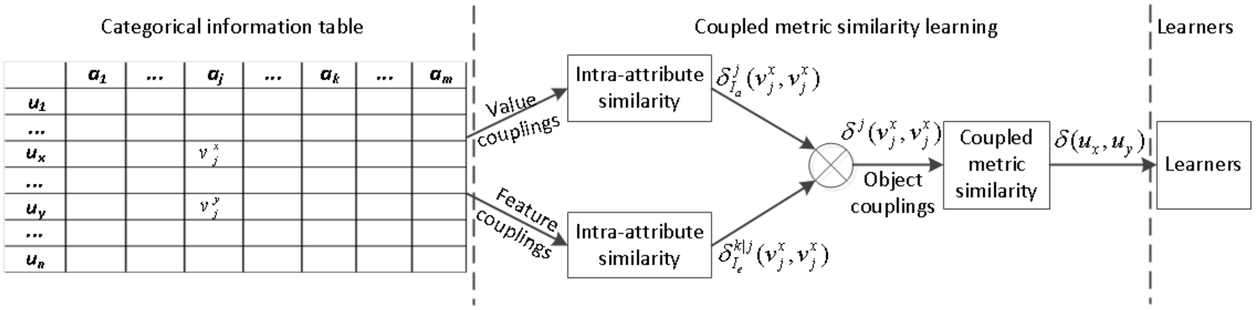
Categorical information table
$a_1$
...
$a_j$
...
$a_k$
...
$a_m$
$u_1$
...
$u_x$
...
$u_y$
...
$u_n$
$v_j^x$
$v_j^y$
Coupled metric similarity learning
Value couplings
Feature couplings
Intra-attribute similarity
$\delta^j_{I_a}(v_j^x, v_j^x)$
Intra-attribute similarity
$\delta^{k|j}_{I_e}(v_j^x, v_j^x)$
$\delta^j(v_j^x, v_j^x)$
Object couplings
Coupled metric similarity
$\delta(u_x, u_y)$
Learners
Learners

Fig. 1. The Framework of Coupling Metric Similarity Learning

between two attribute values $v_j^x$ and $v_j^y$ of attribute $a_j$ with another attribute $a_k$ is:

$$s_{Ie}^{k|j}(v_j^x, v_j^y) \tag{7}$$
$$= \begin{cases} 1, & \text{if } v_j^x = v_j^y \\ \dfrac{\sum_{i=1}^{|W_k|} \max(p_x^i, p_y^i)}{2 \cdot \sum_{i=1}^{|W_k|} \max(p_x^i, p_y^i) - \sum_{i=1}^{|W_k|} \min(p_x^i, p_y^i)} \\ \text{otherwise} \end{cases}$$

where $p_x^i = p(w_k^i | v_j^x)$, $p_y^i = p(w_k^i | v_j^y)$, they are conditional probabilities of $w_k^i$ with respect to $v_j^x$ and $v_j^y$, $p_x^i$ and $p_y^i$ are calculated according to Equation (2). $w_k^i$ is the $i_{th}$ element in $W_k$ which is calculated according to Equation (4). In particular, if $W_k$ is empty, $s_{Ie}^{k|j}(v_j^x, v_j^y) = \epsilon$ where $\epsilon$ is a small positive number.

In Table 2 for example, according to Equation (4), the similarity $s_{Ie}^{2|1}(A_1, A_2)$ depends on the values of attribute $a_2$. $I(A_1) = \{u_1, u_3, u_6\}$ and $I(A_2) = \{u_2, u_4, u_5, \}$, hence $V_2^{I(A_1)} = \{B_1, B_2\}$, $V_2^{I(A_2)} = \{B_1, B_2\}$ and $W_2 = \{B_1, B_2\}$. According to Equation (7), we calculate $\max(p(B_1|A_1), p(B_1|A_2))$, $\max(p(B_2|A_1), p(B_2|A_2))$, $\min(p(B_1|A_1), p(B_1|A_2))$, and $\min(p(B_2|A_1), p(B_2|A_2))$, and obtain $s_{Ie}^{2|1}(A_1, A_2) = 0.57$.

Following the above discussion, we further define the similarity between the value pair $(v_j^x, v_j^y)$ of attribute $a_j$ on top of the Jaccard similarity of other attributes $a_k$ ($j \neq k$).

***Definition 5 (Inter-attribute Similarity).*** The inter-attribute similarity between two attribute values $v_j^x$ and $v_j^y$ of attribute $a_j$ is:

$$s_{Ie}^j(v_j^x, v_j^y) = \sum_{k=1, k \neq j}^{m} \gamma_{k|j} s_{Ie}^{k|j}(v_j^x, v_j^y), \tag{8}$$

where $\gamma_{k|j}$ represents the weight of each attribute $a_k$ ($j \neq k$) to attribute $a_j$, $\sum_{k=1, k\neq j}^{m} \gamma_{k|j} = 1$, $\gamma_{k|j} \in [0, 1]$, and $s_{Ie}^{k|j}(v_j^x, v_j^y)$ is one of the inter-attribute similarity candidates with attribute $a_k$. $\gamma_{k|j}$ reflects the relation between attributes $a_j$ and $a_k$.

Consequently, we have $s_{Ie}^{k|j}(v_j^x, v_j^y) \in [0, 1]$. Particularly, if $W_k$ is not empty, $s_{Ie}^{k|j}(v_j^x, v_j^y) \in [0.5, 1]$. Since $s_{Ie}^{k|j}(v_j^x, v_j^y)$ is in $[0, 1]$, then $s_{Ie}^j(v_j^x, v_j^y) \in (0, 1]$.

In Table 2, for example $s_{Ie}^1(A_1, A_2) = 0.5 \cdot s_{Ie}^{1|2}(A_1, A_2) + 0.5 \cdot s_{Ie}^{1|3}(A_1, A_2) = 0.57$ if $\gamma_2 = \gamma_3 = 0.5$ by taking the equal weight. Furthermore, the coupled metric similarity (see Equation (10) in the following section) is obtained as $s^1(v_j^x, v_j^y) = 0.4904$ if $\alpha = 1$.

### 4.4 Coupled metric similarity

With the above defined intra-attribute similarity measure $s_{Ia}^j(v_j^x, v_j^y)$ and inter-attribute similarity measure $s_{Ie}^j(v_j^x, v_j^y)$, we now define the coupled metric similarity measure for attribute $a_j$.

We believe an ideal similarity measure should adapt to both IID and non-IID [14] data based on the characteristics of given data, hence we introduce a control parameter $\alpha$ in integrating the intra- and inter-attribute similarities. We define the coupled similarity measure of $v_j^x$ and $v_j^y$ as follows.

***Definition 6 (Coupled Metric Attribute Value Similarity).*** The *coupled metric attribute value similarity* (CMAVS) between attribute values $v_j^x$ and $v_j^y$ of attribute $a_j$ is:

$$s^j(v_j^x, v_j^y) = \frac{1}{\alpha \cdot \frac{1}{s_{Ie}^j} + (1 - \alpha) \cdot \frac{1}{s_{Ia}^j}}, \tag{9}$$

where $s_{Ia}^j$ and $s_{Ie}^j$ are respectively the intra-attribute similarity $s_{Ia}^j(v_j^x, v_j^y)$ and inter-attribute similarity $s_{Ie}^j(v_j^x, v_j^y)$ of attribute values $v_j^x$ and $v_j^y$, $\alpha \in [0, 1]$.

We use the weighted harmonic mean of inter-attribute similarity and intra-attribute similarity for the two main reasons. (1) The weighted harmonic mean guarantees the triangle equality of combined similarity (cf. Appendix). (2) It is more robust to outlier values but does not give much weight to the larger value. When $\alpha = 0.5$, the $s^j$ is the harmonic mean of $s_{Ie}^j$ and $s_{Ia}^j$.

Different $\alpha$ values reflect the different proportions of the intra-attribute similarity and inter-attribute similarity in forming the overall object similarity. A larger $\alpha$ indicates that inter-attribute couplings play a more important role in object similarity, i.e., the couplings between attribute $a_j$ and other attributes play a more important role than the couplings between values in $a_j$.

In particular, if all attributes are independent, i.e., $\alpha = 0$, correspondingly $s^j(v_j^x, v_j^y) = s_{Ia}^j$, indicating that only the couplings within an attribute contribute to object similarity. When $\alpha$ increases, $s^j(v_j^x, v_j^y)$ becomes closer to $s_{Ie}^j$. $\alpha = 1$ indicates that attribute values are independent. Therefore, by adjusting $\alpha$, we can control $s^j(v_j^x, v_j^y)$ to flexibly capture the intrinsic couplings in data. Later in Section 6, we will show the selection of parameter $\alpha$ and demonstrate that it may be possible to find an empirically optimal $\alpha$ value for a given dataset, while different datasets may share distinct $\alpha$ values.

We calculate the similarity between two objects $u_x$ and $u_y$ on top of CMAVS defined in Equation (9).

***Definition 7 (Coupled Metric Similarity).*** The *coupled metric similarity* (CMS) between two objects $u_x$ and $u_y$ is $s(u_x, u_y)$:

$$s(u_x, u_y) = \sum_{j=1}^{m} \beta_j s^j(v_j^x, v_j^y), \tag{10}$$

where $\beta_j$ represents the weight of the coupled metric attribute value similarity of an attribute $a_j$, $\sum_{j=1}^{m} \beta_j = 1$, $\beta_j \in [0, 1]$.

## 5 Theoretical analysis

This section proves that CMS is a valid similarity metric and analyses the theoretical properties and computational complexity of CMS.

### 5.1 CMS metric validity

Before we prove the validity of CMS, we first prove several theorems to lay the foundation.

***Theorem 1.*** $s^j(v_j^x, v_j^y) = 1$, if and only if $s_{Ie}^j(v_j^x, v_j^y) = s_{Ia}^j(v_j^x, v_j^y) = 1$ for every attribute $a_j$ and when $\alpha \neq 0$ and $\alpha \neq 1$.

***Theorem 2.*** The coupled metric attribute value similarity $s^j$ satisfies the triangle inequality if both intra-attribute similarity $s_{Ia}^j$ and inter-attribute similarity $s_{Ie}^j$ satisfy the triangle inequality for every attribute $a_j$.

***Theorem 3.*** The intra-attribute similarity $s_{Ia}^j$ satisfies the triangle inequality for any attribute $a_j$.

***Theorem 4.*** The inter-attribute similarity $s_{Ie}^j$ satisfies the triangle inequality for any attribute $a_j$.

These theorems are proved in the Appendix. Consequently, we prove that the validity of the proposed CMS, namely $s(u_x, u_y)$, satisfies the following metric properties.

1) **Positivity**: $0 < s(u_x, u_y) \leq 1$.
   $s^j(v_j^x, v_j^y)$ consists of $s_{Ia}^j(v_j^x, v_j^y)$ and $s_{Ie}^j(v_j^x, v_j^y)$. According to Equation (3), $s_{Ia}^j(v_j^x, v_j^y)$ is in (0,1]. $s_{Ie}^j(v_j^x, v_j^y)$ is based on the linear product of $s_{Ie}^{k|j}(v_j^x, v_j^y)$, and $s_{Ie}^{k|j}(v_j^x, v_j^y)$ is the Jaccard similarity of vectors, accordingly $s_{Ie}^j(v_j^x, v_j^y) \in (0, 1]$. According to Equation (9), $s(u^x, u^y)$ is the weighted sum of all similarity measures for each attribute's $s^j(v_j^x, v_j^y)$ which is the weighted harmonic mean of $s_{Ia}^j(v_j^x, v_j^y)$ and $s_{Ie}^j(v_j^x, v_j^y)$. Therefore, the similarity measure $s(u^x, u^y)$ satisfies the positivity constraint.
2) **Reflexivity**: $s(u_x, u_y) = 1 \Leftrightarrow u_x = u_y$
   We prove the necessity first.
   If $u_x = u_y$ then it means $v_j^x = v_j^y$ for all attributes $\{a_j\}$. According to Equations (3) and (8), if $v_j^x = v_j^y$, then $s_{Ie}^j(v_j^x, v_j^y) = s_{Ia}^j(v_j^x, v_j^y) = 1$, so $s^j(v_j^x, v_j^y) = 1$ and $s^j(u_x, u_y) = 1$. Hence, the similarity measure satisfies the necessity condition.
   We further prove the sufficiency.
   If $s(u_x, u_y) = 1$, we can conclude that $s^j(v_j^x, v_j^y) = 1$ for every attribute $a_j$ according to Equation (10), because $s^j(v_j^x, v_j^y)$ is also in (0,1]. According to Theorem 1, $s^j(v_j^x, v_j^y) = 1$, if and only if $s_{Ie}^j(v_j^x, v_j^y) = s_{Ia}^j(v_j^x, v_j^y) = 1$ and when $\alpha \neq 0$ and $\alpha \neq 1$ . When $\alpha = 0$, $s^j(v_j^x, v_j^y) = s_{Ia}^j(v_j^x, v_j^y) = 1$. From Equation (3), we can conclude that $s_{Ia}^j(v_j^x, v_j^y) = 1$ if and only if $v_j^x = v_j^y$. When $\alpha = 1$, $s^j(v_j^x, v_j^y) = s_{Ie}^j(v_j^x, v_j^y) = 1$. From Equation (8), we can conclude that $s_{Ie}^j(v_j^x, v_j^y) = 1$ if and only if $v_j^x = v_j^y$. For all attributes $a_j$, $v_j^x = v_j^y$ means $u_x = u_y$. The similarity measure satisfies the sufficiency condition, therefore the proposed similarity measure $s(u_x, u_y) = 1$, if and only if $u_x = u_y$.
3) **Commutativity**: $s(u_x, u_y) = s(u_y, u_x)$.
   All operations on our proposed similarity measure are addition, multiplication, maximum selection, and minimum selection. These operations are commutative. Hence the inequality holds implicitly.
4) **Triangle inequality**: $\frac{1}{s(u_x,u_y)} + \frac{1}{s(u_y,u_z)} \geq 1 + \frac{1}{s(u_x,u_z)}$.
   The resultant similarity $s(u_x, u_y)$ is the mean of all similarities $s^j(v_j^x, v_j^x)$ computed for every attribute. If $s^j(v_j^x, v_j^x)$ holds the triangle inequality, so does $s(u_x, u_y)$ (Its proof is similar to the proof of Theorem 2). If we can prove that each component of $s^j(v_j^x, v_j^x)$ (including $s_{Ia}^j(v_j^x, v_j^x)$ and $s_{Ie}^j(v_j^x, v_j^x)$) holds the triangle inequality, then $s^j(v_j^x, v_j^x)$ satisfies the triangle inequality according to Theorem 2. According to Theorem 3 and Theorem 4, $s_{Ia}^j(v_j^x, v_j^x)$ and $s_{Ie}^j(v_j^x, v_j^x)$ satisfy the triangle inequality. Hence, the triangle inequality is satisfied as well.

### 5.2 CMS theoretical property and computational complexity

The CMS measure $s(u_x, u_y)$ is an increasing function of $s_{Ia}^j$ and $s_{Ie}^j$ according to Equation (9). According to Definition 2, $s_{Ia}^j(v_j^x, v_j^x)$ reflects the intra-attribute similarity between two attribute values $v_j^x$ and $v_j^y$. The higher the value $s_{Ia}^j(v_j^x, v_j^x)$ is, the closer the two attribute values are. Equation (7) shows that the inter-attribute similarity $s_{Ie}^{k|j}(v_j^x, v_j^y)$ increases with the size of co-occurrence set $|W_k|$. Hence, the larger $s_{Ie}^j$ is, the more similar the two attribute values $v_j^x$ and $v_j^y$ are. In conclusion, we can obtain the increasing property of CMS, which means that the larger $s(u_x, u_y)$ indicates that two objects $u_x$ and $u_y$ are more similar.

The CMS between two objects captures all intra-attribute and inter-attribute similarities of each attribute value pair in the corresponding information table. Accordingly, the computational complexity linearly depends on the number of attribute values. The most time-consuming element is the calculation of inter-attribute similarity which is quantified by the calculation of $s_{Ie}^{k|j}(v_j^x, v_j^y)$. Hash table is used as the data structure to store $p(v_k|v_j^x)$ of each pair. Suppose the maximal number of distinct values for each attribute is $R$ and $m$ is the number of attributes, the time complexity of calculating the hash table of $p(v_k|v_j^x)$ for all attributes is $mR(R-1)$. The maximal value of $|W_k|$ is the number of objects $n$. According to Equation (7) and Equation (8), the computational complexity of inter-attribute similarity is $nm^2R(R-1)$. Considering Equation (10), the upper bound of the time complexity of CMS for two objects is $O(nm^3R^2)$, and the upper bound of the total CMS complexity for $n$ objects is $O(n^2m^3R^2)$.

## 6 Experiments and evaluation

In this section, we compare CMS with other similarity measures in terms of clustering categorical data by incorporating CMS into popular clustering methods on nineteen datasets.

### 6.1 Baseline clustering methods and measures

The following five state-of-the-art similarity/distance measures are compared with CMS: ALGO_DISTANCE (ALGO for short) [9], the Coupled Object Similarity (COS for short) [10], [22], the Distance Metric (DM for short) in [47], the Hamming Distance (HM for short) [7], and Occurrence Frequency (OF for short) [8].

All the above similarity measures including CMS are incorporated into a typical similarity-based categorical clustering algorithm spectral clustering [48] and a distance-based algorithm k-modes [49]. We compare their clustering performance on categorical data to evaluate which similarity measure achieves better outcomes.

According to the distance-similarity or dissimilarity-similarity mapping function, i.e., Equation (1) in Section 3, we can derive the metric distance or dissimilarity measure from the coupled metric similarity as follows:

$$\delta(u_x, u_y) = \frac{1}{s(u_x, u_y)} - 1, \tag{11}$$

where $\delta(u_x, u_y)$ denotes the distance or dissimilarity between objects $u_x$ and $u_y$, and $s(u_x, u_y)$ is the coupled metric similarity between $u_x$ and $u_y$ defined in Equation (10).

All similarity or distance measures and clustering methods are implemented in MATLAB and performed at 3.4GHz Pheonix Cluster with 32GB memory.

### 6.2 Datasets

19 UCI datasets are used for the experiments[1]. The detailed characteristics of these 19 different datasets are described in terms of four data factors in Table 4. They are $O$ - the number of objects, $A$ - the number of attributes, $V$ - the number of distinct values for all attributes, and $C$ - the number of classes (we include the class information for evaluation only). *Abbr.* refers to the short form of a dataset name. All numerical attributes in the datasets are removed to test the similarity for categorical data only.

The UCI data is used here because it is public, relatively simple and easy to understand compared to more complex real-life data. The assumption made is as follows. If a non-IID-oriented measure can beat its baselines on the UCI data, such a result should hold consistently on real-life data, which is usually non-IID, since the UCI data is not likely to contain more sophisticated non-IID characteristics. Another reason for using the UCI data is the challenge of finding real-life datasets that can be verified as non-IID, since currently no tools are available to verify whether or to what extent a dataset is non-IID.

TABLE 4
The Data Characteristics of 19 UCI Data Sets

| Dataset | $O$ | $A$ | $V$ | $C$ | *Abbr.* |
|---|---|---|---|---|---|
| Soybeansmall | 47 | 35 | 97 | 4 | So |
| Zoo | 101 | 16 | 36 | 7 | Zo |
| DNAPromoter | 106 | 57 | 228 | 2 | Dp |
| Hayesroth | 132 | 4 | 15 | 3 | Ha |
| Lymphography | 148 | 18 | 59 | 4 | Ly |
| Hepatitis | 155 | 13 | 36 | 2 | He |
| Housevotes | 232 | 16 | 32 | 2 | Ho |
| Spect | 267 | 22 | 44 | 2 | Sp |
| Mofn3710 | 300 | 10 | 20 | 2 | Mo |
| Soybeanlarge | 307 | 35 | 132 | 19 | Sol |
| Primarytumor | 339 | 17 | 42 | 21 | Pr |
| Dermatology | 366 | 33 | 129 | 6 | De |
| ThreeOf9 | 512 | 9 | 18 | 2 | Tr |
| Wisconsin | 683 | 9 | 89 | 2 | Wi |
| Crx | 690 | 9 | 45 | 2 | Cr |
| Breastcancer | 699 | 9 | 90 | 2 | Br |
| Mammographic | 830 | 4 | 20 | 2 | Ma |
| Flare | 1066 | 11 | 41 | 6 | Fl |
| Titanic | 2201 | 3 | 6 | 4 | Ti |

### 6.3 Parameter Selection

There are three parameters: $\alpha$, $\beta$ and $\gamma$ in CMS. The $\alpha$ value in Equation (9) reflects the extent of the inter-attribute coupling relationships embedded in a dataset. The larger the value of $\alpha$, the greater the proportion of inter-attribute similarity is. Hence, the coupling relationships in a dataset are stronger. $\beta$ in Equation (10) and $\gamma$ in Equation (7) reflect the importance of each feature which can be learned by feature selection methods [50]. In our experiments, each feature is regarded equally important. We assign the weight vector $(\beta_k)_{1\times m}$ with values $\beta_k = 1/m$, and assign $\gamma_{k|j} = 1/(m-1)$ for every attribute for simplicity. This simple setting is not optimal, but it can test whether the proposed CMS design is effective even in a non-optimal situation.

Since $\alpha$ reflects the combination ratio of intra- and inter-attribute couplings in a dataset, which varies per dataset, customizing the appropriate $\alpha$ fitting a respective dataset is necessary. We use the greedy search [51] on the validation set to choose the optimal $\alpha$ in CMS for each dataset. For large dataset, the validation set can be sampled from the original dataset. However, for unsupervised learning, there is no label to guide the parameter selection process for clustering. We can use some clustering internal criteria to guide the search of an optimal alpha. The clustering internal criteria [52] focus on the compactness and separability of clusters which are dependent on distance or similarity and

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

TABLE 5
The Calinski-Harabasz Index of CMS-enabled Spectral Clustering with Different $\alpha$ Values

| Datasets | $\alpha$ value | | | | | | |
|---|---|---|---|---|---|---|---|
| | 0 | 0.2 | 0.4 | 0.6 | 0.8 | 1 | $\alpha^*$ |
| So | 74.6 | 84.8 | 99.7 | 123.1 | 163.1 | **238.2** | 1 |
| Zo | **67.9** | 56.8 | 42.3 | 34.2 | 63.8 | 53.5 | 0 |
| Dp | 9.7 | 9.8 | 10.0 | 10.2 | 10.6 | **10.8** | 1 |
| Ha | 44.0 | 47.5 | 52.2 | 58.8 | 67.9 | **79.6** | 1 |
| Ly | 27.8 | 28.1 | 28.9 | 29.6 | 30.4 | **34.1** | 1 |
| He | 76.1 | 78.6 | 76.6 | 74.3 | **79.8** | 75.4 | 0.8 |
| Ho | 800.9 | 856.1 | 910.6 | 960.3 | 1005.7 | **1048.1** | 1 |
| Sp | 184.3 | 185.3 | 188.5 | 192.7 | 197.0 | **201.1** | 1 |
| Mo | 33.6 | 33.8 | 36.1 | 39.9 | 52.8 | **90.7** | 1 |
| Sol | 46.8 | 70.4 | **154.9** | 82.9 | 58.9 | 44.1 | 0.4 |
| Pr | 12.5 | 10.9 | 12.8 | **13.9** | 12.7 | 13.2 | 0.6 |
| De | 168.5 | 208.1 | 234.7 | 242.5 | 304.3 | **427.2** | 1 |
| Tr | 40.9 | 40.6 | 40.9 | 40.9 | **44.5** | 43.2 | 0.8 |
| Wi | 2437.8 | 2846.4 | 3267.9 | 3638.4 | 3942.0 | **4253.1** | 1 |
| Cr | 216.7 | 224.0 | 231.7 | 239.6 | **246.1** | 220.3 | 0.8 |
| Br | 2442.9 | 2854.7 | 3275.5 | 3658.6 | 3966.8 | **4282.8** | 1 |
| Ma | 954.2 | 1179.4 | 1432.8 | 1707.5 | 2002.5 | **2321.1** | 1 |
| Fl | 221.6 | 211.1 | 218.4 | 227.3 | 270.5 | **271.1** | 1 |
| Ti | 5837.9 | 5904.3 | 5969.9 | 6034.7 | **6098.5** | 6061.5 | 0.8 |

reflect the quality of resultant clusters to a certain extent. Here, we use the Calinski-Harabasz index [53] based on the clustering results from spectral clustering as the search criterion. The Calinski-Harabasz criterion is sometimes called the variance ratio criterion (VRC) which is defined as:

$$VRC_k = \frac{SS_B}{SS_W} \times \frac{(N-k)}{(k-1)}, \tag{12}$$

where $SS_B$ is the overall between-cluster variance, $SS_W$ is the overall within-cluster variance [53], $k$ is the number of clusters, and $N$ is the number of observations. Well-defined clusters have a large between-cluster variance ($SS_B$) and a small within-cluster variance ($SS_W$). The larger the $VRC_k$ ratio, the better the data partition.

The Calinski-Harabasz index is partially aligned with the purpose of CMS, that is, to maximize the similarity between similar objects and minimize the similarity between dissimilar objects. It is also worth noting that the $\alpha$ value chosen by the Calinski-Harabasz index may not be the optimal value since it only reflects one aspect of similarity measurement and there is no ground truth about the clustering results. Based on the Calinski-Harabasz index, we empirically set the step length to 0.2 in the greedy search and the search space as [0, 0.2, 0.4, 0.6, 0.8, 1] in our experiments, which considers the tradeoff between efficiency and effectiveness.

Table 5 reports the Calinski-Harabasz index of clustering results for different $\alpha$ values taken in spectral clustering. Since the datasets are not very large, we use the original dataset as the validation dataset. The results show that most datasets have inter-attribute coupling relationships between attributes. In the following clustering process, we use the $\alpha$ value which gets the best Calinski-Harabasz index for each dataset.

### 6.4 Evaluation methods

For external criteria, we choose some commonly used criteria to compare the clustering results for different similarity measures. The external criteria estimate the difference between the cluster label of each object assigned by each clustering algorithm and the ground truth indicated by the data labels given in the source data. The criteria include *normalized mutual information* (*NMI*) and *F-score*. The larger these criteria are, the better performance the clustering achieves; the corresponding similarity measure is accordingly more effective. The definitions of these three measures are given below.

- *Normalized Mutual Information*

$$NMI = \frac{\sum_{i=1}^{k}\sum_{j=1}^{c} n_{i,j}\log\left(\frac{n\cdot n_{i,j}}{n_i\cdot n_j}\right))}{\sqrt{\left(\sum_{i=1}^{k} n_i \log\frac{n_i}{n}\right)\left(\sum_{j=1}^{c} n_j \log\frac{n_j}{n}\right)}}, \tag{13}$$

where $c$ stands for the true number of classes, $k$ is the number of clusters obtained by the algorithm, $n_{i,j}$ denotes the number of agreements between cluster $i$ and class $j$, and $n$ is the number of objects in the whole dataset.

- *F-score*

$$F_1 = \frac{2*TP}{2*TP+FP+FN}, \tag{14}$$

where $TP$, $TN$, $FP$, and $FN$ stand for true positive, true negative, false positive, and false negative, respectively.

### 6.5 Comparison of CMS and other similarity measures-enabled spectral clustering

Tables 6 and 7 report the results of spectral clustering driven by the similarity measures CMS, ALGO, COS, DM, OF and HM in terms of performance measures *NMI* and *F-score*. The overall performance is given in the bottom row w.r.t. the mean value. For each dataset, the average performance is obtained by 50 tests of spectral clustering with distinct start points. In the clustering evaluation, the $\alpha^*$ for each dataset, as shown in Table 5, replaces the $\alpha$ parameter in Equation (9). This reflects an acceptable balance between intra- and inter-attribute couplings in a respective dataset.

The clustering results show that the CMS-enabled spectral clustering outperforms the spectral clustering methods empowered by ALGO, COS, DM, OF and HM on seven out of 19 datasets in terms of both *NMI* in Table 6 and *F-score* in Table 7. By contrast, COS, which also captures both intra- and inter-attribute couplings achieves less mean value than CMS in terms of *NMI* and *F-score*. CMS performs better than two best and most recent similarity baselines for categorical data: ALGO and COS by 3.1% and 3.9% respectively, and the worst-performing measure OF by 9.0% in terms of the mean NMI value. In addition, CMS outperforms ALGO and COS by 2.6% and 2.9% respectively in terms of *F-score*.

It is also interesting to note that every other similarity measure outperforms at least one of other measures in one or two datasets. This reflects the difficulty in effectively capturing the intrinsic data characteristics in categorical data and the significant challenge in designing appropriate and generalized similarity measures for categorical data.

TABLE 6
The NMI of CMS vs. ALGO, COS, DM, OF and HM-enabled Spectral Clustering

| Datasets | CMS | ALGO | COS | DM | OF | HM |
|---|---|---|---|---|---|---|
| So | **1** | 0.953 | 0.946 | 0.957 | 0.941 | 0.952 |
| Zo | 0.703 | 0.731 | 0.705 | **0.748** | 0.672 | 0.690 |
| Dp | 0.228 | 0.209 | 0.154 | 0.227 | 0.103 | **0.250** |
| Ha | 0.001 | 0.001 | **0.011** | 0.001 | 0.001 | 0.001 |
| Ly | **0.224** | 0.159 | 0.164 | 0.138 | 0.119 | 0.152 |
| He | **0.196** | 0.183 | 0.179 | 0.185 | 0.129 | 0.171 |
| Ho | **0.526** | 0.522 | 0.524 | 0.522 | 0.493 | 0.493 |
| Sp | 0.103 | **0.106** | 0.102 | 0.105 | 0.094 | **0.106** |
| Mo | **0.055** | 0.054 | 0.054 | 0.017 | 0.017 | 0.017 |
| Sol | 0.697 | 0.736 | **0.768** | 0.666 | 0.632 | 0.673 |
| Pr | 0.346 | 0.348 | 0.337 | **0.366** | 0.351 | 0.344 |
| De | **0.844** | 0.814 | 0.807 | 0.792 | 0.491 | 0.748 |
| Tr | **0.015** | 0.002 | 0.002 | 0.034 | 0.03 | 0.026 |
| Wi | 0.826 | 0.829 | **0.831** | 0.815 | 0.811 | 0.670 |
| Cr | 0.189 | 0.035 | 0.043 | 0.024 | **0.294** | 0.201 |
| Br | 0.806 | 0.818 | **0.82** | 0.805 | 0.801 | 0.749 |
| Ma | 0.336 | 0.329 | **0.361** | 0.332 | 0.326 | 0.331 |
| Fl | 0.260 | 0.318 | 0.269 | 0.192 | **0.374** | 0.280 |
| Ti | 0.115 | 0.101 | 0.101 | 0.122 | **0.128** | 0.114 |
| **Mean** | **0.393** | 0.381 | 0.378 | 0.371 | 0.358 | 0.367 |

TABLE 7
The F-score of CMS vs. ALGO, COS, DM, OF and HM-enabled Spectral Clustering

| Datasets | CMS | ALGO | COS | DM | OF | HM |
|---|---|---|---|---|---|---|
| So | **1** | 0.952 | 0.943 | 0.935 | 0.888 | 0.925 |
| Zo | 0.525 | 0.547 | 0.538 | **0.588** | 0.494 | 0.518 |
| Dp | **0.762** | 0.753 | 0.726 | 0.753 | 0.675 | 0.750 |
| Ha | 0.338 | 0.335 | **0.338** | 0.329 | 0.336 | 0.337 |
| Ly | **0.398** | 0.366 | 0.395 | 0.286 | 0.319 | 0.340 |
| He | **0.696** | 0.662 | 0.622 | **0.695** | 0.633 | 0.649 |
| Ho | 0.892 | 0.888 | **0.893** | 0.888 | 0.884 | 0.884 |
| Sp | 0.547 | 0.572 | **0.582** | 0.563 | 0.565 | 0.559 |
| Mo | **0.567** | **0.567** | **0.567** | 0.509 | 0.509 | 0.509 |
| Sol | 0.528 | 0.553 | **0.609** | 0.476 | 0.48 | 0.504 |
| Pr | 0.213 | 0.209 | 0.196 | **0.230** | 0.213 | 0.205 |
| De | **0.762** | 0.710 | 0.730 | 0.735 | 0.615 | 0.660 |
| Tr | 0.555 | 0.522 | 0.519 | **0.591** | 0.582 | 0.555 |
| Wi | 0.968 | 0.971 | **0.973** | 0.942 | 0.968 | 0.923 |
| Cr | 0.745 | 0.551 | 0.493 | 0.527 | **0.791** | 0.753 |
| Br | 0.966 | 0.969 | **0.97** | 0.937 | 0.966 | 0.921 |
| Ma | 0.817 | 0.818 | **0.822** | 0.814 | 0.817 | 0.801 |
| Fl | 0.365 | 0.392 | 0.352 | 0.321 | **0.444** | 0.359 |
| Ti | 0.325 | **0.375** | 0.358 | 0.354 | 0.306 | 0.298 |
| **Mean** | **0.630** | 0.614 | 0.612 | 0.604 | 0.604 | 0.603 |

### 6.6 Comparison of CMS and other similarity measures-enabled k-modes clustering

Tables 8 and 9 report the *NMI* and *F-score* results of k-modes clustering enabled by the distance measures derived from CMS, ALGO, COS, DM, OF and HM according to Equation (11). The overall performance is given in the bottom row w.r.t. the mean value. For each dataset, the average performance is obtained by 50 tests of k-modes clustering with distinct start points. In k-modes clustering, the $\alpha$ values for respective datasets also follow the $\alpha^*$ in Table 5.

In Table 8, the *NMI* results of CMS-enabled k-modes are superior to other measures-enabled k-modes on nine datasets, compared to five by ALGO, three by COS, one by DM, two by OF, and none by HM. Overall, CMS outperforms ALGO by 1.1%, COS by 5.8%, DM by 9.7%, OF by 45.9%, and HM by 16.0%. The *F-score* results of CMS-enabled k-modes outperform five other measures in ten out of 19 datasets as shown in Table 9, compared to four by ALGO, two by COS, two by HM, one by OF and none by HM. With regard to the mean *F-score*, CMS is superior to ALGO by 6.6%, COS by 9.3%, DM by 9.7%, OF by 18.8%, and HM by 9.8%.

TABLE 8
The NMI of CMS vs. ALGO, COS, DM, OF and HM-enabled K-modes Clustering

| Datasets | CMS | ALGO | COS | DM | OF | HM |
|---|---|---|---|---|---|---|
| So | **1** | 0.887 | 0.860 | 0.858 | 0.745 | 0.828 |
| Zo | **0.842** | 0.788 | 0.803 | 0.757 | 0.736 | 0.759 |
| Dp | 0.002 | **0.08** | 0.071 | 0.018 | 0.048 | 0.06 |
| Ha | 0.012 | 0.014 | **0.056** | 0.012 | 0.037 | 0.015 |
| Ly | **0.252** | 0.159 | 0.164 | 0.138 | 0.119 | 0.152 |
| He | **0.188** | 0.15 | 0.102 | 0.128 | 0.099 | 0.131 |
| Ho | 0.447 | 0.511 | 0.511 | **0.531** | 0.440 | 0.461 |
| Sp | **0.110** | 0.092 | 0.087 | 0.092 | 0.089 | 0.088 |
| Mo | 0.008 | 0.017 | 0.025 | 0.023 | **0.029** | 0.02 |
| Sol | 0.677 | **0.683** | 0.674 | 0.613 | 0.602 | 0.631 |
| Pr | **0.376** | 0.374 | 0.359 | 0.348 | 0.335 | 0.362 |
| De | **0.770** | 0.734 | 0.743 | 0.719 | 0.272 | 0.578 |
| Tr | 0.001 | **0.004** | **0.004** | 0.026 | 0.020 | 0.025 |
| Wi | 0.610 | **0.668** | 0.606 | 0.593 | 0.102 | 0.482 |
| Cr | **0.267** | 0.176 | 0.054 | 0.229 | 0.132 | 0.168 |
| Br | 0.595 | **0.673** | 0.609 | 0.574 | 0.115 | 0.437 |
| Ma | **0.327** | 0.326 | 0.277 | 0.271 | 0.269 | 0.305 |
| Fl | 0.274 | 0.364 | 0.375 | 0.232 | **0.409** | 0.31 |
| Ti | 0.114 | 0.112 | **0.117** | 0.113 | 0.106 | 0.109 |
| **Mean** | **0.362** | 0.359 | 0.342 | 0.330 | 0.248 | 0.312 |

TABLE 9
The F-score of CMS vs. ALGO, COS, DM, OF and HM-enabled K-modes Clustering

| Datasets | CMS | ALGO | COS | DM | OF | HM |
|---|---|---|---|---|---|---|
| So | **1** | 0.854 | 0.780 | 0.744 | 0.745 | 0.799 |
| Zo | **0.713** | 0.554 | 0.571 | 0.563 | 0.514 | 0.534 |
| Dp | 0.498 | **0.611** | 0.564 | 0.358 | 0.578 | 0.606 |
| Ha | 0.403 | 0.374 | **0.421** | 0.375 | 0.398 | 0.359 |
| Ly | **0.396** | 0.366 | 0.395 | 0.324 | 0.319 | 0.34 |
| He | **0.667** | 0.641 | 0.620 | 0.637 | 0.615 | 0.636 |
| Ho | 0.866 | 0.884 | 0.884 | **0.896** | 0.865 | 0.87 |
| Sp | 0.351 | 0.445 | 0.403 | **0.468** | 0.463 | 0.42 |
| Mo | 0.455 | 0.505 | 0.507 | 0.508 | **0.514** | 0.493 |
| Sol | **0.555** | 0.489 | 0.504 | 0.478 | 0.449 | 0.452 |
| Pr | 0.218 | **0.226** | 0.215 | 0.213 | 0.205 | 0.228 |
| De | **0.677** | 0.601 | 0.577 | 0.579 | 0.317 | 0.517 |
| Tr | **0.697** | 0.353 | 0.345 | 0.534 | 0.552 | 0.564 |
| Wi | 0.900 | **0.907** | 0.887 | 0.854 | 0.536 | 0.815 |
| Cr | **0.793** | 0.668 | 0.578 | 0.751 | 0.64 | 0.678 |
| Br | 0.896 | **0.928** | 0.901 | 0.882 | 0.542 | 0.783 |
| Ma | **0.819** | 0.817 | 0.769 | 0.759 | 0.759 | 0.793 |
| Fl | 0.393 | 0.377 | 0.390 | 0.364 | **0.445** | 0.375 |
| Ti | **0.337** | 0.314 | 0.320 | 0.313 | 0.324 | 0.318 |
| **Mean** | **0.612** | 0.574 | 0.560 | 0.558 | 0.515 | 0.557 |

### 6.7 Comparison of CMS and its variants

With different $\alpha$ values, we can obtain multiple CMS variants, e.g., intra-attribute similarity ($\alpha = 0$), inter-attribute similarity ($\alpha = 1$), and combined similarity ($\alpha = 0.5$). Table 10 reports the results of spectral clustering by taking the intra-attribute similarity (denoted by Intra), inter-attribute

This article has been accepted for publication in a future issue of this journal, but has not been fully edited. Content may change prior to final publication. Citation information: DOI 10.1109/TKDE.2018.2808532, IEEE Transactions on Knowledge and Data Engineering

similarity (denoted by Inter), and combined similarity (denoted by Combo).

According to the mean results of all datasets, the combined similarity outperforms pure intra-attribute similarity or inter-attribute similarity. The results in Tables 6 and 7 also show that the combined similarity outperforms other combinations of intra- and inter-attribute similarities in CMS. Though an optimal alpha value may be obtained by the greedy search per criteria such as the Calinski-Harabasz index, it may be highly costly and we thus recommend the empirical value $\alpha = 0.5$ for new datasets.

TABLE 10
The F-score and NMI of Intra-attribute Similarity, Inter-attribute Similarity, and Combined Similarity-enabled Spectral Clustering

| | NMI | | | F-score | | |
|---|---|---|---|---|---|---|
| Datasets | Intra | Inter | Combo | Intra | Inter | Combo |
| Zo | 0.699 | 0.731 | 0.674 | 0.504 | 0.554 | 0.490 |
| Dp | 0.250 | 0.228 | 0.250 | 0.771 | 0.762 | 0.771 |
| Ha | 0.001 | 0.001 | 0.001 | 0.342 | 0.336 | 0.336 |
| Ly | 0.219 | 0.221 | 0.225 | 0.373 | 0.385 | 0.381 |
| He | 0.193 | 0.185 | 0.203 | 0.673 | 0.681 | 0.698 |
| Ho | 0.493 | 0.526 | 0.509 | 0.884 | 0.892 | 0.888 |
| Sp | 0.099 | 0.100 | 0.093 | 0.560 | 0.548 | 0.551 |
| Mo | 0.017 | 0.054 | 0.016 | 0.509 | 0.567 | 0.528 |
| Sol | 0.679 | 0.704 | 0.688 | 0.522 | 0.528 | 0.530 |
| Pr | 0.337 | 0.341 | 0.336 | 0.201 | 0.204 | 0.208 |
| De | 0.766 | 0.847 | 0.788 | 0.713 | 0.757 | 0.757 |
| Tr | 0.012 | 0.003 | 0.038 | 0.550 | 0.526 | 0.596 |
| Wi | 0.731 | 0.816 | 0.797 | 0.945 | 0.968 | 0.964 |
| Cr | 0.201 | 0.024 | 0.195 | 0.753 | 0.527 | 0.749 |
| Br | 0.720 | 0.806 | 0.782 | 0.942 | 0.966 | 0.960 |
| Ma | 0.334 | 0.326 | 0.336 | 0.824 | 0.817 | 0.825 |
| Fl | 0.318 | 0.266 | 0.257 | 0.383 | 0.366 | 0.362 |
| Ti | 0.115 | 0.114 | 0.114 | 0.304 | 0.299 | 0.299 |
| **Mean** | 0.378 | 0.384 | 0.384 | 0.619 | 0.615 | 0.626 |

### 6.8 Scalability Test

Here we use two datasets to test the scalability of the similarity measures. We compare the running time of calculating the similarity between each pair of attribute values in each similarity measure. Except the Hamming distance which does not need to calculate the value distance, we test the scalability of CMS, ALGO, COS, DM and OF.

To test the scalability w.r.t. the number of objects, we generate five synthetic datasets with the smallest size of 1,875 and the largest size of 30,000 from the UCI dataset *Adult* which have 30,162 objects and 8 attributes. To test the scalability w.r.t. the number of attributes, we generate six synthetic data with the smallest dimension of 125 and the largest dimension of 4,000 from a high-dimensional dataset *Wap.wc*[2] which have 346 objects and 4,229 attributes.

In the left panel of Fig. 2, CMS runs significantly faster than ALGO, COS and DM but slower than OF since OF does not consider any coupling relationships between attributes. In the right panel, CMS has similar runtime as ALGO but faster than COS and DM.

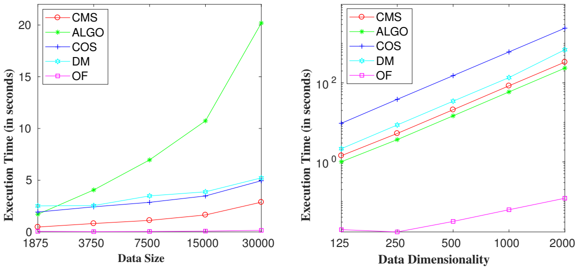

Fig. 2. The Scalability Test Results w.r.t. Data Size and Dimensionality.

### 6.9 Experimental summary

In summary, the above experiments show that CMS in most cases outperforms the other state-of-the-art similarity and distance measures when they are incorporated into spectral clustering and k-modes for clustering categorical data. The experimental results also show that, for most datasets, the similarity/distance measures that involve couplings, i.e., CMS, ALGO, DM and COS, almost always obtain better performance. This shows the importance of capturing the various couplings embedded in complex categorical data [13]. By contrast, CMS significantly outperforms the five state-of-the-art categorical similarity measures in the overall results, indicating that CMS is better at capturing couplings than the other similarity measures.

The results also show that none of the similarity and distance measures can always win on all 19 datasets for unsupervised learning. This indicates the complexity and significance of deeply understanding the intrinsic data characteristics of complex categorical data (which cannot be simply measured by the Hamming measure or the frequency of co-occurrences).

## 7 Discussion about CMS to Adaptively Capture Hierarchical Coupling Relationships

In this section, we empirically analyze why CMS achieves good performance. We explore the intrinsic working mechanisms of CMS, namely, by observing the impact of involving three levels of coupling relationships on clustering performance: the intra-attribute similarity for capturing value couplings, the inter-attribute similarity for capturing attribute couplings, and the coupled similarity between objects which integrates both intra-attribute similarity and inter-attribute similarity. We discuss how the intra- and inter-attribute similarities capture the intrinsic couplings within data.

### 7.1 Balance between intra-attribute and inter-attribute similarities

CMS integrates both intra-attribute similarity and inter-attribute similarity, as shown in Equation (9), in terms of their different contributions and combinations adjustable by parameter $\alpha$. $\alpha = 0$ means we only consider the couplings within an attribute (i.e., intra-attribute similarity). $\alpha = 1$ indicates that we only consider the couplings between attributes (i.e., inter-attribute similarity). The effect of tuning parameter $\alpha$ on the Calinski-Harabasz index is shown in Table 5, although the outcomes only capture partial aspects of data characteristics and may be sub-optimal. The $\alpha$ value corresponding to the highest Calinski-Harabasz index on a dataset strikes a balance between the contributions made by

[2] http://tunedit.org/repo/Data/Text-wc

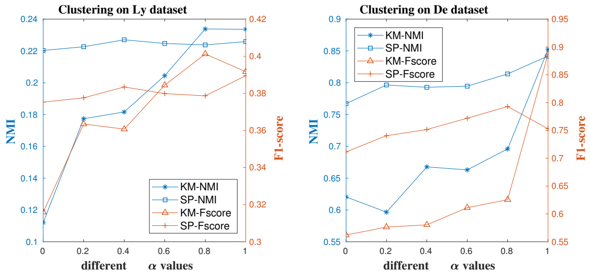

Fig. 3. The clustering results on datasets Ly and De w.r.t. different $\alpha$ values

TABLE 11
The Frequencies and Co-occurrences of Attribute Values

| Attribute Values | a1 | a2 | b1 | b2 | b3 | c1 | c2 | c3 |
|---|---|---|---|---|---|---|---|---|
| a1 | **22** | | 10 | 13 | 0 | 2 | 6 | 14 |
| a2 | | **25** | 0 | 21 | 4 | 15 | 0 | 10 |
| b1 | 10 | 0 | **10** | | | 0 | 6 | 4 |
| b2 | 13 | 21 | | **33** | | 15 | 0 | 18 |
| b3 | 0 | 4 | | | **4** | 2 | 0 | 2 |
| c1 | 2 | 15 | 0 | 15 | 2 | **17** | | |
| c2 | 6 | 0 | 6 | 0 | 0 | | **6** | |
| c3 | 14 | 10 | 4 | 18 | 2 | | | **24** |

intra-attribute similarity and inter-attribute similarity, which explains why the CMS incorporated by the corresponding $\alpha$ value obtains desirable clustering performance.

In our experiments, we also find that the CMS with only inter-attribute similarity obtains better clustering performance than some CMS variants that consider both intra-attribute and inter-attribute similarities on datasets. As shown in Tables 6 and 7 for spectral clustering and Tables 8 and 9 for k-modes clustering, CMS performs consistently well on datasets *Lymphography* and *Dermatology*. Accordingly, we show the clustering performance of CMS-enabled spectral clustering and k-modes clustering w.r.t. all the $\alpha$ values shown in Tables 5, which demonstrates the challenge of balancing intra- and inter-attribute similarities in unsupervised learning.

Fig. 3 reflects the clustering performance on datasets Ly and De. It shows that different $\alpha$ values may lead to different clustering performance, hence, it is necessary to choose the optimal $\alpha$ value. The optimal $\alpha$ value on the Ly dataset is 0.8 for k-modes clustering. Spectral clustering is not sensitive to the change of $\alpha$ value on Ly and the optimal value is 1. For dataset De, the change of $\alpha$ value has a large influence on k-modes clustering and the optimal value is 1. In terms of spectral clustering, the optimal value w.r.t NMI is slightly different from the optimal value w.r.t. F-score. The optimal $\alpha$ value of one dataset is decided by not only data characteristics but also the clustering algorithm. We will study this issue in our future work.

### 7.2 Scrutinizing data characteristics

An effective similarity metric needs to capture the intrinsic data characteristics, which may be quantified in terms of data factors and indicators [54]. This section explores CMS in terms of capturing categorical data factors and hierarchical similarities. We illustrate this exploration by scrutinizing the characteristics of the Soybean-small data in Table 4.

The Soybean-small dataset contains 47 objects, 35 attributes and 100 distinct attribute values. It is clearly a small dataset but it is relatively interesting due to its 'large' numbers of attributes and values compared to very 'small' object number in the UCI data. To illustrate its value and attribute coupling relationships, we select three attributes: *plant-stand*, *precip* and *temp*, and use *a1-a2, b1-b3, and c1-c3* to label the distinct values of these respective attributes.

At the attribute value level, we calculate the occurrence frequency of each value and the co-occurrence frequency of each value pair in Table 11. The boldfaced values in the diagonal correspond to the occurrence frequencies of attribute values, and the other non-empty cells capture the co-occurrences of value pairs from different attributes.

Table 12 shows the intra-attribute similarity and inter-attribute similarity of attribute value pairs, labelled as $s^j_{Ia}$ for the intra-attribute similarity, $s^j_{Ie}$ for the inter-attribute similarity, and $s^j$ for the coupled object similarity, as defined in Equations (3), (8) and (9) with $\alpha = 0.5$. The statistical information shown in Table 11 and the diverse similarities collected in Table 12 enable us to disclose the intrinsic data characteristics in Soybean-small and the power of CMS in terms of capturing such characteristics.

The intra-attribute similarity $s^j_{Ia}$ of pair b1-b2 is 0.5880, which is larger than that of b1-b3. It consists of the relationship between frequencies of b1, b2 and b3 in Table 11, hence the intra-attribute similarity captures the frequency distributions and reflects the couplings between values within an attribute. The inter-attribute similarities $s^j_{Ie}$ of most pairs (except pairs b1-b3 and c1-c2) in Table 12 are larger than their intra-attribute similarities. For pair c1-c2, its inter-attribute similarity is 0.2656, which is smaller than that of other pairs. In Table 11, the co-occurrence frequency of pairs c1-a2, c1-b2 and c1-b3 are 15, 15 and 2 respectively, while the co-occurrence frequencies of pairs c2-a2, c2-b2 and c2-b3 are all 0. This indicates that the co-occurring values of c1 are quite different from those of c2. The inter-attribute similarity $s^j_{Ie}$ consists of the co-occurrence frequencies of attribute value pairs; it captures the latent couplings between different attributes. In this way, the similarity between attributes is transformed to the attribute-value similarity and is then reflected in the similarity on the object level. The results in Table 12 also show the sensitivity of the integration of the intra- and inter-attribute similarities in calculating the value-to-attribute-to-object similarity.

Lastly, as shown in Section 7.1, CMS combines the intra- and inter-attribute similarities. The parameter $\alpha$ adjusts the combination of intra-attribute similarities and inter-attribute similarities. Since different datasets probably own diverse combinations of intra- and inter-attribute couplings, the corresponding optimal $\alpha$ values accordingly are different. An optimal $\alpha$ value reflects the most appropriate distribution of intra- and inter-attribute couplings in a dataset.

## 8 Conclusions and Future Work

Learning for non-IID data significantly challenges existing analytical and learning theories and similarity measures

TABLE 12
The Value-to-Attribute-to-Object Similarities

| | a1-a2 | b1-b2 | b1-b3 | b2-b3 | c1-c2 | c1-c3 | c2-c3 |
|---|---|---|---|---|---|---|---|
| $s^j_{Ia}$ | 0.615 | 0.588 | **0.491** | 0.525 | **0.538** | 0.604 | 0.549 |
| $s^j_{Ie}$ | **0.682** | **0.703** | 0.417 | **0.827** | 0.266 | **0.734** | **0.626** |
| $s^j$ | 0.647 | 0.640 | 0.431 | 0.642 | 0.356 | 0.663 | 0.586 |

in terms of effectively capturing the intrinsic heterogeneity and coupling relationships in non-IID data. The categorical data embedded with value-to-attribute-to-object hierarchical coupling relationships is particularly complex. Learning such data requires the appropriate representation and similarity metrics for capturing such hierarchical coupling relationships from attribute values to attributes and objects.

In this paper, we have proposed and evaluated a novel *coupled metric similarity* measure CMS for learning hierarchical couplings in categorical data. Taking a data-driven approach that integrates the intrinsic coupling relationships from low-level attributes and their values to objects in a dataset, CMS captures both attribute value frequency distribution and attribute dependency similarity to measure attribute value similarity, attribute similarity, and then object similarity.

Compared with the state-of-the-art similarity measures, including ALGO-distance, coupled object similarity, distance matrix, occurrence frequency-based measure, and Hamming-based measure, the incorporation of CMS and the above measures into two representative clustering methods, spectral clustering and k-modes, shows the great advantage of CMS against the baseline similarity measures in representing the above hierarchical couplings. CMS also incorporates a tuning mechanism for both distance-based and similarity-based analysis of either IID or non-IID data.

In addition to the experimental evaluation, we have investigated the driving factors of CMS-enabled performance improvement and soundness supported by satisfying the metric properties and explained by discussions about the underlying working mechanisms of CMS from statistical and data characteristic perspectives. None of the existing categorical similarity and dissimilarity measures provide such a theoretical foundation as CMS.

We are working on designing more effective data structures and strategies for efficient enhancement and scalable clustering of large-scale non-IID categorical data using CMS. Incorporating feature selection or feature weighting into CMS is another open issue for improving the CMS effectiveness and efficiency. Another aspect we are working on is to handle heterogeneous data with value-to-object couplings and quantify the data characteristics to decide the strength of couplings in data automatically.

## Acknowledgments

This work is partially supported by The National Key Research and Development Program of China (No.2016YFB0200401), by program for New Century Excellent Talents in University, by National Science Foundation (NSF) China 61402492, 61402486, 61379146, by the laboratory pre-reseach fund (9140C810106150C81001) and by the Australian Research Council Discovery Grant (DP130102691).

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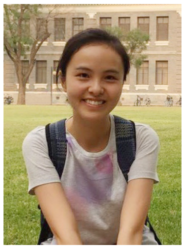

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