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.

- *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.*
  E-mail: jiansonglei@163.com
- *Longbing Cao is with the Advanced Analytics Institute, University of Technology Sydney, Australia. Email: longbing.cao@uts.edu.au (corresponding author).*

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

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

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, δ) where M is a set and δ 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

U \ A	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 $s^j(v_j^x, v_j^y)$, 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_j^x, v_j^y of objects u_x and u_y on attribute a_j is $s_{Ia}^j(v_j^x, v_j^y)$, defined as follows:

$$s_{Ia}^j(v_j^x, v_j^y) = \begin{cases} 1 & \text{if } v_j^x = v_j^y \\ \dfrac{\log p \cdot \log q}{\log(p \cdot q) + \log p \cdot \log q} & \text{otherwise} \end{cases}, \quad (3)$$

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

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 $1 \leq |I(v_j^x)|, |I(v_j^y)| \leq m$, then $s_{Ia}^j(v_j^x, v_j^y) \in (0, 1]$. If $v_j^x \neq v_j^y$, $s_{Ia}^j(v_j^x, v_j^y)$ achieves the maximum value when $|I(v_j^x)| = |I(v_j^y)| = m/2$. For example, in Table 2, $|I(A_1)| = 3$ and $|I(A_2)| = 3$, $s_{Ia}^1(A_1, A_2) = 0.41$.

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_j^x, v_j^y of attribute a_j with the co-occurrence values of attribute a_k ($j \neq k$) is:

$$W_k = V_k^{I(v_j^x)} \cap V_k^{I(v_j^y)}, \quad (4)$$

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

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*

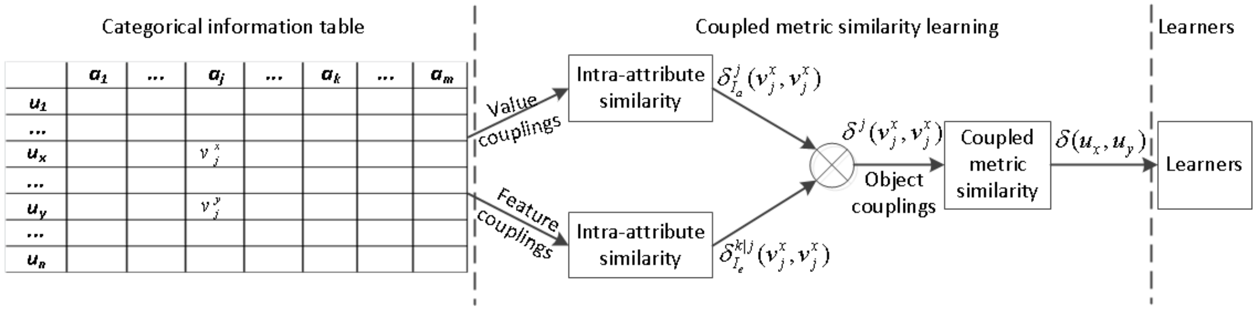


Fig. 1. The Framework of Coupling Metric Similarity Learning

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

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

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 ϵ 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 α 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_{le}^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 α values reflect the different proportions of the intra-attribute similarity and inter-attribute similarity in forming the overall object similarity. A larger α 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 α 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 α, 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 α and demonstrate that it may be possible to find an empirically optimal α value for a given dataset, while different datasets may share distinct α 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 $s(u_x, u_y)$:

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

where β_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.

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

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: α, β and γ in CMS. The α value in Equation (9) reflects the extent of the inter-attribute coupling relationships embedded in a dataset. The larger the value of α, the greater the proportion of inter-attribute similarity is. Hence, the coupling relationships in a dataset are stronger. β in Equation (10) and γ 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 α reflects the combination ratio of intra- and inter-attribute couplings in a dataset, which varies per dataset, customizing the appropriate α fitting a respective dataset is necessary. We use the greedy search [51] on the validation set to choose the optimal α 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

TABLE 5
The Calinski-Harabasz Index of CMS-enabled Spectral Clustering with Different α Values

Datasets	α value						
	0	0.2	0.4	0.6	0.8	1	α^*
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 α 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 α 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 α 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 α^* for each dataset, as shown in Table 5, replaces the α 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 α values for respective datasets also follow the α^* 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 α 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 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.

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).

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

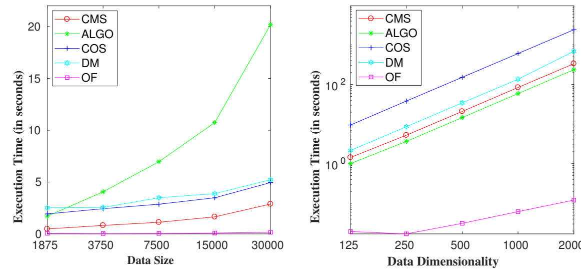


Fig. 2. The Scalability Test Results w.r.t. Data Size and Dimensionality

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 α. $\alpha = 0$ 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 α 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 α value corresponding to the highest Calinski-Harabasz index on a dataset strikes a balance between the contributions made by

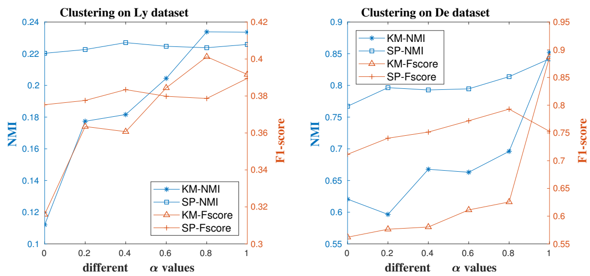


Fig. 3. The clustering results on datasets Ly and De w.r.t. different α values

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 α 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 α 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 α values may lead to different clustering performance, hence, it is necessary to choose the optimal α value. The optimal α value on the Ly dataset is 0.8 for k-modes clustering. Spectral clustering is not sensitive to the change of α value on Ly and the optimal value is 1. For dataset De, the change of α 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 α 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 α 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 α values accordingly are different. An optimal α 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.

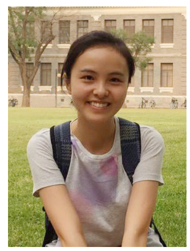
ACKNOWLEDGMENTS

This work is partially supported by the The National Key Research and Development Program of China (2016YFB0200401) by program for New Century Excellent Talents in University by National Science Foundation (NSF) China 61402492, 61402486, 61379146, by the HUNAN Province Science Foundation 2017RS3045, and by the China Scholarship Council (CSC Student ID 201603170310).

REFERENCES

[1] B. McFee and G. Lanckriet, "Learning multi-modal similarity," *The Journal of Machine Learning Research*, vol. 12, pp. 491–523, 2011.
[2] I. Alabdulmohsin, M. Cisse, X. Gao, and X. Zhang, "Large margin classification with indefinite similarities," *Machine Learning*, pp. 1–23, 2016.
[3] H. Gao, X.-W. Liu, Y.-X. Peng, and S.-L. Jian, "Sample-based extreme learning machine with missing data," *Mathematical Problems in Engineering*, 2015.
[4] G. Chechik, V. Sharma, U. Shalit, and S. Bengio, "Large scale online learning of image similarity through ranking," *The Journal of Machine Learning Research*, vol. 11, pp. 1109–1135, 2010.
[5] B. Yang, K. Lu, Y.-h. Gao, X.-p. Wang, and K. Xu, "GPU acceleration of subgraph isomorphism search in large scale graph," *Journal of Central South University*, vol. 22, pp. 2238–2249, 2015.
[6] N. Pradhan, M. Gyanchandani, and R. Wadhvani, "A review on text similarity technique used in ir and its application," *International Journal of Computer Applications*, vol. 120, no. 9, 2015.
[7] E. Diday and H.-H. Bock, "Analysis of symbolic data: Exploratory methods for extracting statistical information from complex data," 2000.
[8] S. Boriah, V. Chandola, and V. Kumar, "Similarity measures for categorical data: A comparative evaluation," *red*, vol. 30, no. 2, p. 3, 2008.
[9] A. Ahmad and L. Dey, "A k-mean clustering algorithm for mixed numeric and categorical data," *Data & Knowledge Engineering*, vol. 63, no. 2, pp. 503–527, 2007.
[10] C. Wang, L. Cao, M. Wang, J. Li, W. Wei, and Y. Ou, "Coupled nominal similarity in unsupervised learning," in *Proceedings of the 20th ACM international conference on Information and knowledge management*. ACM, 2011, pp. 973–978.
[11] L. Cao, Y. Ou, and P. S. Yu, "Coupled behavior analysis with applications," *IEEE Transactions on Knowledge and Data Engineering*, vol. 24, no. 8, pp. 1378–1392, 2012.
[12] T. Xu, J. Sun, and J. Bi, "Longitudinal lasso: Jointly learning features and temporal contingency for outcome prediction," in *Proceedings of the 21th ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*. ACM, 2015, pp. 1345–1354.
[13] L. Cao, "Coupling learning of complex interactions," *Information Processing and Management*, vol. 51, no. 2, pp. 167–186, 2015.
[14] ——, "Non-iidness learning in behavioral and social data," *The Computer Journal*, vol. 57, no. 9, pp. 1358–1370, 2014.
[15] Z.-H. Zhou, Y.-Y. Sun, and Y.-F. Li, "Multi-instance learning by treating instances as non-iid samples," in *Proceedings of the 26th annual International Conference on Machine Learning*. ACM, 2009, pp. 1249–1256.
[16] W. Ping, Y. Xu, K. Ren, C.-H. Chi, and S. Furao, "Non-iid multi-instance dimensionality reduction by learning a maximum bag margin subspace." in *AAAI*, 2010.
[17] M. C. Ganiz, C. George, and W. M. Pottenger, "Higher order Naive Bayes: A novel non-iid approach to text classification," *IEEE Transactions on Knowledge and Data Engineering*, vol. 23, no. 7, pp. 1022–1034, 2011.
[18] Z.-C. Guo and L. Shi, "Classification with non-iid sampling," *Mathematical and Computer Modelling*, vol. 54, no. 5, pp. 1347–1364, 2011.
[19] L. Ralaivola, M. Szafranski, and G. Stempfel, "Chromatic PAC-Bayes bounds for non-iid data: Applications to ranking and stationary β-mixing processes," *The Journal of Machine Learning Research*, vol. 11, pp. 1927–1956, 2010.
[20] I. Steinwart, D. Hush, and C. Scovel, "Learning from dependent observations," *Journal of Multivariate Analysis*, vol. 100, no. 1, pp. 175–194, 2009.
[21] H. Xu and S. Mannor, "Robustness and generalization," *Machine Learning*, vol. 86, no. 3, pp. 391–423, 2012.
[22] C. Wang, X. Dong, F. Zhou, L. Cao, and C.-H. Chi, "Coupled attribute similarity learning on categorical data," *IEEE Transactions on Neural Networks and Learning Systems*, vol. 26, no. 4, pp. 781–797, 2015.
[23] C. Liu and L. Cao, "A coupled k-nearest neighbor algorithm for multi-label classification," *PAKDD2015*, 2015.
[24] X. Cheng, D. Miao, C. Wang, and L. Cao, "Coupled term-term relation analysis for document clustering," pp. 1–8, 2013.

[25] X. Meng, L. Cao, and J. Shao, "Semantic approximate keyword query based on keyword and query coupling relationship analysis," *CIKM 2014*, pp. 529–538, 2014.
[26] F. Li, G. Xu, and L. Cao, "Coupled matrix factorization within non-iid context," *PAKDD2015*, 2015.
[27] L. Cao, H. Zhang, Y. Zhao, D. Luo, and C. Zhang, "Combined mining: Discovering informative knowledge in complex data," *IEEE Transactions on Systems, Man, and Cybernetics, Part B (Cybernetics)*, vol. 41, no. 3, pp. 699 – 712, 2011.
[28] L. Cao, "Combined mining: Analyzing object and pattern relations for discovering and constructing complex but actionable patterns," *WIREs Data Mining and Knowledge Discovery*, vol. 3, no. 2, pp. 140–155, 2013.
[29] Y. Shi, H.-I. Suk, Y. Gao, and D. Shen, "Joint coupled-feature representation and coupled boosting for ad diagnosis," in *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, 2014, pp. 2721–2728.
[30] Y. Shi, W. Li, Y. Gao, L. Cao, and D. Shen, "Beyond iid: Learning to combine non-iid metrics for vision tasks," *AAAI 2017*, pp. 1–7, 2017.
[31] G. Gan, C. Ma, and J. Wu, *Data clustering: theory, algorithms, and applications*. Siam, 2007, vol. 20.
[32] L. Kaufman and P. J. Rousseeuw, *Finding groups in data: an introduction to cluster analysis*. John Wiley & Sons, 2009, vol. 344.
[33] M. K. Ng, M. J. Li, J. Z. Huang, and Z. He, "On the impact of dissimilarity measure in k-modes clustering algorithm," *IEEE Transactions on Pattern Analysis and Machine Intelligence*, vol. 29, no. 3, pp. 503–507, 2007.
[34] K. Sparck Jones, "A statistical interpretation of term specificity and its application in retrieval," *Journal of Documentation*, vol. 28, no. 1, pp. 11–21, 1972.
[35] A. Bellet, A. Habrard, and M. Sebban, "Good edit similarity learning by loss minimization," *Machine Learning*, vol. 89, no. 1-2, pp. 5–35, 2012.
[36] Gray, Katherine R and Aljabar, Paul and Heckemann, Rolf A and Hammers, Alexander and Rueckert, Daniel and Alzheimer's Disease Neuroimaging Initiative and others, "Random forest-based similarity measures for multi-modal classification of alzheimer's disease," *Neuroimage*, vol. 65, pp. 167–175, 2013.
[37] G. Bhattacharya, K. Ghosh, and A. S. Chowdhury, "An affinity-based new local distance function and similarity measure for knn algorithm," *Pattern Recognition Letters*, vol. 33, no. 3, pp. 356–363, 2012.
[38] S. Cost and S. Salzberg, "A weighted nearest neighbor algorithm for learning with symbolic features," *Machine learning*, vol. 10, no. 1, pp. 57–78, 1993.
[39] D. R. Wilson and T. R. Martinez, "Improved heterogeneous distance functions," *JAIR*, vol. 6, pp. 1–34, 1997.
[40] V. Chandola, S. Boriah, and V. Kumar, "Understanding categorical similarity measures for outlier detection," *Technology Report, University of Minnesota*, 2008.
[41] F. Cao, J. Liang, D. Li, L. Bai, and C. Dang, "A dissimilarity measure for the k-modes clustering algorithm," *Knowledge-Based Systems*, vol. 26, pp. 120–127, 2012.
[42] M. E. Houle, V. Oria, and U. Qasim, "Active caching for similarity queries based on shared-neighbor information," in *Proceedings of the 19th ACM International Conference on Information and Knowledge Management*. ACM, 2010, pp. 669–678.
[43] S. Niwattanakul, J. Singthongchai, E. Naenudorn, and S. Wanapu, "Using of jaccard coefficient for keywords similarity," in *Proceedings of the International MultiConference of Engineers and Computer Scientists*, vol. 1, 2013, p. 6.
[44] G. Das and H. Mannila, "Context-based similarity measures for categorical databases," in *Principles of Data Mining and Knowledge Discovery*. Springer, 2000, pp. 201–210.
[45] V. Bryant, *Metric spaces: iteration and application*. Cambridge University Press, 1985.
[46] A. H. Lipkus, "A proof of the triangle inequality for the tanimoto distance," *Journal of Mathematical Chemistry*, vol. 26, no. 1-3, pp. 263–265, 1999.
[47] H. Jia, Y.-m. Cheung, and J. Liu, "A new distance metric for unsupervised learning of categorical data," *IEEE transactions on neural networks and learning systems*, vol. 27, no. 5, pp. 1065–1079, 2016.
[48] U. Von Luxburg, "A tutorial on spectral clustering," *Statistics and computing*, vol. 17, no. 4, pp. 395–416, 2007.
[49] Z. Huang, "Extensions to the k-means algorithm for clustering large data sets with categorical values," *Data mining and knowledge discovery*, vol. 2, no. 3, pp. 283–304, 1998.
[50] J. Li, K. Cheng, S. Wang, F. Morstatter, R. P. Trevino, J. Tang, and H. Liu, "Feature selection: A data perspective," *arXiv preprint arXiv:1601.07996*, 2016.
[51] J. Bergstra and Y. Bengio, "Random search for hyper-parameter optimization," *Journal of Machine Learning Research*, vol. 13, no. Feb, pp. 281–305, 2012.
[52] Y. Liu, Z. Li, H. Xiong, X. Gao, and J. Wu, "Understanding of internal clustering validation measures," in *2010 IEEE International Conference on Data Mining*. IEEE, 2010, pp. 911–916.
[53] T. Caliński and J. Harabasz, "A dendrite method for cluster analysis," *Communications in Statistics-theory and Methods*, vol. 3, no. 1, pp. 1–27, 1974.
[54] L. Cao, X. Dong, and Z. Zheng, "e-nsp: Efficient negative sequential pattern mining," *Artificial Intelligence*, vol. 235, pp. 156–182, 2016.



Songlei Jian Songlei Jian is currently working toward the 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, machine learning and complex network analysis.

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 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 in computer science at the National University of Defense Technology, China. His research interests include machine learning, data analytics, and distributed computing.