PARTIAL MULTI-DIVIDING ONTOLOGY LEARNING ALGORITHM

WEI GAO¹, JUAN L.G. GUIRAO², B. BASAVANAGOUD³ AND JIANZHANG WU⁴

ABSTRACT. As an effective data representation, storage, management, calculation and model for analysis, ontology has attracted more and more attention by researchers and it has been applied to various engineering disciplines. In the background of big data, the ontology is expected to increase the amount of data information and the structure of its corresponding ontology graph has become more important due to its complexity. It demands that the ontology algorithm must be more efficient than before. In a specific engineering application, the ontology algorithm is required to find in a quick way the semantic matching set of the concept and rank it back to the user according to their similarities. Therefore, to use learning tricks to get better ontology algorithms is an open problem nowadays.

The aim of the present paper is to present a partial multi-dividing ontology algorithm with the aim of obtaining an efficient approach to optimize the partial multi-dividing ontology learning model. For doing it we state several theoretical results from a statistical learning theory perspective. Moreover, we present five experiments in different engineering fields to show the precision of our partial multi-dividing algorithm from angles of ontology, similarity measuring and ontology mapping building point of view.

1. INTRODUCTION

The concept of ontology, inspired in the philosophical notion, started to use in sciences in 1980s refers to different properties of a materia and their relations. Later, it was introduced into the field of computer and information technology, and from the 90’s of the last century it became one of the hot research fields in artificial intelligence. Because of its powerful semantic query and concept management ability, the ontology has been applied to other fields in the past 10 years. Now, it is used in nearly all disciplines, such as chemical science (see for instance Vijayasarathi and Sankar [47] or Banchetti-Robino [4]), pharmacology science (see Sarntivijai et al. [36]), biology science (see Kohler et al. [26], Levine et al. [30] and Vishnu et al. [48]), psychology (see Aime and Charlet [1] and Petruria [34]), education system (see Demartini et al. [12], Kruger-Ross [28] and Ochara [33]), geographic information system (GIS) (see Vaccari et al. [46], Delgado et al. [11] and Tahmoorespur et al. [44]), medical science (see Bertaud-Gounot et al. [6] and Lousado et al. [31]), material science

Key words and phrases. Ontology, similarity measuring, ontology mapping, multi-dividing setting, learning.
As a conceptual model, ontology storage and management the information, has been widely concerned in the field of information retrieval. Using the ontology similarity calculation, we can effectively find the semantic similarity concept of the original retrieval concept, carry out the extended query in the retrieval, and return the result to the user. This trick can improve a lot the intelligence of the information retrieval. For example, if we retrieval the keyword “computer”, the traditional way of search will return the computer-related information according to the degree of relevance from high to low and present them to the user. However, this retrieval is based on keyword matching, like a similar information contains the word “laptop” can not be matched to “computer”. But in fact the words “computer” and “laptop” share high semantics similarity. With the help of ontology for query expansion, can be found that the similarity between “laptop” and “computer” is very high. Thus, in order to find information related to the computer, we find laptop-related information, and then return back to the user according to the similarity. The advantage is that the retrieval of query information is intelligent and very comprehensive.

There are several advances in ontology semantic similarity computation. Rodriguez and Egenhofer [35] presented a method to compute semantic similarity which relaxes the demand of a single ontology. Steichen et al. [42] constructed a morphological abnormality ontology in breast pathology to assist inter-observer consensus, and it implemented position-based, content-based and mixed semantic similarity measures between concepts in this ontology. Al-Mubaid and Nguyen [3] proposed a ontology-structure-based trick for measuring semantic similarity across multiple ontologies. By means of human phenotype ontology, Kohler et al. [27] adapted semantic similarity metrics to compute phenotypic similarity between queries and hereditary diseases annotated. Batet et al. [5] studied a measure in view of the exploitation of the taxonomical structure of a biomedical ontology. Albacete et al. [2] gave proposal for computing a similarity function for each dimension of knowledge. Taha [43] presented techniques for determining the semantic relationships among GO terms. Taieb et al. [45] raised an ontology measure for quantifying the degree of the semantic similarity between concepts. Mazandu et al. [32] introduced adaptable gene ontology semantic similarity-based on functional analysis. Lastra-Diaz et al. [29] presented a detailed companion reproducibility article of the trick and experiments proposed by former researchers in a survey where the state of the art on this topic is presented.

Specifically, the framework of ontology can be expressed as a simple graph in which each concept, element or object corresponds to a vertex of the graph and each edge represents a potential link (or potential relationship) between two concepts.
In the previous conditions, let \( G = (V(G), E(G)) \) be a graph corresponding to the ontology \( O \) with vertex set \( V(G) \) and edge set \( E(G) \). In the engineering applications of ontology to various fields, the fundamental goal of the ontology algorithm is to obtain the best ontology function which is applied to measure the similarities between ontology vertices in single ontology or multiple ontologies. The aim of the ontology map is to get the high similarity vertices from different ontologies, i.e., to deduce the similarity between two or multiple ontologies, and it is used to build a bridge between different ontologies thus helps to yield a potential connection among the elements or objects from target ontologies.

At the beginning, the design of the formulas for ontology similarity measuring were heuristic based, i.e., the similarity formula is determined by the researchers according to the structural features of the ontology and the characteristics of the specific application domain. The shortcomings of this method are:

1. It relies on the participate of high-level field experts.
2. The similarity formula contains many man-made parameters.
3. It can not adapt to the dynamic changes in the ontology.
4. It has high complexity, and thus not suited in the specific application with big data background.

In order to overcome these shortcomings, the machine learning techniques are gradually applied to the ontology algorithm. The specific idea is to get the optimal ontology function \( f : V(G) \rightarrow \mathbb{R} \) from the sample learning, which maps each vertex in ontology graph to a real number, and thus maps the whole ontology graph to the one dimension real axis (for multiple ontologies, we put all the graphs into one graph, each ontology is seen as a connected branch of the graph). Then the similarity between the ontology concepts is determined by the distance of their corresponding vertex on the real axis. It means, the similarity between vertices \( v_i \) and \( v_j \) is measured by \( |f(v_i) - f(v_j)| \). To have a closer distance means to have higher similarity. The advantage of this algorithm is that it does not depend on domain experts; the results are intuitive; the parameters set by man-made settings are greatly reduced; and most important, the computational complexity is greatly reduced because there is no pairwise similarity calculating.

Among these ontology learning algorithms, multi-dividing ontology algorithm is the most popular ontology learning approach in which all vertices in ontology graph or multi-ontology graph are divided into \( k \) parts (correspond to the \( k \) classes of rates). Assume that \( f(v^a) > f(v^b) \) if \( v^a \) belongs to rate \( a \) and \( v^b \) belongs to rate \( b \) with \( 1 \leq a < b \leq k \). Note that for ontology graph with tree or tree-like structure, each kind of branch is corresponding to a rate in the dividing. Since most of ontology graphs have tree structure, multi-dividing ontology algorithm method is widely used in various of engineering filed like biology, medicine, chemistry, etc. Gao and Farahani [15] and Wu et al. [49] presented respectively some examples to show how multi-dividing ontology algorithm is applied to some specific engineering applications.

Although there have been several recent advances in the developing of algorithms for various settings on the multi-dividing ontology learning problem, the study of more available tricks and generalization properties of multi-dividing ontology learning algorithms has been largely limited to the special setting. It inspires us to explore more advanced techniques of ontology learning algorithm in multi-dividing setting and theoretical analysis from statistics learning theory.

In this paper, we present a partial multi-dividing ontology learning algorithm and study its statistics characteristics from a mathematical point of view. In this trick, we divide the whole ontology graph into some branches which are corresponding to several rates. The optimal ontology function is obtained by learning the ontology sample set which also can be divided into \( k \) training subsets, and the partial learning framework in multi-dividing setting plays a key role in the implementation process. The structure of the paper is as follows: firstly, we introduce the setting of multi-dividing ontology learning; secondly, the main algorithm is presented in Section 3; and finally, the effectiveness of proposed ontology learning algorithm is stated via five experiments developed in various of engineering applications.

2. Preliminaries, notation and background

For our mathematical discussion and learning setting expression, for each vertex in the ontology graph, we use a \( p \) dimensional vector to express all semantic information of its corresponding ontology concept. We shall use \( v \) to denote the vertex \( v \) and its corresponding vector in \( \mathbb{R}^p \).

Let \( V \subseteq \mathbb{R}^p \) be a vertex space for ontology graph \( G \), and the vertices in \( V \) are drawn independently and randomly according to certain unknown distribution \( \mathcal{D} \). The target of ontology learning algorithms is to predict an ontology function \( f : V \rightarrow \mathbb{R} \) in terms of ontology training set \( S = \{v_1, \cdots, v_n\} \subseteq V \). As an ontology function, it assigns a real number to each vertex in ontology graph, and thus the similarities between two ontology concepts (assume \( v_i \) and
\(v_j\) are corresponding to ontology vertices in ontology graph) are judged in view of the value of \(|f(v_j) - f(v_i)|\). In the multi-dividing ontology setting, ontology vertices are divided into \(k\) parts (corresponding to \(k\) classes or \(k\) rates) and these \(k\) rates are deduced in light of the experts.

Formally, the learner is inferred to an ontology training set

\[
S = (S^1, S^2, \ldots, S^k) \in V^{n_1} \times V^{n_2} \times \cdots \times V^{n_k}
\]

which consists of a sequence of ontology training samples \(S_a = (v_1^a, \ldots, v_{n_a}^a) \in V^{n_a}\) \((1 \leq a \leq k)\). By virtue of ontology sample \(S\), a real-valued ontology function \(f : V \to \mathbb{R}\) is learned which allocates the future \(S^a\) vertices larger value than \(S^b\), where \(a < b\). It means, a real-valued ontology function \(f : V \to \mathbb{R}\) is predicted to assign a value to each vertex satisfies \(f(v^a) > f(v^b)\) for any pair of \((a, b)\) where \(1 \leq a < b \leq k\). On the other hand, it can be regarded as a dimension reduction operator \(f : \mathbb{R}^p \to \mathbb{R}\). Note that the aims of the linear ontology algorithm is to learn a linear ontology function \(f : V \to \mathbb{R}\) denoted by \(f(v) = \beta^T v\) from a given ontology training set \(S = (S^1, S^2, \ldots, S^k) \in V^{n_1} \times V^{n_2} \times \cdots \times V^{n_k}\), where \(\beta \in \mathbb{R}^p\) is the linear ontology sparse vector.

Let \(D_a\) be as the conditional distribution for each rate \(1 \leq a \leq k\) and \(n = \sum_{i=1}^{k} n_i\) as the total size of ontology sample set. In what follows, let \(I\) be the truth function satisfies \(I(\cdot) = 1\) if the assertion is correct and 0 otherwise. For each pair \((a, b)\) with \(1 \leq a < b \leq k\), set false rates \(\alpha_{1}^{a,b}\) and \(\alpha_{2}^{a,b}\), where \(0 \leq \alpha_{1}^{a,b} < \alpha_{2}^{a,b} \leq 1\). Symbols \(\alpha_{1}\) and \(\alpha_{2}\) are denoted as the abstract parameters in our setting which will be changed according to the difference of pair \((a, b)\), i.e., \(\alpha_{1}\)\(_{a,b} = \alpha_{1}^{a,b}\) and \(\alpha_{2}\)\(_{a,b} = \alpha_{2}^{a,b}\). Sign function \(\text{sign}(x)\) is denoted as \(\text{sign}(x) = 1\) if \(x > 0\), and \(-1\) otherwise. For any \(x \in \mathbb{R}\), \((x)_{+} = \max\{x, 0\}\).

For an ontology function \(f : V \to \mathbb{R}\) and threshold \(t \in \mathbb{R}\), the true level rate of the binary classifier \(\text{sign}(f(x) - t)\) as the probability that it correctly classifies a random rate ontology vertices from \(D_a\) (here \(1 \leq a \leq k\)):

\[
\text{TR}_{f}^{a}(t) = \mathbb{P}_{v^a \sim D_a}[f(v^a) > t].
\]

In the multi-dividing ontology (in short, it called MDO) setting, the model to measure the goodness of ontology function \(f\) can be formulated as

\[
\text{MDO}_f = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \int_{0}^{1} \text{TR}_{f}^{a}((\text{TR}_{f}^{b})^{-1}(x))dx,
\]

where \((\text{TR}_{f}^{b})^{-1}(x) = \inf\{t \in \mathbb{R}|\text{TR}_{f}^{b}(t) \leq x\}\). The evaluation model (1) equals to the area under the receiver operating characteristic curve criterion in the regress or classification setting with \(k = 2\), and this is the motivation and rationality of (1).
Assume that there are no ties, then the multi-dividing ontology framework (1) can be expressed as

$$\text{MDO}_f = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \mathbb{P}_{(v^a,v^b) \sim \mathcal{D}_a \times \mathcal{D}_b}(f(v^a) > f(v^b)).$$

For each pair of \((a, b)\) with \(1 \leq a < b \leq k\), we are interested in the area under the curve between \(\alpha_{a}^{a,b}\) and \(\alpha_{b}^{a,b}\). We define the normalized partial MDO of the ontology function \(f\) in the interval \([\alpha_{a}^{a,b}, \alpha_{b}^{a,b}]\) for each pair of \((a, b)\) with \(1 \leq a < b \leq k\) as

$$\text{PMDO}_f = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{\alpha_{a}^{a,b} - \alpha_{b}^{a,b}} \int_{\alpha_{a}^{a,b}}^{\alpha_{b}^{a,b}} \mathcal{T}_f((\mathcal{R}_f)^{-1}(x))dx.$$

Given an ontology sample set \(S = (S^1, S^2, \ldots, S^k) \in V^{n_1} \times V^{n_2} \times \cdots \times V^{n_k}\), the empirical receiver operating characteristic curve corresponding to an ontology function \(f : V \to \mathbb{R}\) is obtained by (here \(a \in \{1, \cdots, k\}\))

$$\widehat{\mathcal{T}}_f^a(t) = \frac{1}{n_a} \sum_{i=1}^{n_a} I(f(v^a_i) > t).$$

Hence, the empirical version of MDO is given by

$$\widehat{\text{MDO}}_f = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a n_b} \sum_{i=1}^{n_a} \sum_{j=1}^{n_b} I(f(v^a_i) > f(v^b_j)).$$

For each pair of \((a, b)\) with \(1 \leq a < b \leq k\), by denoting \(i_{a}^{a,b} = \lfloor n_i \alpha_{a}^{a,b} \rfloor\) and \(j_{a}^{a,b} = \lfloor n_j \alpha_{a}^{a,b} \rfloor\), the normalized empirical partial multi-dividing ontology (PMDO) criterion of ontology function \(f\) in the interval \([\alpha_{a}^{a,b}, \alpha_{b}^{a,b}]\) can then be written as:

$$\widehat{\text{PMDO}}_f = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a (j_{a}^{a,b} - i_{a}^{a,b})} \sum_{i=1}^{n_a} \sum_{j=i_{a}^{a,b}+1}^{j_{a}^{a,b}} I(f(v^a_i) > f(v^b_j)),$$

where \(v^b_j\) denotes the ontology vertices in \(S^b\) ranked (in descending order of values) in the \(j\)-th position by ontology function \(f\).

3. Description of the Partial Multi-Dividing Ontology Algorithm

In this section, we consider ontology function \(f : V \to \mathbb{R}\) denoted by \(f(v) = \beta^\top v\) for some \(\beta \in \mathbb{R}^p\). The contexts in this section is organized as follows: we first introduce the structural SVM based multi-dividing ontology framework with hinge ontology loss; then the partial multi-dividing ontology framework with hinge ontology loss is presented; next, we discuss the optimization methods for partial multi-dividing ontology framework based on structural SVM in interval \([0, \alpha_{a}^{a,b}]\) and \([0, \alpha_{b}^{a,b}]\), respectively in the third and fourth parts; finally, we compute the generalization bound for our ontology algorithm.
3.1. Multi-dividing ontology framework with structural SVM or hinge ontology loss. Given an ontology training set $S = (S^1, S^2, \ldots, S^k) \in V^{n1} \times V^{n2} \times \cdots \times V^{nk}$, the aim here is to search an ontology function that gets maximum empirical MDO on ontology sample $S$, or equivalently minimizes the empirical multi-dividing ontology risk described as follows

$$
\hat{R}_{\text{MDO}}(\beta, S) = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a n_b} \sum_{i=1}^{n_a} \sum_{j=1}^{n_b} I(\beta^T v^a_i \leq \beta^T v^b_j).
$$

In most cases the value of the extremes in the ontology optimization model (2) is difficult since the truth function $I$ is non-differentiable. One trick to solve this problem is using hinge loss function to replace the truth function. For any ontology function $f$ and vertices $v^a$ and $v^b$ from difficult rates, the pair-wise hinge ontology loss is defined as $(1-(\beta^T v^a - \beta^T v^b))^+$ which is convex in $\beta$ and an upper bound on $I(\beta^T v^a \leq \beta^T v^b)$. Thus, ontology optimization framework with pair-wise hinge ontology loss is presented as (which is convex in $\beta$)

$$
\hat{R}_{\text{MDO}}^{\text{hinge}}(\beta, S) = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a n_b} \sum_{i=1}^{n_a} \sum_{j=1}^{n_b} (1-(\beta^T v^a_i - \beta^T v^b_j))^+.
$$

For each pair of $(a, b)$ with $1 \leq a < b \leq k$ and any ordering of the ontology training vertices, we represent the related ordering of the $n_a$ ontology vertices in $S^a$ and $n_b$ ontology vertices in $S^b$ by means of a matrix $\pi^{a,b} = [\pi^{a,b}]_{ij} \in \{0, 1\}^{n_a \times n_b}$ as follows: $[\pi^{a,b}]_{ij} = 1$ if $f(v^a_i) \leq f(v^b_j)$; $[\pi^{a,b}]_{ij} = 0$ if $f(v^a_i) > f(v^b_j)$. Note that for each pair of $(a, b)$ with $1 \leq a < b \leq k$, not all $2^{n_a n_b}$ matrices in $\{0, 1\}^{n_a \times n_b}$ represent a valid relative ordering. Hence, for each pair of $(a, b)$ with $1 \leq a < b \leq k$, set $\Pi^{a,b}_{n_a, n_b}$ as the set of all matrices in $\{0, 1\}^{n_a \times n_b}$ that can express valid orderings, and obviously, for any $i \in \{1, \cdots, n_a\}$ and $j \in \{1, \cdots, n_b\}$ the correct relative ordering $\pi^*$ has $(\pi^*)^{a,b}_{ij} = 0$. In what follows, we always assume $\pi$ as the abstract matrix in our setting, i.e., $\pi_{a,b} = \pi^{a,b}$; similarly, $\Pi$ is the matrix space in our setting with $\Pi_{a,b} = \Pi_{n_a, n_b}^{a,b}$. We can regard $\pi$ and $\Pi$ as the symbols which are well defined in the various pair of $(a, b)$.

Define the multi-dividing ontology loss of $\pi$ with respect to $\pi^*$ as

$$
\Delta_{\text{MDO}}(\pi^*, \pi) = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a n_b} \sum_{i=1}^{n_a} \sum_{j=1}^{n_b} \pi^{a,b}_{i,j}.
$$

Clearly, for any $\pi$ consistent with ontology function $f = \beta^T v$, $\Delta_{\text{MDO}}(\pi^*, \pi)$ evaluates to the multi-dividing ontology risk $\hat{R}_{\text{MDO}}(\beta, S)$ in ontology framework (2). Set a joint feature map between the input ontology training set and
an output ordering matrix \( \phi : (V^{n_1} \times \cdots \times V^{n_k}) \times \Pi_{1 \leq a < b \leq k}^{n_a n_b} \rightarrow \mathbb{R}^p \) as
\[
\phi(S, \pi) = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a n_b} \sum_{i=1}^{n_a} \sum_{j=1}^{n_b} (1 - \pi_{ij}^a)(v_i^a - v_j^b).
\]
Moreover, for each pair of \((a, b)\) with \(1 \leq a < b \leq k\), we set \(\phi_a^b : (V^{n_a} \times V^{n_b}) \times \Pi_{a}^{n_a} \rightarrow \mathbb{R}^p\) as
\[
\phi_a^b(S^a \cup S^b, \pi_a^b) = \frac{1}{n_a n_b} \sum_{i=1}^{n_a} \sum_{j=1}^{n_b} (1 - \pi_{ij}^a)(v_i^a - v_j^b).
\]
The good selection of \(\phi(S, \pi)\) satisfy that for any fixed \(\beta \in \mathbb{R}\), maximizing \(\beta^T \phi(S, \pi)\) over \(\pi\) gets an ordering matrix consistent with the ontology function \(f = \beta^T v\), and thus the loss part evaluates to \(\hat{R}_{\text{MDO}}(\beta, S)\). Now, the ontology problem of optimizing the MDO becomes to searching a \(\beta \in \mathbb{R}^p\) in which the maximizer over \(\pi\) of \(\beta^T \phi(S, \pi)\) has the smallest multi-dividing ontology loss. We now express our ontology problem in light of the following structural SVM based version:
\[
(3) \quad \hat{R}_{\text{MDO}}^{\text{struct}}(\beta, S) = \max_{\pi} \{ \Delta_{\text{MDO}}(\pi^*, \pi) - (\beta^T \phi(S, \pi^*) - \beta^T \phi(S, \pi)) \}.
\]
Obviously, \(\hat{R}_{\text{MDO}}^{\text{struct}}(\beta, S)\) is convex in \(\beta\). Furthermore, if let \(\hat{\pi}\) be the maximizer of \(\beta^T \phi(S, \pi)\) over \(\Pi\), we infer \(\hat{R}_{\text{MDO}}^{\text{struct}}(\beta, S) \geq \Delta_{\text{MDO}}(\pi^*, \pi) - (\beta^T \phi(S, \pi^*) - \beta^T \phi(S, \pi)) \geq \Delta_{\text{MDO}}(\pi^*, \pi) = \hat{R}_{\text{MDO}}(\beta, S)\).

Our first theoretical result stated below shows the equivalent of ontology optimization model by pair-wise hinge loss and structure SVM.

**Theorem 1.** For any \(\beta \in \mathbb{R}^p\) and training sample set \(S = (S^1, S^2, \ldots, S^k) \in V^{n_1} \times V^{n_2} \times \cdots \times V^{n_k}\), we have \(\hat{R}_{\text{MDO}}^{\text{struct}}(\beta, S) = \hat{R}_{\text{MDO}}^{\text{hinge}}(\beta, S)\).

**Proof.** The structural SVM based ontology loss can be simplified into a pair-wise form:
\[
\hat{R}_{\text{MDO}}^{\text{struct}}(\beta, S) = \max_{\pi} \{ \Delta_{\text{MDO}}(\pi^*, \pi) - (\beta^T \phi(S, \pi^*) - \beta^T \phi(S, \pi)) \}
\]
\[
= \max_{\pi} \{ \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} n_a n_b \sum_{i=1}^{n_a} \sum_{j=1}^{n_b} \pi_{ij}^a (1 - \beta^T (v_i^a - v_j^b)) \}
\]
\[
= \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \max_{\pi_{ij} \in \{0,1\}^{n_a n_b}} \left\{ \frac{1}{n_a n_b} \sum_{i=1}^{n_a} \sum_{j=1}^{n_b} \pi_{ij}^a (1 - \beta^T (v_i^a - v_j^b)) \right\}
\]
\[
= \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a n_b} \sum_{i=1}^{n_a} \sum_{j=1}^{n_b} \max_{\pi_{ij} \in \{0,1\}} \left\{ \pi_{ij}^a (1 - \beta^T (v_i^a - v_j^b)) \right\}
\]
\[
= \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a n_b} \sum_{i=1}^{n_a} \sum_{j=1}^{n_b} \pi_{ij}^a (1 - \beta^T (v_i^a - v_j^b)),
\]
where \( \overline{\pi}_{ij} = I(\beta^T(v_i^a - v_j^b) \leq 1) \). Therefore, we deduce

\[
\hat{R}_{\text{MDO}}^{\text{struct}}(\beta, S) = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a n_b} \sum_{i=1}^{n_a} \sum_{j=1}^{n_b} \overline{\pi}_{ij}^a (1 - \beta^T(v_i^a - v_j^b))
\]

\[
= \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a n_b} \sum_{i=1}^{n_a} \sum_{j=1}^{n_b} (1 - \beta^T(v_i^a - v_j^b))_+
\]

\[
= \hat{R}_{\text{MDO}}^{\text{hinge}}(\beta, S).
\]

Hence, we get the desired result. \( \square \)

3.2. Partial multi-dividing ontology framework with hinge ontology loss. For a given ontology training set \( S = (S^1, S^2, \cdots, S^k) \in V^{n_1} \times V^{n_2} \times \cdots \times V^{n_k} \), we try to find an ontology function \( f(v) = \beta^T v \) that maximizes partial multi-dividing ontology risk in \([\alpha_1^{a,b}, \alpha_2^{a,b}]\) (for each pair of \((a, b)\) with \(1 \leq a < b \leq k\)):

\[
(4) \quad \hat{R}_{\text{PMDO}(\alpha_1, \alpha_2)}(\beta, S) = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a} \sum_{i=1}^{n_a} \sum_{j=1}^{n_b} a_{ij}^{a,b} I(\beta^T v_i^a \leq \beta^T v_j^b),
\]

where \( v_{(j)_\beta}^b \) denotes the ontology vertices in \( S^b \) ranked (in descending order of values) in the \( j \)-th position by \( f(v^b) = \beta^T v^b \). Using hinge ontology loss function, the above loss (4) becomes

\[
(5) \quad \hat{R}_{\text{PMDO}(\alpha_1, \alpha_2)}^{\text{hinge}}(\beta, S) = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a} \sum_{i=1}^{n_a} \sum_{j=1}^{n_b} a_{ij}^{a,b} (1 - (\beta^T v_i^a - \beta^T v_{(j)_\beta}^b))_+.
\]

When \( \alpha_1^{a,b} = 0 \) and \( j_{\alpha_1^{a,b}} = |n_b \alpha_1^{a,b}| = 0 \), the ontology risk (5) is manifested as

\[
(6) \quad \hat{R}_{\text{PMDO}(0, \alpha_2)}^{\text{hinge}}(\beta, S) = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a} \sum_{i=1}^{n_a} \sum_{j=1}^{n_b} a_{ij}^{a,b} (1 - (\beta^T v_i^a - \beta^T v_{(j)_\beta}^b))_+. \]

Our next theoretical result shows that the multi-dividing ontology loss depicted in (6) is convex with respect to \( \beta \).

**Theorem 2.** Let \( \alpha_2^{a,b} > 0 \) for each pair of \((a, b)\) with \(1 \leq a < b \leq k\). For any ontology training sample set \( S = (S^1, S^2, \cdots, S^k) \in V^{n_1} \times V^{n_2} \times \cdots \times V^{n_k} \), the \( \hat{R}_{\text{PMDO}(\alpha_2)}^{\text{hinge}}(\beta, S) \) is convex in \( \beta \).

**Proof.** Fix ontology sample \( S = (S^1, S^2, \cdots, S^k) \in V^{n_1} \times V^{n_2} \times \cdots \times V^{n_k} \). Let \( \beta_1, \beta_2 \in \mathbb{R}^p, \lambda \in (0, 1) \), and \( \overline{\beta} = \lambda \beta_1 + (1 - \lambda) \beta_2 \). We aim to show that

\[
\hat{R}_{\text{PMDO}(\alpha_2)}^{\text{hinge}}(\overline{\beta}, S) \leq \lambda \hat{R}_{\text{PMDO}(\alpha_2)}^{\text{hinge}}(\beta_1, S) + (1 - \lambda) \hat{R}_{\text{PMDO}(\alpha_2)}^{\text{hinge}}(\beta_2, S).
\]
For each pair of \((a, b)\) with \(1 \leq a < b \leq k\) and any vertex \(v^b\) \((b \in \{2, \cdots, k\})\), define \(\Psi^{a,b}(\beta, S^a, v^b) = \frac{1}{n_a} \sum_{i=1}^{n_a} I(\beta^\top v_i^a \leq \beta^\top v_i^b)\). In view of \(\Psi^{a,b}(\beta, S^a, v^b)\) is convex in \(\beta\) and is monotonically increasing in the value \(\beta^\top v^b\) assigned to \(v^b\), we yield

\[
\hat{R}_{\text{PMDO}(0, \alpha_2)}(\beta, S) = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a} \sum_{j=1}^{j_{\alpha_2}} \Psi^{a,b}(\beta, S^a, v^b_{(j)\beta})
\]

\[
\leq \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \left\{ \lambda \frac{1}{j_{\alpha_2}} \sum_{j=1}^{j_{\alpha_2}} \Psi^{a,b}(\beta_1, S^a, v^b_{(j)\beta}) + (1 - \lambda) \frac{1}{j_{\alpha_2}} \sum_{j=1}^{j_{\alpha_2}} \Psi^{a,b}(\beta_2, S^a, v^b_{(j)\beta}) \right\}
\]

\[
\leq \lambda \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \left\{ \lambda \frac{1}{j_{\alpha_2}} \sum_{j=1}^{j_{\alpha_2}} \Psi^{a,b}(\beta_1, S^a, v^b_{(j)\beta}) + (1 - \lambda) \frac{1}{j_{\alpha_2}} \sum_{j=1}^{j_{\alpha_2}} \Psi^{a,b}(\beta_2, S^a, v^b_{(j)\beta}) \right\}
\]

\[
= \lambda \hat{R}_{\text{PMDO}(0, \alpha_2)}(\beta_1, S) + (1 - \lambda) \hat{R}_{\text{PMDO}(0, \alpha_2)}(\beta_2, S).
\]

This completes the proof. \(\square\)

We underline that it is still hard to solve the ontology optimization problem directly, although the multi-dividing ontology framework with hinge ontology loss and intervals \([0, \alpha_2]\) for each pair of \((a, b)\) with \(1 \leq a < b \leq k\) been convex.

As a supplement, if we replace the loss term to the structural SVM for the multi-dividing ontology framework in (3) with \([\alpha_1, \alpha_2]\) for each pair of \((a, b)\) with \(1 \leq a < b \leq k\), then we obtain partial multi-dividing ontology framework as follows

\[
\Delta_{\text{PMDO}}(\pi^*, \pi) = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a} \sum_{i=1}^{n_a} \sum_{j=1}^{n_b} \pi_{i,(j)\pi}^{a,b}
\]

where \((j)_{\pi}\) denotes the index of the \(j\)-th ranked ontology vertices in \(S^b\) consistent with \(\pi\). Hence, the resulting ontology risk can be formulated by:

\[
\hat{R}_{\text{PMDO}}(\beta, S) = \max_{\pi} \{\Delta_{\text{PMDO}}(\pi^*, \pi) - (\beta^\top \phi(S, \pi^*) - \beta^\top \phi(S, \pi))\}.
\]

3.3 Partial multi-dividing ontology framework based on structural SVM trick in intervals \([0, \alpha_2]\). In this part, we consider the ontology approach for optimizing the partial multi-dividing ontology framework in intervals \([0, \alpha_2]\) (pair \((a, b)\) satisfies \(1 \leq a < b \leq k\):

\[
\hat{R}_{\text{PMDO}(0, \alpha_2)}(\beta, S) = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a} \sum_{i=1}^{n_a} \sum_{j=1}^{n_b} I(\beta^\top v_i^a \leq \beta^\top v_{(j)\beta}^b).
\]

We shall use the technique of structure SVM here and also provide an algorithm to estate the positions related to value of \(\alpha_2^{a,b}\).
For each pair of \((a, b)\) with \(1 \leq a < b \leq k\) and any subset of negatives \(\Xi^{a,b} \subseteq S^b\), let \(\hat{R}^{a,b}\) be the multi-dividing ontology risk of ontology function \(f = \beta^\top v\) evaluated on an ontology sample containing all the \(S^a\) and the subset of \(\Xi\). Then we obtain the following equivalent result which implies that \(S^b\) can reduce to a subset of size \(j_{a,b}\) for each pair of \((a, b)\) with \(1 \leq a < b \leq k\).

**Theorem 3.** For any \(\beta \in \mathbb{R}^p\) and \(S = (S^1, S^2, \ldots, S^k) \in V^{n_1} \times V^{n_2} \times \cdots \times V^{n_k}\) ontology training sample set, we infer that \(\hat{R}_{PMDO(0,\alpha_2)}(\beta, S) = L\) and

\[
L = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \max_{\Xi^{a,b} \subseteq S^b} \left[ \frac{1}{n_a} \sum_{v^{a,b} \in \Xi^{a,b}} \sum_{i=1}^{n_a} \sum_{j=1}^{n_{a,j}} I(\beta^\top v_i^{a,b} \leq \beta^\top v_j^{a,b}) \right]
\]

(8) \[
\sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \max_{\Xi^{a,b} \subseteq S^b} \left[ \frac{1}{n_{a,j}} \sum_{\pi^{a,b} \in \Xi^{a,b}} \sum_{j=1}^{n_{a,j}} \beta_j^{a,b} S^{a,b} \right]
\]

Note that, for each pair \((a, b)\) with \(1 \leq a < b \leq k\), \(S^a\) and any subset \(\Xi^{a,b} = \{\xi_1^{a,b}, \ldots, \xi_{j_{a,b}}^{a,b}\} \subseteq S^b\), let \(\pi^{a,b} \in \{0, 1\}^{n_a \times j_{a,b}}\) be the truncated ordering matrices defined as \(\pi_{ij}^{a,b} = 1\) if \(f(v_i^{a}) \leq f(v_j^{a})\) and \(\pi_{ij}^{a,b} = 0\) if \(f(v_i^{a}) > f(v_j^{a})\), where \(i \in \{1, \ldots, n_a\}\) and \(j \in \{1, \ldots, j_{a,b}\}\).

Let \(\Pi^{a,b}\) be the collection of all valid orderings for each pair of \((a, b)\) with \(1 \leq a < b \leq k\), and the correct ordering is stated as \((\pi^{a,b})^* = 0_{n_a \times j_{a,b}}\). The joint feature map for \(n_a\) vertices from \(S^a\) and \(j_{a,b}\) vertices from \(S^b\) is redefined as \(\phi^{a,b} : V^{n_a} \times V^{j_{a,b}} \rightarrow \mathbb{R}^p\). In this way, the convex upper bound on the inner multi-dividing ontology part \((\hat{R}^{a,b})_{PMDO(0,\alpha_2)}(\beta, S^a, \Xi^{a,b})\) for each pair of \((a, b)\) with \(1 \leq a < b \leq k\) in (8) can be expressed as

\[
\max_{\pi^{a,b} \in \Pi^{a,b}} \{\Delta^{a,b}_{PMDO(0,\alpha_2)}(\pi^{a,b}) = -\beta^\top (\phi((S^a, \Xi^{a,b}), (\pi^{a,b})^*) - \phi((S^a, \Xi^{a,b}), \pi^{a,b}))\}
\]
By replacing the $\hat{R}_{\text{PMDO}}(\beta, S^a, \Xi^{a,b})$ in (8) with the above expression, we infer

$$\hat{R}_{\text{PMDO}(0, o_2)}(\beta, S) = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \max_{\Xi \subseteq S^b, |\Xi^{a,b}|=j_{a,b}} \max_{\pi^{a,b} \in \Pi_{n_a\cdot j_{a,b}}} \{ \Delta_{\text{PMDO}}((\pi^{a,b})^*, \pi^{a,b}) - \beta^T (\phi((S^a, \Xi^{a,b}), (\pi^{a,b})^*) - \phi((S^a, \Xi^{a,b}), \pi^{a,b})) \},$$

where the $\pi^{a,b}_{ij}'$s indices over all vertices in $S^a$, and over vertices in the corresponding subset $\Xi^{a,b}$ in the outer argmax part.

By means of hinge ontology loss, $\hat{R}_{\text{PMDO}(0, o_2)}(\beta, S)$, i.e. the multi-dividing ontology risk can be simplified as

$$(9) \quad \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \max_{\Xi \subseteq S^b, |\Xi^{a,b}|=j_{a,b}} \max_{\pi^{a,b} \in \Pi_{n_a\cdot j_{a,b}}} \frac{1}{n_a j_{a,b}} \sum_{i=1}^{n_a} \sum_{v^b \in \Xi^{a,b}} (1 - (\beta^T v^a_i - \beta^T v^b))_+.$$

For each pair of $(a, b)$ with $1 \leq a < b \leq k$, let $\Xi^{a,b} = \{\xi_{1}^{a,b}, \ldots, \xi_{j_{a,b}}^{a,b}\}$ be the set of vertices in $S^b$ ranked in the top $j_{a,b}$ positions (in descending order of values) by $f = \beta^T v^b$. Hence, the largest objective value of each pair of $(a, b)$ in (9) is obtained at $\Xi^{a,b}$.

Define $\Psi^{a,b}(\beta, S^a, v^b) = \frac{1}{n_a} \sum_{i=1}^{n_a} (1 - (\beta^T v^a_i - \beta^T v^b))_+$ for each pair of $(a, b)$ with $1 \leq a < b \leq k$ and any $v^b$. For any $\beta \in \mathbb{R}^p$ and ontology training sample set $S = (S^1, S^2, \ldots, S^k) \in V^n \times V^{n_2} \times \cdots \times V^{n_k}$, we yield

$$\hat{R}_{\text{PMDO}(0, o_2)}(\beta, S) = \hat{R}_{\text{PMDO}(0, o_2)}(\beta, S).$$

Now, we present the algorithm to determine the tight set $\Xi^{a,b}$ and truncated ordering matrices $\pi^{a,b}$. The specific ontology optimization problem can be written as:

$$\sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \max_{\Xi \subseteq S^b, |\Xi^{a,b}|=j_{a,b}} \max_{\pi^{a,b} \in \Pi_{n_a\cdot j_{a,b}}} P$$

where $P = \{ \Delta_{\text{PMDO}}((\pi^{a,b})^*, \pi^{a,b}) - \beta^T (\phi((S^a, \Xi^{a,b}), (\pi^{a,b})^*) - \phi((S^a, \Xi^{a,b}), \pi^{a,b})) \}$.

From what we have discussed above, the above inner argmax is attained at the top $j_{a,b}$ vertices $\Xi^{a,b} = \{\xi_{1}^{a,b}, \ldots, \xi_{j_{a,b}}^{a,b}\} \in S^b$ for each pair of $(a, b)$ with $1 \leq a < b \leq k$ in terms of $\beta$. Hence, the rest task is to determine the optimal ordering matrix in $\Pi^{n_a\cdot j_{a,b}}$ with given $\Xi^{a,b}$, and the ontology optimization problem thus be decomposed effectively. Specifically, the ontology optimization problem with given subset $\Xi^{a,b}$ for each pair of $(a, b)$ with $1 \leq a < b \leq k$ can
be represented as

$$\arg\min_{\pi} \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{na_j^{a,b}} \sum_{i=1}^{na_a^{a,b}} \pi_{ij}^{a,b} (1 - \beta^\top (v_i^a - \xi_j^a)),$$

We consider solving a relaxed form of ontology optimization problem (10) over all matrices in $\{0,1\}^{na_a \times j_{a,b}^{a,b}}$, and the optimal ordering matrix is obtained by

$$\pi_{ij}^{a,b} = \mathbf{1}(\beta^\top v_i^a - \beta^\top \xi_j^a \leq 1)$$

for each pair of $(a, b)$ with $1 \leq a < b \leq k$. Furthermore, $\pi$ is also a solution to the original unrelaxed ontology optimization problem (10) for given $\Xi$, and then $(\Xi, \pi)$ provides us the desired conclusion.

**Algorithm 1.** Determine $(\Xi, \pi)$ for partial multi-dividing ontology problem in interval $[0, \alpha^{a,b}_2]$ for each pair:

**Step 1:** Inputs: $S = (S^1, S^2, \cdots, S^k) \in V^{n_1} \times V^{n_2} \times \cdots \times V^{n_k}$, $\alpha^{a,b}_2$ for each pair of $(a, b)$ with $1 \leq a < b \leq k$, $\beta$.

**Step 2:** Set $\Xi_{a,b} = \{\xi_{j_1}^{a,b}, \cdots, \xi_{j_{a,b}^{a,b}}^{a,b}\}$ as the collection of vertices in $S^b$ (for each pair $(a, b)$) ranked in the top $j_{a,b}^{a,b}$ positions (in descending order of values) by $f = \beta^\top v$

**Step 3:** $\pi_{ij}^{a,b} = \mathbf{1}(\beta^\top v_i^a - \beta^\top \xi_j^a \leq 1)$ where $i \in \{1, \cdots, n_a\}$, $j \in \{1, \cdots, j_{a,b}^{a,b}\}$

**Step 4:** Output: $(\Xi, \pi)$

Clearly, computational time for each pair of $(a, b)$ with $1 \leq a < b \leq k$ is $O(n_a j_{a,b}^{a,b} + n_b \log(n_b))$. Thus, the complexity of Algorithm 1 is equal to $O(\sum_{a=1}^{k-1} \sum_{b=a+1}^{k} (n_a j_{a,b}^{a,b} + n_b \log(n_b)))$.

### 3.4. Partial multi-dividing ontology framework based on structural SVM trick in intervals $[\alpha^{a,b}_1, \alpha^{a,b}_2]$.

Recall that the structural SVM based partial multi-dividing ontology risk in $[\alpha^{a,b}_1, \alpha^{a,b}_2]$, $\hat{R}_{\text{PMDO}}(\alpha^{a,b}_1, \alpha^{a,b}_2)(\beta, S)$, is given by:

$$\sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{na_j^{a,b}} \sum_{i=1}^{na_a^{a,b}} \sum_{j=\alpha_b^{a,b}+1}^{\alpha_a^{a,b}} \mathbf{1}(\beta^\top v_i^a \leq \beta^\top v_j^b).$$

Similarly as Theorem 3, the partial multi-dividing ontology risk in interval $[\alpha^{a,b}_1, \alpha^{a,b}_2]$ (for each pair of $(a, b)$ with $1 \leq a < b \leq k$) can be expressed as a maximum of a certain term over subsets of $S^b$ with $j_{a,b}^{a,b}$ vertices.
Theorem 4. For any \( \beta \in \mathbb{R}^p \) and any ontology training sample set \( S = (S^1, S^2, \ldots, S^k) \in V^{n_1} \times V^{n_2} \times \ldots \times V^{n_k} \),

\[
\hat{R}_{PMDO}(\alpha_1, \alpha_2)(\beta, S) = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \max_{\Xi \subseteq S^b, |\Xi| = j_a^b} \hat{R}(\beta, S^a, \Xi^{a,b}),
\]

where for any \( \Xi^{a,b} = \{\xi_{a,b}^1, \ldots, \xi_{a,b}^{j_{a,b}}\} \subseteq S^b \) satisfying \( \beta^\top \xi_{a,b}^1 \geq \cdots \geq \beta^\top \xi_{a,b}^{j_{a,b}} \),

\[
\hat{R}(\beta, S^a, \Xi^{a,b}) = \frac{1}{n_a(j_{a,b} - j_a^b)} \sum_{i=1}^{n_a} \sum_{j=a+1}^{a+b} I(\beta^\top v_i^a \leq \beta^\top \xi_j^{a,b}).
\]

Proof. Inspired by the proof of Theorem 3, for each pair of \( (a, b) \) with \( 1 \leq a < b \leq k \) and any \( v^b \), define \( \Psi^{a,b}(\beta, S^a, v^b) = \frac{1}{n_a} \sum_{i=1}^{n_a} I(\beta^\top v_i^a \leq \beta^\top v^b) \). Then \( \hat{R}(\beta, S^a, \Xi^{a,b}) \) evaluates to the average value of such quantity at the bottom ranked \( j_{a,b} - j_a^b \) vertices in \( \Xi^{a,b} \) by \( \beta \), and \( \Psi^{a,b}(\beta, S^a, v^b) \) is monotonically increasing in the value of \( \beta^\top v^b \). Therefore, \( \hat{R}(\beta, S^a, \Xi^{a,b}) \) takes the largest value if \( \Xi^{a,b} \) includes vertices in the top \( j_{a,b} \) positions in \( S^b \) which ranked by \( \beta \). In terms of (11), this largest value is equal to the partial multi-dividing ontology risk of the ontology function in \([a_1^b, a_2^b]\) for each pair of \((a, b)\) with \( 1 \leq a < b \leq k \).

Our next goal is to discuss the convex upper bound on \( \hat{R} \), and thus get a convex optimization model in the partial multi-dividing setting with interval \([a_1^b, a_2^b]\) for each pair of \((a, b)\) with \( 1 \leq a < b \leq k \). Set the loss of the truncated ordering matrices as follows:

\[
\Delta_{PMDO}^\true(\pi, \pi) = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a(j_{a,b}^a - j_a^b)} \sum_{i=1}^{n_a} \sum_{j=a+1}^{a+b} \pi_{i,j}^{a,b}.
\]

Then, we deduce the convex upper bound on \( \hat{R} \):

\[
\sum_{a=1}^{k-1} \sum_{b=a+1}^{k} Z.
\]

where \( Z = \max_{\pi \in \Pi_{a,b}} \{\Delta_{PMDO}^\true((\pi^{a,b})^*, (\pi^{a,b})^{a,b}) - \beta^\top (\phi((S^a, \Xi^{a,b}), (\pi^{a,b})^*) - \phi((S^a, \Xi^{a,b}), (\pi^{a,b}))\} \). By replacing \( \hat{R} \) in the partial multi-dividing ontology risk part in Theorem 4 with (12), we infer the following upper bounding multi-dividing ontology risk:

\[
\hat{R}_{PMDO}(\alpha_1, \alpha_2)(\beta, S) = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \max_{\Xi \subseteq S^b, |\Xi| = j_a^b} Z.
\]
The risk (13) is the largest value of convex functions in $\beta$, and thus is convex in $\beta$. It reveals that (13) is attained by the top $j_{\alpha_2}^{a,b}$ vertices in $S^b$ according to $\beta$ for each pair of $(a,b)$ with $1 \leq a < b \leq k$.

For any $\Xi^{a,b} = \{\xi_{1}^{a,b}, \cdots, \xi_{j_{\alpha_2}^{a,b}}^{a,b}\} \subseteq S^b$, we assume that $\beta^{\top} \xi_1^{a,b} \geq \cdots \beta^{\top} \xi_{j_{\alpha_2}^{a,b}}^{a,b}$.

In terms of expanding the objective in multi-dividing ontology risk (13), we yield

$$\sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \max_{\Xi^{a,b} = \{\xi_{1}^{a,b}, \cdots, \xi_{j_{\alpha_2}^{a,b}}^{a,b}\} \subseteq S^b} \max_{\pi \in \Pi_{na,j_{\alpha_2}^{a,b}}} \frac{1}{n_a(j_{\alpha_2}^{a,b} - j_{\alpha_1}^{a,b})} \sum_{i=1}^{n_a} \sum_{j=j_{\alpha_1}^{a,b}+1}^{j_{\alpha_2}^{a,b}} \pi_{i}^{a,b} v_i^a - \sum_{j=1}^{j_{\alpha_2}^{a,b}} \pi_{ij}^{a,b} \beta^{\top} v_i^a + \sum_{j=1}^{j_{\alpha_2}^{a,b}} \pi_{ij}^{a,b} \beta^{\top} \xi_{j}^{a,b}].$$

By setting $q_{j}^{a,b} = \sum_{i=1}^{n_a} \pi_{ij}^{a,b}$, the above expression is equivalent to

$$\sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \max_{\Xi^{a,b} = \{\xi_{1}^{a,b}, \cdots, \xi_{j_{\alpha_2}^{a,b}}^{a,b}\} \subseteq S^b} \max_{\pi \in \Pi_{na,j_{\alpha_2}^{a,b}}} \frac{1}{n_a(j_{\alpha_2}^{a,b} - j_{\alpha_1}^{a,b})} \sum_{i=1}^{n_a} \sum_{j=j_{\alpha_1}^{a,b}+1}^{j_{\alpha_2}^{a,b}} \pi_{i}^{a,b} v_i^a - \sum_{j=1}^{j_{\alpha_2}^{a,b}} \pi_{ij}^{a,b} \beta^{\top} v_i^a + \sum_{j=1}^{j_{\alpha_2}^{a,b}} q_{j}^{a,b} \beta^{\top} \xi_{j}^{a,b}].$$

Observe that the only term above which relies on $\Xi^{a,b}$ is the third term, and this term gets the largest value if $\Xi^{a,b}$ contains the $j_{\alpha_2}^{a,b}$ vertices with the highest values by $\beta$. This implies the fact that: let $\Xi^{a,b} = \{\xi_1^{a,b}, \cdots, \xi_{j_{\alpha_2}^{a,b}}^{a,b}\} \subseteq S^b$ be the set of vertices in the top $j_{\alpha_2}^{a,b}$ positions (in descending order of values) by $f = \beta^{\top} v$, then the maximum value of multi-dividing ontology risk (13) is attained at $\Xi^{a,b}$ for each pair of $(a,b)$ with $1 \leq a < b \leq k$.

For finishing this subsection, we characterize the $\hat{R}_{\text{PMDO}(\alpha_1, \alpha_2)}^{\text{tight}}$ which is described in the following theorem.

**Theorem 5.** Let $0 < \alpha_1^{a,b} < \alpha_2^{a,b} \leq 1$ for each pair of $(a,b)$ with $1 \leq a < b \leq k$. Let $\hat{R}_{\text{PMDO}(\alpha_1, \alpha_2)}^{\text{hinge}}$ be the multi-dividing ontology risk with hinge ontology loss in (5). Define $\hat{R}_{\text{PMDO}(\alpha_1, \alpha_2)}^{\text{hinge, +}}(\beta, S)$ as

$$\sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a(j_{\alpha_2}^{a,b} - j_{\alpha_1}^{a,b})} \sum_{i : \beta^{\top} v_i^a \leq \beta^{\top} \xi_{j_{\alpha_1}^{a,b}}^{a,b}} \sum_{j=1}^{j_{\alpha_2}^{a,b}} (1 - \beta^{\top} (v_i^a - v_{j_{\alpha_1}^{a,b}}^b)))^+.$$
\[
\zeta_{[0,\alpha_1]}(\beta) = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a(j_{a,b}^{\alpha_{a,b}} - j_{a,b}^{\alpha_1})} \sum_{i=1}^{n_a} \sum_{j=1}^{j_{a,b}} (-\beta^T(v^a_i - v^b_j))_+ ,
\]

and

\[
\zeta^+_{[0,\alpha_1]}(\beta) = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a(j_{a,b}^{\alpha_{a,b}} - j_{a,b}^{\alpha_1})} \sum_{i: \beta^Tv_i^a < \beta^Tv_{\alpha_{a,b}}^b}^{j_{a,b}} \sum_{j=1}^{j_{a,b}} (-\beta^T(v^a_i - v^b_j))_+ .
\]

Then for any ontology sample set \(S = (S^1, S^2, \cdots, S^k) \in V^{n_1} \times V^{n_2} \times \cdots \times V^{n_k}\) and \(\beta \in \mathbb{R}^p\), we have

\[
\hat{R}_{\text{hinge,}+}^{\text{PMDO}(\alpha_1, \alpha_2)}(\beta, S) + \zeta^+_{[0,\alpha_1]}(\beta) \leq \hat{R}_{\text{PMDO}(\alpha_1, \alpha_2)}^{\text{light}}(\beta, S) \leq \hat{R}_{\text{hinge}}^{\text{PMDO}(\alpha_1, \alpha_2)}(\beta, S) + \zeta_{[0,\alpha_1]}(\beta),
\]

Moreover, if \([\beta^Tv_i^a - \beta^Tv_j^b] \geq 1\) for each pair of \((a, b)\) with \(1 \leq a < b \leq k\) and any \(i \in \{1, \cdots, n_a\}, j \in \{1, \cdots, n_b\}\), then we obtain

\[
\hat{R}_{\text{PMDO}(\alpha_1, \alpha_2)}^{\text{light}}(\beta, S) = \hat{R}_{\text{hinge}}^{\text{PMDO}(\alpha_1, \alpha_2)}(\beta, S) + \zeta_{[0,\alpha_1]}(\beta).
\]

**Proof.** For each pair of \((a, b)\) with \(1 \leq a < b \leq k\), set

\[
\Pi_{n_a,j_{a,b}}^{a,b} = \{ \pi_{a,b} \in \Pi_{n_a,j_{a,b}} | \forall i, j_1 < j_2 : \pi_{i,j_1}^{a,b} \geq \pi_{i,j_2}^{a,b} \},
\]

where as before \((j)_\beta\) denotes the \(j\)-th position ranked vertices in \(S^a\) or equivalently in \(\Xi_{a,b}\) when the vertices are ranked in descending order by \(f = \beta^Tv\).

The structural SVM based multi-dividing ontology risk in interval \([\alpha_1, \alpha_2]\) (for each pair of \((a, b)\) with \(1 \leq a < b \leq k\)) can be deduced in the following
simplified version:

\[
\hat{R}_{\text{PMDO}(\alpha_1, \alpha_2)}^\text{tight}(\beta, S) = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \max_{i, j, a, b, \alpha_1, \alpha_2} \frac{1}{n_a(j_{\alpha_2} - j_{\alpha_1})} \sum_{i=1}^{n_a} \left[ - \sum_{j=1}^{j_{\alpha_2}} \pi_{i(j)\beta}^{a,b} \beta^T (v_i^a - \bar{\xi}_j^{a,b}) \right] \\
+ \sum_{j=j_{\alpha_2}+1}^{j_{\alpha_1}} \pi_{i(j)\beta}^{a,b} (1 - \beta^T (v_i^a - \bar{\xi}_j^{a,b})) \\
= \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \max_{i, j, a, b, \alpha_1, \alpha_2} \frac{1}{n_a(j_{\alpha_2} - j_{\alpha_1})} \sum_{i=1}^{n_a} \left[ - \sum_{j=1}^{j_{\alpha_2}} \pi_{i(j)\beta}^{a,b} \beta^T (v_i^a - v_j^b) \right] \\
+ \sum_{j=j_{\alpha_2}+1}^{j_{\alpha_1}} \pi_{i(j)\beta}^{a,b} (1 - \beta^T (v_i^a - v_j^b)) \\
\leq \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a(j_{\alpha_2} - j_{\alpha_1})} \sum_{i=1}^{n_a} \left[ - \sum_{j=1}^{j_{\alpha_2}} \pi_{i(j)\beta}^{a,b} \beta^T (v_i^a - v_j^b) \right] \\
+ \sum_{j=j_{\alpha_2}+1}^{j_{\alpha_1}} \max_{\pi_{i(j)\beta} \in \{0,1\}} \pi_{i(j)\beta}^{a,b} (1 - \beta^T (v_i^a - v_j^b)) \\
= \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a(j_{\alpha_2} - j_{\alpha_1})} \sum_{i=1}^{n_a} \left[ - \beta^T (v_i^a - v_j^b) \right] \\
+ \sum_{j=j_{\alpha_2}+1}^{j_{\alpha_1}} (1 - \beta^T (v_i^a - v_j^b)).
\]

For each pair of \((a, b)\) with \(1 \leq a < b \leq k\), define \(\hat{\pi}_{a,b}^{a,b} \in \{0,1\}^{n_a \times j_{\alpha_2}^{a,b}}\) as follows: for each \(v_i^a\) such that \(\beta^T v_i^a \leq \beta^T v_j^b\), we have \(\hat{\pi}_{i(j)\beta}^{a,b} = 1\) if \(j \in \{1, \cdots, j_{\alpha_2}^{a,b}\}\) and \(\hat{\pi}_{i(j)\beta}^{a,b} = I(\beta^T v_i^a - \beta^T v_j^b \leq 1)\) otherwise; for each \(v_i^a\) such that \(\beta^T v_i^a > \beta^T v_j^b\), we have \(\hat{\pi}_{i(j)\beta}^{a,b} = I(\beta^T v_i^a - \beta^T v_j^b \leq 0)\) if \(j \in \{1, \cdots, j_{\alpha_2}^{a,b} - 1\}\) and \(\hat{\pi}_{i(j)\beta}^{a,b} = 0\) otherwise.
Obviously, \( \hat{\pi}^{a,b} \) is a valid ordering matrix in \( \Pi^{a,b}_{n_{a,j_{a,b}}} \). Since for each pair of \( (a, b) \) with \( 1 \leq a < b \leq k \) and for \( i \) satisfies \( \beta^T v_i^a \leq \beta^T v_i^b \) and \( j \in \{1, \cdots, j_{a,b}\} \), we get \(-\beta^T (v_i^a - v_i^b) = -\beta^T v_i^a + \beta^T v_i^b \geq -\beta^T v_i^a + \beta^T v_i^b \geq 0\), which means \(-\beta^T (v_i^a - v_i^b) = (-\beta^T (v_i^a - v_i^b))_+ \). Hence, by the definition of \( \hat{\pi}^{a,b} \), we get

\[
\begin{align*}
\mathcal{R}_{\text{PMDO}}^\text{right}(\alpha_1, \alpha_1)(\beta, S) \\
&\geq \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a(j_{a,b} - j_{a,b})} \sum_{i=1}^{n_a} \sum_{j=1}^{j_{a,b}} \hat{\pi}^{a,b}_{i,j}(\beta^T v_i^a - \beta^T v_i^b) \\
&+ \sum_{j=j_{a,b}+1}^{j_{a,b}} \hat{\pi}^{a,b}_{i,j}(1 - \beta^T (v_i^a - v_i^b))_+ \\
&= \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a(j_{a,b} - j_{a,b})} \sum_{i=1}^{n_a} \sum_{j=1}^{j_{a,b}} (-\beta^T (v_i^a - v_i^b))_+
\end{align*}
\]

(14) \[
\mathcal{R}_{\text{PMDO}}^\text{right}(\alpha_1, \alpha_1)(\beta, S) \\
&= \frac{1}{n_a(j_{a,b} - j_{a,b})} \sum_{i=1}^{n_a} \sum_{j=1}^{j_{a,b}} (-\beta^T (v_i^a - v_i^b))_+
\]

Since the last term is not less than zero, the desired bound is obtained.
Now, we shall show that the upper bound on the multi-dividing ontology risk holds if \( |\beta^T v_i^a - \beta^T v_j^b| \geq 1 \) for any \( i \in \{1, \cdots, n_a\} \) and \( j \in \{1, \cdots, n_b\} \). In this case, \( \beta^T (v_i^a - v_j^b) \) is positive for some \( i \in \{1, \cdots, n_a\} \) and \( j \in \{1, \cdots, n_b\} \), then it is also the situation \( \beta^T (v_i^a - v_j^b) \geq 1 \). This implies, for each pair of \((a, b)\) with \( 1 \leq a < b \leq k \), that

\[
\frac{1}{n_a(j_{a,b} - j_{a,b}^1)} \sum_{i:a \leq b \leq a_2} \sum_{j:a \leq b \leq a_1}^{j_{a,b}^1} (1 - \beta^T (v_i^a - v_j^b))_+ = 0.
\]

Combining this to (14), we have

\[
\hat{R}^{\text{tight}}_{\text{PMDO}}(\alpha_1, \alpha_2)(\beta, S) \geq \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \{ \frac{1}{n_a(j_{a,b}^a - j_{a,b}^1)} \sum_{i=1}^{n_a} \sum_{j=1}^{j_{a,b}^1} (-\beta^T (v_i^a - v_j^b))_+ + \sum_{j=j_{a,b}^1+1} (1 - \beta^T (v_i^a - v_j^b))_+ \}.
\]

Therefore, we finish the proof of Theorem 5.

\[ \square \]

3.5. Generalization bound for partial multi-dividing ontology learning algorithm. In this part, we consider the generalization properties of partial multi-dividing ontology learning algorithm, and the uniform convergence generalization bound is derived. By this way, we establish a good training performance generalization performance by virtue of partial multi-dividing ontology learning algorithm. For each pair of \((a, b)\) with \( 1 \leq a < b \leq k \), let \( \Theta_{a,b}^{a_1,a_2}(f, v^b) \) be the indicator function which is 1 if \( P_{\tilde{v}^b} (f(\tilde{v}^b) > f(v^b)) \in [a_1, a_2] \) and is 0 otherwise; \( \tilde{\Theta}_{a,b}^{a_1,a_2}(f, v^b) \) be an indicator function which is 1 if \( v_j^b \) in positions from \( j_{a,b}^1 + 1 \) to \( j_{a,b}^2 \) in the ranking of all vertices in \( S^b \) by ontology function \( f \). For an ontology function \( f : \mathbb{R}^p \rightarrow \mathbb{R} \), define the expectation risk version, \( \hat{R}^{\text{PMDO}}(\alpha_1, \alpha_2)[f, D] \), as

\[
\sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{a_2 - a_1} E_{v^a \sim D_a, v^b \sim D_b} [\mathbf{I}(f(v^a) \leq f(v^b)) \Theta_{a,b}^{a_1,a_2} (f, v^b)],
\]

and for an ontology sample set \( S = (S^1, S^2, \cdots, S^k) \in V^{n_1} \times V^{n_2} \times \cdots \times V^{n_k} \), its corresponding empirical version \( \hat{R}^{\text{PMDO}}(\alpha_1, \alpha_2)[f, S] \) is

\[
\sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a(j_{a,b}^2 - j_{a,b}^1)} \sum_{i=1}^{n_a} \sum_{j=1}^{n_b} \mathbf{I}(f(v_i^a) \leq f(v_j^b)) \tilde{\Theta}_{a,b}^{a_1,a_2} (f, v_j^b).
\]

Let \( \mathcal{F} \) be the ontology function space, and the capacity of \( \mathcal{F} \) will be measured in view of the VC dimension of the kind of classifiers yielded from ontology
functions in the special class: $\mathcal{Y}_F = \{ \text{sign} \circ (f - t) | f \in F, t \in \mathbb{R} \}$. As the last theorem in our paper, we state below the uniform convergence bound for partial multi-dividing ontology algorithm.

**Theorem 6.** Let $F$ be a class of real-valued ontology functions on $V$, and $\mathcal{Y}_F = \{ \text{sign} \circ (f - t) | f \in F, t \in \mathbb{R} \}$. For all pairs of $(a, b)$ with $1 \leq a < b \leq k$, let $n_{a_{\max}} = \max\{ n_1, \ldots, n_k \}$, $n_{b_{\max}} = \max\{ n_2, \ldots, n_k \}$, $(\alpha_{1_{\max}}, \alpha_{2_{\max}}) = \max\{ \alpha_{a_{\max}}^{a, b}, \alpha_{1_{\max}}^{a_{\max}, b_{\max}} | 1 \leq a < b \leq k \}$. Let $\delta > 0$. Then with probability at least $1 - \delta$ over ontology sample $S = (S^1, S^2, \ldots, S^k) \in V^{n_1} \times V^{n_2} \times \cdots \times V^{n_k}$ from $D_1 \times \cdots \times D_k$, we have for all $f \in F$, 

$$R_{\text{PMDO}(\alpha_1, \alpha_2)}[f, \mathcal{D}] \leq \hat{R}_{\text{PMDO}(\alpha_1, \alpha_2)}[f, S] + C\left( \sqrt{\frac{p \ln(n_{a_{\max}}) + \ln\left(\frac{k(k-1)}{2\delta}\right)}{n_{a_{\max}}} + \frac{1}{\alpha_{2_{\max}} - \alpha_{1_{\max}}} \sqrt{\frac{p \ln(n_{b_{\max}}) + \ln\left(\frac{k(k-1)}{2\delta}\right)}{n_{b_{\max}}}} \right),$$

where $p$ is the VC dimension of $\mathcal{Y}_F$, and positive parameter $C$ is distribution-independent.

**Proof.** Assume that $f$ has no ties and $n_b\alpha_2^{a, b}$ is an integer. For each pair of $(a, b)$ with $1 \leq a < b \leq k$, we define 

$$t_{\text{D}_b, f, \alpha_2^{a, b}} = \arg \inf_{t \in \mathbb{R}} \{ t \in \mathbb{R} | P_{v^b \sim \text{D}_b}[f(v^b) > t] = \alpha_2^{a, b} \},$$

and its empirical version as 

$$\hat{t}_{\text{S}^b, f, \alpha_2^{a, b}} = \arg \min_{t \in \mathbb{R}} \{ t \in \mathbb{R} | \frac{1}{n_b} \sum_{j=1}^{n_b} I(f(v_j^b) > t) \geq \alpha_2^{a, b} \}.$$

Clearly, $E_{v^b \sim \text{D}_b}[I(f(v^b) > t_{\text{D}_b, f, \alpha_2^{a, b}})] = \alpha_2^{a, b}$. Since ontology function $f$ has no ties, and $\hat{t}_{\text{S}^b, f, \alpha_2^{a, b}}$ is the threshold on $f$ which $n_b\alpha_2^{a, b}$ vertices in $S^b$ are ranked by $f$, we infer 

$$\sum_{j=1}^{n_b} I(f(v_j^b) > \hat{t}_{\text{S}^b, f, \alpha_2^{a, b}}) = n_b\alpha_2^{a, b}.$$

For any ontology function $f : V \rightarrow \mathbb{R}$, the partial multi-dividing ontology risk in intervals $[0, \alpha_2^{a, b}]$ (pair $(a, b)$ satisfy $1 \leq a < b \leq k$) can be stated as 

$$R_{\alpha_2}[f, \mathcal{D}] = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{\alpha_{2_{\max}}} E_{v^a \sim \text{D}_a, v^b \sim \text{D}_b}[I(f(v^a) \leq f(v^b), f(v^b) > t_{\text{D}_b, f, \alpha_2^{a, b}})],$$

and its empirical version on ontology sample set $S$ can be formulated by 

$$\hat{R}_{\alpha_2}[f, S] = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \frac{1}{n_a n_b \alpha_2^{a, b}} \sum_{i=1}^{n_a} \sum_{j=1}^{n_b} I(f(v_i^a) \leq f(v_j^b), f(v_j^b) > \hat{t}_{\text{S}^b, f, \alpha_2^{a, b}}).$$
For $1 \leq a \leq k$ and fixed any $\epsilon > 0$, using McDiarmid inequality, we get
\begin{equation}
\Pr \left[ \sup_{f \in \mathcal{F}} \Pr_{\alpha_0} \left( \sum_{i=1}^{n_a} I(f(v_i^a) \leq t) - \Pr_{\alpha_0} \left( I(f(v^a) \leq t) \right) \right) \geq \epsilon \right] \leq C^a n_a^p e^{-2n_a \epsilon^2}
\end{equation}
where $p$ is the VC dimension of $\Pr_{\mathcal{F}}$, and positive parameter $C^a$ is distribution-independent.

For each pair of $(a, b)$ with $1 \leq a < b \leq k$, an ontology function $f$ and vertex $v^b$, define $l_{a,b}^2(f, v^b) = \Pr_{\alpha_0} \left( I(f(v^a) \leq f(v^b)) \right)$. Moreover, we set
\begin{align*}
\tilde{R}_{a,b}^{2}(f, D_a \cup D_b, S^b) &= \frac{1}{n_b a_{2,b}} \sum_{j=1}^{n_b} l_{a,b}^2(f, v_j^b) I(f(v_j^b) > l_{a,b}^2 D_b, f, \alpha_{a,b}^2), \\
\tilde{R}_{a,b}^{2}(f, D_a, S^b) &= \frac{1}{n_b a_{2,b}} \sum_{j=1}^{n_b} l_{a,b}^2(f, v_j^b) I(f(v_j^b) > \tilde{l}_{a,b}^2 S^b, f, \alpha_{a,b}^2).
\end{align*}
Hence, for any $f \in \mathcal{F}$, we obtain
\begin{align*}
R_{a,b}^{2}(f, D) - \tilde{R}_{a,b}^{2}(f, S) &= (R_{a,b}^{2}(f, D) - \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \tilde{R}_{a,b}^{2}(f, D_a \cup D_b, S^b)) \\
&\quad + (\sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \tilde{R}_{a,b}^{2}(f, D_a \cup D_b, S^b) - \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \tilde{R}_{a,b}^{2}(f, D_a, S^b)) \\
&\quad + (\sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \tilde{R}_{a,b}^{2}(f, D_a, S^b) - \tilde{R}_{a,b}^{2}(f, S)).
\end{align*}
Thus for any $\epsilon > 0$, we infer
\begin{align*}
\Pr_{S=(S^1, S^2, \ldots, S^k) \in \mathcal{V}^n_1 \times \mathcal{V}^n_2 \times \cdots \times \mathcal{V}^n_k} \left( \sup_{f \in \mathcal{F}} \{ R_{a,b}^{2}(f, D) - \tilde{R}_{a,b}^{2}(f, S) \geq \epsilon \} \right) \\
\leq \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \Pr_{S^a \sim \mathcal{D}_a^{n_a}} \left( \sum_{f \in \mathcal{F}} \frac{1}{n_b a_{2,b}} \Pr_{\alpha_0} \left( I(f(v^a) \leq f(v^b), f(v^b) > l_{a,b}^2 D_b, f, \alpha_{a,b}^2) \right) \right) \\
&\quad - (\sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \Pr_{S^a \sim \mathcal{D}_a^{n_a}} \left( \sum_{f \in \mathcal{F}} \Pr_{\alpha_0} \left( I(f(v^a) \leq f(v^b), f(v^b) > \tilde{l}_{a,b}^2 S^b, f, \alpha_{a,b}^2) \right) \right) \\
&\quad + (\sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \Pr_{S^a \sim \mathcal{D}_a^{n_a} \times S^b \sim \mathcal{D}_b^{n_b}} \left( \sum_{f \in \mathcal{F}} \tilde{R}_{a,b}^{2}(f, D_a, S^b) \right) \\
&\quad - \frac{1}{n_a n_b a_{2,b}} \sum_{i=1}^{n_a} \sum_{j=1}^{n_b} I(f(v_i^a) \leq f(v_j^b), f(v_j^b) > \tilde{l}_{a,b}^2 S^b, f, \alpha_{a,b}^2) \geq \frac{\epsilon}{3} \}).
\end{align*}
Let $N_1$, $N_2$ and $N_3$ be the first, second and third terms of right side of the above inequality. We need to bound $N_1$, $N_2$ and $N_3$ separately. For the first part, according to the assumption that ontology function $f$ has no ties, we have

$$R_{\alpha_2}[f, D] - \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \bar{R}^{a,b}_{\alpha_2}[f, D_a \cup D_{b}, S^b]$$

$$= \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \left\{ \frac{1}{\alpha_2} \mathbb{E}_{v^b} [1_{a,b}(f, v^b) I(f(v^b) > t_{a,b}^{D_{b,f,\alpha_2^a,b})}] \right\}$$

$$- \frac{1}{n_b \alpha_2} \sum_{j=1}^{n_b} \mathbb{I}(f(v^a) \leq f(v^b)) \mathbb{I}(f(v^b) > t_{a,b}^{D_{b,f,\alpha_2^a,b})}]$$

$$= \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \left\{ \frac{1}{\alpha_2} \mathbb{E}_{v^a} [\mathbb{E}_{v^b} [I(f(v^a) \leq f(v^b)) \mathbb{I}(f(v^b) > t_{a,b}^{D_{b,f,\alpha_2^a,b})]]] \right\}$$

$$- \frac{1}{n_b \alpha_2} \sum_{j=1}^{n_b} \mathbb{I}(f(v_j^a) > \max\{f(v^a), t_{a,b}^{D_{b,f,\alpha_2^a,b})}\})]$$

$$\leq \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \left\{ \frac{1}{\alpha_2} \sup_{v^a \in V^a} \mathbb{E}_{v^b} [I(f(v^a) > \max\{f(v^a), t_{a,b}^{D_{b,f,\alpha_2^a,b})}\})] \right\}$$

$$- \frac{1}{n_b \alpha_2} \sum_{j=1}^{n_b} \mathbb{I}(f(v_j^a) > \max\{f(v^a), t_{a,b}^{D_{b,f,\alpha_2^a,b})}\})]$$

$$\leq \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \sup_{v^b \in V^b} \mathbb{E}_{v^b} [I(f(v^b) > t)] - \frac{1}{n_b} \sum_{j=1}^{n_b} \mathbb{I}(f(v_j^b) > t)]$,}
Thus, using (15), we yield

$$N_1 = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \mathbb{P}_{S^b \sim D_b^a} \bigg( \bigcup_{f \in F} \bigg\{ \frac{1}{\alpha_{a,b}^2} \mathbb{P}_{v \sim D_a, v^b \sim D_b} \bigg[ I(f(v^a)) \leq f(v^b), f(v^b) > t_{D_b,f,\alpha_{a,b}}^{a,b} \bigg] \bigg\} - \tilde{R}_{\alpha_{a,b}^2}^{a,b} \bigg[ f, D_a \cup D_b, S^b \bigg] \geq \frac{\epsilon}{3} \bigg) \bigg)$$

$$\leq \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \mathbb{P}_{S^b \sim D_b^a} \bigg( \bigcup_{f \in F} \bigg\{ \frac{1}{n_b} \sum_{j=1}^{n_b} \bigg[ I(f(v_j^b)) > t \bigg] \bigg\} \bigg) \bigg)$$

$$\leq \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \mathbb{P}_{S^b \sim D_b^a} \bigg( \bigcup_{f \in F} \bigg\{ \frac{1}{n_b} \sum_{j=1}^{n_b} \bigg[ I(f(v_j^b)) > t \bigg] \bigg\} \bigg) \bigg)$$

For the second term, for each pair of $(a,b)$ with $1 \leq a < b \leq k$, note that if $t_{D_b,f,\alpha_{a,b}^2}^{a,b} \leq \tilde{R}_{\alpha_{a,b}^2}^{a,b}$, then $I(f(v^b) > t_{D_b,f,\alpha_{a,b}^2}^{a,b}) = I(f(v^b) > \tilde{R}_{\alpha_{a,b}^2}^{a,b}) \geq 0$ for any $v^b \in V$, and if $t_{D_b,f,\alpha_{a,b}^2}^{a,b} > \tilde{R}_{\alpha_{a,b}^2}^{a,b}$, then $I(f(v^b) > t_{D_b,f,\alpha_{a,b}^2}^{a,b}) = I(f(v^b) > \tilde{R}_{\alpha_{a,b}^2}^{a,b}) \leq 0$ for any $v^b \in V$. Since one of these two cases will always hold, and $l$ is bounded by $(0 \leq l^{a,b}(f, v^b) \leq 1$ for any $v^b \in V$), combining with the definition of $t_{D_b,f,\alpha_{a,b}^2}^{a,b}$ and $t_{D_b,f,\alpha_{a,b}^2}^{a,b}$, and (15), we deduce

$$N_2 = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \mathbb{P}_{S^b \sim D_b^a} \bigg( \bigcup_{f \in F} \bigg\{ \frac{1}{n_b} \sum_{j=1}^{n_b} l^{a,b}(f, v_j^b) I(f(v_j^b) > t_{D_b,f,\alpha_{a,b}^2}^{a,b}) \bigg\} \bigg)$$

$$\leq \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \mathbb{P}_{S^b \sim D_b^a} \bigg( \bigcup_{f \in F} \bigg\{ \frac{1}{n_b} \sum_{j=1}^{n_b} l^{a,b}(f, v_j^b) I(f(v_j^b) > t_{D_b,f,\alpha_{a,b}^2}^{a,b}) \bigg\} \bigg)$$

$$\leq \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \mathbb{P}_{S^b \sim D_b^a} \bigg( \bigcup_{f \in F} \bigg\{ \frac{1}{n_b} \sum_{j=1}^{n_b} \bigg[ I(f(v_j^b) > t_{D_b,f,\alpha_{a,b}^2}^{a,b}) \bigg] \bigg\} \bigg)$$

$$\leq \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \mathbb{P}_{S^b \sim D_b^a} \bigg( \bigcup_{f \in F} \bigg\{ \frac{1}{n_b} \sum_{j=1}^{n_b} \bigg[ I(f(v_j^b) > t_{D_b,f,\alpha_{a,b}^2}^{a,b}) \bigg] \bigg\} \bigg)$$
\[
\begin{align*}
&\sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \mathbb{P}_{S^b \sim D_b^{n_b}}(\bigcup_{f \in F} \{ \frac{1}{n_b} \sum_{j=1}^{n_b} I(f(v^b_j) > \nu_{a,b}^{D_b,f,\alpha_2^b}) - \alpha_2^b \geq \frac{\alpha_2^b \epsilon}{3} \}) \\
&- \frac{1}{n_b} \sum_{j=1}^{n_b} I(f(v^b_j) > \nu_{a,b}^{D_b,f,\alpha_2^b}) \geq \frac{\alpha_2^b \epsilon}{3} \}) \\
&= \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \mathbb{P}_{S^b \sim D_b^{n_b}}(\bigcup_{f \in F} \{ \frac{1}{n_b} \sum_{j=1}^{n_b} I(f(v^b_j) > \nu_{a,b}^{D_b,f,\alpha_2^b}) - \alpha_2^b \geq \frac{\alpha_2^b \epsilon}{3} \}) \\
&= \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \mathbb{P}_{S^b \sim D_b^{n_b}}(\bigcup_{f \in F} \{ \frac{1}{n_b} \sum_{j=1}^{n_b} I(f(v^b_j) > \nu_{a,b}^{D_b,f,\alpha_2^b}) - \alpha_2^b \geq \frac{\alpha_2^b \epsilon}{3} \}) \\
&- \mathbb{E}_{\nu_b}[I(f(v^b) > \nu_{a,b}^{D_b,f,\alpha_2^b})] \geq \frac{\alpha_2^b \epsilon}{3} \}) \\
&\leq \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \mathbb{P}_{S^b \sim D_b^{n_b}}(\bigcup_{f \in F} \bigcup_{t \in \mathbb{R}} \{ \frac{1}{n_b} \sum_{j=1}^{n_b} I(f(v^b_j) > t) - \mathbb{E}_{\nu_b}[I(f(v^b) > t)] \geq \frac{\alpha_2^b \epsilon}{3} \}) \\
&\leq \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} C_b n_b^p \epsilon \frac{2n_b^b \alpha_2^{a,b} 2^a \epsilon}{3}.
\end{align*}
\]

Now, we bound the term \( N_3 \).

\[
\begin{align*}
&\sum_{a=1}^{k-1} \sum_{b=a+1}^{k} R_{\alpha_2^{a,b}}[f, D_a, S^b] - \widehat{R}_{\alpha_2}[f, S] \\
&= \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \left\{ \frac{1}{n_a n_b \alpha_2^{a,b}} \sum_{j=1}^{n_b} \sum_{i=1}^{n_a} I(f(v^a_i) \leq f(v^b_j), f(v^b_j) > \nu_{a,b}^{S^b,f,\alpha_2^b}) \right\} \\
&- \frac{1}{n_a n_b \alpha_2^{a,b}} \sum_{j=1}^{n_b} \sum_{i=1}^{n_a} I(f(v^a_i) \leq f(v^b_j), f(v^b_j) > \nu_{a,b}^{S^b,f,\alpha_2^b}) \\
&= \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \left\{ \frac{1}{n_a n_b \alpha_2^{a,b}} \sum_{j=1}^{n_b} I(f(v^b_j) > \nu_{a,b}^{S^b,f,\alpha_2^b}) \sup_{t \in \mathbb{R}} \mathbb{E}_a[I(f(v^a) \leq t)] - \frac{1}{n_a} \sum_{i=1}^{n_a} I(f(v^a_i) \leq f(v^b_j)) \right\} \\
&\leq \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \left\{ \frac{1}{n_a n_b \alpha_2^{a,b}} \sup_{t \in \mathbb{R}} \mathbb{E}_a[I(f(v^a) \leq t)] - \frac{1}{n_a} \sum_{i=1}^{n_a} I(f(v^a_i) \leq t) \right\} \\
&= \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} \left\{ \sup_{t \in \mathbb{R}} \mathbb{E}_a[I(f(v^a) \leq t)] - \frac{1}{n_a} \sum_{i=1}^{n_a} I(f(v^a_i) \leq t) \right\},
\end{align*}
\]
and thus in light of (15), we derive

\[ N_3 = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} P_{S_a \times S_b \rightarrow D_a^n \times D_b^n} \left( \bigcup_{f \in \mathcal{F}} \{ R_{\alpha_2}^a, b[f, D_a, S_b] \} \right) \]

\[ - \frac{1}{n_a n_b} \sum_{i=1}^{n_a} \sum_{j=1}^{n_b} I(f(v_i^a) \leq f(v_j^b), f(v_j^b) > \tilde{p}_{a,b}^{S_a, f, \alpha_2}) \geq \frac{\epsilon}{3} \}

\[ = \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} E_{S_b}[P_{S_a \mid S_b}] \left( \bigcup_{f \in \mathcal{F}} \{ R_{\alpha_2}^a, b[f, D_a, S_b] \} \right) \]

\[ - \frac{1}{n_a n_b} \sum_{i=1}^{n_a} \sum_{j=1}^{n_b} I(f(v_i^a) \leq f(v_j^b), f(v_j^b) > \tilde{p}_{a,b}^{S_a, f, \alpha_2}) \geq \frac{\epsilon}{3} \}

\[ \leq \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} E_{S_b}[P_{S_a \mid S_b}] \left( \bigcup_{f \in \mathcal{F}} \{ \sup_{t \in \mathbb{R}} |E_{v_a}[I(f(v_a) \leq t)]| \geq \frac{\epsilon}{3} \} \right) \]

\[ \leq \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} E_{S_b}[P_{S_a \mid S_b}] \left( \bigcup_{f \in \mathcal{F}} \{ \sup_{t \in \mathbb{R}} |E_{v_a}[I(f(v_a) \leq t)]| \geq \frac{\epsilon}{3} \} \right) \]

\[ \leq \sum_{a=1}^{k-1} \sum_{b=a+1}^{k} C_{n_a}^3 n_a^p e^{-2n_a \frac{\epsilon^2}{9}}. \]

Combining the bounds we show above in three cases, the final result followed by setting the right-hand side equal to \( \delta \) and solving it for \( \epsilon \).

\[ \square \]

4. Experiments

We underline that to implement our algorithm with mathematical learning setting, for each vertex in each ontology in the experiments we shall use fix dimensional vectors to express vertex’s semantic and construct information. All the information of the concept include its name, attribute, instance and structure of vertex in the ontology graph is packaged in its corresponding vector. In this section, five experiments are designed and presented to measure the effectiveness of our partial multi-dividing ontology learning algorithm manifested in the former sections. We use C++ to run our main algorithm, and available LAPACK and BLAS libraries for linear calculating are used. All experiments are implemented on a 32G memory multi-core CPU.

4.1. Ontology similarity measure experiment on plant data. In the field of plant science, “PO” ontology \( O_1 \) (see http://www.plantontology.org for more details, and its basic structure is extracted, draw and depicted in Figure 1) is applied to present plant morphology and anatomy, and development stages for nearly all types of plants. The aim of construction “PO” ontology is to establish a semantic framework for worthy cross-species queries across gene
expressions and phenotype data collections followed from genetics experiments and plant genomics. Indeed, “PO” ontology can be regarded as a dictionary which helps plant scientists to search the concept and understand the potential connection between plant species, biochemical processes and the surrounding climate and environment impact. We use “PO” ontology to test the productivity of our partial multi-dividing ontology algorithm with respect to ontology similarity measuring. Since there are two branches “plant structure development stage” and “plant anatomical entity” in its ontology graph, we set $k = 2$. We use $P@N$ (Precision Ratio, see Craswell and Hawking [8] for more details on this index) to evaluate the equality of the experiment results. The specific procedures can be stated as follows: firstly, with the help of experts, the most similarity $N$ vertices for each vertex are listed; secondly, in terms of our algorithm, other most similarity $N$ for each vertex are obtained; thirdly, the $P@N$ precision ratios for all vertices are inferred; lastly, the average precision ratio for the whole ontology graph is finally calculated. Furthermore, ontology learning technologies proposed in Gao and Zhu [20], Gao et al. [16] and [14] are also acted on the “PO” ontology and their corresponding precision ratios are calculated respectively. Several parts of the compared data can be referred to Table 1.
Table 1. The experiment results of ontology similarity measure on “PO” ontology

<table>
<thead>
<tr>
<th>Algorithm in our paper</th>
<th>0.5383</th>
<th>0.6903</th>
<th>0.9156</th>
<th>0.9705</th>
</tr>
</thead>
<tbody>
<tr>
<td>Algorithm in Gao and Zhu [20]</td>
<td>0.5042</td>
<td>0.6216</td>
<td>0.7853</td>
<td>0.9034</td>
</tr>
<tr>
<td>Algorithm in Gao et al. [16]</td>
<td>0.4921</td>
<td>0.6152</td>
<td>0.8113</td>
<td>0.9174</td>
</tr>
<tr>
<td>Algorithm in Gao et al. [14]</td>
<td>0.5360</td>
<td>0.6664</td>
<td>0.9004</td>
<td>0.9673</td>
</tr>
</tbody>
</table>

In light of the compared data presented in Table 1, we see that the precision ratio using our partial multi-dividing ontology algorithm is clearly higher than the precision ratio determined by algorithms in Gao and Zhu [20], Gao et al. [16] and [14] when N = 3, 5, 10 or 20. Hence, we conclude that our partial multi-dividing ontology algorithm discussed in our paper is superior to the learning techniques that Gao and Zhu [20], Gao et al. [16] and [14] raised.

4.2. Ontology mapping experiment on mathematical data. Mathematical ontologies $O_2$ and $O_3$ (Figure 2 and Figure 3 present the basic structures of $O_2$ and $O_3$, respectively) are employed in our second experiment to test the effectiveness of our new proposed partial multi-dividing algorithm with regard to building ontology mapping between them. This experiment aims to determine the similarity based ontology mapping between $O_2$ and $O_3$ using our ontology learning algorithm. In view of analyzing of ontology graph structures, we set $k = 3$. The $P@N$ criterion is applied as well as criterion to measure the quality of experiment data. Moreover, ontology learning algorithms introduced in Gao and Zhu [20], Wu et al. [49] and Gao et al. [22] are also implemented on mathematical ontologies, and the precision ratios are compared using these methods. Parts of compared experiment data can be referred to Table 2.

<table>
<thead>
<tr>
<th>Algorithm in our paper</th>
<th>$P@1$ average precision ratio</th>
<th>$P@3$ average precision ratio</th>
<th>$P@5$ average precision ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>PMDO Algorithm in our paper</td>
<td>0.4231</td>
<td>0.5128</td>
<td>0.7154</td>
</tr>
<tr>
<td>Algorithm in Gao and Zhu [20]</td>
<td>0.3077</td>
<td>0.4359</td>
<td>0.5615</td>
</tr>
<tr>
<td>Algorithm in Wu et al. [49]</td>
<td>0.3846</td>
<td>0.5000</td>
<td>0.6769</td>
</tr>
<tr>
<td>Algorithm in Gao et al. [22]</td>
<td>0.3462</td>
<td>0.3974</td>
<td>0.5231</td>
</tr>
</tbody>
</table>
Table 2. The experiment results of ontology mapping on mathematical ontologies
The experiment compare results for $N = 1, 3, 5$ presented in Table 2 and it reveals that our partial multi-dividing ontology algorithm performances much more efficient than ontology learning algorithms proposed in Gao and Zhu [20], Wu et al. [49] and Gao et al. [22] especially when $N$ increases.

4.3. **Ontology similarity measure experiment on biology data.** In our third experiment, we aim to utilize the “GO” ontology $O_4$ (see for more details http://www.geneontology.org. Its basic structure is extracted and showed in Figure 4) to test the practicability of our partial multi-dividing ontology learning algorithm on biology engineering application. As a collaborative effort to deal with the need for consistent expressions of gene products across databases, “GO” ontology was founded in 1998. Worked as an encyclopedia, it concludes a great number of databases, and contains various of the world’s major repositories for animal, plant and microbial genomes. Since it contains three main branches: “Molecular function”, “Biological process” and “Cellular Component”, we set $k = 3$. Ontology learning approaches discussed in Gao and Zhu [20], Gao et al. [16] and [14] are implemented on “GO” ontology, and the $P@N$ accuracy rates by these algorithms are determined. Parts of compared the precision ratio data inferred from these techniques are presented in Table 3.
Table 3. The experiment results of ontology similarity measure on “GO” ontology

<table>
<thead>
<tr>
<th>Algorithm in our paper</th>
<th>$P@3$ average precision ratio</th>
<th>$P@5$ average precision ratio</th>
<th>$P@10$ average precision ratio</th>
<th>$P@20$ average precision ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>PMDO Algorithm</td>
<td>0.5670</td>
<td>0.6985</td>
<td>0.8305</td>
<td>0.9671</td>
</tr>
<tr>
<td>Algorithm in Gao and Zhu [20]</td>
<td>0.4988</td>
<td>0.6142</td>
<td>0.7478</td>
<td>0.9101</td>
</tr>
<tr>
<td>Algorithm in Gao et al. [16]</td>
<td>0.4792</td>
<td>0.5409</td>
<td>0.6672</td>
<td>0.8449</td>
</tr>
<tr>
<td>Algorithm in Gao et al. [14]</td>
<td>0.5649</td>
<td>0.6827</td>
<td>0.8124</td>
<td>0.9371</td>
</tr>
</tbody>
</table>

By comparison of experiment results for $N=3, 5, 10$ or $20$ described in Table 3, we see that the partial multi-dividing ontology algorithm depicted in this article is superior to the approaches proposed by Gao and Zhu [20], Gao et al. [16] and [14]. Therefore, our new introduced partial multi-dividing ontology algorithm has more productivity on similarity measuring in biology data applications.

4.4. **Ontology mapping experiment on chemical index data.** The so-called “Chemical Index” ontologies $O_5$ and $O_6$ (the basic structures of $O_5$ and $O_6$ are extracted and presented in Figure 5 and Figure 6, respectively) for our last experiment. The figures only present partial vertices of two ontologies, and in fact $O_5$ and $O_6$ contain 68 concepts and 46 concepts, respectively. There are many concepts of $O_5$ and $O_6$ not displayed in Figure 5 and Figure 6 such as “singly vertex-weighted Wiener number”, “multiplicative Wiener index”, “terminal Wiener index”, “generalized Harary index”, “second atom bond connectivity index”, ···, “General Co-PI index”, “fifth atom bond connectivity index”, “revised edge Szeged index”, “eccentric connectivity polynomial”, “Shultz polynomial”, “second geometric-arithmetic index”, “zeroth-order general Randic index”, ···, “Zagreb polynomial”, “fifth geometric-arithmetic index”, ···, “sixth Zagreb polynomial”, etc.

In chemical graph theory, topological polynomials are defined closely related to topological index. For example, for each vertex (which express an atom) $v$ in molecular graph, the eccentricity of $v$ is denoted by $ec(v) = \max\{u \in V(G)|d(u,v)\}$, then the sixth Zagreb index and the sixth Zagreb polynomial are formulated as

$$Zg_6(G) = \sum_{uv \in E(G)} ec(u)ec(v)$$

and

$$Zg_6(G, x) = \sum_{uv \in E(G)} x^{ec(u)ec(v)}.$$
respectively; the fourth Zagreb index and the fourth Zagreb polynomial are formulated as

$$Z_{g4}(G) = \sum_{uv \in E(G)} (ec(u) + ec(v))$$
and

\[ Zg_4(G, x) = \sum_{uv \in E(G)} x^{ec(u) + ec(v)}, \]

respectively. From this point of view, it is necessary to build the connection between two ontologies. It will help the researchers in theoretical chemistry and mathematical filed to search the related index and polynomial, and find their potential relationship.

The aim of this experiment is to yield the similarity based ontology mapping between ontologies \( O_5 \) and \( O_6 \) in terms of ontology learning algorithm raised in this paper. By virtue of ontology structure analysis, we set \( k = 3 \). Again, the \( P@N \) criterion is applied to study the equality of the experiment result. In order to compare the result data, ontology optimization learning frameworks introduced in Gao and Zhu [20], Wu et al. [49], and Gao et al. [18] are implemented on chemical index ontologies, and the precision ratios obtained from these ontology learning algorithms are manifested in Table 4.

<table>
<thead>
<tr>
<th></th>
<th>( P@1 ) average precision ratio</th>
<th>( P@3 ) average precision ratio</th>
<th>( P@5 ) average precision ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>PMDO Algorithm in our paper</td>
<td>0.4386</td>
<td>0.5263</td>
<td>0.7035</td>
</tr>
<tr>
<td>Algorithm in Gao and Zhu [20]</td>
<td>0.3247</td>
<td>0.4415</td>
<td>0.5667</td>
</tr>
<tr>
<td>Algorithm in Wu et al. [49]</td>
<td>0.4123</td>
<td>0.5058</td>
<td>0.6754</td>
</tr>
<tr>
<td>Algorithm in Gao et al. [18]</td>
<td>0.3947</td>
<td>0.4678</td>
<td>0.5807</td>
</tr>
</tbody>
</table>

Table 4. The experiment results of ontology mapping on chemical index ontologies

In terms of compared data depicted in Table 4, we ensure that our partial multi-dividing ontology algorithm is much more efficient than ontology learning tricks described in Gao and Zhu [20], Wu et al. [49] and Gao et al. [18] especially as \( N \) becoming large.

4.5. **Ontology similarity measuring experiment on energy data.** As matrix and Laplacian spectra parameters, energy related concepts have raised widely attention in physics and chemistry. These energy definitions reflect the atomic and physical-chemical properties of the molecular structure from atomic and microscopic aspects. For instance, the speed that an electron orbits is regarded as the electron energy which is considered as the effect of an electron energy, and it can be formulated as total \( \pi \)-electron energy \( E_\pi \).

In the beginning, the spectral-based energy indicators defined by physicists and chemists were based solely on the experience analysis of physical and chemical experiments. The mathematicians then introduced some new definitions
of energy in terms of modifying the originally defined formula from pure mathematical point of view. Unfortunately, these new energy concepts have only been described intuitively and there is no corresponding experimental objective basis. Although there is a corresponding description of their extreme values and corresponding extreme molecular graphs, there is no corresponding literature to explain whether these energy variables have actual effects on reality physical and chemical engineering. It is reasonable to suspect that many of the defined energy variables, their role in engineering and the original existence of a certain energy concept is repeated, or even no engineering significance. We call this kind of mathematically defined, non-engineering, practical indicator as a “redundant” indicator.

“Redundancy” indicators have increased the workload of engineers to a certain extent, and causing them to waste a lot of time on the useless energy indicators. Hence, “redundant” indicators played the destructive role in the real discipline, and hindered the development of the physical and chemical science. It inspires us to consider this problem and thus construct the energy ontology which contain the following 90 energy related indicators:

- 1) (ordinary) graph energy
- 2) extended adjacency energy
- 3) Laplacian energy
- 4) Laplacian-energy-like invariant
- 5) skew Laplacian energy
- 6) normalized Laplacian energy
- 7) signless Laplacian energy
- 8) additive color Laplacian energy
- 9) Hermitian-Randic energy
- 10) net-Laplacian energy
- 11) eccentric Laplacian energy
- 12) Laplacian minimum boundary dominating energy
- 13) Laplacian incidence energy
- 14) Laplacian distance energy
- 15) Laplacian minimum dominating energy
- 16) Laplacian minimum-covering energy
- 17) color Laplacian energy
- 18) signless Laplacian resolvent energy
- 19) Laplacian resolvent energy
- 20) color signless Laplacian energy
- 21) energy of matrix
- 22) energy of set of vert
- 23) resolvent energy
- 24) Nikiforov energy
- 25) $n$-energy
- 26) iota energy
- 27) Coxeter energy
28) partition energy
29) e-energy
30) Hermitian energy
31) Consonni-Todeschini energies
32) energy of (0,1)-matrix
33) He energy
34) o-energy
35) skew energy
36) so-energy
37) α-incidence energy
38) Randić energy
39) energy of orthogonal matrix
40) color energy
41) (two) reduced color energies
42) energy of polynomial
43) energy of matroid
44) second-stage energy
45) ultimate energy
46) matching energy
47) Kirchhoff energy
48) Seidel energy
49) domination energy
50) minimum dominating
51) minimum robust domination energy
52) minimum-domination energy
53) minimum-covering energy
54) minimum dominating distance energy
55) minimum dominating maximum degree energy
56) minimum boundary dominating energy
57) minimum equitable color dominating energy
58) double dominating energy
59) upper dominating energy
60) minimum-maximal-domination energy
61) complementary dominating energy
62) minimum monopoly energy
63) minimum-covering color energy
64) minimum covering Seidel energy
65) minimum hub energy
66) maximum-degree energy
67) incidence energy
68) oriented incidence energy
69) degree sum energy
70) general Randić energy
71) skew Randić energy
72) Randić incidence energy
We not only describe the semantic information of energy names as the components of the ontology concept vector, but also describe their matrix and the numerical computation of their formulas by means of numerical labelling processing trick and encapsulate them in the ontology vector corresponding to the ontology concept. The essential purpose of constructing this energy ontology is to help chemists and physicists to find redundant energy indices. Note that in the four previous experiments stated in our paper we only paid attention to the calculation of similarity from the perspective of computer algorithms and the specific applications in the field of chemical and physical engineering were not treated.

Since the whole 90 energy concepts can be divided into two subclasses (neighborhood-based energy and distance-based energy), we set $k = 2$. The experiment data are evaluated by $P@N$ criterion. To compare the obtained precision ratios, ontology learning technologies introduced in Gao et al. [21], [14], and [22] are implemented on energy ontology, and the results obtained from these ontology methods are presented in Table 5.
Clearly seen from Table 5, which shows the result data when $N = 3, 5, 10$ or 20, the precision ratio determined by adopting PMDO Algorithm, the newly proposed one, is higher than those from ontology learning algorithms in Gao et al. [21], [14], and [22]. To be specific, the ratios from PMDO Algorithm, the new one, are above 0.5 when $N$ bigger than 6 (approximately), which shows good accuracy and efficiency. In other words, it overshadows the previous ontology learning algorithms in Gao et al. [21], [14], and [22] in efficiency.

5. Conclusions

In recent years, since most ontology structure can be expressed as a tree or analogous to tree, multi-dividing ontology learning becomes a hot topic in ontology research in which all concepts are divided into $k$ parts corresponding to $k$ rates according to the branches of ontology tree, and the rank among these $k$ parts are determined by domain experts. There are several advances both in theoretical and engineering applications in multi-dividing ontology setting, and proved to be in high multidisciplinary special applications.

In our article, we present the partial ontology learning algorithm in multi-dividing setting for both ontology similarity computation and ontology mapping. Several theoretical results on this special learning setting are studied, and the optimal real-valued ontology score function is then yielded. Using this ontology function, each ontology vertex (corresponding to an ontology concept) is mapped into a real number, and the similarity between two vertices $v_i$ and $v_j$ is judged in view of $|f(v_i) - f(v_j)|$. Five experiments are designed to check the practicability and productiveness of our new ontology learning algorithm, and the compared results verify the efficiency of new multi-dividing ontology algorithm.

The biggest advantage of the proposed algorithm is that it maps the entire ontology graph to a one-dimensional real number axis, and replaces the abstract geometric distance calculation in the original abstract high-dimensional
space with the one-dimensional distance between real numbers (which are corresponding to concepts). This allows us to observe the interrelationships between the concepts of the whole ontology from the perspective of a one-dimensional line, which is more intuitive. Since the precondition of the algorithm is the dividing of the vertices in the ontology graph, it leads to the greatest weakness of the algorithm, that is, if the ontology graph is not a tree structure, i.e., a loop situation occurs, then the division of partial vertices can’t be directly determined by the graph structure, but requires the participation of domain experts. Therefore, the algorithm is limited effecting on the non-tree structure of the ontology graph. Since most of the ontology graph are tree structures, the proposed algorithm is still applicable to most of the ontology engineering applications.

Some authors recently focus on the online large scale learning on graphs and other data structures. We leave the ontology learning for ontology semantic similarity calculation and ontology mapping in online large-scale scenarios for our future consideration.

CONFLICT OF INTERESTS

The authors hereby declare that there is no conflict of interests regarding the publication of this paper.

ACKNOWLEDGMENT

We thank the reviewers for their constructive comments in improving the quality of this paper. This work has been partially supported by MINECO grant number MTM2014-51891-P and Fundación Séneca de la Región de Murcia grant number 19219/PI/14 and National Science Foundation of China grant number 11761083.

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1 School of Information Science and Technology, Yunnan Normal University, Kunming 650500, China—Corresponding Author—E-mail address: gaowei@ynnu.edu.cn

2 Departamento de Matemática Aplicada y Estadística. Universidad Politécnica de Cartagena, Hospital de Marina, 30203-Cartagena, Región de Murcia, Spain. E-mail address: juan.garcia@upct.es

3 Department of Mathematics, Karnatak University, Dharwad 580003, India

4 School of Computer Science and Engineer, Southeast University, Nanjing 210096, China