MIML: A Framework for Learning with Ambiguous Objects

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Abstract

In this paper, we propose the MIML (Multi-Instance Multi-Label learning) framework for learning with ambiguous objects, where an example is described by multiple instances and associated with multiple class labels. Comparing with traditional learning frameworks, the MIML framework is more convenient and natural for representing ambiguous objects. To learn MIML examples, we propose the MimlBoost and MimlSvm algorithms based on a simple degeneration strategy, and experiments show that solving problems involving ambiguous objects in the MIML framework can lead to good performances. Considering that the degeneration process may lose information, we propose the D-MimlSvm algorithm which tackles MIML problems directly in a regularization framework. Moreover, we show that even when we do not have access to the raw objects and thus cannot capture more information from raw objects by using the MIML representation, MIML is still useful. We propose the InsDif and SubCod algorithms. InsDif works by transforming single-instances into the MIML representation for learning, while SubCod works by transforming single-label examples into the MIML representation for learning. Experiments show that in some tasks they are able to achieve better performances than learning the single-instances or single-label examples directly.

Key words: MIML, Multi-Instance Multi-Label Learning, Multi-Label Learning, Multi-Instance Learning, Ambiguity

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1 Introduction

In traditional supervised learning, an object is represented by an instance, i.e., a feature vector, and associated with a class label. Formally, let $\mathcal{X}$ denote the instance space (or feature space) and $\mathcal{Y}$ the set of class labels. The task is to learn a function $f : \mathcal{X} \rightarrow \mathcal{Y}$ from a given data set $\{(x_1, y_1), (x_2, y_2), \ldots, (x_m, y_m)\}$, where $x_i \in \mathcal{X}$ is an instance and $y_i \in \mathcal{Y}$ is the known label of $x_i$. Although this formalization is prevailing and successful, there are many real-world problems which do not fit in this framework well. In particular, each object in this framework belongs to only one concept and therefore, the corresponding instance is associated with a single class label. However, many real-world objects are ambiguous, which may belong to multiple concepts simultaneously. For example, an image can belong to several classes simultaneously, e.g., grasslands, lions, Africa, etc.; a text document can be classified to several categories if it is viewed from different aspects, e.g., scientific novel, Jules Verne’s writing or even books on traveling; a web page can be recognized as news page, sports page, soccer page, etc. In a specific real task, maybe only one of the multiple concepts is the right semantic meaning. For example, in image retrieval when a user is interested in an image with lions, s/he may be only interested in the concept lions instead of the other concepts grasslands and Africa associated with that image. The difficulty here is caused by that those objects involve multiple concepts; we call such objects as ambiguous objects. To choose the right semantic meaning for such objects for a specific scenario is the fundamental difficulty of many tasks. In contrast to starting from a large universe of all possible concepts involved in the task, it may be helpful to get the subset of concepts associated with the concerned object at first, and then make a choice in the small subset later. However, getting the subset of concepts, that is, assigning proper class labels to such objects, is still a challenging task.

We notice that as an alternative to representing an object by a single instance, in many cases it is possible to represent an ambiguous object using a set of instances. For example, multiple patches can be extracted from an image where each patch is described by an instance, and thus the image can be represented by a set of instances; multiple sections can be extracted from a document where each section is described by an instance, and thus the document can be represented by a set of instances; multiple links can be extracted from a web page where each link is
described by an instance, and thus the web page can be represented by a set of instances. Using multiple instances to represent those ambiguous objects may be helpful because some inherent patterns which are closely related to some labels may become explicit and clearer. In this paper, we propose the MIML (Multi-Instance Multi-Label learning) framework for learning with ambiguous objects, where an example is described by multiple instances and associated with multiple class labels.

Comparing with traditional learning frameworks, the MIML framework is more convenient and natural for representing ambiguous objects. To exploit the advantages of the MIML representation, new learning algorithms are needed. We propose the MimlBoost algorithm and the MimlSvm algorithm based on a simple degeneration strategy, and experiments show that solving problems involving ambiguous objects under the MIML framework can lead to good performance. Considering that the degeneration process may lose information, we also propose the D-MimlSvm (i.e., Direct MimlSvm) algorithm which tackles MIML problems directly in a regularization framework. Experiments show that this “direct” algorithm outperforms the “indirect” MimlSvm algorithm.

In some practical tasks we do not have access to the raw objects (i.e., the real objects themselves such as the real images and the real web pages; a raw object may be ambiguous or unambiguous, depending on that whether the raw object has multiple class labels or not; traditionally, a raw object is represented by an instance after feature extraction), and instead, we are given observational data where each ambiguous object has already been represented by a single instance. Thus, in such cases we cannot capture more information from the raw objects using the MIML representation. Even in this situation, however, MIML is still useful. We propose the InsDif (i.e., INStance DIFferentiation) algorithm which transforms single-instances into MIML examples to learn. This algorithm is able to achieve a better performance than learning the single-instances directly in some tasks. This is not strange because for an object associated with multiple class labels, if it is described by only a single instance, the information corresponding to these labels are mixed and thus difficult to learn; if we can transform the single-instance into a set of instances in some proper ways, the mixed information might be detached to some extent and thus less difficult to learn.
MIML can also be helpful for learning single-label objects. We propose the SubCod (i.e., SUB-COncept Discovery) algorithm which works by discovering sub-concepts of the target concept at first and then transforming the data into MIML examples to learn. This algorithm is able to achieve a better performance than learning the single-label examples directly in some tasks. This is also not strange because for a label corresponding to a high-level complicated concept, it may be quite difficult to learn this concept directly since many different lower-level concepts are mixed; if we can transform the single-label into a set of labels corresponding to some sub-concepts, which are relatively clearer and easier to learn, we can learn these labels at first and then derive the high-level complicated label based on them with a less difficulty.

The rest of this paper is organized as follows. In Section 2, we review some related works. In Section 3, we propose the MIML framework. Then, in Section 4 we propose the MimlBoost and MimlSvm algorithms, and apply them to tasks where the objects are represented as MIML examples. In Section 5 we present the D-MimlSvm algorithm and compare it with the “indirect” MimlSvm algorithm. In Sections 6 and 7, we study the usefulness of MIML when we do not have access to raw objects. Concretely, in Section 6, we propose the InsDif algorithm and show that using MIML can be better than learning single-instances directly; in Section 7 we propose the SubCod algorithm and show that using MIML can be better than learning single-label examples directly. Finally, we conclude the paper in Section 8.

2 Related Work

Much work has been devoted to the learning of multi-label examples under the umbrella of multi-label learning. Note that multi-label learning studies the problem where a real-world object described by one instance is associated with a number of class labels, which is different from multi-class learning or multi-task learning [28]. In multi-class learning each object is only associated with a single label; while in

1 Most work on multi-label learning assume that an instance can be associated with multiple valid labels, but there are also some work assuming that only one of the labels among those associated with an instance is correct [34].
multi-task learning different tasks may involve different domains and different data sets. Actually, traditional two-class and multi-class problems can both be cast into multi-label problems by restricting that each instance has only one label. The generality of multi-label problems, however, inevitably makes it more difficult to address.

One famous approach to solving multi-label problems is Schapire and Singer’s AdaBoost.MH [55], which is an extension of AdaBoost and is the core of a successful multi-label learning system BoosTexter [55]. This approach maintains a set of weights over both training examples and their labels in the training phase, where training examples and their corresponding labels that are hard (easy) to predict get incrementally higher (lower) weights. Later, De Comité et al. [22] used alternating decision trees [29] which are more powerful than decision stumps used in BoosTexter to handle multi-label data and thus obtained the AdtBoost.MH algorithm. Probabilistic generative models have been found useful in multi-label learning. McCallum [46] proposed a Bayesian approach for multi-label document classification, where a mixture probabilistic model (one mixture component per category) is assumed to generate each document and EM algorithm is employed to learn the mixture weights and the word distributions in each mixture component. Ueda and Saito [65] presented another generative approach, which assumes that the multi-label text has a mixture of characteristic words appearing in single-label text belonging to each of the multi-labels. It is noteworthy that the generative models used in [46] and [65] are both based on learning text frequencies in documents, and are thus specific to text applications.

Many other multi-label learning algorithms have been developed, such as decision trees, neural networks, k-nearest neighbor classifiers, support vector machines, etc. Clare and King [21] developed a multi-label version of C4.5 decision tree through modifying the definition of entropy. Zhang and Zhou [79] presented multi-label neural network Bp-Mll, which is derived from the Backpropagation algorithm by employing an error function to capture the fact that the labels belonging to an instance should be ranked higher than those not belonging to that instance. Zhang and Zhou [80] also proposed the Ml-knn algorithm, which identifies the k nearest neighbors of the concerned instance and then assigns labels according to the maximum a posteriori principle. Elisseeff and Weston [27] proposed the RankSvm
algorithm for multi-label learning by defining a specific cost function and the corresponding margin for multi-label models. Other kinds of multi-label SVMs have been developed by Boutell et al. [11] and Godbole and Sarawagi [32]. In particular, by hierarchically approximating the Bayes optimal classifier for the H-loss, Cesa-Bianchi et al. [15] proposed an algorithm which outperforms simple hierarchical SVMs. Recently, non-negative matrix factorization has also been applied to multi-label learning [42], and multi-label dimensionality reduction methods have been developed [74, 85].

Roughly speaking, earlier approaches to multi-label learning attempt to divide multi-label learning to a number of two-class classification problems [35, 72] or transform it into a label ranking problem [27, 55], while some later approaches try to exploit the correlation between the labels [42, 65, 85].

Majority studies on multi-label learning focus on text categorization [22, 32, 38, 46, 55, 65, 74], and several studies aim to improve the performance of text categorization systems by exploiting additional information given by the hierarchical structure of classes [14, 15, 52] or unlabeled data [42]. In addition to text categorization, multi-label learning has also been found useful in many other tasks such as scene classification [11], image and video annotation [37, 47], bioinformatics [7, 12, 13, 21, 27], and even association rule mining [49, 63].

There is a lot of research on Multi-instance learning, which studies the problem where a real-world object described by a number of instances is associated with a single class label. Here the training set is composed of many bags each containing multiple instances; a bag is labeled positively if it contains at least one positive instance and negatively otherwise. The goal is to label unseen bags correctly. Note that although the training bags are labeled, the labels of their instances are unknown. This learning framework was formalized by Dietterich et al. [24] when they were investigating drug activity prediction.

Long and Tan [43] studied the PAC-learnability of multi-instance learning and showed that if the instances in the bags are independently drawn from product distribution, the APR (Axis-Parallel Rectangle) proposed by Dietterich et al. [24] is PAC-learnable. Auer et al. [5] showed that if the instances in the bags are not independent then APR learning under the multi-instance learning framework is
NP-hard. Moreover, they presented a theoretical algorithm that does not require product distribution, which was transformed into a practical algorithm named MULTINST [4]. Blum and Kalai [10] described a reduction from PAC-learning under the multi-instance learning framework to PAC-learning with one-sided random classification noise. They also presented an algorithm with smaller sample complexity than that of the algorithm of Auer et al. [5].

Many multi-instance learning algorithms have been developed during the past decade. To name a few, DIVERSE DENSITY [44] and EM-DD [83], $k$-nearest neighbor algorithms CITATION-$k$nn and BAYESIAN-$k$nn [67], decision tree algorithms RELIC [53] and MITI [9], neural network algorithms BP-MIP and extensions [77,90] and RBF-MIP [78], rule learning algorithm RIPPER-MI [20], support vector machines and kernel methods MI-SVM and MI-SVM [3], DD-SVM [18], MissSvm [88], MI-Kernel [31], BAG-INSTANCE KERNEL [19], MARGINALIZED MI-KERNEL [41] and convex-hull method CH-FD [30], ensemble algorithms MI-ENSEMBLE [91], MI-BOOSTING [70] and MILBOOSTING [6], logistic regression algorithm MI-LR [50], etc. Actually almost all popular machine learning algorithms have got their multi-instance versions. Most algorithms attempt to adapt single-instance supervised learning algorithms to the multi-instance representation, through shifting their focuses from the discrimination on the instances to the discrimination on the bags [91]. Recently there is some proposal on adapting the multi-instance representation to single-instance algorithms by representation transformation [93].

It is worth mentioning that the standard multi-instance learning [24] assumes that if a bag contains a positive instance then the bag is positive; this implies that there exists a key instance in a positive bag. Many algorithms were designed based on this assumption. For example, the point with maximal diverse density identified by the DIVERSE DENSITY algorithm [44] actually corresponds to a key instance; many SVM algorithms defined the margin of a positive bag by the margin of its most positive instance [3, 19]. As the research of multi-instance learning goes on, however, some other assumptions have been introduced. For example, in contrast to assuming that there is a key instance, some work assumed that there is no key instance and every instance contributes to the bag label [17, 70]. There is also an argument that the instances in the bags should not be treated independently [88]. All those assumptions have been put under the umbrella of multi-instance learning,
and generally, in tackling real tasks it is difficult to know which assumption is the fittest. In other words, in different tasks multi-instance learning algorithms based on different assumptions may have different superiorities.

In the early years of the research of multi-instance learning, most work was on multi-instance classification with discrete-valued outputs. Later, multi-instance regression with real-valued outputs was studied [2, 51], and different versions of generalized multi-instance learning have been defined [57, 68]. The main difference between standard multi-instance learning and generalized multi-instance learning is that in standard multi-instance learning there is a single concept, and a bag is positive if it has an instance satisfying this concept; while in generalized multi-instance learning [57, 68] there are multiple concepts, and a bag is positive only when all concepts are satisfied (i.e., the bag contains instances from every concept). Recently, research on multi-instance clustering [82], multi-instance semi-supervised learning [48] and multi-instance active learning [59] have also been reported.

Multi-instance learning has also attracted the attention of the ILP community. It has been suggested that multi-instance problems could be regarded as a bias on inductive logic programming, and the multi-instance paradigm could be the key between the propositional and relational representations, being more expressive than the former, and much easier to learn than the latter [23]. Alphonse and Matwin [1] approximated a relational learning problem by a multi-instance problem, fed the resulting data to feature selection techniques adapted from propositional representations, and then transformed the filtered data back to relational representation for a relational learner. Thus, the expressive power of relational representation and the ease of feature selection on propositional representation are gracefully combined. This work confirms that multi-instance learning can really act as a bridge between propositional and relational learning.

Multi-instance learning techniques have already been applied to diverse applications including image categorization [17, 18], image retrieval [71, 84], text categorization [3, 59], web mining [86], spam detection [36], computer security [53], face detection [66, 76], computer-aided medical diagnosis [30], etc.
3 The MIML Framework

Let $\mathcal{X}$ denote the instance space and $\mathcal{Y}$ the set of class labels. Then, formally, the MIML task is defined as:

- **MIML** (multi-instance multi-label learning): To learn a function $f : 2^{\mathcal{X}} \to 2^{\mathcal{Y}}$ from a given data set $\{(X_1, Y_1), (X_2, Y_2), \cdots, (X_m, Y_m)\}$, where $X_i \subseteq \mathcal{X}$ is a set of instances $\{x_{i1}, x_{i2}, \cdots, x_{ini}\}$, $x_{ij} \in \mathcal{X}$ ($j = 1, 2, \cdots, n_i$), and $Y_i \subseteq \mathcal{Y}$ is a set of labels $\{y_{i1}, y_{i2}, \cdots, y_{ili}\}$, $y_{ik} \in \mathcal{Y}$ ($k = 1, 2, \cdots, l_i$). Here $n_i$ denotes the number of instances in $X_i$ and $l_i$ the number of labels in $Y_i$.

Note that a basic assumption of MIML is that the labels (or some of the labels) have some correlation. This is a common phenomenon for objects with multiple labels. For example, for an image with labels *grasslands*, *lions* and *Africa*, it is evident that these labels have correlation. Moreover, the way in which the instances trigger different labels may be different. Some label may be triggered by a key instance, some may be triggered by all instances; more generally, labels can be triggered by a subset of instances. Just as the different assumptions on the relationship between instance-labels and bag-labels in multi-instance learning, in tackling different real tasks it is difficult to know which assumption is the fittest one, and algorithms can be designed based on different assumptions.

It is interesting to compare MIML with the existing frameworks of traditional supervised learning, multi-instance learning, and multi-label learning.

- **Traditional supervised learning** (single-instance single-label learning): To learn a function $f : \mathcal{X} \to \mathcal{Y}$ from a given data set $\{(x_1, y_1), (x_2, y_2), \cdots, (x_m, y_m)\}$, where $x_i \in \mathcal{X}$ is an instance and $y_i \in \mathcal{Y}$ is the known label of $x_i$.

- **Multi-instance learning** (multi-instance single-label learning): To learn a function $f : 2^{\mathcal{X}} \to \mathcal{Y}$ from a given data set $\{(X_1, y_1), (X_2, y_2), \cdots, (X_m, y_m)\}$, where $X_i \subseteq \mathcal{X}$ is a set of instances $\{x_{i1}, x_{i2}, \cdots, x_{ini}\}$, $x_{ij} \in \mathcal{X}$ ($j = 1, 2, \cdots, n_i$), and $y_i \in \mathcal{Y}$ is the label of $X_i$. $^2$ Here $n_i$ denotes the number of instances in $X_i$.

- **Multi-label learning** (single-instance multi-label learning): To learn a function $f : \mathcal{X} \to 2^{\mathcal{Y}}$ from a given data set $\{(x_1, Y_1), (x_2, Y_2), \cdots, (x_m, Y_m)\}$, where

$^2$ According to notions used in multi-instance learning, $(X_i, y_i)$ is a labeled bag while $X_i$ an unlabeled bag.
\( x_i \in \mathcal{X} \) is an instance and \( Y_i \subseteq \mathcal{Y} \) is a set of labels \( \{ y_{i1}, y_{i2}, \ldots, y_{il_i} \} \), \( y_{lk} \in \mathcal{Y} \) \((k = 1, 2, \ldots, l_i)\). Here \( l_i \) denotes the number of labels in \( Y_i \).

From Fig. 1 we can see the differences among these learning frameworks. In fact, the multi-learning frameworks are resulted from the ambiguities in representing real-world objects. Multi-instance learning studies the ambiguity in the input space (or instance space), where an object has many alternative input descriptions, i.e., instances; multi-label learning studies the ambiguity in the output space (or label space), where an object has many alternative output descriptions, i.e., labels; while MIML considers the ambiguities in both the input and output spaces simultaneously. In solving real-world problems, having a good representation is often more important than having a strong learning algorithm, because a good representation may capture more meaningful information and make the learning task easier to tackle. Since many real objects are inherited with input ambiguity as well as output ambiguity, MIML is more natural and convenient for tasks involving such objects.

It is worth mentioning that MIML is more reasonable than (single-instance) multi-label learning. Fig. 2(a) shows a multi-label object which is described by one instance but associated with \( l \) number of class labels. The underlying task is to
Fig. 2. Comparing MIML with multi-label learning. In addition to the difference between one-to-many mapping and many-to-many mapping, MIML also offers a possibility for understanding the relationship between instances and labels, e.g., as shown by the red curves, label$_1$ is caused by instance$_n$, label$_l$ is caused by instance$_i$, while label$_j$ is caused by the co-occurrence of instance$_1$ and instance$_i$.

learn an one-to-many mapping, yet one-to-many mappings are not proper mathematical functions. It seems feasible to regard every possible combination of the multiple labels as a “meta-label”, and then the task becomes to learning an one-to-one mapping between the instances and meta-labels. Such a process, however, will suffer seriously from the fact that the number of meta-labels is in exponential to the number of labels. There may be insufficient amount of training examples for learning some meta-labels; more seriously, meta-labels corresponding to label combinations which have not appeared in the training set will have none training example. Another possibility is to decompose the multi-label learning task into a series of two-class problems by treating the labels independently; this has actually been adopted by some multi-label learning algorithms as mentioned in Section 2. Such a process, however, suffers from the neglect of correlations among the labels. Note that in multi-label tasks the labels associated with the same instances are usually with informative correlations which can be leveraged for a better performance. In particular, when there are a large number of labels and small amount of training examples, the correlation information will be important to complement the lack of training data and should not be neglected. Overall, the one-to-many mapping might be the major difficulty in dealing with ambiguous objects. If we represent the multi-label object using a set of instances, however, as Fig. 2(b) illustrates, the underlying task becomes to learn a many-to-many mapping which is realizable by mathematical functions. So, transforming multi-label examples to MIML examples for learning may be beneficial in some tasks, which will be shown
Africa is a complicated high-level concept.

The concept Africa may become easier to learn through exploiting some sub-concepts.

Fig. 3. MIML can be helpful in learning single-label examples involving complicated high-level concepts.

Moreover, note that in some cases, understanding why a concerned object has a certain class label is even more important than simply making an accurate prediction, while MIML offers a possibility for this purpose. For example, the object in Fig. 2(b) has label $l_1$ because it contains instance $n$; it has label $l_t$ because it contains instance $i$; while the occurrence of both instance $i_1$ and instance $i_t$ triggers label $j$.

MIML can also be helpful for learning single-label examples involving complicated high-level concepts. For example, as Fig. 3(a) shows, the concept Africa has a
broad connotation and the images belonging to Africa have great variance, thus it is not easy to classify the top-left image in Fig. 3(a) into the Africa class correctly. However, if we can exploit some low-level sub-concepts that are less ambiguous and easier to learn, such as tree, lions, elephant and grassland shown in Fig. 3(b), it is possible to induce the concept Africa much easier than learning the concept Africa directly. The usefulness of MIML in this process will be shown in Section 7.

4 Solving MIML Problems by Degeneration

It is evident that traditional supervised learning is a degenerated version of multi-instance learning as well as a degenerated version of multi-label learning, while traditional supervised learning, multi-instance learning and multi-label learning are all degenerated versions of MIML. So, a simple idea to tackle MIML is to identify its equivalence in the traditional supervised learning framework, using multi-instance learning or multi-label learning as the bridge, as shown in Fig. 4.

• **Solution A**: Using multi-instance learning as the bridge:

  The MIML learning task, i.e., to learn a function \( f : 2^X \rightarrow 2^Y \), can be transformed into a multi-instance learning task, i.e., to learn a function \( f_{MIL} : 2^X \times Y \rightarrow \{-1,+1\} \). For any \( y \in Y \), \( f_{MIL}(X_i,y) = +1 \) if \( y \in Y_i \) and \(-1\) otherwise. The proper labels for a new example \( X^* \) can be determined according to \( Y^* = \{y | \text{sign}[f_{MIL}(X^*,y)] = +1\} \). This multi-instance learning task can be further transformed into a traditional supervised learning task, i.e., to learn a function \( f_{SISL} : X \times Y \rightarrow \{-1,+1\} \), under a constraint specifying how to derive \( f_{MIL}(X_i,y) \) from \( f_{SISL}(x_{ij},y) \) \((j = 1,2,\ldots,n_i)\). For any \( y \in Y \), \( f_{SISL}(x_{ij},y) = +1 \) if \( y \in Y_i \) and \(-1\) otherwise. Here the constraint can be
\[ f_{MIL}(X_i, y) = \text{sign} \left[ \sum_{j=1}^{n_i} f_{SISL}(x_{ij}, y) \right] \]
which has been used by Xu and Frank [70] in transforming multi-instance learning tasks into traditional supervised learning tasks. Note that other kinds of constraint can also be used here.

- **Solution B**: Using multi-label learning as the bridge:

  The MIML learning task, i.e., to learn a function \( f : 2^X \rightarrow 2^Y \), can be transformed into a multi-label learning task, i.e., to learn a function \( f_{MLL} : \mathcal{Z} \rightarrow 2^Y \).

  For any \( z_i \in \mathcal{Z} \), \( f_{MLL}(z_i) = f_{MIML}(X_i) \) if \( z_i = \phi(X_i), \phi : 2^X \rightarrow \mathcal{Z} \). The proper labels for a new example \( X^* \) can be determined according to \( Y^* = f_{MLL}(\phi(X^*)) \).

  This multi-label learning task can be further transformed into a traditional supervised learning task, i.e., to learn a function \( f_{SISL} : \mathcal{Z} \times Y \rightarrow \{-1, +1\} \). For any \( y \in \mathcal{Y} \), \( f_{SISL}(z_i, y) = +1 \) if \( y \in Y_i \) and \(-1\) otherwise. That is, \( f_{MLL}(z_i) = \{y | f_{SISL}(z_i, y) = +1\} \). Here the mapping \( \phi \) can be implemented with constructive clustering which was proposed by Zhou and Zhang [93] in transforming multi-instance bags into traditional single-instances. Note that other kinds of mappings can also be used here.

In the rest of this section we will propose two MIML algorithms, MimlBoost and MimlSvm. MimlBoost is an illustration of Solution A, which uses *category-wise decomposition* for the A1 step in Fig. 4 and MiBoosting for A2; MimlSvm is an illustration of Solution B, which uses *clustering-based representation transformation* for the B1 step and Mlsvm for B2. Other MIML algorithms can be developed by taking alternative options.

### 4.1 MimlBoost

Now we propose the MimlBoost algorithm according to the first solution mentioned above, that is, identifying the equivalence in the traditional supervised learning framework using multi-instance learning as the bridge. Note that this strategy can also be used to derive other kinds of MIML algorithms.

Given any set \( \Omega \), let \(|\Omega|\) denote its size, i.e., the number of elements in \( \Omega \); given any predicate \( \pi \), let \([\pi]\) be \(1\) if \( \pi \) holds and \(0\) otherwise; given \((X_i, Y_i)\), for any \( y \in \mathcal{Y} \), let \( \Psi(X_i, y) = +1 \) if \( y \in Y_i \) and \(-1\) otherwise, where \( \Psi \) is a function \( \Psi : 2^X \times \mathcal{Y} \rightarrow \{-1, +1\} \) which judges whether a label \( y \) is a proper label of \( X_i \) or
Table 1
The MIMLBoost algorithm

1 Transform each MIML example \((X_u, Y_u) \ (u = 1, 2, \cdots , m)\) into \(|\mathcal{Y}|\) number of multi-instance bags \(\{[(X_u, y_1), \Psi(X_u, y_1)], \cdots , [(X_u, y_{|\mathcal{Y}|}), \Psi(X_u, y_{|\mathcal{Y}|})]\}\). Thus, the original data set is transformed into a multi-instance data set containing \(m \times |\mathcal{Y}|\) number of multi-instance bags, denoted by \(\{[(X^{(i)}, y^{(i)}), \Psi(X^{(i)}, y^{(i)})] \ (i = 1, 2, \cdots , m \times |\mathcal{Y}|)\}.

2 Initialize weight of each bag to \(W^{(i)} = \frac{1}{m \times |\mathcal{Y}|} (i = 1, 2, \cdots , m \times |\mathcal{Y}|)\).

3 Repeat for \(t = 1, 2, \cdots , T\) iterations:

3a Assign the bag’s label \(\Psi(X^{(i)}, y^{(i)})\) to each of its instances \((x^{(i)}_j, y^{(i)}) \ (i = 1, 2, \cdots , m \times |\mathcal{Y}|; j = 1, 2, \cdots , n_i)\), set the weight of the \(j\)-th instance of the \(i\)-th bag \(W^{(i)} = W^{(i)}/n_i\), and build an instance-level predictor \(h_i[(x^{(i)}_j, y^{(i)})] \in \{-1, +1\}\).

3b For the \(i\)-th bag, compute the error rate \(e^{(i)} \in [0, 1]\) by counting the number of misclassified instances within the bag, i.e. \(e^{(i)} = \sum_{j=1}^{n_i} \frac{[h_i(x^{(i)}_j, y^{(i)})] \neq \Psi(x^{(i)}_j, y^{(i)})]}{n_i}\).

3c If \(e^{(i)} < 0.5\) for all \(i \in \{1, 2, \cdots , m \times |\mathcal{Y}|\}\), go to Step 4.

3d Compute \(c_t = \arg \min_{c_t} \sum_{i=1}^{m \times |\mathcal{Y}|} W^{(i)} \exp[(2e^{(i)} - 1)c_t]\).

3e If \(c_t \leq 0\), go to Step 4.

3f Set \(W^{(i)} = W^{(i)} \exp[(2e^{(i)} - 1)c_t] (i = 1, 2, \cdots , m \times |\mathcal{Y}|)\) and re-normalize such that \(0 \leq W^{(i)} \leq 1\) and \(\sum_{i=1}^{m \times |\mathcal{Y}|} W^{(i)} = 1\).

4 Return \(Y^* = \{y|\text{sign} \left( \sum_j \sum_{t} c_t h_i[(x^{(i)}_j, y)] \right) = +1\}\) \((x^{(i)}_j\) is \(X^*\)'s \(j\)th instance).

not. The pseudo-code of MIMLBoost is summarized in Table 1.

In the first step of MIMLBoost, each MIML example \((X_u, Y_u) \ (u = 1, 2, \cdots, m)\) is transformed into a set of \(|\mathcal{Y}|\) number of multi-instance bags, i.e., \(\{(X_u, y_1), \Psi(X_u, y_1)\}, [(X_u, y_2), \Psi(X_u, y_2)], \cdots , [(X_u, y_{|\mathcal{Y}|}), \Psi(X_u, y_{|\mathcal{Y}|})]\). Note that \(\{(X_u, y_v), \Psi(X_u, y_v)\} (v = 1, 2, \cdots , |\mathcal{Y}|)\) is a labeled multi-instance bag where \((X_u, y_v)\) is a bag containing \(n_u\) number of instances, i.e., \(\{(x_{u1}, y_v), (x_{u2}, y_v), \cdots , (x_{u, n_u}, y_v)\}\), and \(\Psi(X_u, y_v) \in \{-1, +1\}\) is the label of this bag.

Thus, the original MIML data set is transformed into a multi-instance data set containing \(m \times |\mathcal{Y}|\) number of bags. We order them as \(\{(X_1, y_1), \Psi(X_1, y_1)\}, \cdots , [(X_1, y_{|\mathcal{Y}|}), \Psi(X_1, y_{|\mathcal{Y}|})], [(X_2, y_1), \Psi(X_2, y_1)], \cdots , [(X_m, y_{|\mathcal{Y}|}), \Psi(X_m, y_{|\mathcal{Y}|})]\), and let
[(X(i), y(i)), Ψ(X(i), y(i))] denote the i-th of these m × |Y| number of bags which contains n_i number of instances.

Then, from the data set a multi-instance learning function f_{MIL} can be learned, which can accomplish the desired MIML function because f_{MIML}(X) = \{y | \text{sign} [f_{MIL}(X, y)] = +1\}. In this paper, the MiBOOTING algorithm [70] is used to implement f_{MIL}. Note that by using MiBOOTING, the MIMLBoost algorithm assumes that all instances in a bag contribute independently in an equal way to the label of that bag.

For convenience, let (B, g) denote the bag [(X, y), Ψ(X, y)], B ∈ B, g ∈ G, and E denotes the expectation. Then, here the goal is to learn a function F(B) minimizing the bag-level exponential loss \( E_B E_{g|B} [\exp(-g F(B))] \), which ultimately estimates the bag-level log-odds function \( \frac{1}{2} \log \frac{Pr(g=1|B)}{Pr(g=-1|B)} \) on the training set. In each boosting round, the aim is to expand F(B) into F(B) + cf(B), i.e., adding a new weak classifier, so that the exponential loss is minimized. Assuming that all instances in a bag contribute equally and independently to the bag’s label, f(B) = \( \frac{1}{n_B} \sum_j h(b_j) \) can be derived, where \( h(b_j) \in \{-1, +1\} \) is the prediction of the instance-level classifier h(·) for the jth instance of the bag B, and n_B is the number of instances in B.

It has been shown by [70] that the best f(B) to be added can be achieved by seeking h(·) which maximizes \( \sum_i \sum_{j=1}^{n_i} [\frac{1}{n_i} W^{(i)} g^{(i)} h(b_j^{(i)})] \), given the bag-level weights W = \( \exp(-g F(B)) \). By assigning each instance the label of its bag and the corresponding weight \( W^{(i)} / n_i \), h(·) can be learned by minimizing the weighted instance-level classification error. This actually corresponds to the Step 3a of MIMLBoost. When f(B) is found, the best multiplier c > 0 can be got by directly optimizing the exponential loss:

\[
E_B E_{g|B} [\exp(-g F(B) + c(-g f(B)))] = \sum_i W^{(i)} \exp \left[ c \left( -\frac{g^{(i)} \sum_j h(b_j^{(i)})}{n_i} \right) \right] \\
= \sum_i W^{(i)} \exp[(2e^{(i)} - 1)c],
\]

where \( e^{(i)} = \frac{1}{n_i} \sum_j [(h(b_j^{(i)}) \neq g^{(i)})] \) (computed in Step 3b). Minimization of this expectation actually corresponds to Step 3d, where numeric optimization techniques such as quasi-Newton method can be used. Note that in Step 3c if \( e^{(i)} \geq 0.5 \), the


Boosting process will stop [89]. Finally, the bag-level weights are updated in Step 3f according to the additive structure of $\mathcal{F}(B)$.

### 4.2 MimlSvm

Now we propose the MimlSvm algorithm according to the second solution mentioned before, that is, identifying the equivalence in the traditional supervised learning framework using multi-label learning as the bridge. Note that this strategy can also be used to derive other kinds of MIML algorithms.

Again, given any set $\Omega$, let $|\Omega|$ denote its size, i.e., the number of elements in $\Omega$; given $(X_i, Y_i)$ and $z_i = \phi(X_i)$ where $\phi : 2^X \rightarrow Z$, for any $y \in \mathcal{Y}$, let $\Phi(z_i, y) = +1$ if $y \in Y_i$ and $-1$ otherwise, where $\Phi$ is a function $\Phi : Z \times \mathcal{Y} \rightarrow \{-1, +1\}$. The pseudo-code of MimlSvm is summarized in Table 2. This algorithm assumes that the structure of the bags carries relevant information. It tries to identify representative training bags by clustering, and then represent all bags by the vector of their distances to the representatives.

In the first step of MimlSvm, the $X_u$ of each MIML example $(X_u, Y_u)$ ($u = 1, 2, \cdots, m$) is collected and put into a data set $\Gamma$. Then, in the second step, $k$-medoids clustering is performed on $\Gamma$. Since each data item in $\Gamma$, i.e. $X_u$, is an unlabeled multi-instance bag instead of a single instance, Hausdorff distance [26] is employed to measure the distance. The Hausdorff distance is a famous metric for measuring the distance between two bags of points, which has often been used in computer vision tasks; other techniques that can measure the distance between bags of points, such as the set kernel [31], can also be used here. In detail, given two bags $A = \{a_1, a_2, \cdots, a_n\}$ and $B = \{b_1, b_2, \cdots, b_n\}$, the Hausdorff distance between $A$ and $B$ is defined as

$$d_H(A, B) = \max\{\max_{a \in A} \min_{b \in B} \|a - b\|, \max_{b \in B} \min_{a \in A} \|b - a\|\},$$

where $\|a - b\|$ measures the distance between the instances $a$ and $b$, which takes the form of Euclidean distance here.

After the clustering process, the data set $\Gamma$ is divided into $k$ partitions, whose medoids are $M_t$ ($t = 1, 2, \cdots, k$), respectively. With the help of these medoids,
Table 2
The MIML-SVM algorithm

1. For MIML examples $(X_u, Y_u) (u = 1, 2, \cdots, m)$, $\Gamma = \{X_u | u = 1, 2, \cdots, m\}$.

2. Randomly select $k$ elements from $\Gamma$ to initialize the medoids $M_t$ ($t = 1, 2, \cdots, k$), repeat until all $M_t$ do not change:

   2a. $\Gamma_t = \{M_t\} (t = 1, 2, \cdots, k)$.

   2b. Repeat for each $X_u \in (\Gamma - \{M_t | t = 1, 2, \cdots, k\})$:

      2b1. $index = \arg \min_{t \in \{1, \cdots, k\}} d_H(X_u, M_t)$, $\Gamma_{index} = \Gamma_{index} \cup \{X_u\}$.

   2c. $M_t = \arg \min_{A \in \Gamma_t} \sum_{B \in \Gamma_t} d_H(A, B) (t = 1, 2, \cdots, k)$.

3. Transform $(X_u, Y_u)$ into a multi-label example $(z_u, Y_u) (u = 1, 2, \cdots, m)$, where

   $z_u = (z_{u1}, z_{u2}, \cdots, z_{uk}) = (d_H(X_u, M_1), d_H(X_u, M_2), \cdots, d_H(X_u, M_k))$.

4. For each $y \in \mathcal{Y}$, derive a data set $D_y = \{(z_u, \Phi(z_u, y)) | u = 1, 2, \cdots, m\}$, and then train an SVM $h_y = SVMTrain(D_y)$.

5. Return $Y^* = \{\arg \max_{y \in \mathcal{Y}} h_y(z^*)\} \cup \{y | h_y(z^*) \geq 0, y \in \mathcal{Y}\}$, where $z^* = (d_H(X^*, M_1), d_H(X^*, M_2), \cdots, d_H(X^*, M_k))$.

Then, from the data set a multi-label learning function $f_{MLL}$ can be learned, which can accomplish the desired MIML function because $f_{MIML}(X^*) = f_{MLL}(z^*)$. In this paper, the MLSVM algorithm [11] is used to implement $f_{MLL}$. Concretely, MLSVM decomposes the multi-label learning problem into multiple independent
binary classification problems (one per class), where each example associated with
the label set \( Y \) is regarded as a positive example when building SVM for any
class \( y \in Y \), while regarded as a negative example when building SVM for any
class \( y \notin Y \), as shown in the Step 4 of MIMLSVM. In making predictions, the \( T-
Criterion \) [11] is used, which actually corresponds to the Step 5 of the MIMLSVM
algorithm. That is, the test example is labeled by all the class labels with positive
SVM scores, except that when all the SVM scores are negative, the test example is
labeled by the class label which is with the \( top \) (least negative) score.

4.3 Experiments

4.3.1 Multi-Label Evaluation Criteria

In traditional supervised learning where each object has only one class label, \( accuracy \) is often used as the performance evaluation criterion. Typically, accuracy
is defined as the percentage of test examples that are correctly classified. When
learning with ambiguous objects associated with multiple labels simultaneously,
however, accuracy becomes less meaningful. For example, if approach \( A \) missed
one proper label while approach \( B \) missed four proper labels for a test example
having five labels, it is obvious that \( A \) is better than \( B \), but the accuracy of \( A \) and
\( B \) may be identical because both of them incorrectly classified the test example.

Five criteria are often used for evaluating the performance of learning with multi-
label examples [55,92]; they are \( hamming loss, one-error, coverage, ranking loss \) and
\( average precision \). Using the same denotation as that in Sections 3 and 4, given
a test set \( S = \{(X_1,Y_1),(X_2,Y_2),\cdots,(X_p,Y_p)\} \), these five criteria are defined as
below. Here, \( h(X_i) \) returns a set of proper labels of \( X_i \); \( h(X_i,y) \) returns a real-value
indicating the confidence for \( y \) to be a proper label of \( X_i \); \( rank^h(X_i,y) \) returns the
rank of \( y \) derived from \( h(X_i,y) \).

- \( hloss_S(h) = \frac{1}{p} \sum_{i=1}^{p} \frac{1}{|Y|} |h(X_i) \Delta Y_i| \), where \( \Delta \) stands for the symmetric difference
  between two sets. The \( hamming loss \) evaluates how many times an object-
  label pair is misclassified, i.e., a proper label is missed or a wrong label is pre-
  dicted. The performance is perfect when \( hloss_S(h) = 0 \); the smaller the value of
  \( hloss_S(h) \), the better the performance of \( h \).
• one-error\(_S(h) = \frac{1}{p} \sum_{i=1}^{p} \left\lfloor \arg \max_{y \in \mathcal{Y}} h(X_i, y) \right\rfloor \notin Y_i \right\rfloor. \) The one-error evaluates how many times the top-ranked label is not a proper label of the object. The performance is perfect when one-error\(_S(h) = 0; \) the smaller the value of one-error\(_S(h), \) the better the performance of \( h. \)

• coverage\(_S(h) = \frac{1}{p} \sum_{i=1}^{p} \max_{y \in Y_i} \text{rank}^h(X_i, y) - 1. \) The coverage evaluates how far it is needed, on the average, to go down the list of labels in order to cover all the proper labels of the object. It is loosely related to precision at the level of perfect recall. The smaller the value of coverage\(_S(h), \) the better the performance of \( h. \)

• rloss\(_S(h) = \frac{1}{p} \sum_{i=1}^{p} \frac{1}{|Y_i|} \frac{|\{(y_1, y_2) \mid h(X_i, y_1) \leq h(X_i, y_2), (y_1, y_2) \in Y_i \times \overline{Y}_i\}|}{|Y_i|}. \) The ranking loss evaluates the average fraction of label pairs that are misordered for the object. The performance is perfect when rloss\(_S(h) = 0; \) the smaller the value of rloss\(_S(h), \) the better the performance of \( h. \)

• avgprec\(_S(h) = \frac{1}{p} \sum_{i=1}^{p} \frac{1}{|Y_i|} \sum_{y \in Y_i} \frac{|\{y' \mid \text{rank}^h(X_i, y') \leq \text{rank}^h(X_i, y), y' \in Y_i\}|}{|Y_i|}. \) The average precision evaluates the average fraction of labels ranked above a particular label \( y \in Y_i. \) The performance is perfect when avgprec\(_S(h) = 1; \) the larger the value of avgprec\(_S(h), \) the better the performance of \( h. \)

In addition to the above criteria, we design two new multi-label criteria, average recall and average F1, as below.

• avgrecl\(_S(h) = \frac{1}{p} \sum_{i=1}^{p} \frac{1}{|Y_i|} \frac{|\{(y \mid \text{rank}^h(X_i, y) \leq \text{rank}^h(X_i, y), y \in Y_i\)}|}{|Y_i|}. \) The average recall evaluates the average fraction of proper labels that have been predicted. The performance is perfect when avgrecl\(_S(h) = 1; \) the larger the value of avgrecl\(_S(h), \) the better the performance of \( h. \)

• avgF1\(_S(h) = \frac{2 \times \text{avgprec}_S(h) \times \text{avgrecl}_S(h)}{\text{avgprec}_S(h) + \text{avgrecl}_S(h)}. \) The average F1 expresses a tradeoff between the average precision and the average recall. The performance is perfect when avgF1\(_S(h) = 1; \) the larger the value of avgF1\(_S(h), \) the better the performance of \( h. \)
Note that since the above seven criteria measure the performance from different aspects, usually one algorithm is difficult to outperform another algorithm on all these criteria.

4.3.2 Scene Classification

The scene classification data set consists of 2,000 natural scene images belonging to the classes desert, mountains, sea, sunset and trees. Over 22% images belong to multiple classes simultaneously. Each image has already been represented as a bag of nine instances generated by the Sbn method [45], which uses a Gaussian filter to smooth the image and then subsamples the image to an $8 \times 8$ matrix of color blobs where each blob is a $2 \times 2$ set of pixels within the matrix. An instance corresponds to the combination of a single blob with its four neighboring blobs (up, down, left, right), which is described with 15 features. The first three features represent the mean R, G, B values of the central blobs and the remaining twelve features express the differences in mean color values between the central blob and other four neighboring blobs respectively.

We evaluate the performances of the MIML algorithms MimlBoost and MimlSvm. Note that MimlBoost and MimlSvm are just proposed to illustrate the two general degeneration solutions to MIML problems shown in Fig. 4, and we do not claim that they are the best algorithms that can be developed through the degeneration paths. There may exist other processes for transforming MIML examples into multi-instance single-label (MISL) examples or single-instance multi-label (SIML) examples. Even by using the same degeneration process as that used in MimlBoost and MimlSvm, there are also many alternatives to realize the second step. For example, by using mi-Svm [3] to replace the MiBOOSTING used in MimlBoost, we get MimlSvm$_{mi}$ and it is also evaluated in our experiments.

We compare the MIML algorithms with several state-of-the-art algorithms for learning with multi-label examples, including AdtBoost.MH [22], RankSvm [27], MLSvm [11] and ML-knn [80]; these algorithms have been introduced briefly in Section 2. Note that these are single-instance algorithms that regard each image

\footnote{The data set is available at \url{http://cs.nju.edu.cn/zhouzh/zhouzh.files/publication/annex/miml-image-data.htm}}
Table 3
Results (mean±std.) on scene classification (‘↓’ indicates ‘the smaller the better’; ‘↑’ indicates ‘the larger the better’)
Figure 5. Performances of MIMLBoost and AdtBoost.MH at different rounds.

Fig. 6. Performances of MIMLSvm with different $k$ values.

criteria measure the learning performance from different aspects and one algorithm rarely outperforms another algorithm on all criteria. Both MIMLSvm and MIMLSvm$_{mi}$ are significantly better than RANKSvm on all the evaluation criteria. MIMLBoost is significantly better than RANKSvm on the first five criteria. Both MIMLBoost and MIMLSvm$_{mi}$ are significantly better than ML-knn on all criteria except hamming loss. MIMLSvm is significantly better than ML-knn on one-error, average precision, average recall and average F1, while there are ties on the other criteria. Moreover, note that the best performances on all evaluation criteria are always attained by MIML algorithms. Overall, comparison on the scene classification task shows that the MIML algorithms can be significantly better than the non-MIML algorithms; this validates the powerfulness of the MIML framework.
4.3.3 Text Categorization

The Reuters-21578 data set is used in the experiment. The seven most frequent categories are considered. After removing documents that do not have labels or main texts, and randomly removing some documents that have only one label, a data set containing 2,000 documents is obtained, where over 14.9% documents have multiple labels. Each document is represented as a bag of instances according to the method used in [3]. Briefly, the instances are obtained by splitting each document into passages using overlapping windows of maximal 50 words each. As a result, there are 2,000 bags and the number of instances in each bag varies from 2 to 26 (3.6 on average). The instances are represented based on term frequency. The words with high frequencies are considered, excluding “function words” that have been removed from the vocabulary using the SMART stop-list [54]. It has been found that based on term frequency, the dimensionality of the data set can be reduced to 1-10% without loss of effectiveness [73]. Thus, we use the top 2% frequent words, and therefore each instance is a 243-dimensional feature vector.

The compared algorithms are as same as those in Section 4.3.2. Linear kernels are used. The single-instance algorithms regard each document as a 243-dimensional feature vector which is obtained by aggregating all the instances in the same bag; this is equivalent to represent the document using a sole term frequency feature vector.

Here in the experiments, 1,500 documents are used as training examples while the remaining 500 documents are used for testing. Experiments are repeated for thirty runs by using random training/test partitions, and the average and standard deviation are summarized in Table 4, where the best performance on each criterion has been highlighted in boldface.

Pairwise $t$-tests with 95% significance level disclose that, impressively, both MIMLSvm and MIMLSvm$_{mi}$ are significantly better than all the non-MIML algorithms. MIMLBoost is significantly better than AdtBoost.MH on all criteria except that there is a tie on hamming loss; significantly better than RankSvm on all criteria; significantly better than MLSvm on average recall and there is a tie on average $F1$;

5 The data set is available at [http://cs.nju.edu.cn/zhouzh/zhouzh.files/publication/annex/miml-text-data.html](http://cs.nju.edu.cn/zhouzh/zhouzh.files/publication/annex/miml-text-data.html)
significantly better than ML-knn on one-error, coverage, ranking loss and average precision. Moreover, note that the best performances on all evaluation criteria are always attained by MIML algorithms. Overall, comparison on the text categorization task shows that the MIML algorithms are better than the non-MIML algorithms; this validates the powerfulness of the MIML framework.

5 Solving MIML Problems by Regularization

The degeneration methods presented in Section 4 may lose information during the degeneration process, and thus a “direct” MIML algorithm is desirable. In this section we propose a regularization method for MIML. This method considers the loss between the labels and the predictions on the bags as well as on the constituent instances. It also considers the relatedness between the labels associated to the same example. Moreover, considering that for any class label the number of positive examples is much fewer than that of negative examples, this method incorporates a mechanism to deal with class imbalance. We employ the constrained concave-convex procedure (CCCP) which has well-studied convergence properties [61] to solve the resultant non-linear optimization problem. We also present a cutting plane algorithm that finds the solution efficiently. In contrast to MIMLSvm, this method is developed from the regularization framework directly and so we call it D-MIMLSvm.
5.1 The Loss Function

Suppose \( f_t(X_i) \) can judge that whether the \( t \)-th element of \( Y \) is a proper label of \( X_i \) or not. By learning such a function for every element in \( Y \), i.e., by learning \( f = (f_1, f_2, \ldots, f_T) \), the proper labels of an unseen bag \( X^* \) can be determined. Here \( T \) is the number of labels in \( Y \). It is worth noting that each instance \( x_{ij} \) in a bag can be viewed as a bag \( \{x_{ij}\} \) containing only one instance, and so \( f(\{x_{ij}\}) \) is also a well-defined function for each instance \( x_{ij} \). For convenience, we write \( f(x_{ij}) \) for \( f(\{x_{ij}\}) \).

In order to learn \( f_t \), it is needed to consider the relationship between the bag \( X_i \) and its instances \( \{x_{i1}, x_{i2}, \ldots, x_{in_i}\} \). In multi-instance learning, it is usually assumed that the strength for \( X_i \) to hold a label is equal to the maximum strength for its instances to hold the label, i.e., \( f_t(X_i) = \max_{j=1, \ldots, n_i} f_t(x_{ij}) \). The above requirement, however, is usually too restrictive. One reason is that there are many cases where the label of the bag does not only rely on the instance with the maximum prediction, as discussed in Section 2; another reason is that, in classification only the sign of prediction is important [19], i.e., \( \text{sign}(f_t(X_i)) = \text{sign}(\max_{j=1, \ldots, n_i} f_t(x_{ij})) \). Thus, we introduce the general loss function \( V \) for MIML setting as shown in Eq. 3.

\[
V((X_i)_{i=1}^m, (Y_i)_{i=1}^m, f) = \frac{1}{mT} \sum_{i=1}^m \sum_{t=1}^T (1 - y_{it}f_t(X_i))_+ \\
+ \frac{\lambda}{mT} \sum_{i=1}^m \sum_{t=1}^T l \left( f_t(X_i), \max_{j=1, \ldots, n_i} f_t(x_{ij}) \right). \tag{3}
\]

The loss function \( V \) involves two parts balanced by \( \lambda \). The first part considers the loss between the bag \( X_i \)'s labels and its corresponding predictions \( f(X_i) \), such as the hinge loss \( (1 - y_{it}f_t(X_i))_+ \) where \((z)_+ = \max(0, z)\). The second part considers the loss between \( f(X_i) \) and the predictions of \( X_i \)'s constituent instances \( \{f(x_{ij})\} \), such as \( l \left( f_t(X_i), \max_{j=1, \ldots, n_i} f_t(x_{ij}) \right) \). Here \( l(v_1, v_2) \) can be defined in various ways, such as \( l_1 \) loss

\[
l(v_1, v_2) = |v_1 - v_2|. \tag{4}
\]
5.2 Representer Theorem for MIML

For simplicity, we assume that each function $f_t$ is a linear model, i.e., $f_t(x) = \langle w_t, \phi(x) \rangle$ where $\phi$ is the feature map induced by a kernel function $k$ and $\langle \cdot, \cdot \rangle$ denotes the standard inner product in the Reproducing Kernel Hilbert Space (RKHS) $\mathcal{H}$ induced by the kernel $k$. Remind that an instance can be regarded as a bag containing only one instance, the kernel $k$ can be any kernel defined on set of instances, such as the set kernel [31]. In the case of classification, objects (bags or instances) are classified according to the sign of $f_t$.

It is evident that the labels associated with a bag should have some relatedness; otherwise they should not be associated with the bag simultaneously. Inspired by [28], we assume that all the $w_t$’s come from a particular Gaussian distribution, with the mean denoted as $w_0$,

$$w_0 = \frac{1}{T} \sum_{t=1}^{T} w_t. \quad (5)$$

The original idea in [28] is to minimize $\sum_{i=1}^{T} ||w_i - w_0||^2$ and meanwhile minimize $||w_0||^2$, which is a bit complicated. Note that, according to Eq.5 we have

$$\sum_{t=1}^{T} ||w_t - w_0||^2 = \sum_{t=1}^{T} ||w_t||^2 - T||w_0||^2. \quad (6)$$

Therefore, minimizing $\sum_{i=1}^{T} ||w_i - w_0||^2$ and meanwhile minimizing $||w_0||^2$ can be simplified by minimizing $\sum_{t=1}^{T} ||w_t||^2$ and $||w_0||^2$ simultaneously.

Further note that $\sum_{t=1}^{T} ||w_t||^2 = \sum_{t=1}^{T} ||f_t||^2_{\mathcal{H}}$ and $||w_0||^2 = ||\frac{\sum_{t=1}^{T} f_t}{T}||^2_{\mathcal{H}}$, using Eq. 3 and $w_0$ in Eq. 5, we have the regularized framework for MIML in Eq. 7,

$$\min_{f \in \mathcal{H}} \frac{1}{T} \sum_{t=1}^{T} ||f_t||^2_{\mathcal{H}} + \mu ||\frac{\sum_{t=1}^{T} f_t}{T}||^2_{\mathcal{H}} + \gamma V (\{X_i\}_{i=1}^{m}, \{Y_i\}_{i=1}^{m}, f), \quad (7)$$

where $\gamma$ is a regularization parameter that balances the model complexity and the empirical risk, and $\mu$ is a parameter to trade off the discrepancy and commonness among the labels. Intuitively, when $\mu$ is large, the commonness among the labels is more important, and vice versa.

Given the above setup, we can prove the following representer theorem.
Theorem 1 The minimizer of the optimization problem Eq. 7 admits an expansion
\[ f_t(x) = \sum_{i=1}^{m} \left( \alpha_{t,i} k(x, X_i) + \sum_{j=1}^{n_i} \alpha_{t,ij} k(x, x_{ij}) \right) \]
where all \( \alpha_{t,i0}, \alpha_{t,ij} \in \mathcal{R} \).

Proof. Analogous to [28], we first introduce a combined feature map
\[ \Psi(x, t) = \begin{pmatrix} \phi(x) \sqrt{T}, 0, \ldots, 0, 0, \ldots, 0 \end{pmatrix} \]
and its decision function, i.e., \( \hat{f}(x, t) = \langle \hat{w}, \Psi(x, t) \rangle \) where
\[ \hat{w} = (\sqrt{r} w_0, w_1 - w_0, \ldots, w_T - w_0). \]
Here \( r = \mu T + T. \) Let \( \hat{k} \) denote the kernel function induced by \( \Psi \) and \( \mathcal{H} \) is its corresponding RKHS. We have Eqs. 8 and 9.
\[ \hat{f}(x, t) = \langle \hat{w}, \Psi(x, t) \rangle = \langle (w_0 + w_t - w_0), \phi(x) \rangle = \langle w_t, \phi(x) \rangle = f_t(x) \quad (8) \]
\[ \|\hat{f}\|_{\mathcal{H}}^2 = \|\hat{w}\|^2 = \sum_{i=1}^{T} ||w_t - w_0||^2 + r||w_0||^2 = \sum_{i=1}^{T} ||w_t||^2 + \mu T||w_0||^2 \quad (9) \]
Therefore, loss function in Eq.3 can be represented by \( \hat{V}(\{X_i\}_{i=1}^{m}, \{Y_i\}_{i=1}^{m}, \hat{f}) \), i.e.,
\[ \hat{V}(\{X_i\}_{i=1}^{m}, \{Y_i\}_{i=1}^{m}, \hat{f}) = \frac{1}{mT} \sum_{i=1}^{m} \sum_{t=1}^{T} \left( 1 - y_{it} \hat{f}((X_i, t)) \right) + \frac{\lambda}{mT} \sum_{i=1}^{m} \sum_{t=1}^{T} t \left( \hat{f}(X_i, t), \max_{j=1, \ldots, n_i} \hat{f}(x_{ij}, t) \right). \quad (10) \]
Thus, Eq. 7 is equivalent to
\[ \min_{\hat{f} \in \mathcal{H}} \frac{1}{T} \|\hat{f}\|_{\mathcal{H}}^2 + \gamma \hat{V}(\{X_i\}_{i=1}^{m}, \{Y_i\}_{i=1}^{m}, \hat{f}). \quad (11) \]
Note that \( \Omega(||\hat{f}\|_{\mathcal{H}}) = ||\hat{f}\|_{\mathcal{H}}^2 : [0, \infty) \rightarrow \mathcal{R} \) is a strictly monotonically increasing function. According to representer theorem (Theorem 4.2 in [56]), each minimizer \( \hat{f} \) of the functional risk in Eq. 11 admits a representation of the form
\[ \hat{f}(x, t) = \sum_{t=1}^{T} \sum_{i=1}^{m} \left( \beta_{t,i0} \hat{k}((X_i, t), (x, t)) + \sum_{j=1}^{n_i} \beta_{t,ij} \hat{k}((x_{ij}, t), (x, t)) \right), \quad (12) \]
where $\beta_{t,ij} \in \mathcal{R}$ and the corresponding weight vector $\hat{w}$ is represented as

$$\hat{w} = \sum_{t=1}^{T} \sum_{i=1}^{m} \left( \beta_{t,00} \Psi(X_i, t) + \sum_{j=1}^{n_i} \beta_{t,ij} \Psi(x_{ij}, t) \right).$$

(13)

Finally, with Eqs. 8 and 13, we have

$$f_t(x) = \langle w_t, \phi(x) \rangle = \langle w, \Psi(x, t) \rangle = \sum_{i=1}^{m} \left( \alpha_{t,00} k(x, X_i) + \sum_{j=1}^{n_i} \alpha_{t,ij} k(x, x_{ij}) \right)$$

(14)

where $\alpha_{t,ij} = \frac{1}{\sqrt{r}}(\sum_t \beta_{t,ij}) + \beta_{t,ij}/r$.

Note that $x$ in Eq. 14 can be regarded not only as a bag $X_i$ but also an instance $x_{ij}$. In other words, both $f_t(X_i)$ and $f_t(x_{ij})$ can be obtained by Eq. 14.

5.3 Optimization

Considering the use of $l_1$ loss for $l(v_1, v_2)$, Eq.7 can be re-written as

$$\min_{f \in \mathcal{H}, \xi, \delta} \frac{1}{T} \sum_{t=1}^{T} \|f_t\|^2_{\theta_t} + \mu \left\| \sum_{t=1}^{T} f_t \right\|^2_{\theta_t} + \gamma \frac{1}{mT} \xi' 1 + \gamma \frac{1}{mT} \delta' 1$$

s.t. $y_{it} f_t(X_i) \geq 1 - \xi_{it}$,

$$\xi \geq 0,$$

$$-\delta_{it} \leq f_t(X_i) - \max_{j=1,\ldots,n_i} f_t(x_{ij}) \leq \delta_{it}$$

(15)

where $\xi = [\xi_{11}, \xi_{12}, \ldots, \xi_{it}, \ldots, \xi_{mT}]'$ are slack variables for the errors on the training bags for each label, $\delta = [\delta_{11}, \delta_{12}, \ldots, \delta_{it}, \ldots, \delta_{mT}]'$, and $0$ and $1$ are all-zero and all-one vector, respectively.

Without loss of generality, assume that the bags and instances are ordered in the order $(X_1, \ldots, X_m, x_{11}, \ldots, x_{1,n_1}, \ldots, x_{m,1}, \ldots, x_{m,n_m})$. Thus, each object (bag or instance) in the training set can then be indexed by the following function $I$, i.e.,

$$\begin{cases} I(X_i) = i \\ I(x_{ij}) = m + \sum_{l=1}^{i-1} n_l + j \end{cases}$$
for \( j = 1, \cdots, n_i \) and \( i = 1, \cdots, m \). With this ordering, we can obtain the \((m + n) \times (m + n)\) kernel matrix \( K \) defined on all objects in the training set, where \( n = \sum_{i=1}^{m} n_i \). Denote the \( i \)-th column of \( K \) by \( k_i \). We have \( f_t(X_i) = k_{t(X_i)}^T \alpha_t + b_t \) and \( f_t(x_{ij}) = k_{t(x_{ij})}^T \alpha_t + b_t \). Here, the bias \( b_t \) for each label is included.

The weight vector corresponding to \( f_t \) can be re-written as \( w_t = \Phi \alpha_t \), where \( \Phi \) is the matrix with all the mapped bags and instances stacked as columns, thus \( \Phi^T \Phi = K \).

According to definition of \( f_t \) in Eq. 14, Eq. 15 can be cast as the optimization problem

\[
\begin{align*}
\min_{\alpha, \xi, \delta, b} & \quad \frac{1}{2T} \sum_{t=1}^{T} \alpha_t^T K \alpha_t + \frac{\mu}{T^2} 1^T A^T K A + \frac{\gamma}{mT} \xi^T 1 + \frac{\gamma\lambda}{mT} \delta^T 1 \\
\text{s.t.} & \quad y_{it}(k_{t(X_i)}^T \alpha_t + b_t) \geq 1 - \xi_{it}, \\
& \quad \xi \geq 0, \\
& \quad k_{t(x_{ij})}^T \alpha_t - \delta_{it} \leq k_{t(X_i)}^T \alpha_t, \\
& \quad k_{t(X_i)}^T \alpha_t - \max_{j=1, \cdots, n_i} k_{t(x_{ij})}^T \alpha_t \leq \delta_{it},
\end{align*}
\]

where \( A = [\alpha_1, \alpha_2, \cdots, \alpha_T] \) and \( b = [b_1, b_2, \cdots, b_T]^T \).

The above optimization problem is a non-convex optimization problem since the last constraint is non-convex. Note that this non-convex constraint is a difference between two convex functions, and thus the optimization problem can be solved by CCCP [19,61], which is one of the most standard techniques to solve such kind of non-convex optimization problems. CCCP is guaranteed to converge to a local minimal [75], and in many cases it can even converge to a global solution [25].

In particular, CCCP needs to solve a sequential convex quadratic problem. Suppose given the initial subgradient \( \sum_{j=1}^{n_i} \rho_{ij} k_{t(x_{ij})}^T \alpha_t \) of \( \max_{j=1, \cdots, n_i} k_{t(x_{ij})}^T \alpha_t \), then we solve the convex quadratic optimization problem

\[
\begin{align*}
\min_{\alpha, \xi, \delta, b} & \quad \frac{1}{2T} \sum_{t=1}^{T} \alpha_t^T K \alpha_t + \frac{\mu}{T^2} 1^T A^T K A + \frac{\gamma}{mT} \xi^T 1 + \frac{\gamma\lambda}{mT} \delta^T 1 \\
\text{s.t.} & \quad y_{it}(k_{t(X_i)}^T \alpha_t + b_t) \geq 1 - \xi_{it}, \\
& \quad \xi \geq 0, \\
& \quad k_{t(x_{ij})}^T \alpha_t - \delta_{it} \leq k_{t(X_i)}^T \alpha_t, \\
& \quad k_{t(X_i)}^T \alpha_t - \sum_{j=1}^{n_i} \rho_{ij} k_{t(x_{ij})}^T \alpha_t \leq \delta_{it},
\end{align*}
\]
In the next iteration, we update $\rho_{ijk}$ according to

$$\rho_{ijt} = \begin{cases} 
0, & \text{if } k' I(x_{ij}) \alpha_t \neq \max_{k=1,\ldots,n_i} (k' I(x_{ik}) \alpha_t), \\
1/n_d, & \text{otherwise},
\end{cases}$$

where $n_d$ is the number of active $x_{ij}$'s. It holds $\sum_{j=1}^{n_i} \rho_{ijt} = 1$ for any $t$'s. This procedure is guaranteed to converge to a local minimum.

5.4 Handling Class-Imbalance

The above solution may be improved further if we explicitly take into account the instance-level class-imbalance, that is, for any class label the number of positive instances is much fewer than the number of negative instances in MIML problems.

We can roughly estimate the imbalance rate, which is the ratio of the number of positive instances to that of negative instances, for each class label using the strategy adopted by [40]. In detail, for a specific label $y \in \mathcal{Y}$, we can divide the training bags $\{(X_1, Y_1), (X_2, Y_2), \ldots, (X_m, Y_m)\}$ into two subsets, $A_1 = \{(X_i, Y_i) | y \in Y_i\}$ and $A_2 = \{(X_i, Y_i) | y \notin Y_i\}$. It is obvious that all the instances in $A_2$ are negative to $y$. Then, for every $(X_i, Y_i)$ in $A_1$, assuming that the instances of different labels is roughly equally distributed, the number of positive instances of $y$ in $(X_i, Y_i)$ is roughly $n_i \times \frac{1}{|Y_i|}$ where $|Y_i|$ returns the number of labels in $Y_i$. Thus, the imbalance rate of $y$ is:

$$ibr(y) = \sum_{i=1}^{m} \frac{n_i}{|Y_i|} \times \frac{1}{\sum_{i=1}^{m} n_i} = \sum_{i=1}^{m} \frac{n_i}{n \times |Y_i|}.$$ 

There are many class-imbalance learning methods [69]. One of the most popular and effective methods is rescaling [87], which can be incorporated into our framework easily. In short, after obtaining the estimated imbalance rate for every class label, we can use these rates to modulate the loss caused by different misclassifications.

In detail, $\xi$ in Eq. 17 is directly related to the hinge loss $(1 - y_{it}f_t(X_i))_+$. According to the rescaling method [87], without loss of generality, we can rewrite the loss function into Eq. 18:

$$\left(\frac{y_{it} + 1}{2} - y_{it} \times ibr(y_{it})\right) (1 - y_{it}f_t(X_i)).$$

(18)
Let $\tau = [\tau_{11}, \tau_{12}, \ldots, \tau_{it}, \ldots, \tau_{mT}]$, where $\tau_{it} = \left(\frac{y_{it+1}}{2} - y_{it} \times \text{ibr}(y_{it})\right)$. Then, to minimize the loss defined in Eq. 18, Eq. 17 becomes Eq. 19. Here $\xi^T\tau$ indicates the weighted loss after considering the instance-level class-imbalance. It is evident that the problem in Eq. 19 is still a standard QP problem.

$$
\min_{A, \xi, \delta, b} \frac{1}{2T} \sum_{t=1}^{T} \alpha_t^T K \alpha_t + \frac{\mu}{T^2} 1^T A^T K A 1 + \frac{\gamma}{mT} \xi^T \tau + \frac{\gamma \lambda}{mT} \delta^T 1
$$

s.t. $y_{it}(k'_{I(X_i)} \alpha_t + b_t) \geq 1 - \xi_{it}$,
$\xi \geq 0$,
$k'_{I(x_{ij})} \alpha_t - \delta_{it} \leq k'_{I(X_i)} \alpha_t$,
$k'_{I(X_i)} \alpha_t - \sum_{j=1}^{n_i} \rho_{ij} k'_{I(x_{ij})} \alpha_t \leq \delta_{it}$.

5.5 Efficient Algorithm

Eq. 19 is a large-scale quadratic programming problem which involves lots of constraints and variables. To make it tractable and scalable, and on observing that most of the constraints in Eq. 19 are redundant, we present an efficient algorithm which constructs a nested sequence of tighter relaxations of the original problem using the cutting plane method [39].

Similar to its use with structured prediction [64], we add a constraint (or a cut) that is most violated by the current solution, and then find the solution in the updated feasible region. Such procedure will converge to an optimal (or $\varepsilon$-suboptimal) solution of the original problem. Moreover, Eq. 19 supports a natural problem decomposition since its constraint matrix is a block diagonal matrix, i.e., each block corresponds to one label.

The pseudo-code of the algorithm is shown in Table 5. We first initialize the working sets $S_i$'s as empty sets and the solutions as all zeros (Line 1). Then, instead of testing all the constraints, which is rather expensive when there are lots of constraints, we use the speedup heuristic as described in [60], i.e., we use $p$ constraints to approximate the whole constraints (Line 4). Smola and Schölkopf [60] have shown that when $p$ is larger than 59, the most violated constraint in $I$ is with probability 0.95 among the 5% most violated constraints among all constraints.

The Loss $i$ (Line 5) is calculated as $\max\{0, u'x - d\}$ where $u$ and $d$ are the linear
Table 5
Efficient Algorithm for Eq. 19

**Input:** \( K, \lambda, \mu, \gamma, \epsilon, \{X_i, Y_i\}_{i=1}^m \)

1. \( \forall t, S_t = \emptyset, v_t = (\alpha_t^T, \xi_{t1}, \cdots, \xi_{tm}, \delta_{t1}, \cdots, \delta_{tm}, b_t) = 0 \)
2. Repeat
   3. For \( t = 1, \cdots, T \)
   4. Pick \( p \) indexes of constraints that are not in \( S_t \) randomly, denoted by \( I \);
   5. Compute \( \text{Loss}_i \) for every constraint in \( I \);
   6. \% find out the cutting plane
   7. \( q = \arg\max_{i \in I} \text{Loss}_i \)
   8. If \( \text{Loss}_q > \epsilon \)
   9. \( S_t = S_t \cup \{q\} \);
10. \( v_t \leftarrow \text{optimized over } S_t \);
11. End If
12. End For
13. Until no \( S_t \) changes

coefficients and bias of the \( i \)-th linear constraint, respectively. If the maximal \( \text{Loss} \) is lower than the given stopping criteria \( \epsilon \) (we simply set \( \epsilon \) as \( 10^{-4} \) in our experiments), no update will be taken for the working set \( S_t \); otherwise the constraint with the maximal \( \text{Loss} \) will be added into \( S_t \) (lines 8 and 9). Once a new constraint is added, the solution will be re-computed with respect to \( S_t \) via solving a smaller quadratic program problem (line 10). The algorithm stops when there is no update for all \( S_t \)'s.

5.6 Experiments

In this section, we compare the two SVM algorithms for MIML, that is, the “direct" algorithm D-MimlSVM and the “indirect" algorithm MimlSVM, on the scene classification data set used in Section 4.3.2 and the text categorization data set used in Section 4.3.3.

To study the behavior of D-MimlSVM and MimlSVM under different amounts of multi-label data, we derive five data sets from the scene data. By randomly removing some single-label images, we obtain a data set where 30% (or 40%, or
50%) images belonging to multiple classes simultaneously; by randomly removing some multi-label images, we obtain a data set where 10% (or 20%) images belong to multiple classes simultaneously. A similar process is applied to the text data to derive five data sets. On the derived data sets we use 25% data for training and the remaining 75% data for testing, and experiments are repeated for thirty runs with random training/test partitions. The parameters of both MIMLSVM and D-MIMLSVM are set by hold-out tests on training sets. Since D-MIMLSVM needs to solve a large optimization problem, although we have incorporated advanced mechanisms such as cutting-plane algorithm, the current D-MIMLSVM can only deal with moderate size of training set.

The seven criteria introduced in Section 4.3.1 are used to evaluate the performance. The average and standard deviation are plotted in Figs. 7 and 8. Note that in the figures we plot $1$−average precision, $1$−average recall and $1$−average F1 such that in all the figures, the lower the curve, the better the performance.

From Figs. 7 and 8 we can find that the performance of D-MIMLSVM is apparently better than that of MIMLSVM. The results suggest that D-MIMLSVM is a good choice for learning with moderate number of MIML examples.
Fig. 8. Results on text categorization with different percentage of multi-label data. The lower the curve, the better the performance.

5.7 Discussion

The regularization framework presented in this section has an important assumption, that is, all the class labels share some commonness, i.e., the $w_0$ in Eq. 5. This assumption makes the regularization easier to realize, however, it over-simplifies the real scenario. In fact, in real applications it is rare that all class labels share some commonness; it is more typical that some class labels share some commonness, but the commonness shared by different labels may be different. For example, class label $y_1$ may share something with class label $y_2$, and $y_2$ may share something with $y_3$, but maybe $y_1$ shares nothing with $y_3$. So, a more reasonable assumption is that different pairs of labels share different things (or even nothing). By taking this assumption, a more powerful method may be developed.

Actually, it is not difficult to modify the framework of Eq. 7 by replacing the role of $w_0$ by $W$ whose element $W_{ij}$ expresses the relatedness between the $i$-th and $j$-th class labels, that is,

$$
\min \frac{1}{2T^2} \sum_{i,j} \| w_i - W_{ij} \|^2 + \frac{1}{T^2} \sum_{i,j} \mu_{ij} \| W_{ij} \|^2 + \gamma V .
$$

Note that $W$ is a tensor and $W_{ij}$ is a vector.
To minimize Eq. 20, taking derivative to \( W_{ij} \), we have

\[-(w_i - W_{ij}) - (w_j - W_{ji}) + 2\mu_{ij}W_{ij} + 2\mu_{ji}W_{ji} = 0.\]

Considering \( W_{ij} = W_{ji} \) and \( \mu_{ij} = \mu_{ji} \), we have

\[-(w_i - W_{ij}) - (w_j - W_{ij}) + 4\mu_{ij}W_{ij} = 0,\]

and so,

\[W_{ij} = \frac{w_i + w_j}{4\mu_{ji} + 2}. \tag{21}\]

Put Eq. 21 into Eq. 20, we have

\[
\min \frac{1}{2T^2} \sum_{i,j} \frac{1}{4\mu_{ij} + 2} \| w_i - w_j \|^2 + \frac{1}{T^2} \sum_{i,j} \mu_{ij} \left\| \frac{w_i + w_j}{4\mu_{ij} + 2} \right\|^2 + \gamma V. \tag{22}
\]

After simplification, Eq. 20 becomes

\[
\min \frac{1}{8T^2} \sum_{i,j} \left( \frac{16\mu_{ij}^2 + 10\mu_{ij} + 1}{(2\mu_{ij} + 1)^2} \| w_i \|^2 + \frac{2\mu_{ij} + 1}{(2\mu_{ij} + 1)^2} \| w_j \|^2 \right)
- \frac{1}{4T^2} \sum_{i,j} \frac{2\mu_{ij} + 1}{(2\mu_{ij} + 1)^2} (w_i, w_j) + \gamma V.
\]

So, the new optimization task becomes

\[
\min_{A,\ell,b} \frac{1}{8T^2} \sum_{i=1}^{T} \sum_{j=1}^{T} \left( \frac{16\mu_{ij}^2 + 10\mu_{ij} + 1}{(2\mu_{ij} + 1)^2} \alpha_i^\prime K \alpha_i + \frac{2\mu_{ij} + 1}{(2\mu_{ij} + 1)^2} \alpha_j^\prime K \alpha_j \right)
- \frac{1}{4T^2} \sum_{i=1}^{T} \sum_{j=1}^{T} \frac{2\mu_{ij} + 1}{(2\mu_{ij} + 1)^2} \alpha_i^\prime K \alpha_j + \frac{\gamma}{mT} \ell^\prime \ell + \frac{\gamma\lambda}{mT} \delta^\prime \delta
\]

\[\text{s.t. } y_{it}(k_{I(X_i)}^\prime \alpha_t + b_t) \geq 1 - \xi_{it},\]
\[\xi \geq 0,\]
\[k_{I(x_{ij})}^\prime \alpha_t - \delta_{it} \leq k_{I(X_i)}^\prime \alpha_t,\]
\[k_{I(X_i)}^\prime \alpha_t - \max_{j=1,\ldots,n_i} k_{I(x_{ij})}^\prime \alpha_t \leq \delta_{it}.\]

By solving Eq. 23 we can get not only a MIML learner, but also some understanding on the relatedness between pairs of labels from \( W_{ij} \), and some understanding on the different importance of the \( W_{ij} \)'s in determining the concerned class label from \( \mu_{ij} \)'s; this may be very helpful for understanding the ambiguous concepts underlying the task. Eq. 23, however, is difficult to solve since it involves too
many variables. Thus, how to exploit/understand the pairwise relatedness between different pairs of labels remains an open problem.

6 Solving Single-Instance Multi-Label Problems through MIML Transformation

The previous sections show that when we have access to the raw objects and are able to represent ambiguous objects as MIML examples, using the MIML framework is beneficial. However, in many practical tasks we are given observational data where each ambiguous object has already been represented by a single instance, and we do not have access to the raw objects. In such case, we cannot capture more information from the raw objects using the MIML representation. Even in this situation, however, MIML is still useful. Here we propose the InsDif (i.e., INStance DIFferentiation) algorithm which transforms single-instance multi-label examples into MIML examples to exploit the power of MIML.

6.1 InsDif

For an object associated with multiple class labels, if it is described by only a single instance, the information corresponding to these labels are mixed and thus difficult to learn; if we can transform the single-instance into a set of instances in some proper ways, the mixed information might be detached to some extent and thus less difficult to learn. This is the motivation of InsDif.

InsDif is a two-stage algorithm, which is based on instance differentiation. In the first stage, InsDif transforms each example into a bag of instances, by deriving one instance for each class label, in order to explicitly express the ambiguity of the example in the input space; in the second stage, an MIML learner is utilized to learn from the transformed data set. For the consistency with our previous description of the algorithm [85], in the current version of InsDif we use a two-level classification strategy, but note that other MIML algorithms such as D-MIML SVM can also be applied.

Using the same denotation as that in Sections 3 and 4, that is, given data set $S = \{(x_1, Y_1), (x_2, Y_2), \cdots, (x_m, Y_m)\}$, where $x_i \in \mathcal{X}$ is an instance and $Y_i \subseteq \mathcal{Y}$
a set of labels \( \{y_{i1}, y_{i2}, \ldots, y_{il} \} \), \( y_{ik} \in \mathcal{Y} \) \( (k = 1, 2, \ldots, l) \). Here \( l_i \) denotes the number of labels in \( Y_i \). For the ease of discussion, assume that the number of possible labels \( |\mathcal{Y}| = T \), and the dimensionality of \( \mathbf{x}_i \) \( (i = 1, 2, \ldots, m) \) is \( d \).

In the first stage, \textsc{InsDif} derives a prototype vector \( \mathbf{v}_l \) for each class label \( l \in \mathcal{Y} \) by averaging all the training instances belonging to \( l \), i.e.,

\[
\mathbf{v}_l = \frac{1}{|S_l|} \left( \sum_{x_i \in S_l} x_i \right),
\]

(24)

where

\[
S_l = \{x_i | \{x_i, Y_i\} \in S, l \in Y_i\}, l \in \mathcal{Y}.
\]

Here \( \mathbf{v}_l \) can be approximately regarded as a profile-style vector describing common characteristics of the class \( l \). Actually, this kind of prototype vectors have already shown their usefulness in solving text categorization problems. For example, the \textsc{Rocchio} method \cite{33, 58} forms a prototype vector for each class by averaging all the documents (represented by weight vectors) of this class, and then classifies the test document by calculating the dot-products between the weight vector representing the document and each of the prototype vectors. Here we use such kind of prototype vectors to facilitate bag generation. After obtaining the prototype vectors, each example \( \mathbf{x}_i \) is re-represented by a bag of instances \( B_i \), where each instance in \( B_i \) expresses the difference between \( \mathbf{x}_i \) and a prototype vector according to Eq. 25. In this way, each example is transformed into a bag whose size equals to the number of class labels.

\[
B_i = \{\mathbf{x}_i - \mathbf{v}_l | l \in \mathcal{Y}\}
\]

(25)

In fact, such a process attempts to exploit the spatial distribution since \( \mathbf{x}_i - \mathbf{v}_l \) in Eq. 25 is a kind of distance between \( \mathbf{x}_i \) and \( \mathbf{v}_l \). The transformation can also be realized in other ways. For example, other than referring to the prototype vector of each class, we can also go along with the following way. For each possible class \( l \), identify the \( k \)-nearest neighbors of \( \mathbf{x}_i \) among training instances that have \( l \) as a proper label. Then, the mean vector of these neighbors can be regarded as an instance in the bag. Note that the transformation of a single instance into a bag of instances can be realized as a general pre-processing method which can be plugged into many learning systems.
In the second stage, InsDif learns from the transformed training set $S^* = \{(B_1, Y_1), (B_2, Y_2), \ldots, (B_m, Y_m)\}$. This task is accomplished by the two-level classification structure shown in Fig. 9. Input to the structure is a bag $B$ consisting of $n$ instances $\{b_1, b_2, \ldots, b_n\}$, where each instance $b_i$ is a $d$-dimensional feature vector $[b_{i1}, b_{i2}, \ldots, b_{id}]^T$. Outputs of the structure consist of $T$ real values $\{y_1, y_2, \ldots, y_T\}$, where each output $y_l$ corresponds to a label $l \in \mathcal{Y}$. The first level is composed of $M$ bags $\{C_1, C_2, \ldots, C_M\}$, where each bag $C_j$ is the medoid of group $G_j$. Here $\{G_1, G_2, \ldots, G_M\}$ partition the transformed training set $S^*$ into disjoint groups of bags with $\bigcup_{j=1}^M G_j = \{B_1, B_2, \ldots, B_m\}$ and $G_i \cap_{i \neq j} G_j = \emptyset$. The second level weights $\mathbf{W} = [w_{jl}]_{j=1}^M_{l=1}^T$ connect each medoid $C_j$ in the first level to each output $y_l$.

By regarding each bag as an atomic object, we adapt the popular $k$-medoids algorithm to cluster $S^*$ into $M$ disjoint groups of bags. Here, we employ the Hausdorff distance [26] shown in Eq. 2 to measure the distance between bags. For categorical data, distance metric such as the Value Difference Metric ($\text{VDM}$) [62] can be used. After this process, $S^*$ is divided into $M$ partitions and the medoids $C_j$ ($j = 1, 2, \ldots, M$) are

$$C_j = \arg \min_{A \in G_j} \sum_{B \in G_j} d_H(A, B).$$

Since clustering can help to find the underlying structure of a data set, the medoid of each group may encode some distributional information of different bags. With the help of these medoids, each bag $B$ can be converted into an $M$-dimensional
feature vector \([\phi_1(B), \phi_2(B), \cdots, \phi_M(B)]^\top\) with \(\phi_j(B) = d_H(B, C_j)\). The second level weights \(W = [w_{jl}]_{M \times T}\) are optimized by minimizing the following sum-of-squares error function

\[
E = \frac{1}{2} \sum_{i=1}^{m} \sum_{l=1}^{T} (y_l(B_i) - d^i_l)^2,
\]

(27)

where \(y_l(B_i) = \sum_{j=1}^{M} w_{jl} \phi_j(B_i)\) is the actual output of the structure on \(B_i\) on the class \(l\); \(d^i_l\) is the desired output of \(B_i\) on the class \(l\), which takes the value of +1 if \(l \in Y_i\) and −1 otherwise. Differentiating the objective function in Eq. 27 with respect to \(w_{jl}\) and setting the derivative to zero gives the normal equations for the least-squares problem as

\[
(\Phi^\top \Phi) W = \Phi^\top T,
\]

(28)

where \(\Phi = [\phi_{ij}]_{m \times M}\) is with elements \(\phi_{ij} = \phi_j(B_i)\) and \(T = [t^i_l]_{m \times T}\) is with elements \(t^i_l = d^i_l\). Here we compute the second layer weights \(W\) by solving Eq. 28 using singular value decomposition.

The pseudo-code of InsDif is summarized in Table 6. In the first stage (Steps 1 to 2), InsDif transforms each example into a bag of instances by querying the class prototype vectors. In the second stage (Steps 3 to 5), the two-level classification structure is used to learn from the transformed data. Note that the two-level classification structure is actually a MIML learner, and any MIML algorithm can be used to realize the second stage of InsDif. Test example \(x^*\) is transformed into the corresponding bag representation \(B^*\) and then fed to the learned classification structure for prediction.

### 6.2 Experiments

We compare InsDif with several state-of-the-art multi-label learning algorithms, including AdtBoost.MH [22], RankSvm [27], MLSVM [11], ML-knn [80] and Cnmf [42]; these algorithms have been introduced briefly in Section 2.

Note that the experiments here are very different from that in Sections 4.3 and 5.6. In Sections 4.3 and 5.6, it is assumed that the data are MIML examples; while in this section, it is assumed that we are given observational data where each raw object has already been represented as a single instance. In other words, in
Table 6
The INSdif algorithm

1. For single-instance multi-label examples \((x_u, Y_u)\) \((u = 1, 2, \cdots, m)\), compute the prototype vectors \(v_l (l \in Y)\) using Eq. 24.

2. Derive the new training set \(S^*\) by transforming each \(x_i\) into a bag of instances \(B_i\) using Eq. 25.

3. Divide \(\{B_1, B_2, \cdots, B_m\}\) into \(M\) partitions using \(k\)-medoids algorithm employing Hausdorff distance.

4. Determine the medoids \(C_j (j = 1, 2, \cdots, M)\) using Eq. 26.

5. Compute the weights \(W\) by solving Eq. 28 using singular value decomposition.

6. Return \(Y^* = \{l | y_l(B^*) = \sum_{j=1}^{M} w_{jl} \phi_j(B^*) > 0, l \in Y\}\), where \(B^* = \{x^* - v_l | l \in Y\}\).

This section we are trying to learn from single-instance multi-label examples, and therefore the experimental data sets are different from those used in Sections 4.3 and 5.6.

6.2.1 Yeast Gene Functional Analysis

The task here is to predict the gene functional classes of the Yeast \textit{Saccharomyces cerevisiae}, which is one of the best studied organisms. Specifically, the Yeast data set investigated in [27,80] is studied. Each gene is represented by a 103-dimensional feature vector generated by concatenating a gene expression vector and the corresponding phylogenetic profile. Each 79-element gene expression vector reflects the expression levels of a particular gene under two different experimental conditions, while the phylogenetic profile is a Boolean string each bit indicating whether the concerned gene has a close homolog in the corresponding genome. Each gene is associated with a set of functional classes whose maximum size can be potentially more than 190. Elisseeff and Weston [27] have preprocessed the data set where only the known structure of the functional classes are used. Actually, the whole set of functional classes is structured into hierarchies up to 4 levels deep. The first level of the hierarchy is shown in Fig. 10. The resulting multi-label data set contains

\[^{6}\text{See http://mips.gsf.de/proj/yeast/catalogues/funct/ for more details.}\]
Fig. 10. The first level of the hierarchy of the Yeast gene functional classes. One gene, for instance the one named YAL062w, can belong to several classes (shaded in gray) of the fourteen possible classes.

2,417 genes, fourteen possible class labels and the average number of labels for each gene is $4.24 \pm 1.57$.

For InsDif, the parameter $M$ is set to be 20% of the size of training set; it can be found from Fig. 11 that the performance of InsDif is not sensitive to the setting of $M$. The number of boosting rounds of AdtBoost.MH is set to 50 according to Section 4.3.2. For RankSVM, MLSVM, ML-knn and Cnmf, the best performed parameters reported in [27], [11], [80] and [42] are used, respectively. The criteria introduced in Section 4.3.1 are used to evaluate the learning performance. Ten-fold cross-validation is conducted on this data set and the results are summarized in Table 7, where the best performance on each criterion has been highlighted in boldface.

Table 7 shows that InsDif performs quite well on all evaluation criteria. Pairwise $t$-tests with 95% significance level disclose that InsDif is significantly better than

---

7 Hamming loss, average recall and average F1 are not available for Cnmf; ranking loss, average recall and average F1 are not available for AdtBoost.MH.
Table 7
Results (mean±std.) on yeast gene data set (‘↓’ indicates ‘the smaller the better’; ‘↑’ indicates ‘the larger the better’)

| Compared Algorithms | Evaluation Criteria |
|---------------------|---------------------|
|                     | $hloss$ $↓$ | $one-error$ $↓$ | $coverage$ $↓$ | $rloss$ $↓$ | $aveprec$ $↑$ | $avgrecl$ $↑$ | $avgF1$ $↑$ |
| INSDiff             | .189±.010 | .214±.030 | 6.288±0.240 | .163±.017 | .774±.019 | .602±.026 | .677±.023 |
| ADTBoost.MH         | .207±.010 | .244±.035 | 6.390±0.203 | N/A | .744±.025 | N/A | N/A |
| RANKSVM             | .207±.013 | .243±.039 | 7.090±0.503 | .195±.021 | .749±.026 | .500±.047 | .600±.041 |
| ML-KNN              | .199±.009 | .227±.032 | 7.220±0.338 | .201±.019 | .749±.021 | .572±.023 | .649±.022 |
| Ml-Svm              | .194±.010 | .230±.030 | 6.275±0.240 | .167±.016 | .765±.021 | .574±.022 | .656±.021 |
| Cnmf                | N/A | .354±.184 | 7.930±1.089 | .268±.062 | .668±.093 | N/A | N/A |

Fig. 11. Performances of INSDiff with different $M$ settings.

all the compared algorithm on all criteria, except that on coverage it is worse than ML-kNN but the difference is not statistical significant. It is noteworthy that Cnmf performs quite poor compared to other algorithms although it has used test set information. The reason may be that the key assumption of Cnmf, i.e., two examples with high similarity in the input space tend to have large overlap in the output space, does not hold on this gene data since there are some genes whose functions are quite different but the physical appearances are similar.

Overall, results on the Yeast gene functional analysis task suggest that MIML can be useful when we are given observational data where each ambiguous object has already been represented by a single instance.
Table 8
Characteristics of the web page data sets (after term selection). **PMC** denotes the percentage of documents belonging to more than one category; **ANL** denotes the average number of labels for each document; **PRC** denotes the percentage of rare categories, i.e., the kind of category where only less than 1% instances in the data set belong to it.

| Data Set             | Number of Categories | Vocabulary Size | Training Set | Test Set |
|---------------------|----------------------|-----------------|--------------|----------|
|                     |                      | PMC            | ANL          | PRC      | PMC     | ANL     | PRC      |
| Arts&Humanities    | 26                   | 462            | 44.50%       | 1.627    | 19.23%  | 43.63%  | 1.642    | 19.23%  |
| Business&Economy   | 30                   | 438            | 42.20%       | 1.590    | 50.00%  | 41.93%  | 1.586    | 43.33%  |
| Computers&Internet | 33                   | 681            | 29.60%       | 1.487    | 39.39%  | 31.27%  | 1.522    | 36.36%  |
| Education           | 33                   | 550            | 33.50%       | 1.465    | 57.58%  | 33.73%  | 1.458    | 57.58%  |
| Entertainment       | 21                   | 640            | 29.30%       | 1.426    | 28.57%  | 28.20%  | 1.417    | 33.33%  |
| Health              | 32                   | 612            | 48.05%       | 1.467    | 53.13%  | 47.20%  | 1.459    | 53.13%  |
| Recreation&Sports   | 22                   | 606            | 30.20%       | 1.414    | 18.18%  | 31.20%  | 1.429    | 18.18%  |
| Reference           | 33                   | 793            | 13.75%       | 1.159    | 51.52%  | 14.60%  | 1.177    | 54.55%  |
| Science             | 40                   | 743            | 34.85%       | 1.489    | 35.00%  | 30.57%  | 1.425    | 40.00%  |
| Social&Science      | 39                   | 1047           | 20.95%       | 1.274    | 56.41%  | 22.83%  | 1.290    | 58.97%  |
| Society&Culture     | 27                   | 636            | 41.90%       | 1.705    | 25.93%  | 39.97%  | 1.684    | 22.22%  |

6.2.2 Web Page Categorization

The web page categorization task has been studied in [38, 65, 80]. The web pages were collected from the “yahoo.com” domain and then divided into 11 data sets based on Yahoo’s top-level categories. After that, each page is classified into a number of Yahoo’s second-level subcategories. Each data set contains 2,000 training documents and 3,000 test documents. The simple term selection method based on document frequency (the number of documents containing a specific term) was applied to each data set to reduce the dimensionality. Actually, only 2% words with the highest document frequency were retained in the final vocabulary. Other term selection methods such as information gain and mutual information can also be adopted. After term selection, each document in the data set is described as a feature vector using the “Bag-of-Words” representation, i.e., each feature expresses the number of times a vocabulary word appearing in the document.

Table 8 summarizes the characteristics of the web page data sets. Comparing with the Yeast data in Section 6.2.1, here the instances are represented by much higher...
dimensional feature vectors and a large portion of them (about 20% ~ 45%) are multi-labeled. Moreover, here the number of categories (21 ~ 40) are much larger and many of them are rare categories (about 20% ~ 55%). So, the web page data sets are more difficult than the Yeast data to learn.

In the experiments the parameter settings are similar as that in Section 6.2.1. Results of the eleven data sets are shown in Fig. 12, and the average results are summarized in Table 9 where the best performance on each criterion has been highlighted in boldface.
Table 9 shows that InsDif performs quite well on almost all evaluation criteria. Pairwise $t$-tests with 95% significance level disclose that InsDif is significantly better than all the compared algorithm on hamming loss, average precision and average $F1$; on ranking loss it is comparable to Ml-$k$NN, significantly better than all other algorithms; on average recall it is comparable to MlSvm, significantly better than all other algorithms; on one-error it is worse than MlSvm, but significantly better than all the other three algorithms; on coverage it is worse than AdtBoost.MH and Ml-$k$NN, but significantly better than the other three algorithms.

Overall, results on the web page categorization task suggest that MIML can be useful when we are given observational data where each ambiguous object has already been represented by a single instance.

7 Solving Multi-Instance Single-Label Problems through MIML Transformation

In many tasks we are given observational data where each object has already been represented as a multi-instance single-label example, and we do not have access to the raw objects. In such case, we cannot capture more information from the raw objects using the MIML representation. Even in this situation, however, MIML is still useful. Here we propose the SubCod (i.e., SUB-COncept Discovery) algorithm which transforms multi-instance single-label examples into MIML examples to exploit the power of MIML.
7.1 SubCod

For an object that has been described by multi-instances, if it is associated with a label corresponding to a high-level complicated concept such as Africa in Fig. 3(a), it may be quite difficult to learn this concept directly since many different lower-level concepts are mixed. If we can transform the single-label into a set of labels corresponding to some sub-concepts, which are relatively clearer and easier to learn, we can learn these labels at first and then derive the high-level complicated label based on them, as illustrated in Fig. 3(b). This is the motivation of SubCod.

SubCod is a two-stage algorithm, which is based on sub-concept discovery. In the first stage, SubCod transforms each single-label example into a multi-label example by discovering and exploiting sub-concepts involved by the original label; this is realized by constructing multiple labels through unsupervised clustering all instances and then treating each cluster as a set of instances of a separate sub-concept. In the second stage, the outputs learned from the transformed data set are used to derived the original labels that are to be predicted; this is realized by using a supervised learning algorithm to predict the original labels from the sub-concepts predicted by an MIML learner.

Using the same denotation as that in Sections 3 and 4, that is, given data set \( \{(X_1, y_1), (X_2, y_2), \ldots, (X_m, y_m)\} \), where \( X_i \subseteq \mathcal{X} \) is a set of instances \( \{x_{i1}, x_{i2}, \ldots, x_{in_i}\} \), \( x_{ij} \in \mathcal{X} \) (\( j = 1, 2, \ldots, n_i \)), and \( y_i \in \mathcal{Y} \) is the label of \( X_i \). Here \( n_i \) denotes the number of instances in \( X_i \).

In the first stage, SubCod collects all instances from all the bags to compose a data set \( D = \{x_{11}, \ldots, x_{1n_1}, x_{21}, \ldots, x_{2n_2}, \ldots, x_{m1}, \ldots, x_{m,n_m}\} \). For the ease of discussion, let \( N = \sum_{i=1}^{m} n_i \) and re-index the instances in \( D \) as \( \{x_1, x_2, \ldots, x_N\} \).

A Gaussian mixture model with \( M \) mixture components is to be learned from \( D \) by the EM algorithm, and the mixture components are regarded as sub-concepts. The parameters of the mixture components, i.e., the means \( \mu_k \), covariances \( \Sigma_k \) and mixing coefficients \( \pi_k \) (\( k = 1, 2, \ldots, M \)), are randomly initialized and the initial value of the log-likelihood is evaluated. In the E-step, the responsibilities
are measured according to
\[
\gamma_{ik} = \frac{\pi_k N(x_i | \mu_k, \Sigma_k)}{\sum_{j=1}^{M} \pi_j N(x_i | \mu_j, \Sigma_j)} \quad (i = 1, 2, \cdots, N).
\] (29)

In the M-step, the parameters are re-estimated according to
\[
\mu_{k}^{\text{new}} = \frac{\sum_{i=1}^{N} \gamma_{ik} x_i}{\sum_{i=1}^{N} \gamma_{ik}},
\] (30)
\[
\Sigma_{k}^{\text{new}} = \frac{\sum_{i=1}^{N} \gamma_{ik} (x_i - \mu_{k}^{\text{new}})(x_i - \mu_{k}^{\text{new}})^T}{\sum_{i=1}^{N} \gamma_{ik}},
\] (31)
\[
\pi_{k}^{\text{new}} = \frac{\sum_{i=1}^{N} \gamma_{ik}}{N},
\] (32)
and the log-likelihood is evaluated according to
\[
\ln p(D | \mu, \Sigma, \pi) = \sum_{i=1}^{N} \ln \left( \sum_{k=1}^{M} \pi_{k}^{\text{new}} N(x_i | \mu_{k}^{\text{new}}, \Sigma_{k}^{\text{new}}) \right).
\] (33)

After the convergence of the EM process (or after a pre-specified number of iterations), we can estimate the associated sub-concept for every instance \(x_i \in D \) (\(i = 1, 2, \cdots, N\)) by
\[
sc(x_i) = \arg \max_k \gamma_{ik} \quad (k = 1, 2, \cdots, M).
\] (34)

Then, we can derive the multi-label for each \(X_i \) \((i = 1, 2, \cdots, m)\) by considering the sub-concept belongingness. Let \(c_i\) denotes a \(M\)-dimensional binary vector where each element is either +1 or -1. For \(j = 1, 2, \cdots, M\), \(c_{ij} = +1\) means that the sub-concept corresponding to the \(j\)-th Gaussian mixture component appears in \(X_i\), while \(c_{ij} = -1\) means that this sub-concept does not appear in \(X_i\). Here the value of \(c_{ij}\) can be determined according to a simple rule that \(c_{ij} = +1\) if \(X_i\) has at least one instance which takes the \(j\)-th sub-concept (i.e., satisfying Eq. 34); otherwise \(c_{ij} = -1\). Note that for examples with identical single-label, the derived multi-labels for them may be different.
The above process works in an unsupervised way which does not consider the original labels of the bags $X_i$'s. Thus, the derived multi-labels $c_i$ need to be polished by incorporating the relation between the sub-concepts and the original label of $X_i$. Here the maximum margin criterion is used. In detail, consider a vector $z_i$ with elements $z_{ij} \in [-1.0, +1.0]$ ($j = 1, 2, \cdots, M$); $z_{ij} = +1$ means that the label $c_{ij}$ should not be modified while $z_{ij} = -1$ means that the label $c_{ij}$ should be inverted. Denote $q_i = c_i \odot z_i$ as that for $j = 1, 2, \cdots, M$, $q_{ij} = c_{ij}z_{ij}$. Let $\theta$ denote the smallest number of labels that cannot be inverted. SubCod attempts to optimize the objective

$$
\min_{w, b, \xi, Z} \frac{1}{2} \|w\|^2 + C \sum_{i=1}^{m} \xi_i \tag{35}
$$

s.t. $y_i((w^T(c_i \odot z_i) + b) \geq 1 - \xi_i$, 
$\xi \geq 0$, 
$\sum_{i,j} z_{ij} \geq 2\theta - 1$ ,

where $Z = [z_1, z_2, \cdots, z_m]$.

By solving Eq. 35 we will get the vector $z_i$ which maximizes the margin of the prediction of the proper labels of $X_i$. Here we solve Eq. 35 iteratively. We initialize $Z$ with all 1's. First, we fix $Z$ to get the optimal $w$ and $b$; this is a standard QP problem. Then, we fix $w$ and $b$ to get the optimal $Z$; this is a standard LP problem. These two steps are iterated till convergence. Finally, we set the multi-label vector’s elements which correspond to positive $c_{ij}z_{ij}$’s ($i = 1, 2, \cdots, m; j = 1, 2, \cdots, M$) to $+1$, and set the remaining ones to $-1$. Thus, we get all the polished multi-label vector $\tilde{c}_i$ for the bags $X_i$. Thus, the original data set $\{(X_1, y_1), (X_2, y_2), \cdots, (X_m, y_m)\}$ is transformed to a MIML data set $\{(\tilde{c}_1), (\tilde{c}_2), \cdots, (\tilde{c}_m)\}$, and any MIML algorithms can be applied.

To map the multi-labels predicted by the MIML classifier for a test example to the original single-labels $y \in \mathcal{Y}$, in the second stage of SubCod, a traditional classifier $f : \{+1, -1\}^M \rightarrow \mathcal{Y}$ is generated from the data set $\{ (\tilde{c}_1, y_1), (\tilde{c}_2, y_2), \cdots, (\tilde{c}_m, y_m) \}$. This is relatively simple and traditional supervised learning algorithms can be applied.

The pseudo-code of SubCod is summarized in Table 10. In the first stage (Steps
The **SubCod** algorithm

1. For multi-instance single-label examples \((X_u, y_u)\) \((u = 1, 2, \cdots, m)\), collect all the instances \(x \in X_u\) together and identify the Gaussian mixture components through the EM process detailed in Eqs. 29 to 33.

2. Determine the sub-concept for every instance \(x \in X_u\) according to Eq. 34, and then derive the label vector \(c_u\) for \(X_u\).

3. Make corrections to \(c_u\) by optimizing Eq. 35, which results in \(\tilde{c}_u\) for \(X_u\), and then train a MIML learner \(h_t(X)\) on \(\{(X_u, \tilde{c}_u)\}\) \((u = 1, 2, \cdots, m)\).

4. Train a classifier \(h_y(\tilde{c})\) on \(\{\tilde{c}_u, y_u\}\) \((u = 1, 2, \cdots, m)\), which maps the derived multi-labels to the original single-labels.

5. Return \(y^* = h_y(h_t(X^*))\).

1 to 3), **SubCod** derives multi-labels via sub-concept discovery and transforms single-label examples into a MIML examples, from which a MIML learner is generated. In the second stage (Steps 4), a traditional classifier is trained to map the derived multi-labels to the original single-labels. Test example \(X^*\) is fed to the MIML learner to get its multi-labels, and the multi-labels are then fed to the supervised classifier to get the label \(y^*\) predicted for \(X^*\).

### 7.2 Experiments

We compare **SubCod** with several state-of-the-art multi-instance learning algorithms, including **Diverse Density** [44], **Em-dd** [83], **mi-Svm** and **Mi-Svm** [3], and **Ch-Fd** [30]; these algorithms have been introduced briefly in Section 2.

Note that the experiments here are very different from that in Sections 4.3, 5.6 and 6.2. Both Sections 4.3 and 5.6 deal with learning from MIML examples, Section 6.2 deals with learning from single-instance multi-label examples, while this section deals with learning from multi-instance single-label examples, and therefore the experimental data sets in this section are different from those used in Sections 4.3, 5.6 and 6.2.
Table 11
Predictive accuracy on five multi-instance benchmark data sets

| Compared Algorithms | Data sets |
|--------------------|----------|
|                    | Musk1   | Musk2 | Elephant | Tiger | Fox  |
| **SubCod**         | 85.0%   | **92.1%** | 83.6%    | 80.8% | **61.6%** |
| **Diverse Density**| 88.0%   | 84.0% | N/A      | N/A   | N/A  |
| **Em-DD**          | 84.8%   | 84.9% | 78.3%    | 72.1% | 56.1% |
| **mi-Svm**         | 87.4%   | 83.6% | 82.0%    | 78.9% | 58.2% |
| **Mi-Svm**         | 77.9%   | 84.3% | 81.4%    | **84.0%** | 59.4% |
| **Ch-Fd**          | **88.8%** | 85.7% | **82.4%** | 82.2% | **60.4%** |

Five benchmark multi-instance learning data sets are used, including Musk1, Musk2, Elephant, Tiger and Fox. Both Musk1 and Musk2 are drug activity prediction data sets, publicly available at the UCI machine learning repository [8]. Here every bag corresponds to a molecule, while every instance corresponds to a low-energy shape of the molecule [24]. Musk1 contains 47 positive bags and 45 negative bags, and the number of instances contained in each bag ranges from 2 to 40. Musk2 contains 39 positive bags and 63 negative bags, and the number of instances contained in each bag ranges from 1 to 1,044. Each instance is a 166-dimensional feature vector. Elephant, Tiger and Fox are three image annotation data sets generated by [3] for multi-instance learning. Here every bag is an image, while every instance corresponds to a segmented region in the image [3]. Each data set contains 100 positive and 100 negative bags, and each instance is a 230-dimensional feature vector. These data sets are popularly used in evaluating the performance of multi-instance learning algorithms.

We follow the benchmark experiment design and report average accuracy of 10 runs of ten-fold cross validation. Here the parameters of SubCod are determined by hold-out tests on training sets, and the candidate value ranges are [10, 70] for $M$, the number of Gaussian mixture components, and [10% $\times$ #labels, 70% $\times$ #labels] for $\theta$, the smallest number of derived labels that cannot be inverted. MIMLSvm is used to realize the MIML learner in Step 3 of SubCod, and the candidate value range is [200, 400] for parameter $k$, the number of intermediate clusters in MIMLSvm. The classifier $h_y$ in Step 4 of SubCod is realized by SMO with default parameters. The
results of the compared algorithms are the best performance reported in literatures [3, 30]. The comparison is summarized in Table 11, where the best performance on each data set has been highlighted in boldface.

Table 11 shows that SubCod is very competitive to state-of-the-art multi-instance learning algorithms. In particular, on Musk2 its performance is much better than other algorithms. This is expectable because Musk2 is a complicated data set which has the largest number of instances, while on such data set the sub-concept discovery process of SubCod may be more effective.

Overall, the experimental results suggest that MIML can be useful when we are given observational data where each object has already been represented as a multi-instance single-label example.

8 Conclusion

This paper extends our preliminary work [81, 92] to formalize the MIML Multi-Instance Multi-Label learning framework for learning with ambiguous objects, where an example is described by multiple instances and associated with multiple class labels. It was inspired by the recognition that when solving real-world problems, having a good representation is often more important than having a strong learning algorithm because a good representation may capture more meaningful information and make the learning task easier to tackle. Since many real objects are inherited with input ambiguity as well as output ambiguity, MIML is more natural and convenient for tasks involving such objects.

To exploit the advantages of the MIML representation, we propose the MIIMLBoost algorithm and the MIIMLSvm algorithm based on a simple degeneration strategy. Experiments on scene classification and text categorization show that solving problems involving ambiguous objects under the MIML framework can lead to good performance. Considering that the degeneration process may lose information, we also propose the D-MIIMLSvm algorithm which tackles MIML problems directly in a regularization framework. Experiments show that this “direct” SVM algorithm outperforms the “indirect” MIIMLSvm algorithm.
In some practical tasks we are given observational data where each ambiguous object has already been represented by a single instance, and we do not have access to the raw objects such that we cannot capture more information from the raw objects using the MIML representation. For such scenario, we propose the \textbf{InsDif} algorithm which transforms single-instances into MIML examples to learn. Experiments on Yeast gene functional analysis and web page categorization show that such algorithm is able to achieve a better performance than learning the single-instances directly. This is not difficult to understand. Actually, the underlying task of (single-instance) multi-label learning is to learn an \textit{one-to-many} mapping yet one-to-many mappings are not mathematical functions. If we represent the multi-label object using multi-instances, the underlying task becomes to learn a \textit{many-to-many} mapping which is realizable by mathematical functions. So, transforming multi-label examples to MIML examples for learning may be beneficial in some tasks.

MIML can also be helpful for learning single-label examples involving complicated high-level concepts. Usually it may be quite difficult to learn such concepts directly since many different lower-level concepts are mixed together. If we can transform the single-label into a set of labels corresponding to some sub-concepts, which are relatively clearer and easier to learn, we can learn these labels at first and then derive the high-level complicated label based on them. Inspired by this recognition, we propose the \textbf{SubCod} algorithm which works by discovering sub-concepts of the target concept at first and then transforming the data into MIML examples to learn. Experiments show that this algorithm is able to achieve better performance than learning the single-label examples directly in some tasks.

We believe that semantics exist in the connections between atomic input patterns and atomic output patterns; while a prominent usefulness of MIML, which has not been realized in this paper, is the possibility of identifying such connection. As illustrated in Fig. 2(b), in the MIML framework it is possible to understand why a concerned object has a certain class label; this may be more important than simply making an accurate prediction, because the results could be helpful for understanding the source of ambiguous semantics.
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