MetaMIML: Meta Multi-Instance Multi-Label Learning

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Abstract

Multi-Instance Multi-Label learning (MIML) models complex objects (bags), each of which is associated with a set of interrelated labels and composed with a set of instances. Current MIML solutions still focus on a single-type of objects and assumes an IID distribution of training data. But these objects are linked with objects of other types, which also encode the semantics of target objects. In addition, they generally need abundant labeled data for training. To effectively mine interdependent MIML objects of different types, we propose a network embedding and meta learning based approach (MetaMIML). MetaMIML introduces the context learner with network embedding to capture semantic information of objects of different types, and the task learner to extract the meta knowledge for fast adapting to new tasks. In this way, MetaMIML can naturally deal with MIML objects at data level improving, but also exploit the power of meta-learning at the model enhancing. Experiments on benchmark datasets demonstrate that MetaMIML achieves a significantly better performance than state-of-the-art algorithms.

1 Introduction

In many real-world applications, a complex object of interest has its inherent structure, is represented as a bag of instances and associated with multiple labels simultaneously. Multi-Instance Multi-Label learning (MIML) [Zhou et al., 2012] provides a framework for handling such complex bags and instances. MIML focuses on mining the association between a bag and its instances, labels of bags and label correlations to differentiate the labels of individual instances. MIML solutions have been extensively applied for many tasks, such as image classification [Wu et al., 2015], text categorization [Briggs et al., 2012], gene function prediction [Yu et al., 2020a] and so on. Multi-view MIML (M3L) solutions have been invented to fuse multiple feature views of MIML objects [Nguyen et al., 2013; Yang et al., 2018; Xing et al., 2019], which further model the varying associations between bags and instances across views.

However, these MIML/M3L solutions still model homogeneous bags and neglect these bags linked with objects of other types, which reflect the semantic labels of target bags. As shown in Fig. 2 (i), the topic of a research paper in the academic network is not only reflected by its own textual features, but also depends on its authors and published venue. These multi-types objects are interdependent, while most MIML methods build on the promise of MIML objects with IID distribution [Zhou et al., 2008; Zhou et al., 2012]. To effectively mine the target bags, a natural idea is to encode these bags and their links with other types of objects via a heterogeneous network, and then applies network representation learning to form the composite feature representation of bags or instances. Recently, Multi-types objects Multi-view Multi-instance Multi-label Learning (M4L) is proposed to model interconnected complex objects of different types, and a joint matrix factorization based solution (M4L-JMF) is introduced [Yang et al., 2020b]. M4L-JMF uses low-rank representation learning on a heterogeneous network composed with multiple types of objects to aggregate the information of other types of objects toward the target bags and to complete the bag/instance-label associations. M4L-JMF proves the necessity and power of fusing multi-types linked MIML objects.

However, existing MIML algorithms and even the more advanced M3L and M4L approaches often require a large amount of training data to achieve good results on such complex dataset, but sufficient labeled bags/instances are hard and even infeasible to collect in practice. Furthermore, they suffer a vulnerable performance when dealing with new tasks, where the training data are even fewer but a good generalization is expected.

Meta learning can extract meta knowledge through learning from multi-related tasks, and then quickly adapt to new tasks with the aid of meta knowledge and few support training samples [Vanschoren, 2019]. Although it has achieved good results in various tasks [Finn et al., 2017; Sung et al., 2018; Snell et al., 2017], it is still a non-trivial problem to apply meta learning on multi-types MIML objects encoded by heterogeneous network. **Challenge 1:** Existing meta learning algorithms are mainly designed for single-type of objects, there is no principle way to apply meta-learning on multi-types MIML objects and to quickly adapt for a new task with
Figure 1: (i) An exemplar Heterogeneous Multi-Instance Network (HMIN) composed with papers, authors and published venues, the paper is the complex object further made instances of abstract, references and paragraphs. These papers can be associated with different but related topics (i.e. AI, NLP, CV and DM). (ii) The Meta-path, the meta-path ‘A-P-A’ indicates two authors have co-authored relation. (iii) The schematic framework of MetaMIML, which first uses the context learner with different meta-paths to learn context embeddings of target objects/instances and to generate multiple cross-tasks (meta-training support samples) from these embeddings. At the same time, it uses task learner to extract meta-knowledge from these tasks and optimizes the embeddings in an iterative manner. The meta-testing phase utilizes the extracted meta-knowledge, embeddings and few meta-test support samples to quickly adapt to new task.

just a few training samples. **Challenge 2:** How to learn different context representations of bags from heterogeneous multi-instance network for building meta-training tasks and extracting meta knowledge extraction? **Challenge 3:** How to leverage the extracted meta-knowledge and fuse the structure and attribute information of linked objects to predict the labels of target bags/instances.

To address the above challenges, we propose an approach called Meta Multi-Instance Multi-Label learning (MetaMIML). MetaMIML firstly constructs a heterogeneous multi-instance network (HMIN) with multiple types of bags, and then trains a context learner and a task learner. Context learner works in the bag contextual semantic space to generate different semantic representations of bags (tasks) from HMIN, while task learner operates in the task space to achieve meta knowledge acquisition from different tasks (for Challenges 1 and 2). MetaMIML then leverage random embedding and meta knowledge to obtain effective instance/bag embedding representations, and utilizes the task learner to predict the labels of bags/instances (for Challenge 3).

The main contributions of our work are summarized as:

- We focus on how to integrate meta learning with MIML to quickly adapt to new task with a few labeled MIML objects, which is a practical but largely unexplored topic of meta learning and of MIML. This studied problem has its distinctive challenges and application values.

- We propose the MetaMIML with a context learner for fusing multiple objects of HMIN and generating multiple context tasks, and with a task learner for acquiring knowledge from multiple context tasks. MetaMIML not only performs well in the meta learning setting, but also in the typical MIML settings, by multi-types objects fusion and meta knowledge.

- Experimental results on benchmark datasets under different scenarios show that MetaMIML outperforms both the representative MIML algorithms (MIMLfast [Huang et al., 2019], MIMLSVM [Zhou et al., 2012] and MIMLNN [Zhou et al., 2008]), and matrix factorization based data fusion solutions (MFDF [Zitnik and Zupan, 2015] and SelDFMF [Wang et al., 2019]) and network embedding-based methods (M4L-JMF [Yang et al., 2020], Metapath2vec[Dong et al., 2017] and HANE [Wang et al., 2019]).

2 Related work

Our work has close connections with MIML and Meta Learning. Diverse MIML methods have been proposed in the past decades [Zhou et al., 2012]. To name a few, MIML-Boost [Zhou et al., 2012] degrades the MIML problem into multiple multi-instance single-label tasks; and MIMLSVM [Zhou et al., 2012] uses a bag transformation strategy to convert bags into single instances and then degrades MIML into a single-instance multi-label learning task. MIMLNN [Zhou et al., 2008] utilizes two-layer neural network structure to replace the multi-label SVM used in MIMLSVM. Fast Multi-instance Multi-label learning (MIMLfast) [Huang et al., 2019] naturally detect key instance for each label by exploiting label relations in a shared space and discovering sub-concepts for complicated labels. Multi-instance multi-label learning with spatio-temporal pre-trimming (PreTrim-Net) [Zhang et al., 2020] learns from the given video-level labels to construct action recognition model, discover the underlying relevance between input patterns (instances) and semantic labels. Multi-modal Multi-instance Multi-label LDA (M3LDA) [Nguyen et al., 2013] learns a visual-label part from the visual features and a text-label part from the textual features, and forces these two parts having consistent labels.
Weakly-supervised M3L (WSM3L) [Xing et al., 2020] concerns with unpaired multi-view MIML objects with missing labels by multi-modal dictionary learning. However, these MIML methods can only consider single-type of bags, while in practice, these bags are also linked with objects of other types, which also reflect the semantic labels of target bags.

Heterogeneous network provides a natural way to represent linked objects of multi-types, as such network embedding-based solutions have been proposed to mine rich semantics between objects by matrix factorization [Yu et al., 2020b; Yang et al., 2020b] or by graph neural networks [Dong et al., 2017; Yang et al., 2020a]. These solutions aim at mapping the topological proximity of network nodes into continuous low dimensional vector representations for follow-up tasks, such as node classification/clustering, and link prediction. Although these network embedding based solutions can fuse objects of different types and reduce information bottleneck of target objects at the data level, they ignore that a complex object can be composed of multiple instances, whose feature representations also encode the semantics of target objects. For example, different salient regions (instances) of a web image often carry different semantics, which give the global semantic of this image.

Meta learning (also called learn to learning) [Vanschoren, 2019] aims to use the general knowledge previously learnt from multiple meta-training tasks and a small amount of training data for quickly adapting to new tasks. Diverse meta-learning techniques have been invented, and they can be categorized into three types: (i) metric-based methods learn a metric or distance function over tasks [Snell et al., 2017; Sung et al., 2018]; (ii) model-based methods [Santoro et al., 2016; Munkhdalai and Yu, 2017] aim to design an architecture or training process for rapid generalization across tasks; and (iii) optimization-based methods directly adjust the optimization algorithm to enable quick adaptation with just a few examples [Finn et al., 2017; Lee et al., 2019]. These meta learning algorithms still focus on single-type of objects. On the other hand, existing MIML methods performs the optimization of parameter from scratch for every task, and the pre-specified scratch can drastically affect the performance. In contrast, MetaMIML considers multi-types of objects, and it extracts cross-task knowledge (or meta-knowledge) by a task learner, which help specifying and adaptive optimizing the parameter for target task using just several training samples.

3 Method

3.1 Problem statement and overview

Let \( \mathcal{G} = \{ \mathcal{V}, \mathcal{E} \} \) be a Heterogeneous Multiple Instance Network (HMIN). \( \mathcal{V} \) includes a set of nodes of different types, \( \mathcal{E} \) stores links between nodes in \( \mathcal{V} \). HMIN contains at least one type of bags (i.e. papers in Fig. 2(ii)), which are further composed with a variable number of instances, \( \mathcal{X}_i = \{ \mathbf{x}_{i,1}, \mathbf{x}_{i,2}, \cdots, \mathbf{x}_{i,n_i} \} \), where \( \mathbf{x}_{i,j} \in \mathbb{R}^d \) is the \( j \)-instance and \( n_i \) is the number of instances affiliated with the \( i \)-th bag, and \( d \) is the dimension of instance. In contrast, a typical Heterogeneous Information Network (HIN) only includes objects of different types, or views a multi-instance bag as a plain node, without considering its composition of instances. As such, HMIN encodes richer relations among complex objects, instances and labels; it enables a more fine-grained analysis of real-world objects.

MetaMIML aims to explore the fusion of linked objects of different types to enhance the bag-instance representation, and to boost the prediction of labels of target bags/instances. In addition, it has to just leverage a few labeled bags/instances and meta-knowledge to induce an accurate model with good generalization. The optimization-based meta-learning [Finn et al., 2017; Lee et al., 2019] optimizes globally shared parameters over tasks, which can rapidly adapt to a new task with just one or few gradient steps. Inspired by this advantage, we build MetaMIML on a set of source tasks as \( \mathcal{D}_s = \{ (G^s_t, G^s_{val}) \}_{i=1}^N \), and a set of target tasks as \( \mathcal{D}_t = \{ (G^t_i, G^t_{val}) \}_{i=1}^M \). Suppose \( B \in \mathcal{V} \) denote the target type of bags and \( N + M = n, n = |B| \) is the number of bags. More details of data split are explained in Section 4.2.

In our MIML setting, a task \( T^s_t = (G^s_t, G^s_{val}) \) involves with one bag, consists of a training and a validation data. Note that the source training and validation datasets are respectively termed as support and query sets. We aim to learn meta-knowledge from a set of meta-training tasks \( \mathcal{D}_s \), and quickly adapt to new tasks (as meta-test tasks \( \mathcal{D}_t \)) using the meta knowledge. In the meta-training stage: for each task \( T^s_t \), its training and validation data sampled from the set of target objects (e.g. topics/labels in Fig. 2). The task learner adjusts the global task-wise prior parameters \( \omega \) with the loss on the training data \( G^s_{tr} \). Next, it calculates the loss with \( \omega \) on the validation data \( G^s_{val} \), backward propagates the loss to update \( \omega \) as follows:

\[
\min_{\phi} \mathbb{E}_{T^s_t \in \mathcal{D}_s} L(G^s_{val}, \phi - \gamma \nabla_{\phi} L(G^s_{tr}, \phi))
\]

where \( L(G^s_{tr}, \phi) \) measures the performance of an MIML model trained by \( \phi \) on \( G^s_{tr} \). \( L \) is the loss function and \( \gamma \) is the learning rate. \( \phi - \gamma \nabla_{\phi} L(G^s_{tr}, \phi) \) is the task parameter adapted for \( T^s_t \) by one gradient step from \( \phi \) (local update in Fig. 2(ii)). In the meta-test stage, a target task \( T^t_i \in \mathcal{D}_t \) also contains a small number of training data \( G^t_{tr} \), while the validation set contains \( G^t_{val} \). Conceptually, the base model initialized by meta-knowledge \( \phi \) on each unseen target task \( T^t_i \) is fast adapted as follows:

\[
\min L(G^t_{tr}, \omega | \phi)
\]

We can evaluate the performance of a meta-learner by \( \omega \) on \( G^t_{val} \) of each target task.

3.2 Context Learner

Our base model \( h_\phi = \{ f_\theta, g_\omega \} \) contains two components: context learner \( f_\theta \) and task learner \( g_\omega \). \( f_\theta \) aims to learn the semantic context information, and \( g_\omega \) aims to predict the labels of bags/instances. \( \phi = \{ \theta, \omega \} \) denotes the global prior.

To explore the network structure information of multi-types linked objects and to obtain the context representation of bags, we use the meta-path sampling on the bag-level to capture HMIN. As a form of higher-order graph structure, meta-path has been widely used to explore the semantics in a HIN [Dong et al., 2017; Yang et al., 2020a]. For example the meta-path ‘A-P-A’/‘A-C-A’ indicates two authors
have co-authored/co-attended a paper/conference. Given a HMIN with \(|\mathcal{V}| = m\) object types and \(|\mathcal{E}|\) relation types, a meta-path of length \(l\) is defined as a composite relation \(p = v_1 \stackrel{\phi_1}{\rightarrow} v_2 \stackrel{\phi_2}{\rightarrow} \cdots \stackrel{\phi_l}{\rightarrow} v_{l+1}\), where \(v_i \in \mathcal{V}\) and \(\phi_j \in \mathcal{E}\).

Towards effective meta-learning on HMIN, it is important to incorporate multi-aspect semantic contexts with tasks via different meta-paths. Given a task \(T_s\), \(G_{s,i}^{tr} = (G_{s,i}^{tr,dir}, G_{s,i}^{tr,ind})\) gathers direct and indirect information of the bag object as:

\[
G_{s}^{tr} = (G_{s,i}^{tr,dir}, G_{s,i}^{tr,ind}) = (G_{i}^{tr,dir}, G_{i}^{tr,P})
\]

where \(G_{s,i}^{tr,ind}\) is a set of objects that directly connect with objects of type \(\mathcal{V}_b\) (bag object), and \(G_{s,i}^{tr,ind} = G_{s,i}^{tr,dir}\) is a set of objects that indirectly connect with target objects by meta-paths, \(G_{s,i}^{tr,dir}\) is like a transfer station for \(G_{i}^{tr,ind}\) to connect different objects. Since each task \(T_s\) may interact with multiple target objects, we build multiple meta-paths based semantic contexts for task \(T_s\) as follows:

\[
G_{i}^{tr,P} = \{G_{i}^{P_1}, G_{i}^{P_2}, \cdots, G_{i}^{P_s}\}
\]

where \(G_{s,i}^{tr,P}\) encodes semantic contexts induced by meta-path \(p\). Since we want to obtain the context representation of bags, each meta-path starts with target bags in \(\mathcal{V}_b\). Therefore, \(G_{s,i}^{tr,P}\) contains diverse contextual information from target bags to other objects by walking along different meta-paths. Similarly, we can build the query set \(G_{i}^{val} = (G_{i}^{val,dir}, G_{i}^{val,ind}, G_{i}^{val,P})\). The support and query set in a task \(T_s\) are mutually exclusive, namely \(G_{i}^{tr,dir} \cap G_{i}^{val,dir} = \emptyset\).

In context leaner, the bag information are aggregated from its contexts. Inspired by Word2Vec [Mikolov et al., 2013], we use the Skip-Gram model to get the bag object embedding \(X_i\) induced by meta-path \(p\) as follows:

\[
X_i = f_\theta(G_{i}^{P}) = \sigma(SG(G_{i}^{P}, \theta))
\]

where \(X_i \in \mathbb{R}^{d_i}\) and \(p \in \mathcal{P}\). \(\sigma\) is the activation function (such as LeaklyReLU). \(f_\theta\) is the embedding function and \(SG(\cdot)\) is the Skip-gram model parameterized by \(\theta \in \mathbb{R}^{d \times d_i}\) (also called look up table), \(b \in \mathbb{R}^{d_i}\). \(l\) is the length of meta-path \(p\) and \(d_i\) is the embedding dimension. To obtain the aggregated representation of instances, we merge the context representation of bags with instance features through random projection embedding as follows:

\[
\hat{x}_{ij} = (x_{ij} \oplus X_i^p)^T \cdot E
\]

where \(\{x_{ij}\}_{r=1}^{n}\) is the set of instances affiliated with the \(i\)-th bag, \(\oplus\) denotes the concatenation operation, \(\hat{x}_{ij}^p \in \mathbb{R}^k\) is the instance representation for the \(j\)-th instance of this bag, and \(k\) is the dimension of final embedding. \(E \in \mathbb{R}^{u \times k}\) is the sparse random projection matrix and \(u = d_i + d\). In this way, we can obtain a bag’s context representation \(X_i^p = \{\hat{x}_{i,1}^p, \hat{x}_{i,2}^p, \cdots, \hat{x}_{i,n_i}^p\}\) w.r.t. meta-path \(p\).

Random projection is a simple but powerful technique of dimensionality reduction, which can preserve the pairwise distance between data points. The sparse random projection we use is a variant of random projection, it can achieve a significant speedup with little loss in accuracy. Formally, each entry of \(E \in \mathbb{R}^{u \times k}\) is IID drawn from:

\[
e_{ij} = \begin{cases} 
1, & \text{with prob. } \frac{1}{s} \\
0, & \text{with prob. } 1 - \frac{1}{s} \\
-1, & \text{with prob. } \frac{1}{s} 
\end{cases}
\]

where \(s = \sqrt{n}\) or \(s = \frac{n}{\log n}\) is the number of bags. Eq. (7) can achieve a \(\sqrt{n}\)-fold speedup, and only \(1/\sqrt{n}\) entries need to be processed when \(s = \sqrt{n}\) [Li et al., 2006].

### 3.3 Task Learner

Through the context leaner introduced above, we have obtained an instance representation that combines semantic contexts and instance features. Because different semantic context representations have different degrees of importance for different objects, the change in semantics also changes the representation of instances. Similarly, new tasks have different preferences for semantic representations. Given that, we firstly use the task leaner to predict the labels of bags/instances, then the support loss locally updates parameters via gradient descent and back-propagation.

In the meta-path \(p\) induced semantic space, we can calculate the loss on the support set \(G_{s}^{tr}\) and task \(T_s\) as:

\[
\mathcal{L}_{T_s}(\omega, \hat{X}_i^p, G_{s,i}^{tr,dir}) = ||y - g_{\omega}(\hat{X}_i^p)||^2 + ||g_{\omega}(\hat{X}_i^p) - MP(z_{\omega}(\hat{X}_i^p))||^2
\]

where \(y \in \mathbb{R}^{q_r}\) is the ground truth bag-label vector of one task, \(q_r^{tr} + q_r^{val} = q_r\), \(q_r^{tr}\) and \(q_r^{val}\) are the label space sizes of support set and query set in a source task, respectively. \(g_{\omega}(\hat{X}_i^p) = MP(Soft(MLP(\hat{X}_i^p)))\) predicts the labels of bags. \(MLP(\cdot)\) is a three-layer Multi-Layer Perceptron, \(Soft(\cdot)\) is the Softmax operation and \(MP(\cdot)\) is the column-wise Max Pooling operation to aggregate the labels of instances to their hosting bags. \(g_{\omega}\) predicts the labels of bags and is parameterized by \(\omega\). \(z_{\omega}(\hat{X}_i^p)\) predicts the labels of instances. So the first term on the right of Eq. (8) pursues the label prediction of bags by referring to known labels of bags. The second term pursues the consistent labels from the bag-level and instance-level, and distributes the bag-level labels to individual instances of \(X_i^p\).

To obtain the prior information on meta-path \(p\) from the global prior \(\phi\), we perform gradient descent on loss in the meta-path \(p\) induced semantic space for task \(T_s\). Here \(\phi^p = \{\theta^p, \omega^p\}\), and \(\theta^p\) indicate semantic-specific parameters and \(\omega^p\) denotes task-specific parameters. In this way, MetaMIML can learn multiple aspects of meta-knowledge as follows:

\[
\theta^p_i = \theta - \alpha \frac{\partial \mathcal{L}_{T_s}(\omega, \hat{X}_i^p, G_{s,i}^{tr,dir})}{\partial \theta}
\]

\[
\omega^p_i = \omega - \alpha \frac{\partial \mathcal{L}_{T_s}(\omega, \hat{X}_i^p, G_{s,i}^{tr,dir})}{\partial \theta}
\]

where \(\alpha\) is the learning rate. Different meta-path spaces encode different semantic information, and the semantic information extracted by different tasks are of different importance and relevance. To gather different semantic contexts, we apply attention mechanism on different meta-paths to reduce the redundancy as follows:

\[
a^p_i = Soft(\mathcal{L}_{T_s}(\omega, \hat{X}_i^p, G_{s,i}^{tr,dir}))
\]
where \( d_p^i \) is the weight of semantic space \( p \) for task \( T_i \). This attention strategy also retains different semantics while quickly adapts to a new task. In this way, we can get the attention weights of all meta-paths \( \mathcal{P} \).

To achieve cross-task knowledge across multiple meta-paths \( \mathcal{P} \), we set \( \omega_i = \sum_{p \in \mathcal{P}} d_p^i \omega_i^p \) and \( \hat{X}_i = \sum_{p \in \mathcal{P}} d_p^i \hat{X}_i^p \). Next, the task-wise can be adapted by the global prior knowledge \( \omega \) and attention based \( \omega_i \), which help predicting the labels of bags. The prediction task \( T_i \) with meta-path \( p \) is adapted as follows:

\[
\omega_i^p = \omega \odot \omega_i - \beta \frac{\partial L_{T_i}(\omega_i^p, \hat{X}_i, G_i^{tr,dir})}{\partial \omega_i^p}
\]

(11)

where \( \beta \) is the learning rate and \( \odot \) is the element-wise product. As shown in Fig. 2(ii), the global prior \( \phi = \{\theta, \omega\} \) can then be optimized through query loss:

\[
\min_{\phi \in \mathcal{T}_s \in \mathcal{D}_s} E_{T_s \in \mathcal{D}_s} L_{T_s}(\omega_i^p, \hat{X}_i, G_i^{val,dir})
\]

(12)

Note the label space of a query bag is \( y \in \mathbb{R}^{q^val} \), \( q^val \) is the number of distinct labels in a query set of a source task.

To this end, MetaMIML not only learns different semantic representations of bags/instances via different meta-paths \( p \), and generates multiple meta-training tasks from these semantic representations to acquire prior knowledge, but also can quickly adapt to new tasks from task-wise by prior knowledge using one (or a few) gradient descent step. The pseudo code of the training procedure for MetaMIML is detailed in Algorithm 1.

We conduct a complexity analysis of our training procedure, which include the context learner, random embedding operation and task learner. The complexity of context learner and task learner are both \( O(|\mathcal{T}_s| \cdot |\mathcal{P}| \cdot d \cdot d_l \cdot n_m) \), and the complexity of random embedding operation is \( O((d + d_l) \cdot k \cdot n_m) \). Thus the time complexity of MetaMIML is \( O(e |\mathcal{T}_s| \cdot |\mathcal{P}| \cdot d \cdot d_l + (d + d_l) \cdot k \cdot n_m) \), where \( e \) is the number of epochs, \( |\mathcal{T}_s| \) and \( |\mathcal{P}| \) are the number of meta-training tasks and meta-paths, respectively, \( d \) and \( d_l \) are the dimension of instance and semantic context, and \( k \) and \( n_m \) are the dimension of instance embeddings and the number of instances. \( |\mathcal{P}| \), \( d \), \( d_l \) and \( k \) are usually small and random embedding operation can carry out \( \sqrt{n} \)-fold speedup, so the complexity of MetaMIML is about linear with the number of tasks, w.r.t. \( O(|\mathcal{T}_s| \cdot \log(n_m)) \).

4 Experimental Results and Analysis

4.1 Experimental Setup

Datasets: We use six benchmark datasets: Isoform, LncRNA, Birds, MSRC v2, Letter Carroll and Letter Frost. Isoform and LncRNA are two biological datasets naturally linked with multi-types of molecules; they were used to predict the associations between isoforms/LncRNAs and functions/diseases. The last four are widely-used MIML datasets [Briggs et al., 2012; Huang et al., 2019]. Table 1 gives the statistics of these datasets.

Baselines: To comparatively evaluate the performance of our MetaMIML, we compare it against eight methods of different categories, which include three MIML algorithms (MIMLfast [Huang et al., 2019], MIMLSVM [Zhou et al., 2012] and MIMLNN [Zhou et al., 2008]) for MIML objects, two data fusion solutions based on matrix factorization (MFDF [Žitnik and Zupan, 2015] and SelDFMF [Wang et al., 2019a]) and three network embedding based methods (Metapath2vec[Dong et al., 2017], HANE[Wang et al., 2019b] and M4L-JMF[Yang et al., 2020b]) for linked objects as follows:

- **MIMLSVM** [Zhou et al., 2012] uses a bag transformation strategy to convert bags into single instances and then degenerates MIML into a single-instance multi-label learning task. We set \( ratio = 0.2 \) (parameter \( k \) is set to be 20% of the number of training bags), \( svm.para = 0.2 \) (the value of ‘gamma’) and \( svm.type = Linear \) for Isoform dataset; \( ratio = 0.3 \), \( svm.para = 0.2 \) and \( svm.type = Poly \) for four MIML datasets; and \( cost = 1 \) (the value of \( C \)) for all datasets.
- **MIMLNN** [Zhou et al., 2008] utilizes two-layer neural network structure to replace the MLSVMiZhao and Zhou, 2007] used in MIMLSVM, then predicts the labels of bags. We follow the configuration \( ratio = 0.4 \) and \( \lambda = 0.5 \) for Isoform dataset; \( ratio = 0.2 \) and
\( \lambda = 0.3 \) for four MIML datasets;

- **MIMLfast** [Huang et al., 2019] first constructs a low-dimensional subspace shared by all labels, then trains label specific linear models to optimize approximated ranking loss via stochastic gradient descent. It can naturally detect key instance for each label by exploiting label relations in a shared space and discovering subconcepts for complicated labels. We follow the configuration \( d = 300 \) (dimension of the shared space), \( \text{norm}_\text{up} = 10 \) (norm of each vector), \( \text{step}_\text{size} = 0.005 \) (step size of SGD), \( \lambda = 0.0001 \) and \( \text{num}_\text{sub} = 20 \) (number of sub concepts) for Isoform; \( d = 100 \), \( \text{norm}_\text{up} = 10 \), \( \text{step}_\text{size} = 0.003 \), \( \lambda = 0.0005 \) and \( \text{num}_\text{sub} = 5 \) for four MIML datasets; \( \text{opts.norm} = 1 \), \( \text{opts.average.size} = 10 \) and \( \text{opts.average.begin} = 0 \) for all datasets.

- **DFMF** [Žitnik and Zupan, 2015] collaboratively factorizes block matrices of a heterogeneous information network into low-rank matrices and then reconstructs the target relational matrix to predict the relations between bags and labels. We follow the configuration \( d = 300 \) for Isoform dataset, while \( d = 20 \) for MIML datasets and \( d = 170 \) for LncRNA dataset.

- **SelDFMF** [Wang et al., 2019a] can select and integrate inter-relational data sources by assigning different weights to them. We set \( \alpha = 10^6 \), \( d = 300 \) and \( \text{nTypes} = 5 \) for Isoform dataset, \( \alpha = 10^5 \), \( d = 20 \) and \( \text{nTypes} = 3 \) for four MIML datasets and \( \alpha = 10^5 \), \( d = 160 \) and \( \text{nTypes} = 5 \) for the LncRNA dataset.

- **M4L-JMF** [Yang et al., 2020b] firstly uses multiple data matrices to separately store the attributes and multiple inter/intra-associations of objects, and then jointly factorizes these matrices into low-rank ones to explore the latent representation of each bag and its instances. We set \( \alpha = 10^6 \), \( \beta = 10^6 \), \( d = 240 \) and \( \text{nTypes} = 5 \) for Isoform dataset; \( \alpha = 10^5 \), \( \beta = 10^6 \), \( d = 20 \) and \( \text{nTypes} = 3 \) for four MIML datasets, and \( \alpha = 10^7 \), \( \beta = 10^6 \), \( d = 160 \) and \( \text{nTypes} = 5 \) for the LncRNA dataset.

- **Metapath2vec** [Dong et al., 2017] is a classic heterogeneous information network representation learning method, which samples meta-path based random walks, then leverages a heterogeneous skip-gram model to perform node embedding. We set the length of random walks, the number of walks and the size of windows to \( l = 40 \), \( w = 10 \) and \( \text{size} = 4 \) respectively for Isoform and LncRNA datasets. These parameter also was set for MetaMIML for walking.

- **HANE** [Wang et al., 2019b] uses an attention mechanism on Graph Convolutional Networks (GCN) to encode the structure and attribute information of nodes to generate high-quality embedding. We set \( d = 270 \) for Isoform dataset, \( d = 150 \) for LncRNA dataset.

The input parameters of these comparison methods are specified (or optimized) according to the recommendations of the authors in their codes or papers. All the experiments are performed on a server with following configurations: CentOS 7.3, 256GB RAM, Intel Xeon E5-2678 v3 and NVIDIA Corporation GK110BGL [Tesla K40s]. We implement the proposed MetaMIML with deep learning library PyTorch. The Python and PyTorch versions are 3.6.5 and 1.3.1, respectively. We perform experiments on the six benchmark datasets to quantitatively study the performance of the proposed MetaMIML, and compare it against eight representative and related approaches as follows:

The first three compared methods are Multi-Instance Multi-Label (MIML) solutions, while the two methods (DFMF and SelDFMF) address the fusion of linked multi-types objects via matrix factorization, two network embedding methods (Metapath2vec and HANE) disregard the bag-instance associations. M4L-JMF also use heterogeneous multi-instance information network (HMIN). The input parameters of these comparison methods are specified (or optimized) according to the recommendations of the authors in their codes or papers. For the proposed MetaMIML, we adopt Adaptive Moment Estimation (Adam) to optimize our MetaMIML. For all datasets, we use a batch size 32 and set the meta-learning rate to 0.005 (\( \gamma = 0.005 \)). We set both the context learner and task learner learning rate to 0.005 (\( \alpha = \beta = 0.005 \)) for Isoform and LncRNA dataset, while \( \alpha = \beta = 0.003 \) for four MIML datasets. We perform one step gradient descent update in both context learner and task learner adaptations. We use the meta-path set \{G\text{DG},G\text{GdG},G\text{MGD}\} and \{G\text{DG},G\text{LG},G\text{LDG}\} for Isofrom and LncRNA datasets (G: gene, D: disease, L: LncRNA, M: miRNA and G\text{Gd}: Gene Ontology) respectively to MetaMIML and Metapath2vec. The maximum number of epochs are set as \( e = 100 \) and \( e = 80 \), \( k = 240 \) and \( k = 100 \) for Isofrom and LncRNA, respectively, \( e = 20 \) and \( k = 8 \) for Birds, we set \( e = 15 \) and \( k = 10 \) for other MIML datasets.

**Evaluation metrics:** To quantify the performance of MetaMIML, we adopted four canonical evaluation metrics, namely the average area under the precision-recall curve (AUPRC), the average area under the receiver operating curve (AUROC), the average F1-score (AvgF1) of all classes, and Hamming Loss (HL). Unlike other metrics, the smaller the value of HL, the better the performance is, so we report 1-HL. For each bag (instance), we use the top \( K \) labels with the largest probability as the relevant labels of the bag (instance). Here \( K \) is the average number of labels per bag/instance. We report the average results (10 random partitions of each dataset) and standard deviations for each method.

We conducted three types of experiments to study the performance of MetaMIML. In the first experiments, we apply MetaMIML on Isoform dataset to study two questions: how does MetaMIML perform compared with related methods? How does MetaMIML benefit from HMIN. In the second experiments, we compare MetaMIML against traditional MIML methods on four benchmark MIML datasets. In the third experiment, we explore the performance of MetaMIML and network embedding methods on LncRNA dataset with linked objects of multi-types.
4.2 Results on Isoform

In the first experiment, we use the Isoform dataset composed of 5 types of objects (miRNAs(495), genes(8,000), isoforms(76,244), Gene Ontology(6,428), Disease Ontology(8,450)) and 5 link types, the more detailed information can be found in [Yu et al., 2020a]. Follow the experimental protocol (recommend items to users) in [Lee et al., 2019], we divided the samples and labels into two groups: source and target as the meta-training and meta-test data. We randomly divided the Gene Ontology labels (functional annotations of genes) into two sets (approximately 8:2), the first 80% labels serve as source tasks and the remaining as the target tasks. Then we randomly selected 80% of the bags (genes) as the source bags and the rest as target bags. For each bag, five labels are randomly selected as the query set and rest as the support set from source labels during meta-training. The same way to split target labels for each task (bag) during meta-test stage.

Because MIML methods (MIMLSVM, MIMLNN and MIMLfast) cannot directly handle linked objects of multi-types, we first project other objects (except Gene Ontology labels) towards the genes to form MIML Isoform data, and then apply these MIML methods. For matrix factorization based data fusion (except M4L-JMF) and heterogeneous network embedding methods, we adopt the transformation used in [Yang et al., 2020b], disregarding the bag-instance associations.

Table 2 reports results of on Isoform dataset. From these results, we have some important observations:
(i) MetaMIML has clear better (or comparable) performance results than most competitive methods. This facts the effectiveness of our MetaMIML for fast adapting to new tasks using few training samples. We find that the fusion of multi-types objects in HMIN improves the representation of bags/instances and contributes to a significantly increased AvgF1 and AUROC by at least 3% and 1.3%. MIMLSVM and MIMLNN often have the lowest performance in terms of AUROC and AUPRC, that is because they both degenerate an MIML problem into a single-instance multi-label learning problem, which causes information loss. None of these compared methods consistently holds the best performance across the four evaluation metrics, that is because these metrics quantify the performance of multi-label learning from different perspectives, and a learner can not always outperform another one across all the metrics. This fact also signifies the complexity and hardship of MIML problems.
(ii) Heterogeneous multi-instance information network helps the fusion of linked objects of multi-types. This is supported by classical MIML methods have a lower performance than the network embedding based methods. The former cannot utilize the network structure information. MIMLfast is relatively better than the other two MIML methods (MIMLSVM and MIMLNN), since it trains label specific linear models to optimize approximated ranking loss by stochastic gradient descent. However, MIMLfast can not model linked objects of different types. So its often loses to data fusion based solutions. Metapath2vec also performs meta-path based random walks and uses heterogeneous skip-gram model to learn the representation of bags, but it disregards the instance information. As such, it beats by M4L-JMF and MetaMIL, which consider the bag-instance associations. For the similar reason, matrix factorization based data fusion methods (DFMF and SelDFMF) also often have a lower performance than MetaMIML. Although M4L-JMF can fuse multi-types of objects and model the bag-instance associations, its avgF1 and AUROC values are lower than MetaMIML, since it can not extract and use meta-knowledge for fast adapting to new tasks M4L-JMF has higher values of AUPRC and 1-HL than MetaMIML, since it uses an aggregation term to push the labels of bags to their affiliated instances in a coherent manner. HANE uses an attention mechanism with graph convolutional networks to mine the structure and attribute information of network nodes, but it loses to MetaMIML by a large margin, due to its inability to extract meta-knowledge for new tasks.

In summary, MetaMIML can not only utilize HMIN to fuse multi-types of objects, but also can leverage context learner and task leaner to extract meta knowledge from multiple semantic contexts induced by different meta-paths, and fast adapt to new tasks. For these advantages, it frequently outperforms those competitive compared methods.

4.3 Results on MIML data

In the second experiment, we use four MIML datasets listed Table 1 to study the performance of MetaMIML and related methods on typical MIML tasks. Here, we randomly partition the samples of each dataset into a training set (70%) and a testing set (30%). Following the protocol in [Xing et al., 2019], we construct a heterogeneous network of bags and instances, and then use this network as input for matrix factorization/network embedding based compared methods. Table 3 reports the bag-level evaluation results. Compared with other methods, MetaMIML often has the best performance on each dataset, and improves the AUPRC and AUPRC more obviously.
Table 2: Results of compared methods on Isoform. */* indicates whether MetaMIML is statistically (pairwise t-test at 95% significance level) superior/inferior to the other method.

| Metric   | MIMLfast | MIMLSVM | MIMLNN | M4L-JMF | DFMF | SelDFMF | MetaMIML |
|----------|----------|---------|--------|---------|------|---------|----------|
| AvgF1    | .295±.005 | .325±.002 | .516±.003 | .268±.014 | .252±.012 | .261±.009 | .575±.003 |
| AUROC    | .518±.002 | .743±.002 | .774±.005 | .944±.002 | .902±.009 | .912±.003 | .906±.002 |
| AUPRC    | .235±.000 | .535±.007 | .713±.013 | .963±.008 | .886±.045 | .891±.018 | .965±.003 |
| 1-HL     | .756±.005 | .846±.007 | .865±.004 | .972±.001 | .971±.001 | .972±.000 | .985±.002 |

Table 3: Bag-level results of compared methods on four datasets with known bag/instance-level labels. */* indicates whether MetaMIML is statistically (pairwise t-test at 95% significance level) superior/inferior to the other method.

We report the experimental results at instance-level in Table 4. MetaMIML has the highest AvgF1 values, and MetaMIML improves AvgF1 by at least 14% compared with MIMLfast. That is because MetaMIML can learn a good representation for instances. M4L-JMF has a higher AUROC values than MetaMIML on Birds and MSRC v2 datasets. That is because M4L-JMF not only can push the labels of bags to their affiliated instances, but also can reversely aggregate the labels of instances to their hosting bags. But compared with the results at bag-level and at instance-level, MetaMIML beats M4L-JMF in terms of other evaluation metrics. This fact proves that MetaMIML can also make a competitive instance-level label prediction. The instance-level evaluation results also prove that MetaMIML outperforms compared methods, due to the improved instance representation via fusion of bag-level context semantics.

In the third experiment, we further study the performance of MetaMIML on linked objects of different types. We use the LncRNA dataset [Wang et al., 2019a], which is composed of 6 types of objects (LncRNA(240), genes(15,527), miRNAs(495), Gene Ontology(6,428), Disease Ontology(412) and Drug(8,283)) and 9 types of links. We report the results in Table 5. Overall, MetaMIML has a relatively stable performance and frequently outperforms competitive compared methods. These experiment results not only demonstrate the flexibility of MetaMIML in diverse settings, but also prove the effectiveness of the context leaner for exacting the network structure information via different meta-paths. Overall, these results also confirm that MetaMIML can also work on traditional MIML tasks.

4.4 Parameter Sensitivity Analysis

In this paper, parameter $k$ (the column size of sparse random projection embedding matrix $E$) (in Eq. (6) of the main text) should be specified for our proposed MetaMIML. We observe from Fig. 2 that a too small $k$ can not sufficiently encode multi-types objects, and while a too large $k$ brings in some noises and thus leads to a low AUROC value. From the above analysis, we adopt $k = 155$ and $k = 18$ for experiments on
Table 4: Results of MetaMIML and compared methods on four datasets with instance-level labels. •/◦ indicates whether MetaMIML is statistically (according to pairwise t-test at 95% significance level) superior/inferior to the other method.

5 Conclusions

In this paper, we investigate how to perform meta learning on multi-instance multi-label data, which is a challenging and practical, but under-studied problem. We introduce an approach called MetaMIML for naturally linked MIML objects of multi-types. Experimental results on real-world datasets show that MetaMIML can quickly adapt to new tasks and achieve a better performance than other competitive and related methods. MetaMIML also outperforms these methods in the typical MIML tasks.

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| Method          | AvgF1     | AUROC     | AUPRC     | I-HL     |
|-----------------|-----------|-----------|-----------|----------|
| DFMF            | 0.062±0.001● | 0.872±0.007● | 0.546±0.091● | 0.982±0.001 |
| SelMFDF         | 0.066±0.003● | 0.887±0.003 | 0.604±0.015 | 0.986±0.001 |
| M4L-JMF         | 0.067±0.002● | 0.895±0.004● | 0.616±0.026 | 0.989±0.001 ○ |
| metapath2vec    | 0.096±0.002● | 0.771±0.013 | 0.375±0.014● | 0.952±0.006 ○ |
| HANE            | 0.224±0.002● | 0.867±0.008● | 0.471±0.008● | 0.975±0.005● |
| MetaMIML        | 0.282±0.003 | 0.886±0.002 | 0.611±0.008 | 0.984±0.002● |

Table 5: Results of MetaMIML, matrix factorization based and network embedding methods on the LncRNA dataset. ●○/●○ indicates whether MetaMIML is statistically (according to pairwise t-test at 95% significance level) superior/inferior to the other method.

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