# Learning Label-Specifc Multiple Local Metrics for Multi-Label Classifcation

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# Abstract

Multi-label metric learning serve as an effective strategy to facilitate multi-label classifcation, aiming to learn better similarity metrics from multilabel examples. Existing multi-label metric learning approaches learn consistent metrics across all multi-label instances in the label space. However, such consistent metric learning approaches are suboptimal as they neglect the nonlinear distribution characteristics of multi-label instances. In this paper, we present LSMM, *a Label-Specifc Multi-Metric learning framework for multi-label classifcation*, where nonlinear distribution characteristics of multi-label examples are considered by learning label-specifc multiple local metrics for different instances on the shoulder of a global one. Specifcally, multi-label instances within each label space can be divided into several disjoint partitions through either semantic-based or cluster-based partition strategies, in each of which a local metric is trained to separate the instances locally. Besides, a global metric is introduced to implicitly exploit high-order label correlations across all labels. The combination of the global metric and labelspecifc local metrics is utilized to measure the semantic similarities between multi-label instances in each label space, under which similar intra-class instances are pushed closer and inter-class instances are pulled apart. Comprehensive experiments on benchmark multi-label datasets validate the superiority of LSMM in learning effective similarity metrics for multi-label classifcation.

# 1 Introduction

Different from multi-class classifcation[Jia *et al.*[, 2023\]](#page-7-0), multi-label classifcation aims to model real-world objects with rich semantics, where each multi-label example is represented by an instance while associated with multiple labels simultaneously [\[Zhang and Zhou, 2014;](#page-8-0) Liu *et al.*[, 2021\]](#page-7-1). As a practical machine learning paradigm, multi-label classifcation has been widely applied in various real-world application, such as text categorization [Xu *et al.*[, 2023\]](#page-7-2), bioinformatics analysis [Li *et al.*[, 2023\]](#page-7-3), etc.

Similarity is a crucial concept in machine learning that reveals the degree of connectedness between objects. The predefned similarity metric, such as the Euclidean distance, face challenges in universal adaptation across diverse scenarios. In response, Distance metric learning [Xing *et al.*[, 2002\]](#page-7-4) has emerged as a solution to learn task-specifc distance metrics by leveraging side information such as linkages and comparisons derived from examples. This approach autonomously refnes similarity measurements beyond the limitations of the predefned metric. The learned distance metrics align with the inherent relationships between examples, ensuring that similar intra-class instances exhibit proximity, while distances between dissimilar inter-class instances are sufficiently large. Through the utilization of adaptively learned distance metrics, the effcacy of distance metric learning has been substantiated in enhancing  $k$ -nearest neighbor (KNN) classifiers on single-label examples[Song *et al.*[, 2021;](#page-7-5) [Li and Lu, 2022;](#page-7-6) Chen *et al.*[, 2023\]](#page-7-7). Given the effective modeling of semantic similarity among examples achieved through distance metric learning, there exist the potential for simple KNN classifers to achieve state-of-the-art classifcation performance.

In light of the remarkable capability for measuring semantic similarities, distance metric learning has been extended to multi-label scenarios in recent years, a.k.a. *multi-label metric learning* [\[Liu and Tsang, 2015;](#page-7-8) Gouk *et al.*[, 2016;](#page-7-9) [Sun and Zhang, 2021;](#page-7-10) Mao *et al.*[, 2023\]](#page-7-11). Multi-label metric learning aims to assess the more intricate semantic similarities among examples with rich semantics. Experimental evidence has demonstrated its capability to enhance the performance of KNN-based multi-label classifers, such as BR-KNN [\[Boutell](#page-7-12) *et al.*, 2004] and ML-KNN [\[Zhang and Zhou,](#page-8-1) [2007\]](#page-8-1), thereby facilitating multi-label classifcation. Existing multi-label metric learning approaches learn consistent metrics across all multi-label instances in the label space. Although such consistent multi-label metric learning framework has achieved favorable outcomes, it might be suboptimal as they neglect the fact that multi-label instances exhibit nonlinear distribution characteristics in each label space. For example, in multimedia annotation, the label "sun" is applicable to images depicting forests as well as those representing urban environments. Likewise, in text categorization, the label "president" manifests in both political and economic textual

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contexts. This implies that in each label space, the distribution of multi-label instances exhibits a high degree of nonlinearity. Consequently, in such cases, employing a single consistent metric encounters formidable challenges in simultaneously pushing similar instances closer while pulling dissimilar instances further away.

With the above observations, we present LSMM, *a Label-Specifc Multi-Metric learning framework for multi-label classifcation*, where nonlinear distribution characteristics of multi-label instances are considered by learning label-specifc multiple local metrics for different instances on the shoulder of a global one. Specifcally, multi-label instances within each label space can be divided into several disjoint partitions through either semantic-based or cluster-based partition strategies, in each of which a local metric is trained to separate the instances locally. To take label correlation into consideration, a global metric is introduced to implicitly exploit high-order label correlations across all labels. The global metric serves as the foundation to reveal the common characteristics among multi-label examples, while the label-specifc local metrics act as local biases, depicting the individuality of different instances in each label space. The combination of the global metric and label-specifc local metrics is utilized to measure the semantic similarities between multi-label instances in each label space, under which similar intra-class instances are pushed closer and inter-class instances are pulled apart. Comprehensive experiments on benchmark multi-label datasets validate the superiority of LSMM in learning effective similarity metrics for multi-label classifcation.

The rest of this paper is organized as follows. Section 2 briefy reviews related works. Section 3 presents details of the proposed LSMM framework. Section 4 reports experimental results of comparative studies over benchmark multilabel datasets. Section 5 concludes this paper.

# 2 Related Work

Multi-Label Classifcation. In the last decades, numerous approaches have been proposed to tackle multi-label classifcation problem [\[Zhang and Zhou, 2014;](#page-8-0) Liu *et al.*[, 2021\]](#page-7-1). To deal with the challenge of an exponential-sized output space, modeling label correlations has become a mainstream strategy to solve this problem. Generally speaking, these approaches can be grouped into three categories, differing in the order of label correlations under consideration. The order of label correlations can be considered in a frst-order manner by treating each label independently [\[Boutell](#page-7-12) *et al.*, 2004; [Zhang and Zhou, 2007\]](#page-8-1), a second-order manner by exploiting pairwise interactions between labels [Zhu *et al.*[, 2017;](#page-8-2) [Yu and Zhang, 2021\]](#page-8-3), and a high-order manner by exploiting relations among a subset or all labels [\[Zhang](#page-8-4) *et al.*, 2021; Si *et al.*[, 2023\]](#page-7-13). BR-KNN [\[Boutell](#page-7-12) *et al.*, 2004] and ML-KNN [\[Zhang and Zhou, 2007\]](#page-8-1), as the most classic frst-order multi-label classifcation methods, extend KNN to the multilabel scenario and have achieved certain results in multi-label classifcation tasks. However, due to the neglect of label correlations, their performance is usually inferior to secondorder and high-order methods. In addition, another signifcant reason for their insufficient performance is their heavy reliance on the chosen similarity metric. In the absence of prior knowledge, the predefned Euclidean metric used in BR-KNN and ML-KNN is often unsuitable for all scenarios.

Distance Metric Learning. To address the limitations imposed by predefned metrics, distance metric learning is proposed to learn task-specifc similarity metrics, mainly for single-label examples [Xing *et al.*[, 2002;](#page-7-4) [Weinberger](#page-7-14) *et al.*, [2005;](#page-7-14) [Schroff](#page-7-15) *et al.*, 2015]. By leveraging various types of supervision extracted from examples, such as linkages and comparisons, distance metric learning aims to align the learned distance metrics with the intrinsic relationships between examples, i.e. similar instances are close to each other and dissimilar instances are far away from each other. In distance metric learning, the Mahalanobis metric is extensively employed as a substitute for the Euclidean metric due to its broad applicability as a general form of the Euclidean metric and its effcient optimization capabilities [Ye *et al.*[, 2019;](#page-8-5) Ye *et al.*[, 2020;](#page-8-6) Ren *et al.*[, 2022;](#page-7-16) [Zhao and Yang, 2023\]](#page-8-7). The Mahalanobis distance between instances is essentially equivalent to the Euclidean distance within the metric space. The superiority of distance metric learning has been substantiated in improving KNN classifers on single-label examples [Liao *et al.*[, 2021;](#page-7-17) Song *et al.*[, 2021;](#page-7-5) Li *et al.*[, 2022;](#page-7-18) Chen *et al.*[, 2023\]](#page-7-7). With the effective modeling of semantic similarity among examples accomplished by distance metric learning, there is the potential for simple KNN classifers to achieve state-of-the-art classifcation performance.

Multi-Label Metric Learning. In recent years, distance metric learning has been extended to the multi-label scenario to measure the more complicated semantic similarities between multi-label examples. To the best of our knowledge, there are four available multi-label metric learning approaches, namely LM [\[Liu and Tsang, 2015\]](#page-7-8), LJE [\[Gouk](#page-7-9) *et al.*[, 2016\]](#page-7-9), COMMU [\[Sun and Zhang, 2021\]](#page-7-10), and LIMIC [\[Mao](#page-7-11) *et al.*[, 2023\]](#page-7-11). LM utilizes a large margin formulation to create a shared metric space, preserving the similarity relationships from the feature space to the label space. LJE learns a metric that projects instances into a metric space, where the Euclidean distance is a good approximation of the Jaccard distance between labels. COMMU constructs a compositional metric by modeling structural interactions between the feature and label spaces, exploring the integrated semantics of all labels. LIMIC learns a consistent metric in each label space and employs label co-occurrence to constrain the dependencies between multiple metrics. The multi-label metric learning approaches above all learn consistent metrics across all instances in the label space, which might be suboptimal as they neglect the fact that multi-label instances exhibit nonlinear distribution characteristics in each label space. In the next section, our proposed LSMM framework is introduced.

### 3 The LSMM Framework

### 3.1 Preliminaries

Let  $\mathcal{X} = \mathbb{R}^d$  denote the input space and  $\mathcal{Y} = \{l_1, l_2, \dots, l_q\}$ denote the label space with  $q$  labels. A multi-label example is denoted as  $(x, Y)$ , where  $x \in \mathcal{X}$  is its feature vector and  $Y \subseteq Y$  corresponds to the set of its relevant labels. Here, a *q*dimensional indicator vector  $y = [y^1, y^2, \dots, y^q] \in \{0, 1\}^q$ 

is utilized to denote Y, where  $y^p = 1$  when  $l_p \in Y$  and  $y^p =$ 0 otherwise. Generally speaking, multi-label classifcation aims to induce a multi-label prediction function  $h: \mathcal{X} \to 2^{\mathcal{Y}}$ from a multi-label data set  $\mathcal{D} = \{(\boldsymbol{x}_i, Y_i) \mid 1 \leq i \leq n\}.$ Given an unseen instance  $x' \in \mathcal{X}$ , its associated label set is predicted as  $h(x') \subseteq Y$ .

Let  $\mathbb{S}^d_+$  denotes the cone of Positive Semi-Definite (PSD)  $d \times d$  matrices. Given a metric  $\mathbf{M} \in \mathbb{S}^d_+$ , the (squared) Mahalanobis distance between a pair  $(\boldsymbol{x}_i,\boldsymbol{x}_j)$  is  $(\boldsymbol{x}_i{-}\boldsymbol{x}_j)^\top \mathbf{M} (\boldsymbol{x}_i{-}$  $\mathbf{x}_j = \langle \mathbf{M}, \mathbf{A}_{ij} \rangle = \text{Tr}(\mathbf{M} \mathbf{A}_{ij})$ . The outer product of the pair difference is  $\mathbf{A}_{ij} = (\mathbf{x}_i - \mathbf{x}_j)(\mathbf{x}_i - \mathbf{x}_j)^{\top} \in \mathbb{S}^d_+$  [\[Bellet](#page-7-19) *et al.*, [2015\]](#page-7-19). By decomposing the metric into the inner product of transformations  $\mathbf{L}(\mathbf{L} \in \mathbb{R}^{d \times d'}, d' \leq d)$  as  $\mathbf{M} = \mathbf{L}\mathbf{L}^{\top}$ , the (square) Mahalanobis distance between two instances is equal to their Euclidean distance in a projected space, i.e.

$$
\mathrm{Dis}_{\mathbf{M}}^{2}(\boldsymbol{x}_{i}, \boldsymbol{x}_{j}) = (\boldsymbol{x}_{i} - \boldsymbol{x}_{j})^{\top} \mathbf{M}(\boldsymbol{x}_{i} - \boldsymbol{x}_{j})
$$
\n
$$
\iff \mathrm{Dis}_{\mathbf{L}}^{2}(\boldsymbol{x}_{i}, \boldsymbol{x}_{j}) = (\boldsymbol{x}_{i} - \boldsymbol{x}_{j})^{\top} \mathbf{L} \mathbf{L}^{\top}(\boldsymbol{x}_{i} - \boldsymbol{x}_{j}) \qquad (1)
$$
\n
$$
= ||\mathbf{L}^{\top}(\boldsymbol{x}_{i} - \boldsymbol{x}_{j})||_{2}^{2}.
$$

Generally speaking, there are several advantages to learning transformation L rather than metric M. On one hand, transformation L does not have a PSD constraint, eliminating the need for a PSD projection step, in turn, accelerates the optimization process [\[Kulis, 2013\]](#page-7-20). In addition, the transformation decomposition often leads to low-rank metrics, proving advantageous in many real-world applications [\[Zhang and](#page-8-8) [Zhang, 2017\]](#page-8-8). It is also noteworthy that although the decomposition leads to non-convex problems, satisfactory solutions can still be obtained. Based on the above consideration, we learn transformation L rather than metric M in this paper.

#### 3.2 Label-Specifc Multi-Metric Learning

To begin with, we introduce the construction procedure of label-specifc side information, which is used to direct the learning process of metrics.

For the p-th label  $l_p$ , the set of positive examples  $\mathcal{P}_p$  as well as the set of negative examples  $\mathcal{N}_p$  are determined by considering the relevance of each example to  $l_p$ , i.e.

$$
\mathcal{P}_p = \{ \boldsymbol{x}_i | (\boldsymbol{x}_i, Y_i) \in \mathcal{D}, l_p \in Y_i \},
$$
  
\n
$$
\mathcal{N}_p = \{ \boldsymbol{x}_i | (\boldsymbol{x}_i, Y_i) \in \mathcal{D}, l_p \notin Y_i \}.
$$
\n(2)

The label-specific side information w.r.t the label  $l_p$  is constructed from all possible pairwise combinations of training examples, denoted as  $\mathcal{T}_p = \{ (x_i, x_j, \theta_{ij}^p) \}$ , where  $\theta_{ij}^p \in$  $\{-1, 1\}$  indicates whether  $x_i$  and  $x_j$  share relevance w.r.t the label  $l_p$ . Specifically,  $\theta_{ij}^p = 1$  implies that instances  $x_i$  and  $x_j$  are considered similar due to their simultaneous presence (or absence) of the label  $l_p$ , i.e.  $(\mathbf{x}_i \in \mathcal{P}_p \land \mathbf{x}_j \in \mathcal{P}_p) \lor (\mathbf{x}_i \in \mathcal{P}_p)$  $\mathcal{N}_p \wedge \mathbf{x}_j \in \mathcal{N}_p$ , while  $\theta_{ij}^p$  equals -1 otherwise. Let  $T_p$  represent the number of pairs in  $\mathcal{T}_p$ , and  $(x_i, x_j) \sim \mathcal{T}_p$  denote the enumeration of a total of  $T_p$  pairs from the label-specific side information  $\mathcal{T}_p$ . In practice, there is no need to compute all pairs of side information, as this may lead to substantial computational burden. Opting for a judicious selection of targets (denoted as  $k_t$ ) and imposters (denoted as  $k_i$ ) among the nearest neighbors can mitigate computational load and enhance the efficiency of the training procedure, where targets indicate instances similar to an anchor and imposters otherwise. [\[Weinberger and Saul, 2009;](#page-7-21) Ye *et al.*[, 2019;](#page-8-5) Ye *et al.*[, 2020\]](#page-8-6). In this paper,  $k_t$  and  $k_i$  are set to 20.

Next, we present two simple yet effective partition strategies, i.e. semantic-based partition and cluster-based partition, designed to divide each label space into several disjoint partitions. In each partition, a local metric is trained to separate the instances locally. Furthermore, a global metric is introduced to implicitly exploit high-order label correlations across all labels. In this way, different instances can be measured with the combination of a global metric and corresponding labelspecifc local metrics, as opposed to a consistent metric.

Semantic-based Partition. The first strategy is to assign different local metrics to positive and negative examples in each label space. For the  $p$ -th label  $l_p$ , the (squared) distance between a pair  $(\boldsymbol{x}_i, \boldsymbol{x}_j)$  is calculated as

<span id="page-2-1"></span>
$$
Dis_{\mathbf{L}_0+\mathbf{L}_p^{s(\mathbf{x}_i)}}^2(\mathbf{x}_i,\mathbf{x}_j)=||(\mathbf{L}_0+\mathbf{L}_p^{s(\mathbf{x}_i)})^\top(\mathbf{x}_i-\mathbf{x}_j)||_2^2.
$$
 (3)

Here,  $s(x_i) = y_i^p \in \{0, 1\}$  is a semantic indicator function.  $L_0$  serves as the foundation to reveal the common characteristics among multi-label examples, while the label-specifc local metric  $\mathbf{L}_p^{s(x_i)}$  act as a local bias, depicting the individuality of  $x_i$  in the p-th label space. Our purpose is to push similar instances closer, while dissimilar instances far away from each other. Therefore, we formulate the following optimization problem:

<span id="page-2-0"></span>
$$
\ell_{\text{pos}}^{p} = \frac{1}{|\mathcal{P}_p|} \sum_{\substack{(\boldsymbol{x}_i, \boldsymbol{x}_j) \sim \mathcal{T}_p \\ \boldsymbol{x}_i \in \mathcal{P}_p}} \ell\left(\theta_{ij}^p \left(\gamma - \alpha \text{Dis}_{\mathbf{L}_0 + \mathbf{L}_p^1}^2(\boldsymbol{x}_i, \boldsymbol{x}_j)\right)\right)
$$

$$
\ell_{\text{neg}}^p = \frac{1}{|\mathcal{N}_p|} \sum_{\substack{(\boldsymbol{x}_i, \boldsymbol{x}_j) \sim \mathcal{T}_p \\ \boldsymbol{x}_i \in \mathcal{N}_p}} \ell\left(\theta_{ij}^p \left(\gamma - \alpha \text{Dis}_{\mathbf{L}_0 + \mathbf{L}_p^0}^2(\boldsymbol{x}_i, \boldsymbol{x}_j)\right)\right)
$$

$$
\min_{\mathbf{L}_0, \{\mathbf{L}_p^1, \mathbf{L}_p^0\}_{p=1}^q} \frac{1}{q} \sum_{p=1}^q \left(\ell_{\text{pos}}^p + \ell_{\text{neg}}^p\right) + \frac{\lambda_1}{2q} \sum_{p=1}^q \sum_{t=0}^1 ||\mathbf{L}_p^t||_F^2
$$

$$
+\lambda_2||{\bf L}_0||_F^2. \qquad (4)
$$

Here,  $\gamma$  and  $\alpha$  are predefined non-negative threshold values, which can differ for similar and dissimilar pairs.  $\ell(\cdot)$  is a convex and non-increasing loss function. If two instances  $x_i, x_j$ possess (or do not possess) the label  $l_p$  simultaneously, i.e.  $\theta_{ij}^p = 1$ , then the loss equals 0 when their distance is smaller than  $\gamma/\alpha$ . Conversely, when they are dissimilar  $(\theta_{ij}^p = -1)$ , their distance should exceed  $\gamma/\alpha$ . By optimizing Eq.[\(4\)](#page-2-0), the learned metrics require that similar instances have small distances, while dissimilar instances are sufficiently far apart. Besides,  $\lambda_1$  and  $\lambda_2$  serve as non-negative weights to balance the impact of the regularization terms. Intuitively, for a fxed value of  $\lambda_2$ , a large value of the ratio  $\lambda_1/\lambda_2$  tends to make the model learn a single global metric  $\mathbf{L}_0$  across all labels ( $\mathbf{L}_p^t$ are nearly equal to zero). Conversely, for a fixed  $\lambda_1$ , a small value of the ratio  $\lambda_1/\lambda_2$  tends to make all label-specific local metrics unrelated  $(L_0$  nearly equal to zero). In this paper,  $\gamma$  and  $\alpha$  are fixed to 2 and 0.4 respectively, and the smooth hinge loss is used to instantiate  $\ell(\cdot)$ , which is defined as

$$
\ell(x) = \begin{cases} 0, & \text{if } x > 1 \\ \frac{1}{2}(x-1)^2, & \text{if } 0 \le x \le 1 \\ \frac{1}{2} - x, & \text{if } x < 0. \end{cases}
$$
 (5)

The smoothness property of this loss function will facilitate the optimization process. Besides,  $\ell(\cdot)$  also keeps a small margin besides  $\gamma$  and  $\alpha$ , which further improves the generalization ability of the learned metrics.

Cluster-based Partition. The second strategy is to assign different metrics to different clusters. In this paper, the popular k-means algorithm [Jain *et al.*[, 1999\]](#page-7-22) is adopted due to its effectiveness and simplicity. Assuming that all multi-label instances are divided into C disjoint clusters  $\mathcal{D} = \mathcal{C}^1 \cup \mathcal{C}^2 \ldots \cup$  $\mathcal{C}^C$ , the (squared) distance between a pair  $(x_i, x_j)$  in the p-th label space is calculated as

$$
\text{Dis}_{\mathbf{L}_0 + \mathbf{L}_p^{c(\mathbf{x}_i)}}^2(\mathbf{x}_i, \mathbf{x}_j) = ||(\mathbf{L}_0 + \mathbf{L}_p^{c(\mathbf{x}_i)})^\top(\mathbf{x}_i - \mathbf{x}_j)||_2^2.
$$
 (6)

Here,  $c(\mathbf{x}_i) \in \{0, 1, \dots, C\}$  is a cluster indicator function. The optimization problem is formulated as follows:

<span id="page-3-0"></span>
$$
\ell_m^p = \frac{1}{|\mathcal{C}^m|} \sum_{\substack{(\boldsymbol{x}_i, \boldsymbol{x}_j) \sim \mathcal{T}_p \\ \boldsymbol{x}_i \in \mathcal{C}^m}} \ell\left(\theta_{ij}^p \left(\gamma - \alpha \text{Dis}_{\mathbf{L}_0 + \mathbf{L}_p^m}^2(\boldsymbol{x}_i, \boldsymbol{x}_j)\right)\right)
$$
  

$$
\min_{\mathbf{L}_0, \{\mathbf{L}_p^1, \mathbf{L}_p^2, \dots, \mathbf{L}_p^C\}_{p=1}^q} \frac{1}{q} \sum_{p=1}^q \sum_{m=1}^C \ell_m^p + \frac{\lambda_1}{Cq} \sum_{p=1}^q \sum_{t=1}^C ||\mathbf{L}_p^t||_F^2 + \lambda_2 ||\mathbf{L}_0||_F^2. \tag{7}
$$

In this paper,  $C$  is set to 3. Besides, the similar instantiations and properties have been elaborated on in the previous paragraph. Therefore, we do not repeat them here.

#### 3.3 Optimization Procedure

In order to solve the unconstrained nonlinear optimization problems as shown in Eq. $(4)$  and Eq. $(7)$ , we employ the *Limited-memory Broyde-Fletcher-Golfarb-Shanno* (L-BFGS) algorithm [\[Liu and Nocedal, 1989\]](#page-7-23), which is particularly suited for problems with a large number of optimization variables. Let  $\mathcal{L}_{se}$  and  $\mathcal{L}_{cl}$  denote the objective functions of the semantic-based and cluster-based partition strategies in Eq.[\(4\)](#page-2-0) and Eq.[\(7\)](#page-3-0) respectively. L-BFGS iteratively optimizes the objective functions with resort to the frst-order derivatives of the functions.

For the semantic-based partition strategy, the frst-order derivatives of  $\mathcal{L}_{se}$  w.r.t  $\mathbf{L}_0$  and  $\left\{ \mathbf{L}_p^1, \mathbf{L}_p^0 \right\}_{p=1}^q$  respectively are

$$
\frac{\partial \mathcal{L}_{se}}{\partial \mathbf{L}_{0}} = \frac{2}{q} \sum_{p=1}^{q} \left( \frac{1}{|\mathcal{P}_{p}|} \sum_{\substack{(\mathbf{x}_{i}, \mathbf{x}_{j}) \sim \mathcal{T}_{p} \\ \mathbf{x}_{i} \in \mathcal{P}_{p}}} \sigma_{ij}^{p} \theta_{ij}^{p} \mathbf{A}_{ij} \left( \mathbf{L}_{0} + \mathbf{L}_{p}^{1} \right) \right) \n+ \frac{1}{|\mathcal{N}_{p}|} \sum_{\substack{(\mathbf{x}_{i}, \mathbf{x}_{j}) \sim \mathcal{T}_{p} \\ \mathbf{x}_{i} \in \mathcal{N}_{p}}} \sigma_{ij}^{p} \theta_{ij}^{p} \mathbf{A}_{ij} \left( \mathbf{L}_{0} + \mathbf{L}_{p}^{0} \right) \right) + 2 \lambda_{2} \mathbf{L}_{0}
$$
\n(8)

$$
\frac{\partial \mathcal{L}_{se}}{\partial \mathbf{L}_{p}^{1}} = \frac{2}{q|\mathcal{P}_{p}|} \sum_{\substack{(\mathbf{x}_{i}, \mathbf{x}_{j}) \sim \mathcal{T}_{p} \\ \mathbf{x}_{i} \in \mathcal{P}_{p}}} \sigma_{ij}^{p} \theta_{ij}^{p} \mathbf{A}_{ij} \left( \mathbf{L}_{0} + \mathbf{L}_{p}^{1} \right) + \frac{\lambda_{1}}{q} \mathbf{L}_{p}^{1}
$$
\n(9)

$$
\frac{\partial \mathcal{L}_{se}}{\partial \mathbf{L}_{p}^{0}} = \frac{2}{q|\mathcal{N}_{p}|} \sum_{\substack{(\mathbf{x}_{i}, \mathbf{x}_{j}) \sim \mathcal{T}_{p} \\ \mathbf{x}_{i} \in \mathcal{N}_{p}}} \sigma_{ij}^{p} \theta_{ij}^{p} \mathbf{A}_{ij} \left( \mathbf{L}_{0} + \mathbf{L}_{p}^{0} \right) + \frac{\lambda_{1}}{q} \mathbf{L}_{p}^{0}
$$
\n(10)

<span id="page-3-1"></span>where  $\sigma_{ij}^p$  is a piecewise function defined as follows:

$$
\sigma_{ij}^p = \begin{cases}\n0, & \text{if } \delta_{ij}^p > 1 \\
\alpha \left(1 - \delta_{ij}^p\right), & \text{if } 0 \le \delta_{ij}^p \le 1 \\
\alpha, & \text{if } \delta_{ij}^p < 0.\n\end{cases}
$$
\n(11)

$$
\delta_{ij}^p = \theta_{ij}^p \left( \gamma - \alpha \text{Dis}_{\mathbf{L}_0 + \mathbf{L}_p^{s(\mathbf{x}_i)}}^2(\mathbf{x}_i, \mathbf{x}_j) \right)
$$
(12)

For the cluster-based partition strategy, the frst-order derivatives of  $\mathcal{L}_{cl}$  w.r.t  $\mathbf{L}_0$  and  $\left\{ \mathbf{L}_p^1, \mathbf{L}_p^2, \ldots, \mathbf{L}_p^C \right\}_{p=1}^q$  respectively are

$$
\frac{\partial \mathcal{L}_{cl}}{\partial \mathbf{L}_0} = \frac{2}{q} \sum_{p=1}^q \sum_{m=1}^C \frac{1}{|\mathcal{C}^m|} \sum_{\substack{(\mathbf{x}_i, \mathbf{x}_j) \sim \mathcal{T}_p \\ \mathbf{x}_i \in \mathcal{C}^m}} \zeta_{ij}^p \theta_{ij}^p \mathbf{A}_{ij} \left( \mathbf{L}_0 + \mathbf{L}_p^m \right) + 2\lambda_2 \mathbf{L}_0
$$
\n(13)

$$
\frac{\partial \mathcal{L}_{cl}}{\partial \mathbf{L}_{p}^{m}} = \frac{2}{q|\mathcal{C}^{m}|} \sum_{\substack{(\boldsymbol{x}_{i}, \boldsymbol{x}_{j}) \sim \mathcal{T}_{p} \\ \boldsymbol{x}_{i} \in \mathcal{C}^{m}}} \zeta_{ij}^{p} \theta_{ij}^{p} \mathbf{A}_{ij} \left( \mathbf{L}_{0} + \mathbf{L}_{p}^{m} \right) + \frac{2\lambda_{1}}{Cq} \mathbf{L}_{p}^{m}
$$
\n(14)

where  $\zeta_{ij}^p$  is a piecewise function defined as follows:

$$
\zeta_{ij}^p = \begin{cases}\n0, & \text{if } \xi_{ij}^p > 1 \\
\alpha \left(1 - \xi_{ij}^p\right), & \text{if } 0 \le \xi_{ij}^p \le 1 \\
\alpha, & \text{if } \xi_{ij}^p < 0.\n\end{cases}
$$
\n(15)

$$
\xi_{ij}^p = \theta_{ij}^p \left( \gamma - \alpha \text{Dis}_{\mathbf{L}_0 + \mathbf{L}_p^{c(\mathbf{x}_i)}}^2(\mathbf{x}_i, \mathbf{x}_j) \right)
$$
(16)

The complete procedure of LSMM can be found in Appendix A. After learning the global metric and label-specifc multiple local metrics with the above LSMM framework, the distances between multi-label instances can be measured with the combination of the global metric and corresponding labelspecifc local metrics according to Eq.[\(3\)](#page-2-1) and Eq.[\(6\)](#page-3-1). Therefore, the associated label set of an unseen multi-label instance can be easily predicted by resorting to KNN-based multi-label classifers, such as BR-KNN and ML-KNN.

<span id="page-4-0"></span>

1 <http://mulan.sourceforge.net/datasets.html>

2 <http://palm.seu.edu.cn/zhangml/Resources.htm#data>

3 <https://waikato.github.io/meka/datasets/>

Table 1: Characteristics of experimental datasets.

# 4 Experiments

#### 4.1 Experimental Setup

Datasets. Nine benchmark multi-label datasets with diversifed properties are employed for comprehensive performance evaluation. Table [1](#page-4-0) summarizes the characteristics of each experimental dataset  $D$ , including the number of examples  $|\mathcal{D}|$ , number of features  $dim(\mathcal{D})$ , number of labels  $L(\mathcal{D})$ , label cardinality  $LCard(\mathcal{D})$ , and domain of datasets. For all the datasets except emotions and birds, we use principal component analysis as a preprocessing to reduce the dimensionality and retain 95% of the information.

Evaluation metrics. For performance evaluation, six widely-used evaluation metrics are utilized for multi-label classifcation, including *Hamming loss*, *Ranking loss*, *Coverage*, *Average precision*, *Macro-F1*, and *Macro-averaging AUC*. Detailed defnitions of these metrics can be found in [\[Zhang and Zhou, 2014\]](#page-8-0).

#### 4.2 Comparative Studies

To validate the effectiveness of the proposed LSMM framework in learning effective similarity metrics for multi-label classifcation, BR-KNN [\[Boutell](#page-7-12) *et al.*, 2004] and ML-KNN [\[Zhang and Zhou, 2007\]](#page-8-1) are introduced as subsequent multilabel classifcation methods after learning similarity metrics. Our semantic-based and cluster-based partition approaches are denoted as LSMM-SE and LSMM-CL respectively.

Given a KNN-based multi-label classifcation approach  $A \in \{BR-KNN, ML-KNN\}$  and a multi-label metric learning algorithm  $\beta$ , the coupling version of them is denoted as  $A-B$ . The predictive performance of  $A$ -LSMM-SE and  $A$ -LSMM-CL are compared against other state-of-the-art multilabel metric learning algorithms coupled with  $A$  to manifest whether the proposed LSMM framework does learn effective similarity metrics and improve the generalization performance of KNN-based multi-label classifcation.

In this paper, four state-of-the-art multi-label metric learning algorithms are employed to instantiate  $\beta$  with suggested parameter confgurations in respective literature:

• LM [\[Liu and Tsang, 2015\]](#page-7-8): A margin-based multi-label metric learning approach that learns a shared metric by preserving the similarity relation from the feature to label space [suggested configuration:  $\eta = 0.4$ ,  $C = 10$ ].

- LJE [Gouk *et al.*[, 2016\]](#page-7-9): An integration-based multilabel metric learning approach that employs Jaccard distance between labels to provide more fne-grained side information [suggested configuration:  $t = 32$ ,  $e = 5$ ].
- COMMU [\[Sun and Zhang, 2021\]](#page-7-10): A composition-based multi-label metric learning approach that learns a compositional metric by modeling structural interactions between the feature and label space [suggested confguration:  $\alpha, \theta \in \{0.2, 0.4, \ldots, 0.8\}, C = 10$ .
- LIMIC [Mao *et al.*[, 2023\]](#page-7-11): A decomposition-based multi-label metric learning approach that learns a consistent metric in each label space and employs label cooccurrence to constrain the dependencies between multiple metrics [suggested configuration:  $\gamma = 2$ ,  $\lambda_1, \lambda_2 \in$  $\{10^{-3}, 10^{-1}, \ldots, 10^{3}\}.$

For the proposed LSMM-SE and LSMM-CL approaches, regularization parameters  $\lambda_1$  and  $\lambda_2$  are searched in  $\{10^{-1}, 1, \ldots, 10^3\}$  and  $\{10^{-3}, 10^{-2}, \ldots, 10\}$  respectively. The number of nearest neighbors (denoted as  $k$ ) in KNN and ML-KNN is set to 10, which is consistent with previous multilabel metric learning works for fair comparisons. We take out 10% examples in each dataset as a hold out validation set for hyperparameter searching and perform ten-fold crossvalidation on the remaining 90% examples to evaluate the above approaches on the nine benchmark multi-label datasets.

Due to page limit, Table [2](#page-5-0) reports detailed experimental results in terms of *Hamming loss* and *Ranking loss*. The results on other metrics can be found in Appendix B.1. Furthermore, pairwise t-test [\[Dietterich, 1998\]](#page-7-24) at 0.05 signifcance level is conducted to demonstrate whether the performance difference between LSMM-SE (LSMM-CL) and other comparing multi-label metric learning algorithms coupled with  $A \in \{BR-KNN, ML-KNN\}$  is significant statistically, where the resulting win/tie/loss counts are also reported in Appendix B.1. Based on these results, it is impressive to observe that:

- The prediction performance of BR-KNN and ML-KNN is signifcantly improved after coupling multi-label metric learning algorithms. In particular, our proposed LSMM-SE (LSMM-CL) approach signifcantly enhances the performance of BR-KNN and ML-KNN in 88.9% (92.6%) and 94.4% (92.6%) of cases, respectively. The results clearly demonstrate the effectiveness of multi-label metric learning for improving KNN-based multi-label classifcation methods.
- Across all evaluation metrics, our proposed LSMM-SE and LSMM-CL approaches have demonstrated signifcantly improved performance compared to other multilabel metric learning algorithms. One one hand, in terms of BR-KNN, LSMM-SE (LSMM-CL) signifcantly outperforms LM, LJE, COMMU, and LIMIC in 75.9% (87%), 94.4% (100%), 87% (88.9%), and 77.8% (85.2%) of cases, respectively. On the other hand, in terms of ML-KNN, LSMM-SE (LSMM-CL) signifcantly outperforms them in 81.5% (85.2%), 100% (100%), 94.4% (94.4%), and 72.2% (75.9%) of cases, respectively. The superior

Proceedings of the Thirty-Third International Joint Conference on Artificial Intelligence (IJCAI-24)

<span id="page-5-0"></span>

Compared	<b>Datasets</b>								
Algorithms	emotions	birds	medical	enron	image	scene	slashdot	arts	education
	Hamming Loss $\downarrow$								
<b>BR-KNN</b>	$0.263 \pm 0.023$	$0.056 + 0.007$	$0.016 + 0.002$ $0.055 + 0.002$ $0.167 + 0.016$ $0.088 + 0.008$ $0.065 + 0.001$					$0.073 + 0.002$	$0.038 \pm 0.001$
BR-KNN-LM	$0.270 + 0.019$	$0.065 + 0.009$	$0.011 + 0.002$ $0.048 + 0.003$		$0.180 + 0.016$ $0.088 + 0.012$		$0.044 + 0.003$	$0.055 + 0.002$	$0.038 \pm 0.001$
<b>BR-KNN-LJE</b>	$0.219 + 0.022$	$0.055 + 0.007$	$0.022 + 0.003$	$0.059 + 0.003$	$0.184 + 0.018$ $0.110 + 0.011$		$0.060 + 0.002$	$0.061 + 0.001$	$0.043 \pm 0.002$
<b>BR-KNN-COMMU</b>	$0.263 + 0.023$	$0.056 + 0.007$	$0.016 + 0.002$ $0.055 + 0.002$		$0.167 + 0.016$ $0.088 + 0.008$		$0.056 + 0.001$	$0.072 \pm 0.002$	$0.038 \pm 0.001$
BR-KNN-LIMIC	$0.212 + 0.008$		$0.053 + 0.006$ $0.014 + 0.002$ $0.049 + 0.003$ $0.165 + 0.016$ $0.083 + 0.008$				$0.045 \pm 0.002$	$0.058 + 0.002$	$0.039 + 0.001$
BR-KNN-LSMM-SE	$0.204 + 0.018$		$0.051 + 0.006$ $0.014 + 0.003$ $0.045 + 0.003$ $0.162 + 0.013$			$0.081 + 0.007$	$0.035 + 0.002$	$0.054 \pm 0.001$	$0.037 + 0.002$
BR-KNN-LSMM-CL	$0.202 \pm 0.017$	$0.050\!\pm\!0.007$	$0.012 \pm 0.002$ 0.044 $\pm$ 0.003		$0.157 \pm 0.017$	$0.079 \pm 0.009$	$0.037 \pm 0.002$	$0.052 \pm 0.002$	$0.038 \pm 0.001$
ML-KNN	$0.262 + 0.022$		$0.054 \pm 0.006$ $0.016 \pm 0.002$ $0.052 \pm 0.003$ $0.171 \pm 0.013$ $0.084 \pm 0.009$				$0.058 + 0.001$	$0.060 + 0.001$	$0.038 \pm 0.001$
ML-KNN-LM	$0.254 + 0.017$	$0.054 + 0.007$	$0.013 + 0.002$ $0.048 + 0.002$ $0.174 + 0.015$			$0.086 + 0.010$	$0.045 + 0.003$	$0.054 \pm 0.001$	$0.038 \pm 0.001$
ML-KNN-LJE	$0.227 + 0.022$	$0.054 + 0.007$	$0.023 + 0.003$	$0.058 + 0.002$ $0.184 + 0.017$		$0.109 + 0.009$	$0.056 + 0.001$	$0.060 + 0.001$	$0.042 + 0.002$
ML-KNN-COMMU	$0.262 + 0.022$		$0.054 + 0.006$ $0.015 + 0.002$ $0.052 + 0.003$		$0.171 + 0.013$	$0.084 \pm 0.009$	$0.050 + 0.001$	$0.059 + 0.001$	$0.038 \pm 0.001$
ML-KNN-LIMIC			$0.215 + 0.009$ $0.053 + 0.006$ $0.013 + 0.002$ $0.050 + 0.003$ $0.164 + 0.017$			$0.082 + 0.007$	$0.050 + 0.003$	$0.057 + 0.002$	$0.038 \pm 0.002$
ML-KNN-LSMM-SE			$0.204 \pm 0.016$ $0.050 \pm 0.005$ $0.012 \pm 0.003$ $0.043 \pm 0.002$ $0.159 \pm 0.014$			$0.080 \pm 0.007$	$0.041 \pm 0.002$	$0.053 \pm 0.001$	$0.037 \pm 0.001$
ML-KNN-LSMM-CL			$0.209 \pm 0.018$ $0.051 \pm 0.006$ $0.012 \pm 0.002$ $0.045 \pm 0.003$ $0.155 \pm 0.013$ $0.078 \pm 0.007$				$0.039 \pm 0.003$	$0.052 + 0.001$	$0.038 + 0.001$
					Ranking Loss $\downarrow$				
<b>BR-KNN</b>			$0.272+0.048$ $0.516+0.064$ $0.081+0.028$ $0.228+0.023$ $0.180+0.020$ $0.095+0.014$ $0.417+0.026$ $0.354+0.029$ $0.244+0.013$						
BR-KNN-LM			$0.256 + 0.030$ $0.527 + 0.066$ $0.105 + 0.033$ $0.201 + 0.011$ $0.191 + 0.020$ $0.097 + 0.016$ $0.221 + 0.021$ $0.257 + 0.015$ $0.222 + 0.014$						
<b>BR-KNN-LJE</b>		$0.202 + 0.035$ 0.497 + 0.067	$0.114 + 0.037$ $0.244 + 0.027$		$0.205 + 0.020$ $0.124 + 0.019$		$0.345 + 0.024$	$0.265 + 0.015$ $0.234 + 0.012$	
BR-KNN-COMMU			$0.272 + 0.048$ $0.516 + 0.064$ $0.088 + 0.031$ $0.230 + 0.023$ $0.180 + 0.020$			$0.095 \pm 0.014$	$0.407 + 0.027$	$0.357 + 0.033$ $0.244 + 0.013$	
BR-KNN-LIMIC	$0.182 + 0.028$		$0.513 + 0.066$ $0.077 + 0.023$ $0.245 + 0.020$		$0.171 + 0.024$	$0.102 \pm 0.011$	$0.393 + 0.023$	$0.348 + 0.021$	$0.220 + 0.015$
BR-KNN-LSMM-SE		$0.170 + 0.033$ $0.472 + 0.061$	0.065 $\pm$ 0.018 0.194 $\pm$ 0.026 0.157 $\pm$ 0.021			$0.092 + 0.011$		$0.201 \pm 0.018$ $0.263 \pm 0.010$ $0.210 \pm 0.010$	
BR-KNN-LSMM-CL			$0.178 \pm 0.034$ $0.487 \pm 0.058$ $0.071 \pm 0.023$ $0.192 \pm 0.022$		$0.150\!\pm\!0.025$	$0.090 \pm 0.013$ $0.190 \pm 0.025$		$0.258 \pm 0.027$	$0.205 \pm 0.012$
ML-KNN	$0.258 + 0.038$		$0.295 + 0.035$ $0.032 + 0.009$ $0.091 + 0.010$ $0.173 + 0.018$ $0.075 + 0.011$				$0.182 + 0.013$	$0.148 + 0.008$	$0.097 + 0.004$
ML-KNN-LM		$0.240 + 0.026$ $0.298 + 0.047$	$0.034 + 0.015$ $0.090 + 0.008$ $0.177 + 0.018$ $0.078 + 0.012$ $0.112 + 0.008$					$0.129 + 0.007$	$0.078 + 0.005$
ML-KNN-LJE		$0.201 + 0.030$ $0.299 + 0.047$	$0.053 + 0.017$ $0.111 + 0.011$ $0.201 + 0.022$			$0.110 + 0.017$	$0.198 + 0.013$	$0.145 + 0.009$ $0.089 + 0.003$	
ML-KNN-COMMU		$0.258 + 0.038$ $0.295 + 0.035$	$0.038 + 0.013$ $0.091 + 0.010$ $0.173 + 0.018$			$0.075 + 0.011$		$0.159 + 0.012$ $0.147 + 0.008$ $0.097 + 0.004$	
ML-KNN-LIMIC	$0.184 \pm 0.020$	$0.263 + 0.039$		$0.031 + 0.012$ $0.088 + 0.010$	$0.163 + 0.022$	$0.072 + 0.007$	$0.133 + 0.009$	$0.137 + 0.006$ $0.079 + 0.004$	
ML-KNN-LSMM-SE			$0.166 + 0.033$ $0.256 + 0.034$ $0.034 + 0.015$ $0.075 + 0.007$		$0.157 + 0.021$	$0.072 + 0.004$	$0.095 + 0.008$	$0.123 + 0.006$ $0.078 + 0.004$	
ML-KNN-LSMM-CL 0.170 $\pm$ 0.036 0.260 $\pm$ 0.038 0.038 $\pm$ 0.013 0.073 $\pm$ 0.009 0.146 $\pm$ 0.020 0.069 $\pm$ 0.005							$0.083 \pm 0.007$	$0.120 + 0.005$ $0.074 + 0.004$	

Table 2: Predictive performance (mean $\pm$ std) of  $A(A \in \{BR\text{-KNN}, ML\text{-KNN}\})$  coupled with our proposed approaches and state-of-the-art multi-label metric learning approaches in terms of *Hamming Loss* and *Ranking Loss*. ↑ (↓) indicates the larger (smaller) the value, the better the performance. The best and second best results are highlighted in **boldface** and underline respectively.

performance provides persuasive evidence for our proposed LSMM framework in learning effective similarity metrics for multi-label classifcation.

In addition to comparing our proposed LSMM-SE and LSMM-CL with state-of-the-art multi-label metric learning algorithms, we further evaluate LSMM-enhanced BR-KNN and ML-KNN against four state-of-the-art non-metric learning multi-label classifcation approaches with different order of label correlations under consideration:

- LIFT [\[Zhang and Wu, 2014\]](#page-8-9): A frst-order multi-label classifcation approach that exploits label-specifc features [suggested configuration:  $r = 0.1$ ].
- RELIAB [\[Zhang](#page-8-4) *et al.*, 2021]: A high-order multi-label classifcation approach that leverages implicit relative labeling-importance information [suggested confguration: mode = *global*,  $\tau \in \{0.1, 0.2, \ldots, 0.5\}$ , and  $\lambda \in$  $\{10^{-3}, 10^{-2}, \ldots, 10\}$ ].
- WRAP [\[Yu and Zhang, 2021\]](#page-8-3): A second-order multi-label classifcation approach that jointly performs label-specifc feature generation and classifcation model induction [suggested configuration:  $\lambda_1, \lambda_2 \in$  $\{0, 1, \ldots, 10\}, \lambda_3 = 10$ , and  $\alpha = 0.9$ ].
- HOMI [Si *et al.*[, 2023\]](#page-7-13):A high-order multi-label classifcation approach that constrains the high-rank of

the label matrix and depict high-order label correlations explicitly [suggested configuration:  $\beta, \gamma, \in$  $\{10^{-2}, 10^{-1}, \ldots, 10^{2}\}, \lambda = 1, s = 10$ ].

Detailed experimental results and resulting win/tie/loss counts of pairwise  $t$ -test at 0.05 significance in terms of six evaluation metrics are reported in Table [3](#page-6-0) and Appendix B.2. The results clearly demonstrate that, although the performance of simple BR-KNN and ML-KNN are inferior to stateof-the-art multi-label classifcation approaches, the LSMMenhanced version achieve statistically superior or at least comparable performance against state-of-the-art multi-label classifcation approaches. The results once again validate the superiority of our proposed LSMM framework in learning effective similarity metrics for multi-label classifcation.

### 4.3 Further Analysis

Ablation study. To validate the usefulness of the introduced global metric when learning label-specifc multiple local metrics, two variants called LSMM-SE-N and LSMM-CL-N are implemented by learning label-specifc multiple local metrics directly. Table [4](#page-6-1) reports detailed experimental results of BR-KNN coupled with LSMM-SE, LSMM-CL, and variants in terms of *Average precision*. We can observe clear performance degradation with variants, demonstrating the usefulness of the global metric in LSMM framework. Similar results can be observed on other evaluation metrics.

<span id="page-6-0"></span>

Compared	Datasets								
Algorithms	emotions	birds	medical	enron	image	scene	slashdot	arts	education
	Hamming Loss $\downarrow$								
LIFT	$0.267 + 0.015$	$0.074 + 0.026$	$0.012 + 0.002$	$0.046 + 0.002$ $0.159 + 0.014$		$0.079 + 0.007$	$0.042 + 0.001$	$0.053 + 0.001$	$0.037 + 0.001$
<b>RELIAB</b>	$0.260 + 0.031$	$0.074 + 0.007$	$0.016 + 0.001$	$0.059 + 0.003$	$0.178 + 0.015$	$0.110 + 0.015$	$0.051 + 0.003$	$0.055 + 0.003$	$0.037 + 0.002$
WRAP	$0.242 + 0.019$	$0.053 + 0.008$	$0.010 + 0.001$	$0.047 + 0.002$	$0.186 + 0.009$	$0.114 + 0.007$	$0.037 + 0.001$	$0.054 + 0.002$	$0.037 + 0.001$
HOMI	$0.238 + 0.018$	$0.073 + 0.025$	$0.013 + 0.002$ $0.045 + 0.002$ $0.162 + 0.017$			$0.085 + 0.006$	$0.044 + 0.003$	$0.057 + 0.002$	$0.038 + 0.001$
BR-KNN-LSMM-SE	$0.204 + 0.018$	$0.051 + 0.006$	$0.014 + 0.003$	$0.045 + 0.003$	$0.162 + 0.013$	$0.081 + 0.007$	$0.035 + 0.002$	$0.054 + 0.001$	$0.037 + 0.002$
BR-KNN-LSMM-CL	$0.202 + 0.017$	$0.050 + 0.007$	$0.012 \pm 0.002$	$0.044 + 0.003$	$0.157 + 0.017$	$0.079 \pm 0.009$	$0.037 + 0.002$	$0.052 + 0.002$	$0.038 + 0.001$
ML-KNN-LSMM-SE	$0.204 + 0.016$	$0.050 + 0.005$	$0.012 + 0.003$	$0.043 + 0.002$	$0.159 + 0.014$	$0.080 + 0.007$	$0.041 + 0.002$	$0.053 + 0.001$	$0.037 + 0.001$
ML-KNN-LSMM-CL	$0.209 + 0.018$	$0.051 \pm 0.006$ $0.012 \pm 0.002$		$0.045 + 0.003$	$0.155 \!\pm\! 0.013$	$0.078 + 0.007$	$0.039 + 0.003$	$0.052 + 0.001$	$0.038 + 0.001$
					Ranking Loss $\downarrow$				
LIFT	$0.254 + 0.046$	$0.323 + 0.050$	$0.028 + 0.011$	$0.079 + 0.006$	$0.156 + 0.020$	$0.074 + 0.009$	$0.096 + 0.008$	$0.124 + 0.006$	$0.084 + 0.003$
<b>RELIAB</b>	$0.256 + 0.040$	$0.427 + 0.036$	$0.014 + 0.009$	$0.085 + 0.009$	$0.181 + 0.025$	$0.091 + 0.009$	$0.117 + 0.017$	$0.145 + 0.006$	$0.097 + 0.008$
WRAP	$0.229 + 0.029$	$0.322 + 0.030$	$0.017 + 0.008$	$0.090 + 0.009$	$0.173 + 0.023$	$0.085 + 0.008$	$0.092 + 0.012$	$0.128 + 0.009$	$0.086 + 0.006$
HOMI	$0.237 + 0.032$	$0.329 + 0.046$	$0.041 + 0.012$	$0.098 + 0.013$ $0.196 + 0.021$		$0.084 + 0.010$	$0.103 + 0.009$	$0.186 + 0.010$ $0.132 + 0.004$	
BR-KNN-LSMM-SE	$0.170 + 0.033$	$0.472 + 0.061$	$0.065 + 0.018$ $0.194 + 0.026$ $0.157 + 0.021$			$0.092 + 0.011$	$0.201 + 0.018$	$0.263 + 0.010$ $0.210 + 0.010$	
BR-KNN-LSMM-CL	$0.178 + 0.034$	$0.487 + 0.058$	$0.071 + 0.023$	$0.192 + 0.022$	$0.150 + 0.025$	$0.090 + 0.013$	$0.190 + 0.025$	$0.258 + 0.027$	$0.205 + 0.012$
ML-KNN-LSMM-SE	$0.166 + 0.033$	.256+0.034 0	$0.034 + 0.015$	$0.075 + 0.007$	$0.157 + 0.021$	$0.072 \pm 0.004$	$0.095 + 0.008$	$0.123 + 0.006$	$0.078 + 0.004$
ML-KNN-LSMM-CL	$0.170 + 0.036$	$0.260 \pm 0.038$	$0.038 \pm 0.013$	$0.073 \!\pm\! 0.009$	$0.146 \!\pm\! 0.020$	$0.069 \pm 0.005$	$0.083 + 0.007$	$0.120 + 0.005$	$0.074 + 0.004$

Table 3: Predictive performance (mean $\pm$ std) of  $A$  ( $A \in \{BR-KNN, ML-KNN\}$ ) coupled with our proposed approaches and state-of-the-art non-metric learning multi-label classifcation approaches in terms of *Hamming Loss* and *Ranking Loss*. ↑ (↓) indicates the larger (smaller) the value, the better the performance. The best and second best results are highlighted in boldface and underline respectively.

<span id="page-6-1"></span>

Data sets	Average precision $\uparrow$								
	LSMM-SE	LSMM-SE-N	LSMM-CL	LSMM-CL-N					
emotions	$0.795 + 0.039$	$0.772 \pm 0.035 \bullet$ 0.797 $\pm$ 0.038		$0.768 + 0.032 \bullet$					
<b>birds</b>	$0.438 + 0.063$	$0.397+0.057 \bullet 0.427+0.058$		$0.386 + 0.061 \bullet$					
medical	$0.882 + 0.036$	$0.833+0.031 \bullet 0.878+0.030$		$0.836 + 0.027$					
enron	$0.637 + 0.029$	$0.624 + 0.022 \bullet 0.648 + 0.032$		$0.637+0.030\bullet$					
image	$0.817 + 0.023$	$0.805 + 0.021 \bullet$	$0.820 + 0.018$	$0.808 + 0.023$					
scene	$0.857 + 0.012$	$0.855 + 0.013$	$0.868 + 0.017$	$0.860 + 0.020$					
slashdot	$0.678 + 0.021$	$0.596 \pm 0.019 \bullet$	$0.677+0.025$	$0.611 + 0.024 \bullet$					
arts	$0.593 + 0.020$	$0.521 + 0.017 \bullet 0.602 + 0.018$		$0.535 + 0.023$					
education	$0.612 + 0.015$	$0.587+0.014 \bullet 0.619+0.017$		$0.591 \pm 0.019$					

Table 4: Predictive performance (mean±std) of BR-KNN coupled with LSMM-SE, LSMM-CL, and variants in terms of *Average precision*. •/◦ indicates whether BR-KNN-LSMM-SE and BR-KNN-LSMM-CL achieve signifcantly superior/inferior to the variants on each dataset (pairwise t-test at 0.05 signifcance level).

**Sensitivity analysis.**  $\lambda_1$  and  $\lambda_2$  serve as primary trade-off parameters in LSMM, balancing the impact of the global and label-specifc multiple local metrics. Figure [1](#page-6-2) provides an illustrative example of how the performance of BR-KNN-LSMM-SE changes with varying values of  $\lambda_1$  and  $\lambda_2$  (dataset: emotions, image; evaluation metric: *Average precision*). As shown in Figure [1,](#page-6-2) the performance of BR-KNN-LSMM-SE is quite sensitive to the values of  $\lambda_1$  and  $\lambda_2$ . This demonstrates again the effectiveness of the global metric in exploiting label correlation. Similar results can be found in other cases.

Complexity analysis. In LSMM, the main computation lies in the gradient calculation and update for the global and labelspecifc multiple local metrics. The training complexity of one iteration for LSMM-SE, LSMM-CL are  $\mathcal{O}(q(nk_t k_i d^2 +$  $(2dn^2+2d^3)$ ),  $\mathcal{O}(q(nk_t k_i d^2 + Cdn^2 + Cd^3))$  respectively. It is noteworthy that LSMM learns multiple metrics of which the number equals  $2q + 1$  (for LSMM-SE) or  $Cq + 1$  (for LSMM-CL), which could be hard to generalize to datasets with huge

<span id="page-6-2"></span>

Figure 1: Performance of BR-KNN-LSMM-SE with varying values of  $\lambda_1$  and  $\lambda_2$  in terms of *Average precision*.

labels, i.e. extreme multi-label learning [Liu *et al.*[, 2021\]](#page-7-1). This is unavoidable if considering label-specifc metrics. We will leave efficiency improvement for future work.

# 5 Conclusion

In this paper, we present a novel label-specifc multi-metric learning framework LSMM for multi-label classifcation, where nonlinear distribution characteristics of multi-label instances are considered by learning label-specifc multiple local metrics for different instances on the shoulder of a global one. Comprehensive experiments verify LSMM outperforms existing consistent multi-label metric learning algorithms in learning effective similarity metrics. Furthermore, we observe that when coupled with LSMM, simple BR-KNN and ML-KNN also have the potential to approach or even surpass state-of-the-art multi-label classifcation methods. However, LSMM learns multiple metrics, which could be hard to generalize to extreme multi-label learning. This is unavoidable if considering label-specifc metrics. It is interesting to investigate towards this dilemma to achieve better performance and tolerable scalability for multi-label metric learning.

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