Deep Multi-Dimensional Classification with Pairwise Dimension-Specific Features

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Abstract

In multi-dimensional classification (MDC), each instance is associated with multiple class variables characterizing the semantics of objects from different dimensions. To consider the dependencies among class variables and the specific characteristics contained in different semantic dimensions, a novel deep MDC approach named PIST is proposed to jointly deal with the two issues via learning pairwise dimension-specific features. Specifically, PIST conducts pairwise grouping to model the dependencies between each pair of class variables, which are more reliable with limited training samples. For extracting pairwise dimension-specific features, PIST weights the feature embedding with a feature importance vector, which is learned via utilizing a global loss measurement based on intra-class and inter-class covariance. Final prediction w.r.t. each dimension is determined by combining the joint probabilities related to this dimension. Comparative studies with eleven real-world MDC data sets clearly validate the effectiveness of the proposed approach.

1 Introduction

In multi-dimensional classification (MDC), each object is represented by a single instance while associated with multiple class variables. Here, each class variable corresponds to one label space characterizing the rich semantics of objects from some specific dimension. Take landscape paintings classification as an example, each picture can be classified from `time` dimension (with possible labels *morning*, *afternoon*, *night*, etc.), from `weather` dimension (with possible labels *sunny*, *rainy*, *cloudy*, etc.), and from `scene` dimension (with possible labels *desert*, *mountain*, *grass*, etc.). Specifically, the needs of learning from MDC objects widely exist in diverse real-world applications, including text mining [Lertnattee and Theeramunkong, 2004; Shatkay *et al.*, 2008], computer vision [Song *et al.*, 2018; Lian *et al.*, 2020; Shi *et al.*, 2025], bioinformatics [Borchani *et al.*, 2013; Fernandez Gonzalez *et al.*, 2015], etc.

Formally speaking, given a feature space $\mathcal{X} = \mathbb{R}^d$ and an output space $\mathcal{Y} = C_1 \times C_2 \times \cdots \times C_q$ corresponding to the Cartesian product of q label spaces, each label space $C_j = \{c_1^j, c_2^j, \ldots, c_{K_j}^j\}$ includes K_j possible labels $(1 \leq j \leq q)$ to characterize the semantics along one dimension. Let $\mathcal{D} = \{(\boldsymbol{x}_i, \boldsymbol{y}_i) | 1 \leq i \leq m\}$ be the training set and each sample $(\boldsymbol{x}_i, \boldsymbol{y}_i)$ corresponds to a d-dimensional feature vector $\boldsymbol{x}_i = [x_{i1}, x_{i2}, \ldots, x_{id}]^{\mathrm{T}} \in \mathcal{X}$ associated with a q-dimensional label vector $\boldsymbol{y}_i = [y_{i1}, y_{i2}, \ldots, y_{iq}]^{\mathrm{T}} \in \mathcal{Y}$. Given an unseen instance $\boldsymbol{x}_*$, the task of MDC is to learn a mapping function $f : \mathcal{X} \mapsto \mathcal{Y}$ from the training set $\mathcal{D}$ which can return a proper label vector $f(\boldsymbol{x}_*)$.

One popular solution to MDC tasks is to independently deal with each dimension as a traditional multi-class classification problem. Nonetheless, this strategy completely ignores the dependencies among class variables and then the performance of the induced predictive model might degenerate. To tackle this issue, existing MDC approaches are designed to consider class dependencies in either explicit manner with some structures (e.g., directed acyclic graph [Bielza *et al.*, 2011; Gil-Begue *et al.*, 2021], chaining order [Zaragoza *et al.*, 2011] and pairwise interaction [Jia and Zhang, 2020b]) or in implicit manner via manipulating feature space [Jia and Zhang, 2020a; Jia and Zhang, 2022] or label space [Jia and Zhang, 2021b; Tang *et al.*, 2024].

Although these existing approaches have successfully considered class dependencies, they might obtain suboptimal performances since the predictive models for different dimensions are induced based on the same feature space [Jia *et al.*, 2023]. However, different semantics in each dimension might prefer different feature characteristics. Take the aforementioned landscape painting as an example, the level of luminance would be preferred in discriminating labels in `time` dimension; abrupt color changes are more likely to reveal the labels in `scene` dimension and the upper part of a picture is supposed to be more related to `weather` dimension. Moreover, samples belonging to the same class should be similar in the feature space generally, but it is very common that two MDC samples belong to the same class in one dimension while different classes in another dimension.

To consider the specific characteristics contained in different semantic dimensions as well as the dependencies among class variables, we propose a novel MDC approach named PIST (i.e., *Pairwise dImension-Specific feaTures*) based on

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deep learning techniques. Specifically, PIST aims to model class dependencies between each pair of class variables via pairwise grouping. Firstly, to construct pairwise dimensional embeddings, a combinatorial encoding procedure is conducted for pairwise class variables via optimizing the intra-class and inter-class covariance. Then an element-wise selection mechanism is used to extract pairwise dimension-specific features, which are considered better capturing the correlation between feature space and heterogeneous label semantics in respective dimension pairs. Finally, joint probabilities predicted by pairwise neural networks are integrated to accomplish the final discrimination collectively. To the best of our knowledge, PIST serves as the first attempt towards learning dimension-specific features as well as considering class dependencies. Comprehensive experiments on eleven benchmark data sets show that PIST performs better than existing well-established MDC approaches.

The rest of this paper is organized as follows. Firstly, Section 2 briefly reviews related works. Then Section 3 presents the proposed PIST approach at length. After that, Section 4 reports the results of empirical studies over a wide range of MDC data sets. Finally, Section 5 concludes this paper.

2 Related Work

On one hand, MDC can be regarded as a set of multi-class classification problems, one per dimension. Thus, we can solve the MDC problem by learning an independent multi-class classifier for each dimension, which is known as binary relevance (BR) [Zhang *et al.*, 2018] but ignores all possible class dependencies. To exploit class dependencies among dimensions, on the other hand, one straightforward strategy is to regard each distinct label combination as a new class, which is known as class powerset (CP). However, the combinatorial nature of CP induces high complexity and is also prone to class-imbalance and overfitting problem. According to the strategy of dependency modeling, existing MDC works can be roughly categorized into two categories, including explicit and implicit dependency modeling methods.

The MDC methods of explicit category attempt to model class dependencies with some explicit structures. Chaining-based classifiers improve BR by learning a chain of multi-class classifiers, where subsequent classifiers on the chain will augment predictions of preceding one as features [Zaragoza *et al.*, 2011; Read *et al.*, 2014b]. Multi-dimensional Bayesian classifiers construct directed acyclic graph over class variable to explicitly consider the class dependencies [Bielza *et al.*, 2011; Gil-Begue *et al.*, 2021]. Generally, the dependencies among many class variables are hard to model due to limited samples in training set. SEEM [Jia and Zhang, 2020b] and MDKNN [Jia and Zhang, 2021a] suggest that pairwise dependencies can be modeled more reliably than modeling the dependencies among all class variables.

The MDC methods of implicit category attempt to transform the original MDC problem into a new one without some explicit dependency modeling mechanism in the transformation procedure. gMML [Ma and Chen, 2018] transforms the original categorical output space into a binary one and then induce the predictive model based on metric learning. SLEM [Jia and Zhang, 2021b] encodes the original class vectors into real-valued ones and decodes the predicted class vectors over the outputs of learned multi-output regression model. To extract more powerful features, KRAM [Jia and Zhang, 2020a] manipulates the feature space via utilizing kNN information to enrich the original feature space.

LEFA [Wang *et al.*, 2020] is the first MDC approach that utilizes deep learning techniques. It learns an augmented feature vector for each instance via assuming that the representations of features and labels should be aligned in some latent space. ADVAE-FLOW [Zhang *et al.*, 2022] encodes both feature and class variables to probabilistic latent spaces by normalizing flows, in which the one-hot representation for the label vectors w.r.t. different dimensions are directly stacked. DSOC [Saleh and Li, 2023] is formed of multiple neural networks and a hypercube classifier, where the former are responsible for feature selection and the latter aims to accommodate the model for rare sample classification.

However, all these works only aim to consider class dependencies but cannot consider the specific characteristics contained in different semantic dimensions. In the next section, we will present the technical details of the proposed PIST approach, which considers not only class dependencies but also pairwise dimension-specific characteristics.

3 The PIST Approach

As shown in Figure 1, PIST includes two key modules: pairwise dimension encoding and dimension-specific feature extraction. Briefly, a weighted sum-pooling is conducted to obtain pairwise dimension embeddings in the first module and the outputs will further guide the dimension-specific feature extraction in the second module. The final classification is enabled by the returned probabilities of softmax regression.

3.1 Pairwise Dimension Encoding

To consider pairwise interactions, PIST considers each pair of dimensions as an entirety. Without loss of generality, we will carry out the following discussions in the case of C_1 and C_2. To extract dimension-specific features for this dimension pair, PIST learns a corresponding pairwise dimension embedding with a weighted sum-pooling as follows:

$$\boldsymbol{l}^{(12)} = \sum_{a_1=1}^{K_1} \sum_{a_2=1}^{K_2} \frac{f_{a_1 a_2}}{m} \boldsymbol{l}_{a_1 a_2} \tag{1}$$

where $f_{a_1 a_2}$ is the number of samples labeled by $c^1_{a_1}$ and $c^2_{a_2}$ in the training set and $\boldsymbol{l}_{a_1 a_2} \in \mathbb{R}^t$ is a latent label embedding vector related to $c^1_{a_1}$ and $c^2_{a_2}$. Here, t is a hyper-parameter to be set (cf. Section 4.3 for further discussions).

For each component $\boldsymbol{l}_{a_1 a_2}$ in Eq.(1), a natural cluster assumption is that $\boldsymbol{l}_{a_1 1}, \boldsymbol{l}_{a_1 2}, \ldots, \boldsymbol{l}_{a_1 K_2}$ are close to each other and far from $\boldsymbol{l}_{\tilde{a}_1 1}, \boldsymbol{l}_{\tilde{a}_1 2}, \ldots, \boldsymbol{l}_{\tilde{a}_1 K_2}$ where $a_1 \in \{1, 2, \ldots, K_1\}$ and $\tilde{a}_1 \in \{1, 2, \ldots, K_1\} \setminus \{a_1\}$. For this purpose, good embeddings $\boldsymbol{l}_{a_1 a_2}$ should minimize the intra-class covariance and maximize inter-class covariance, which can be implemented via minimizing the following objective $\mathcal{L}^{(12)}_{le-\text{part1}}$:

$$\mathcal{L}^{(12)}_{le-\text{part1}} = \frac{\sum_{a_1=1}^{K_1} \sum_{a_2=1}^{K_2} ||\boldsymbol{l}_{a_1 a_2} - \bar{\boldsymbol{l}}_{a_1}||_2^2}{\sum_{a_1=1}^{K_1} K_2 ||\bar{\boldsymbol{l}}_{a_1} - \bar{\boldsymbol{l}}||_2^2} \tag{2}$$

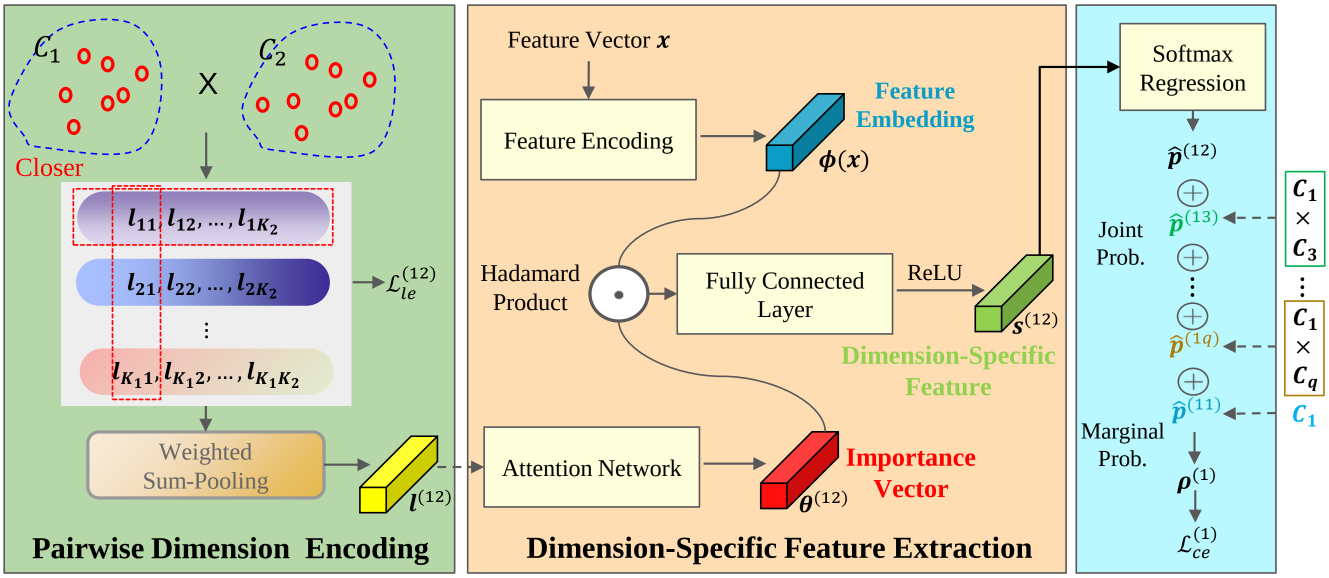


Figure 1: The workflow of the proposed PIST approach by taking the pair of label spaces C_1 and C_2 as an example.

where $\bar{\boldsymbol{l}}_{a_1} = \frac{1}{K_2}\sum_{a_2=1}^{K_2} \boldsymbol{l}_{a_1a_2}$ is the intra-class mean and $\bar{\boldsymbol{l}} = \frac{1}{K_1K_2}\sum_{a_1=1}^{K_1}\sum_{a_2=1}^{K_2} \boldsymbol{l}_{a_1a_2}$ is the global mean.

It is worth noting that the above discussions on similarity of latent label embeddings have another 'dual' form with an exchange of subscript a_1 and a_2. Then another objective $\mathcal{L}_{le-\text{part2}}^{(12)}$ is as follows:

$$\mathcal{L}_{le-\text{part2}}^{(12)} = \frac{\sum_{a_2=1}^{K_2}\sum_{a_1=1}^{K_1} ||\boldsymbol{l}_{a_1a_2} - \bar{\boldsymbol{l}}'_{a_2}||_2^2}{\sum_{a_2=1}^{K_2} K_1 ||\bar{\boldsymbol{l}}'_{a_2} - \bar{\boldsymbol{l}}||_2^2} \tag{3}$$

where $\bar{\boldsymbol{l}}'_{a_2} = \frac{1}{K_1}\sum_{a_1=1}^{K_1} \boldsymbol{l}_{a_1a_2}$ is the 'dual' intra-class mean. By combining the two above objectives together, the final label embedding loss $\mathcal{L}_{le}^{(12)}$ w.r.t. C_1 and C_2 can be defined as follows:

$$\mathcal{L}_{le}^{(12)} = \mathcal{L}_{le-\text{part1}}^{(12)} + \mathcal{L}_{le-\text{part2}}^{(12)} \tag{4}$$

3.2 Dimension-Specific Feature Extraction

For each example $\boldsymbol{x}$, numerous early works [Yeh *et al.*, 2017; Wang *et al.*, 2016; Zhang *et al.*, 2023] have proved that it is significant to exploit powerful feature embeddings in latent spaces. Thus we firstly encode $\boldsymbol{x}$ into a latent space based on neural networks which is denoted by $\phi(\boldsymbol{x}) \in \mathbb{R}^{d'}$. To extract pairwise dimension-specific feature, decode $\boldsymbol{l}^{(12)}$ into a feature importance vector with an attention network:

$$\boldsymbol{\theta}^{(12)} = \sigma(\mathbf{W}_l \boldsymbol{l}^{(12)} + \boldsymbol{b}_l) \tag{5}$$

where $\boldsymbol{\theta}^{(12)}, \boldsymbol{b}_l \in \mathbb{R}^{d'}$ and $\mathbf{W}_l \in \mathbb{R}^{d' \times t}$. σ is the ReLU activation function. Here, note that $\mathbf{W}_l$ and $\boldsymbol{b}_l$ are shared parameters for all pairwise dimensions.

PIST further assumes that $\phi(\boldsymbol{x})$ could be transformed via an element-wise selection mechanism. Then for dimensions C_1 and C_2, the latent feature embedding is transformed into $\phi(\boldsymbol{x}) \odot \boldsymbol{\theta}^{(12)}$, where $\odot$ is the Hadamard product. With a fully-connected network used, the final pairwise dimension-specific feature is obtained:

$$\boldsymbol{s}^{(12)} = \sigma[\mathbf{W}_s(\phi(\boldsymbol{x}) \odot \boldsymbol{\theta}^{(12)}) + \boldsymbol{b}_s] \tag{6}$$

where $\boldsymbol{s}^{(12)}, \boldsymbol{b}_s \in \mathbb{R}^{d'}$, $\mathbf{W}_s \in \mathbb{R}^{d' \times d'}$.

In addition, it is possible that one dimension is irrelevant to others. PIST also seeks to acquire single dimension-specific features by a similar procedure. Take the j-th dimension as an example ($1 \leq j \leq q$):

$$\boldsymbol{l}^{(jj)} = \sum_{a=1}^{K_j} \frac{f_a}{m} \boldsymbol{l}_a \tag{7}$$

$$\boldsymbol{\theta}^{(jj)} = \sigma(\mathbf{W}_l \boldsymbol{l}^{(jj)} + \boldsymbol{b}_l) \tag{8}$$

$$\boldsymbol{s}^{(jj)} = \sigma[\mathbf{W}_s(\phi(\boldsymbol{x}) \odot \boldsymbol{\theta}^{(jj)}) + \boldsymbol{b}_s] \tag{9}$$

Here, we denote j by jj for notation consistency with the aforementioned pairwise case.

3.3 Classification

For classification, we simply obtain probabilities of all K_1K_2 class combinations w.r.t the first two dimensions with a softmax regression as follows:

$$\boldsymbol{o}^{(12)} \quad = \mathbf{W}_o^{(12)} \boldsymbol{s}^{(12)} + \boldsymbol{b}_o^{(12)} \tag{10}$$

where $\boldsymbol{o}^{(12)}, \boldsymbol{b}_o^{(12)} \in \mathbb{R}^{K_1K_2}$ and $\mathbf{W}_o^{(12)} \in \mathbb{R}^{K_1K_2 \times d'}$. Define an injective function $\psi(\cdot,\cdot) : \{1, 2, \dots, K_1\} \times \{1, 2, \dots, K_2\} \to \{1, 2, \dots, K_1K_2\}$ and further assume that $\psi(a_1, a_2) = w$. The predicted probability of any instance $\boldsymbol{x}$ is as follows:

$$\hat{\boldsymbol{p}}^{(12)} = softmax(\boldsymbol{o}^{(12)}) \tag{11}$$

where the w-th element $\hat{p}_w^{(12)}$ in $\hat{\boldsymbol{p}}^{(12)}$ corresponds to:

$$\hat{p}_w^{(12)} = \frac{\exp(o_w^{(12)})}{\sum_{a=1}^{K_1K_2}\exp(o_a^{(12)})} \tag{12}$$

Here, $o_a^{(12)}$ denotes the a-th element in vector $\boldsymbol{o}_a^{(12)}$. It is easy to know that $\hat{p}_w^{(12)}$ indicates the probability that $\boldsymbol{x}$ is labeled by $c_{a_1}^1$ and $c_{a_2}^2$ w.r.t. C_1 and C_2, respectively.

Similar derivation can apply to the case of a single dimension. Take the j-th dimension as an example ($1 \leq j \leq q$):

$$\boldsymbol{o}^{(jj)} \quad = \mathbf{W}_o^{(jj)}\boldsymbol{s}^{(jj)} + \boldsymbol{b}_o^{(jj)} \tag{13}$$

where $\boldsymbol{o}^{(jj)}, \boldsymbol{b}_o^{(jj)} \in \mathbb{R}^{K_j}$ and $\mathbf{W}_o^{(jj)} \in \mathbb{R}^{K_j \times d'}$. The corresponding predicted probability of any instance $\boldsymbol{x}$ is as follows:

$$\hat{\boldsymbol{p}}^{(jj)} = softmax(\boldsymbol{o}^{(jj)}) \tag{14}$$

where the a_j-th element $\hat{p}_a^{(jj)}$ in $\hat{\boldsymbol{p}}^{(jj)}$ corresponds to:

$$\hat{p}_{a_j}^{(jj)} = \frac{\exp(o_{a_j}^{(jj)})}{\sum_{a=1}^{K_j}\exp(o_a^{(jj)})} \tag{15}$$

After traversing all dimension pairs, we can obtain $\binom{q}{2} + q$ predicted probabilities $\{\hat{\boldsymbol{p}}^{(rs)} | 1 \leq r \leq s \leq q\}$, the final confidence score $\rho_{a_r}^{(r)}$ for the a_r-th label in the r-th dimension is determined as follows ($a_r \in \{1, 2, \ldots, K_r\}, 1 \leq r \leq q$):

$$\rho_{a_r}^{(r)} = \hat{p}_{a_r}^{(rr)} + \sum_{a_s=1}^{K_s}\left(\sum_{s=1}^{r-1}\hat{p}_{\psi(a_s,a_r)}^{(sr)} + \sum_{s=r+1}^{q}\hat{p}_{\psi(a_r,a_s)}^{(rs)}\right) \tag{16}$$

It is not hard to verify that $\sum_{a_r=1}^{K_r}\rho_{a_r}^{(r)} = q$ holds. To render $\rho_{a_r}^{(r)}$ probabilistic and facilitate cross-entropy loss, we further normalize it with softmax operation:

$$Q_{a_r}^r = \frac{\exp(\rho_{a_r}^{(r)})}{\sum_{a=1}^{K_r}\exp(\rho_a^{(r)})} \tag{17}$$

Based on $Q_{a_r}^r$, assuming ground-truth label of $\boldsymbol{x}$ in the r-th dimension is c_γ^r, the cross-entropy loss w.r.t. the r-th dimension is defined as follows ($1 \leq r \leq q$):

$$\mathcal{L}_{ce}^{(r)} = -\sum_{a_r=1}^{K_r}[\![a_r = \gamma]\!] \cdot \log(Q_{a_r}^r) \tag{18}$$

where $[\![\pi]\!]$ returns 1 if π holds and 0 otherwise. The final loss corresponds to the sum of the average of the dimension-wise cross-entropy loss $\mathcal{L}_{ce}^{(r)}$ in Eq.(18) as well as the average of pairwise label embedding loss $\mathcal{L}_{le}^{(rs)}$ in Eq.(4):

$$\mathcal{L} = \frac{1}{q}\sum_{1\leq r\leq q}\mathcal{L}_{ce}^{(r)} + \frac{2}{q(q-1)}\sum_{1\leq r<s\leq q}\mathcal{L}_{le}^{(rs)} \tag{19}$$

Given an unseen instance $\boldsymbol{x}_*$, its predicted label $\hat{y}_{*j}$ w.r.t. the j-th dimension is determined as follows ($1 \leq j \leq q$):

$$\hat{y}_{*j} = c_\omega^j, \text{where } \omega = \arg\max_{1\leq a\leq K_j} Q_a^j, \tag{20}$$

The final predicted vector can be obtained after traversing all dimensions, i.e., $\hat{\boldsymbol{y}} = [\hat{y}_{*1}, \hat{y}_{*2}, \ldots, \hat{y}_{*q}]^{\mathrm{T}}$.

Data set	#Exam.	#Dim.	#Labels/Dim.	#Feat.
WQplants	1060	7	4	$16n$
WQanimals	1060	7	4	$16n$
WaterQuality	1060	14	4	$16n$
BeLaE	1930	5	5	$1n, 44x$
Voice	3136	2	4,2	$19n$
Scm20d	8966	16	4	$61n$
CoIL2000	9822	5	6,10,10,4,2	$81x$
TIC2000	9822	3	6,4,2	$83x$
Flickr	12198	5	3,4,3,4,4	$1536n$
Adult	18419	4	7,7,5,2	$5n, 5x$
Default	28779	4	2,7,4,2	$14n, 6x$

Table 1: Basic information for data sets. Here, n and x in last column represent numeric and nominal type features.

4 Experiments

4.1 Experimental Setting

Data Sets

In this paper, we use eleven real-world MDC data sets for experimental studies. Table 1 summarizes basic characteristics, including the number of examples (#Exam.), the number of dimensions (#Dim.), the number of labels in each dimension (#Labels/Dim.) and the number of features (#Feat.).

Evaluation Metrics

In this paper, three commonly used metrics for performance evaluation are adopted, i.e. *hamming score* (HS), *exact match* (EM) and *sub-exact match* (SEM) [Read *et al.*, 2014a; Zhu *et al.*, 2016]. Given the test set $\mathcal{S} = \{(\boldsymbol{x}_i, \boldsymbol{y}_i) \mid 1 \leq i \leq p\}$ and the MDC model f to be evaluated, the definitions of these three evaluation metrics are given as follows:

1. Hamming Score:

$$\mathrm{HS}_{\mathcal{S}}(f) = \frac{1}{p}\sum_{i=1}^{p}\frac{1}{q}\cdot r^{(i)}$$

2. Exact Match:

$$\mathrm{EM}_{\mathcal{S}}(f) = \frac{1}{p}\sum_{i=1}^{p}[\![r^{(i)} = q]\!]$$

3. Sub-Exact Match:

$$\mathrm{SEM}_{\mathcal{S}}(f) = \frac{1}{p}\sum_{i=1}^{p}[\![r^{(i)} \geq q-1]\!]$$

Here, $r^{(i)} = \sum_{j=1}^{q}[\![y_{ij} = \hat{y}_{ij}]\!]$ denotes the number of dimensions which are predicted correctly, y_{ij} and $\hat{y}_{ij}$ denote the ground-truth and predicted label w.r.t. the j-th dimension for the i-th test sample. Ten-fold cross validation are conducted for all data sets where the mean metric value as well as the standard derivation are recorded for comparison.

Comparing Approaches

We compare PIST against eight state-of-the-art MDC approaches with parameter configurations suggested in respective literatures:

(a) Hamming Score

Data Set	PIST	BR	CP	ECC	gMML	KRAM	LEFA	MDKNN	SEEM
WQplants	.661±.013	.649±.016●	.576±.018●	.648±.015●	.655±.014	.663±.016	.653±.014●	.660±.013	.666±.015
WQanimals	.632±.014	.628±.012	.558±.014●	.628±.012	.630±.014	.638±.012	.625±.015	.631±.013	.630±.017
WaterQuality	.647±.012	.639±.012●	.567±.012●	.638±.012●	.643±.012	.651±.011○	.643±.012	.646±.009	.648±.012
BeLaE	.452±.015	.423±.021●	.357±.019●	.408±.021●	.417±.019●	.415±.017●	.410±.012●	.395±.011●	.398±.022●
Voice	.954±.008	.940±.009●	.938±.006●	.930±.008●	.842±.008●	.944±.008●	.932±.015●	.943±.008●	.936±.011●
Scm20d	.845±.012	.632±.006●	.862±.003○	.608±.007●	.600±.007●	.872±.002○	.855±.005○	.866±.004○	.770±.005●
CoIL2000	.957±.004	.874±.005●	.897±.005●	.858±.005●	.894±.004●	.929±.004●	.949±.009●	.877±.005●	.921±.004●
TIC2000	.945±.004	.892±.007●	.875±.006●	.884±.007●	.895±.006●	.942±.003●	.936±.006●	.864±.005●	.916±.006●
Flickr	.795±.003	.715±.005●	.675±.006●	.693±.005●	.779±.004●	.749±.006●	.748±.007●	.735±.006●	.734±.006●
Adult	.725±.003	.701±.004●	.638±.005●	.702±.005●	.705±.004●	.705±.005●	.657±.007●	.699±.005●	.706±.004●
Default	.676±.003	.665±.003●	.587±.004●	.666±.003●	.666±.004●	.665±.004●	.625±.015●	.654±.003●	.668±.003●

(b) Exact Match

Data Set	PIST	BR	CP	ECC	gMML	KRAM	LEFA	MDKNN	SEEM
WQplants	.094±.021	.092±.028	.048±.020●	.094±.028	.092±.033	.096±.033	.094±.030	.096±.029	.100±.030
WQanimals	.057±.015	.056±.023	.025±.015●	.056±.023	.062±.022	.059±.013	.048±.024	.057±.013	.039±.013●
WaterQuality	.009±.006	.006±.008	.005±.006	.006±.008	.006±.008	.008±.006	.008±.007	.006±.008	.008±.007
BeLaE	.035±.019	.028±.009	.013±.009●	.035±.012	.022±.009●	.030±.012	.017±.008●	.023±.008	.023±.011●
Voice	.910±.016	.884±.016●	.878±.010●	.866±.014●	.699±.016●	.892±.017●	.872±.021●	.889±.014●	.877±.020●
Scm20d	.199±.019	.054±.005●	.219±.012○	.073±.008●	.052±.007●	.245±.009○	.210±.012	.231±.011○	.104±.007●
CoIL2000	.822±.014	.515±.011●	.616±.013●	.466±.013●	.576±.014●	.743±.010●	.786±.036●	.552±.014●	.701±.013●
TIC2000	.843±.013	.698±.018●	.665±.010●	.675±.016●	.706±.017●	.835±.008●	.819±.016●	.632±.017●	.764±.015●
Flickr	.330±.013	.187±.010●	.158±.008●	.168±.010●	.287±.008●	.244±.009●	.246±.010●	.228±.013●	.211±.011●
Adult	.288±.006	.228±.006●	.206±.007●	.251±.009●	.230±.009●	.275±.009●	.202±.014●	.260±.010●	.256±.009●
Default	.195±.006	.177±.007●	.124±.006●	.179±.006●	.177±.007●	.186±.006●	.134±.018●	.177±.004●	.185±.006●

(c) Sub-Exact Match

Data Set	PIST	BR	CP	ECC	gMML	KRAM	LEFA	MDKNN	SEEM
WQplants	.285±.050	.284±.049	.171±.030●	.282±.047	.286±.050	.291±.041	.286±.033	.288±.029	.287±.031
WQanimals	.223±.042	.226±.029	.132±.023●	.226±.029	.227±.031	.253±.023	.209±.039	.225±.028	.223±.041
WaterQuality	.053±.011	.044±.023	.016±.013●	.045±.022	.049±.023	.057±.022	.048±.018	.046±.017	.045±.022
BeLaE	.160±.024	.132±.023●	.070±.021●	.134±.015●	.130±.019●	.121±.019●	.117±.017●	.111±.019●	.116±.019●
Voice	.997±.003	.996±.004	.998±.003	.995±.005	.985±.010●	.997±.003	.992±.011	.997±.004	.995±.004
Scm20d	.403±.025	.105±.007●	.442±.015○	.128±.010●	.100±.009●	.483±.012○	.425±.016○	.472±.020○	.225±.007●
CoIL2000	.966±.006	.873±.015●	.905±.010●	.851±.013●	.903±.009●	.922±.010●	.963±.007	.872±.010●	.923±.005●
TIC2000	.993±.002	.979±.004●	.961±.007●	.977±.005●	.978±.003●	.992±.003	.989±.004●	.962±.003●	.985±.004●
Flickr	.723±.009	.543±.015●	.483±.010●	.494±.013●	.689±.015●	.629±.019●	.627±.021●	.597±.015●	.595±.018●
Adult	.693±.007	.657±.009●	.532±.010●	.651±.010●	.669±.007●	.652±.008●	.575±.011●	.638±.009●	.660±.007●
Default	.610±.007	.590±.008●	.446±.008●	.593±.008●	.593±.008●	.588±.008●	.518±.032●	.568±.007●	.596±.007●

Table 2: Experimental results (mean±std.) of each MDC approach. In addition, ●/○ indicates whether PIST is significantly superior/inferior to other compared approaches on each data set with pairwise t-test at 0.05 significance level.

- BR: Learn an independent multi-class classifier for each dimension one by one.
- CP: Learn a multi-class classifier via treating each distinct label combination as a new label.
- ECC [Zaragoza *et al.*, 2011]: Ensemble of several multi-class classifier chains with random dimension orders. Predicted results generated by preceding classifiers are taken as augmented inputs of the subsequent classifier.
- gMML [Ma and Chen, 2018]: Mapping the output space in MDC into a binary one via one-vs-rest strategy. The resulted problem is solved by learning regression models based on metric learning.
- KRAM [Jia and Zhang, 2020a]: Count the number of instances in the k nearest neighbors of each sample which is associated with exactly each label respectively w.r.t. each dimension. These counted numbers are concatenated to form augmented features.
- LEFA [Wang *et al.*, 2020]: Introduce a cross correlation aware network to learn low-dimensional latent label embeddings which are considered close to latent feature embeddings. Aligned label embeddings are used to augment the original feature space. Multi-class algorithms

Evaluation	PIST against								
Metric	BR	CP	ECC	gMML	KRAM	LEFA	MDKNN	SEEM	In Total
HS	10/1/0	10/0/1	10/1/0	8/3/0	7/2/2	8/2/1	7/3/1	8/3/0	68/15/5
EM	7/4/0	9/1/1	7/4/0	8/3/0	6/4/1	7/4/0	6/4/1	9/2/0	59/26/3
SEM	7/4/0	9/1/1	7/4/0	8/3/0	5/5/1	5/5/1	6/4/1	7/4/0	54/30/4
In Total	24/9/0	28/2/3	24/9/0	24/9/0	18/11/4	20/11/2	19/11/3	24/9/0	181/71/12

Table 3: Win/tie/loss counts of pairwise t-test (at 0.05 significance level) between PIST and each comparing approach.

are also used for subsequent classification.

- MDKNN [Jia and Zhang, 2021a]: Obtain kNN counting statistics as KRAM and consider class dependencies for each pair of label spaces. Predictions are determined by the best learned classifier which achieve the highest accuracy in the k nearest neighbors.
- SEEM [Jia and Zhang, 2020b]: Learn pairwise classifiers in the first level and stack corresponding predicted outputs according to the accuracy in the k nearest neighbors to generate second-level data sets for subsequent multi-class models.

For comparing approaches which necessitate a multi-class algorithms, LIBSVM [Chang and Lin, 2011] is used to implement the base classifier as suggested in literatures. While PIST is based on neural networks, to make fair comparison and eliminate the impact exerted by difference of base classifiers, we further investigate 5 adjusted approaches including BR, KRAM, LEFA, MDKNN and SEEM by replacing the multi-class classifier with neural networks as PIST. In the context below, these methods with changed base classifiers are denoted by the original name plus a subscript δ. Detailed implementation will be elaborated in the next section.

Implementation Details

For our proposed method, feature embeddings are generated by a fully-connected layer and ReLU activation. Label embeddings $\{\boldsymbol{l}_{a_r a_s} | 1 \leq r \leq s \leq q, 1 \leq a_r \leq K_r, 1 \leq a_s \leq K_s\}$ are initialized by standard normal distribution. It is worth noting that we adopt a dropout-like strategy for all label embeddings used for weighted sum-pooling, i.e. randomly drop 80% of them to alleviate overfitting. The latent dimensions of label embeddings t, feature embeddings d' and all hidden layers are empirically set as 32, 512 and 512, respectively. All activation functions are fixed as ReLU followed by a dropout layer [Srivastava *et al.*, 2014] with dropping probability of 0.5. For network optimization, SGD with a batch size of 512 and momentum of 0.9 is employed. We set the learning rate as 0.1 and the weight decay as 10^{-4}.

For comparing approaches, all recommended parameters in their literatures are employed. Given that in PIST, the subsequent networks adopted on transformed features $\{\phi(\boldsymbol{x}) \odot \boldsymbol{\theta}^{rs} | (1 \leq r \leq s \leq q)\}$ are actually equivalent to a multi-layer perceptron with one hidden layer (Eq.(6) and Eq.(10)), thus for changed base classifiers, we replace all LIBSVM implemented classifiers with the exact same multi-layer perceptron for all comparing approaches.

Evalu.	PIST against					
Metric	BR$_\delta$	KRAM$_\delta$	LEFA$_\delta$	MDKNN$_\delta$	SEEM$_\delta$	In Total
HS	7/4/0	8/2/1	8/3/0	10/0/1	9/2/0	42/11/2
EM	5/6/0	9/1/1	7/4/0	10/0/1	7/4/0	38/15/2
SEM	7/4/0	8/3/0	7/4/0	9/1/1	6/5/0	37/17/1
In Total	19/14/0	25/6/2	22/11/0	29/1/3	22/11/0	117/43/5

Table 4: Win/tie/loss counts of pairwise t-test (at 0.05 significance level) between PIST and each comparing approach with replaced base classifiers.

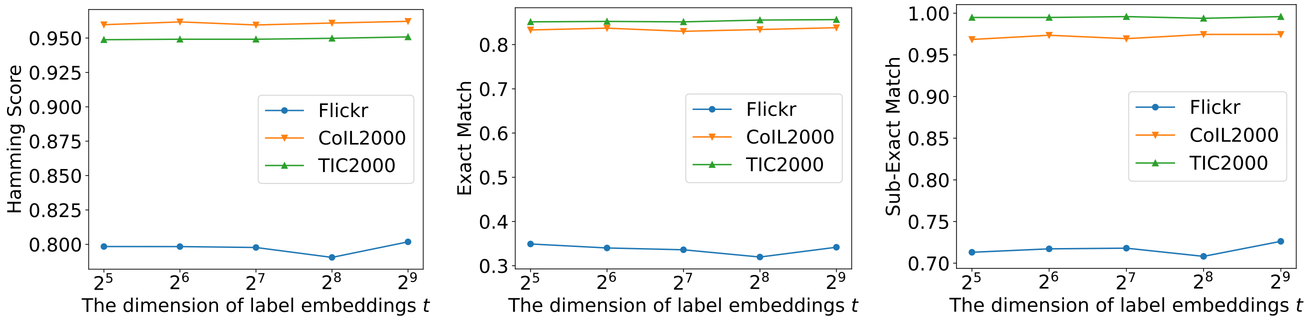
4.2 Experimental Results

The detailed experimental results are reported in Table 2. Due to the space limitation, the detailed experimental results of MDC approaches with replaced base classifiers are deferred into the supplementary materials. Moreover, pairwise t-test [Demšar, 2006] at 0.05 significance level is conducted to show whether PIST achieves significantly superior/inferior performance against other comparing approaches on each data set. Accordingly, the resulting win/tie/loss counts are summarized in Table 3 and Table 4.

According to the reported experimental results, observations can be made as follows:

- Evaluated by three metrics, PIST respectively significantly outperforms the 13 comparing approaches (8 original approaches plus 5 approaches with neural network based classifiers) in 84.6%, 74.6% and 70.0% cases across all the 130 configurations (11 data sets × 13 comparing approaches).
- PIST achieves greater advantage on large-scale data sets than on small-scale data sets probably because deep learning technique is more suitable for sufficient data. Relatively poor performance on *Scm20d* might be attributed to the large number of dimensions which is a challenging circumstance for pairwise strategy.
- Substituting neural network based classifiers for SVM presents overall degeneration of performance, which might be caused by the inconsistency between the transformed data sets generated by original MDC approaches and neural networks.

To summarize, PIST achieves highly competitive performance against other well-established MDC approaches, which validates the effectiveness of our proposed pairwise dimension-specific feature learning approach.



(a) Hamming Score (b) Exact Match (c) Sub-Exact Match

Figure 2: Performance of PIST changes as the dimension of label embeddings t varies in the range of $\{2^5, 2^6, 2^7, 2^8, 2^9\}$.

PIST against	HS	EM	SEM
PAIR	**win**[2.44e-02]	**win**[2.44e-02]	**tie**[8.84e-02]
RAND	**win**[1.41e-02]	**win**[4.20e-02]	**tie**[9.69e-02]
STACK	**win**[9.77e-04]	**win**[9.77e-04]	**win**[1.44e-02]
MONO	**win**[9.77e-04]	**win**[5.06e-03]	**win**[2.93e-03]

Table 5: Summary of the Wilcoxon signed-ranks test for PIST against its variants in terms of each evaluation metric at 0.05 significance level. The p-values are shown in the brackets.

4.3 Further Analysis

Ablation Studies

In this section, we conduct ablation studies on all the eleven MDC benchmark data sets. The four variants are denoted as PAIR, RAND, STACK, and MONO.

- PAIR. Use original features to induce pairwise classifiers instead of learning dimension-specific features.
- RAND. Initialize pairwise dimension embeddings $\boldsymbol{l}^{(ij)}$ by standard normal distribution without combinatorial strategy in Eq.(1) and thus remove the embedding loss (i.e. the second term in Eq.(19)).
- STACK. To reduce the number of neural network based classifiers, stack the dimension-specific features for all dimension pairs. Specifically, for the j-th $(1 \leq j \leq q)$ dimension, the stacked dimension-specific feature is:

  $$\boldsymbol{s}^{(j)} = [\boldsymbol{s}^{(1j)}; \ldots; \boldsymbol{s}^{((j-1)j)}; \boldsymbol{s}^{(jj)}; \boldsymbol{s}^{(j(j+1))}; \ldots; \boldsymbol{s}^{(jq)}]$$

  Here, $\boldsymbol{s}^{(1j)}, \ldots, \boldsymbol{s}^{(jq)}$ are obtained in Eq.(6) and Eq.(9). Then for the obtained q dimension-specific features $\{\boldsymbol{s}^{(j)} | 1 \leq j \leq q\}$, q fully-connected layers are respectively used to output probabilities w.r.t. corresponding dimensions.
- MONO. Get rid of all pairwise parts, i.e., only employ Eq.(7)$\sim$Eq.(9), Eq.(13)$\sim$Eq.(15).

Wilcoxon signed-ranks test [Demšar, 2006] at significance level $\alpha = 0.05$ is conducted to analyze whether PIST performs statistically better than variant models. Table 5 summarizes the p-value statistics on each evaluation metric. Compared with these four variant models, we observe that PIST achieves statistically superior performance against them in terms of each metric, which validates effectiveness of PIST in the following aspects:

- It is beneficial to use pairwise dimension-specific features than original ones.
- Our proposed combinatorial encoding method with embedding loss generates better label embeddings for capturing the correlation between features and their corresponding dimensions compared to random initialization of label embeddings.
- Combining probabilistic predictions w.r.t. pairwise dimensions can effectively leverage class dependencies, surpassing the strategy of stacking dimension-specific features and obtaining prediction in each respective dimension directly.
- Single dimension-specific features are insufficient to model class dependencies and our proposed pairwise dependencies modeling is one of the most essential approaches for designing MDC algorithms.

Parameter Sensitivity

Figure 2 shows how the performance of PIST fluctuates with different values of t, i.e. the dimension of latent label embeddings as mentioned in Eq.(1). It is shown that PIST achieves relatively stable performance when the value of t changed in the range of $\{2^5, 2^6, 2^7, 2^8, 2^9\}$. In this paper, the value of t is set to 2^5 in light of lower complexity which can be used as the default parameter setting.

5 Conclusion

The main contributions of this paper are two-fold. (1) We propose to consider the specific characteristics contained in different semantic dimensions for MDC which is as important as modeling class dependencies. (2) We proposed a novel MDC approach named PIST which learns pairwise dimension-specific features for MDC to consider both the specific characteristics in each dimension and the dependencies among different dimensions. Experiments clearly validate the effectiveness of the proposed PIST approach.

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