Multi-Dimensional Classification via *k*NN Feature Augmentation

Bin-Bin Jia[1,2,3], **Min-Ling Zhang**[1,3,4,*]
[1] School of Computer Science and Engineering, Southeast University, Nanjing 210096, China
[2] College of Electrical and Information Engineering, Lanzhou University of Technology, Lanzhou 730050, China
[3] Key Laboratory of Computer Network and Information Integration (Southeast University), Ministry of Education, China
[4] Collaborative Innovation Center of Wireless Communications Technology, China
jiabb@seu.edu.cn, zhangml@seu.edu.cn* (corresponding author)

Abstract

Multi-dimensional classification (MDC) deals with the problem where one instance is associated with multiple class variables, each of which specifies its class membership w.r.t. one specific class space. Existing approaches learn from MDC examples by focusing on modeling dependencies among class variables, while the potential usefulness of manipulating feature space hasn't been investigated. In this paper, a first attempt towards feature manipulation for MDC is proposed which enriches the original feature space with kNN-augmented features. Specifically, simple counting statistics on the class membership of neighboring MDC examples are used to generate augmented feature vector. In this way, discriminative information from class space is encoded into the feature space to help train the multi-dimensional classification model. To validate the effectiveness of the proposed feature augmentation techniques, extensive experiments over eleven benchmark data sets as well as four state-of-the-art MDC approaches are conducted. Experimental results clearly show that, compared to the original feature space, classification performance of existing MDC approaches can be significantly improved by incorporating kNN-augmented features.

Introduction

Multi-dimensional classification aims at modeling real-world objects with rich semantics, which assumes a number of class spaces to characterize the object's semantics from different dimensions. Here, an MDC example is associated with multiple class variables with each of them specifying its class membership w.r.t. one specific class space. Specifically, the need of learning from MDC examples naturally arises in many scenarios (Theeramunkong and Lertnattee 2002; Rodríguez et al. 2012; Borchani et al. 2013; Sagarna et al. 2014; Hernández-González, Inza, and Lozano 2015; Serafino et al. 2015). For example, the semantics of a natural scene image can be characterized from the `season` dimension (with possible classes *spring*, *summer*, *autumn*, and *winter*), and from the `landscape` dimension (with possible classes *mountain*, *grassland*, *lake*, etc.). For another example, the semantics of a piece of music can be characterized from the `genre` dimension (with possible classes *rock*, *popular*, *classical*, etc.), from the `instrument` dimension (with possible classes *piano*, *violin*, *guitar*, etc.), and from the `language` dimension (with possible classes *English*, *Chinese*, *Spanish*, etc.).

Formally, let $\mathcal{X} = \mathbb{R}^d$ denote the d-dimensional input (feature) space and $\mathcal{Y} = C_1 \times C_2 \times \cdots \times C_q$ denote the output space which corresponds to the Cartesian product of q class spaces. Here, each class space C_j $(1 \leq j \leq q)$ consists of K_j possible classes, i.e. $C_j = \{c_1^j, c_2^j, \ldots, c_{K_j}^j\}$. Given a set of MDC training examples $\mathcal{D} = \{(\boldsymbol{x}_i, \boldsymbol{y}_i) \mid 1 \leq i \leq m\}$, where $\boldsymbol{x}_i = [x_{i1}, x_{i2}, \ldots, x_{id}]^\top \in \mathcal{X}$ is a d-dimensional feature vector and $\boldsymbol{y}_i = [y_{i1}, y_{i2}, \ldots, y_{iq}]^\top \in \mathcal{Y}$ is the associated class vector with each component class variable y_{ij} assuming one possible value in C_j, the task of multi-dimensional classification is to learn a predictive function $f : \mathcal{X} \mapsto \mathcal{Y}$ from $\mathcal{D}$ which can assign a proper class vector $f(\boldsymbol{x}) \in \mathcal{Y}$ for unseen instance $\boldsymbol{x}$.

To learn from MDC examples, an intuitive solution is to decompose the multi-dimensional classification problem into a number of independent multi-class classification problems, one per class space. Nonetheless, dependencies among class spaces are ignored in this case which would impact the generalization performance of induced predictive model. Therefore, existing MDC approaches work by modeling dependencies among class variables from different dimensions in various ways, such as capturing pairwise interactions between class variables (Arias et al. 2016), specifying chaining order over class variables (Zaragoza et al. 2011; Read, Martino, and Luengo 2014), assuming directed acyclic graph (DAG) structure over class variables (Bielza, Li, and Larrañaga 2011; Batal, Hong, and Hauskrecht 2013; Zhu, Liu, and Jiang 2016; Bolt and van der Gaag 2017; Benjumeda, Bielza, and Larrañaga 2018), and partitioning class variables into groups (Read, Bielza, and Larrañaga 2014), etc.

Other than modeling dependencies among class variables in the output space, we show the potential usefulness of manipulating feature space for multi-dimensional classification. In this paper, a simple yet effective approach named KRAM, i.e. *kNN featuRe Augmentation for Multi-dimensional classification*, is proposed. KRAM manipulates the feature space of MDC examples by making use of the popular kNN techniques, where specific counting statistics on the class membership of neighboring MDC examples are employed to enrich the original feature space. In this way,

Copyright © 2019, Association for the Advancement of Artificial Intelligence (www.aaai.org). All rights reserved.

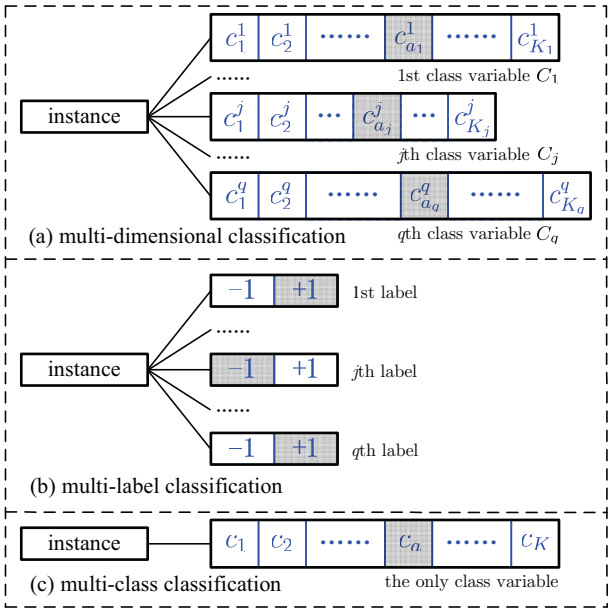


Figure 1: Relationships among multi-dimensional classification, multi-label classification, and multi-class classification.

discriminative information from class space is encoded into the feature space to facilitate subsequent induction of MDC predictive model. Extensive experiments clearly validate the effectiveness of KRAM in improving predictive performance of existing MDC approaches with kNN-augmented features.

The rest of this paper is organized as follows. Firstly, related works on multi-dimensional classification are briefly discussed. Secondly, technical details of the proposed approach are introduced. Thirdly, experimental results of comparative studies are reported. Finally, we conclude this paper.

Related Work

In multi-dimensional classification each instance is associated with multiple class variables, whose most related learning frameworks include traditional multi-class classification and multi-label classification (MLC) (Zhang and Zhou 2014; Gibaja and Ventura 2015).

As shown in Figure 1, MDC corresponds to a set of joint multi-class classification problems while MLC corresponds to a set of joint binary classification problems. Nonetheless, the major differences between MDC and MLC do not just lie in whether the joint problem to be solved is multi-class or binary class. Conceptually speaking, MDC usually assumes *heterogenous* semantic spaces where each class variable corresponds to one possible class space, while MLC assumes *homogeneous* semantic space where each label specifies the relevancy of one concept in the class space. Formally speaking, MLC can be regarded as a degenerated version of MDC by restricting binary-valued class variable in each dimension.

MDC can be decomposed into multiple traditional multi-class classification problems, i.e. training an independent multi-class classifier w.r.t. each class space. However, this intuitive strategy doesn't consider possible dependencies among class spaces and may lead to suboptimal MDC solution. Therefore, modeling dependencies among class spaces is one of the core goals when designing MDC learning approaches.

Pairwise interactions between class spaces can be encoded using a collection of base classifiers, where predictions from base classifiers are combined via Markov random field for subsequent multi-dimensional inference (Arias et al. 2016). Following the idea of classifier chain (CC) for MLC (Read et al. 2011), the MDC problem can be transformed into a chain of multi-class classification problems where the chaining order over class variables are specified in random manner (Read, Martino, and Luengo 2014) or deterministic manner (Zaragoza et al. 2011).

Moreover, dependencies among class spaces can be explicitly modeled with directed acyclic graph (DAG) with different families of DAG structures (Bielza, Li, and Larrañaga 2011; Batal, Hong, and Hauskrecht 2013; Zhu, Liu, and Jiang 2016; Bolt and van der Gaag 2017; Benjumeda, Bielza, and Larrañaga 2018). Class powerset (CP) models dependencies by transforming the MDC problem into a single multi-class classification problem, where each possible combination of class variables $\boldsymbol{y} \in \mathcal{Y}$ is treated as a new class in the transformed problem. In light of the huge class space (with $\prod_{j=1}^{q} K_j$ classes after CP transformation), it is helpful to partition MDC class variables into groups so as to expedite subsequent MDC model induction (Read, Bielza, and Larrañaga 2014).

The KRAM Approach

Although modeling dependencies among class spaces plays a crucial role in learning from MDC examples, the importance of manipulating feature space for model induction hasn't been well studied for MDC researches. In this section, we present technical details of the KRAM approach which aims to improve the generalization ability of learned MDC models by enriching the original feature space with kNN techniques.

Following the same notations given in previous section, let $\mathcal{D} = \{(\boldsymbol{x}_i, \boldsymbol{y}_i) \mid 1 \leq i \leq m\}$ be the MDC training set where $\boldsymbol{y}_i = [y_{i1}, y_{i2}, \ldots, y_{iq}]^\top \in \mathcal{Y}$ corresponds to the class vector associated with $\boldsymbol{x}_i$. For each instance $\boldsymbol{x}$, let $\mathcal{N}(\boldsymbol{x}) = \{i_r \mid 1 \leq r \leq k\}$ denote the set of indices for the k nearest neighbors of $\boldsymbol{x}$ identified in $\mathcal{D}$. Then, the following counting statistics $\boldsymbol{\delta}_j^{\boldsymbol{x}} = [\delta_{j1}^{\boldsymbol{x}}, \delta_{j2}^{\boldsymbol{x}}, \ldots, \delta_{jK_j}^{\boldsymbol{x}}]^\top$ can be defined for the j-th class space by considering the class membership of neighboring MDC examples:

$$\delta_{ja}^{\boldsymbol{x}} = \sum_{i_r \in \mathcal{N}(\boldsymbol{x})} [\![y_{i_r j} = c_a^j]\!] \quad (1 \leq a \leq K_j) \qquad (1)$$

Here, $\boldsymbol{y}_{i_r} = [y_{i_r 1}, y_{i_r 2}, \ldots, y_{i_r q}]^\top$ corresponds to the class vector of the neighboring MDC example $\boldsymbol{x}_{i_r}$ for $\boldsymbol{x}$. The predicate $[\![\pi]\!]$ returns 1 if π holds and 0 otherwise. Therefore, $\delta_{ja}^{\boldsymbol{x}}$ records the number of $\boldsymbol{x}$'s neighboring MDC examples which has class value of c_a^j in the j-th class space. According to Eq.(1), it is easy to verify that $\sum_{a=1}^{K_j} \delta_{ja}^{\boldsymbol{x}} = k$ holds.

Table 1: The pseudo-code of KRAM.

Inputs:

$\mathcal{D}$: MDC training set $\{(\boldsymbol{x}_i, \boldsymbol{y}_i) \mid 1 \leq i \leq m\}$
k: number of nearest neighbors considered
$\mathcal{L}$: MDC training algorithm
$\boldsymbol{x}^*$: unseen instance

Outputs:

$\boldsymbol{y}^*$: predicted class vector for $\boldsymbol{x}^*$

Process:

1: **for** $i = 1$ to m **do**
2: Identify k nearest neighbors of $\boldsymbol{x}_i$ in $\mathcal{D}$ and store their indices in $\mathcal{N}(\boldsymbol{x}_i)$;
3: **for** $j = 1$ to q **do**
4: **for** $a = 1$ to K_j **do**
5: Calculate $\delta_{ja}^{\boldsymbol{x}_i}$ according to Eq.(1);
6: **end for**
7: Set $\boldsymbol{\delta}_j^{\boldsymbol{x}_i} = [\delta_{j1}^{\boldsymbol{x}_i}, \delta_{j2}^{\boldsymbol{x}_i}, \ldots, \delta_{jK_j}^{\boldsymbol{x}_i}]^\top$;
8: **end for**
9: Set $\boldsymbol{\Delta}_{\boldsymbol{x}_i} = \left[\boldsymbol{\delta}_1^{\boldsymbol{x}_i}, \boldsymbol{\delta}_2^{\boldsymbol{x}_i}, \ldots, \boldsymbol{\delta}_q^{\boldsymbol{x}_i}\right]$;
10: **end for**
11: Form the transformed MDC training set $\widetilde{\mathcal{D}} = \{(\widetilde{\boldsymbol{x}}_i, \boldsymbol{y}_i) \mid 1 \leq i \leq m\}$ according to Eq.(3);
12: Induce MDC predictive function f based on $\widetilde{\mathcal{D}}$: $f \leftarrow\!\shortmid \mathcal{L}(\widetilde{\mathcal{D}})$;
13: Identify k nearest neighbors of $\boldsymbol{x}^*$ in $\mathcal{D}$ and store their indices in $\mathcal{N}(\boldsymbol{x}^*)$;
14: Generate augmented instance $\tilde{\boldsymbol{x}}^* = [\boldsymbol{x}^*, \boldsymbol{\Delta}_{\boldsymbol{x}^*}]$ with $\boldsymbol{\Delta}_{\boldsymbol{x}^*}$ being calculated according to Eq.(2) and Eq.(1);
15: Return $\boldsymbol{y}^* = f(\tilde{\boldsymbol{x}}^*)$.

Therefore, a total of q counting statistics $\boldsymbol{\delta}_j^{\boldsymbol{x}}$ $(1 \leq j \leq q)$ each containing K_j elements can be generated by traversing all class spaces. By concatenating all counting statistics, an augmented feature vector $\boldsymbol{\Delta}_{\boldsymbol{x}}$ for $\boldsymbol{x}$ is defined as follows:

$$\boldsymbol{\Delta}_{\boldsymbol{x}} = \left[\boldsymbol{\delta}_1^{\boldsymbol{x}}, \boldsymbol{\delta}_2^{\boldsymbol{x}}, \ldots, \boldsymbol{\delta}_q^{\boldsymbol{x}}\right] \tag{2}$$

Then, the original MDC training set $\mathcal{D}$ is transformed into:

$$\widetilde{\mathcal{D}} = \{(\tilde{\boldsymbol{x}}_i, \boldsymbol{y}_i) \mid 1 \leq i \leq m\}, \quad \text{where } \tilde{\boldsymbol{x}}_i = [\boldsymbol{x}_i, \boldsymbol{\Delta}_{\boldsymbol{x}_i}] \tag{3}$$

Here, each instance $\tilde{\boldsymbol{x}}_i$ belongs to the augmented feature space $\widetilde{\mathcal{X}}$ which is the Cartesian product between $\mathcal{X}$ and a $(\sum_{j=1}^{q} K_j)$-dimensional feature space. Thereafter, an MDC predictive function $f : \widetilde{\mathcal{X}} \mapsto \mathcal{Y}$ can be induced from $\widetilde{\mathcal{D}}$ by applying any MDC training algorithm $\mathcal{L}$, i.e. $f \leftarrow\!\shortmid \mathcal{L}(\widetilde{\mathcal{D}})$. For unseen instance $\boldsymbol{x}^*$, its class vector $\boldsymbol{y}^*$ can be predicted by feeding the augmented instance $\tilde{\boldsymbol{x}}^*$ into f.

In summary, Table 1 presents the complete procedure of KRAM. Firstly, the original feature space is enriched by kNN feature augmentation based on simple counting statistics derived from neighboring MDC examples (steps 1-10). After that, an MDC predictive function is induced by learning from the transformed MDC training set (steps 11-12). Finally, the class vector for unseen instance is predicted based on the augmented features as well (steps 13-15).

Table 2: Characteristics of the experimental data sets.

Data Set	#Exam.	#Dim.	#Values/Dim.	#Features†
Edm	154	2	3	$16n$
Flare1	323	3	2-4	$10x$
Song	785	3	3	$98n$
WQplants	1060	7	4	$16n$
WQanimals	1060	7	4	$16n$
WaterQuality	1060	14	4	$16n$
Thyroid	9172	7	2-5	$7n$, $20b$, $2x$
Music	591	6	2	$71n$
Image	2000	5	2	$294n$
Scene	2407	6	2	$294n$
Yeast	2417	14	2	$103n$

† n, b and x denote numeric, binary, and nominal features respectively.

It is worth noting that the proposed KRAM approach should be regarded as a meta-strategy to learn from MDC examples, where any off-the-shelf MDC training algorithm $\mathcal{L}$ can be utilized to instantiate KRAM. Moreover, the kNN-based techniques proposed in this paper only represent as a first attempt towards MDC feature augmentation, which is not meant to be the best possible practice among other feasible choices. Nevertheless, experimental studies reported in the next section clearly validate the effectiveness of KRAM in improving the generalization performance of multi-dimensional classification.

Experiments

Experimental Setup

Data Sets To evaluate the effectiveness of KRAM in improving the generalization performance of MDC predictive model, a number of MDC data sets have been employed for experimental studies. Table 2 summarizes characteristics of the experimental data sets, including *number of examples* (#Exam.), *number of class spaces* (#Dim.), *number of class values per class space* (#Values/Dim.), and *number of features* (#Features).

The first seven data sets in Table 2 are collected from different real-world MDC tasks:[1]

- `Edm` deals with the task of predicting control operations during electrical discharge machining process (Karalič and Bratko 1997), where the 2 class spaces correspond to two controlling parameters gap and flow.
- `Flare1` deals with the task of predicting the number of times certain types of solar flare occurred within 24 hours period (Dheeru and Karra Taniskidou 2017), where the 3 class spaces correspond to common, moderate, and severe solar flares.

[1]To the best of our knowledge, the number of real-world MDC data sets employed in this paper is larger than most state-of-the-art multi-dimensional classification studies (Bielza, Li, and Larrañaga 2011; Read, Bielza, and Larrañaga 2014; Ma and Chen 2018).

Table 3: Experimental results (mean±std. deviation) of each MDC approach and its KRAM counterpart in terms of *hamming score*. In addition, •/○ indicates whether the KRAM counterpart is significantly superior/inferior to the MDC approach on each data set (pairwise t-test at 0.05 significance level).

(a) Multi-class classifier: SVM

Data Set	BR	KRAM-BR	ECC	KRAM-ECC	ECP	KRAM-ECP	ESC	KRAM-ESC
Edm	.689±.070	.734±.083•	.695±.065	.769±.087•	.721±.082	.763±.107•	.698±.089	.751±.102•
Flare1	.922±.034	.922±.033	.922±.034	.922±.034	.921±.036	.922±.034	.923±.033	.923±.036
Song	.793±.023	.787±.023○	.790±.024	.788±.026	.786±.029	.781±.028	.790±.029	.788±.029
WQplants	.657±.016	.664±.013	.654±.016	.663±.014•	.647±.015	.585±.027○	.651±.017	.664±.016•
WQanimals	.630±.014	.635±.012•	.630±.014	.637±.014•	.629±.013	.556±.014○	.631±.014	.635±.014
WaterQuality	.644±.013	.646±.010	.643±.013	.644±.013	.628±.015	.557±.010○	.641±.013	.636±.013
Thyroid	.965±.002	.969±.003•	.965±.002	.969±.003•	.965±.002	.968±.002•	.965±.002	.969±.002•
Music	.808±.023	.818±.022•	.814±.025	.810±.022	.799±.032	.802±.025	.813±.028	.809±.029
Image	.828±.010	.841±.011•	.831±.012	.844±.012•	.832±.012	.842±.009•	.838±.009	.844±.015
Scene	.895±.009	.918±.008•	.905±.011	.921±.008•	.914±.009	.925±.008•	.910±.011	.923±.008•
Yeast	.801±.006	.811±.007•	.797±.007	.808±.007•	.795±.007	.795±.007	.802±.006	.808±.008•

(b) Multi-class classifier: NB

Data Set	BR	KRAM-BR	ECC	KRAM-ECC	ECP	KRAM-ECP	ESC	KRAM-ESC
Edm	.677±.096	.680±.088	.690±.084	.674±.097	.731±.062	.722±.089	.674±.095	.674±.101
Flare1	.886±.061	.872±.051	.883±.059	.875±.053	.908±.045	.903±.046	.896±.059	.892±.053
Song	.626±.038	.629±.034	.621±.036	.623±.034	.674±.044	.684±.042	.646±.031	.666±.037•
WQplants	.397±.028	.506±.033•	.353±.033	.494±.038•	.607±.015	.647±.019•	.442±.034	.549±.031•
WQanimals	.381±.021	.419±.019•	.377±.024	.416±.020•	.590±.020	.625±.017•	.577±.022	.598±.013•
WaterQuality	.389±.017	.488±.022•	.360±.020	.487±.021•	.599±.018	.597±.018	.609±.017	.609±.017
Thyroid	.926±.005	.925±.003	.926±.007	.929±.004	.966±.003	.963±.003○	.958±.004	.952±.006○
Music	.743±.018	.761±.023•	.745±.020	.761±.023•	.770±.029	.784±.019•	.738±.023	.764±.030•
Image	.573±.016	.586±.018•	.576±.014	.587±.014•	.746±.012	.754±.011•	.593±.017	.608±.015•
Scene	.763±.009	.777±.009•	.767±.010	.780±.010•	.867±.011	.875±.013•	.866±.010	.868±.013
Yeast	.699±.010	.695±.014	.696±.009	.698±.013	.773±.011	.787±.008•	.716±.006	.743±.006•

- `Song` deals with the task of predicting properties of songs which are collected and annotated by ourselves, where the 3 class spaces correspond to the emotion, genre and scenarios of one song.
- `Water Quality` deals with the task of predicting plant and animal species in Slovenian rivers (Džeroski, Demšar, and Grbović 2000), where the 14 class spaces correspond to relative representation of different species. By focusing on the 7 class spaces on plant or the 7 class spaces on animal, we have the `WQplants` and `WQanimals` data sets respectively (Kocev et al. 2007).
- `Thyroid` deals with the task of estimating types of thyroid problems based on patient information (Dheeru and Karra Taniskidou 2017), where the 7 class spaces correspond to diagnosis of seven different conditions.

The last four data sets in Table 2 are collected from benchmark multi-label learning tasks including audio classification: `Music` (Read, Bielza, and Larrañaga 2014), image classification: `Image`, `Scene` (Zhang and Zhou 2007; Boutell et al. 2004), and gene functional analysis: `Yeast` (Elisseeff and Weston 2002). Here, each class space corresponds to a binary-valued class variable which specifies whether one concept is relevant to the example or not.

Evaluation Metrics Let $\mathcal{S} = \{(\boldsymbol{x}_i, \boldsymbol{y}_i) \mid 1 \leq i \leq p\}$ be the test set with p MDC examples, where $\boldsymbol{y}_i = [y_{i1}, y_{i2}, \ldots, y_{iq}]^\top \in \mathcal{Y}$ is the class vector associated with $\boldsymbol{x}_i$. Furthermore, let $f : \mathcal{X} \mapsto \mathcal{Y}$ be the induced MDC predictive function where $\hat{\boldsymbol{y}}_i = f(\boldsymbol{x}_i) = [\hat{y}_{i1}, \hat{y}_{i2}, \ldots, \hat{y}_{iq}]^\top$ is the predicted class vector for $\boldsymbol{x}_i$.

For each MDC test example $(\boldsymbol{x}_i, \boldsymbol{y}_i)$, let $r^{(i)} = \sum_{j=1}^{q} [\![y_{ij} = \hat{y}_{ij}]\!]$ denote the number of class spaces on which f makes correct classification. Then, the following three metrics are utilized in this paper to measure the generalization performance of MDC approaches:

- *Hamming Score*:

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

The hamming score measures the average fraction of class spaces which have been correctly classified by the MDC predictor.

Table 4: Experimental results (mean±std. deviation) of each MDC approach and its KRAM counterpart in terms of *exact match*. In addition, •/○ indicates whether the KRAM counterpart is significantly superior/inferior to the MDC approach on each data set (pairwise t-test at 0.05 significance level).

(a) Multi-class classifier: SVM

Data Set	BR	KRAM-BR	ECC	KRAM-ECC	ECP	KRAM-ECP	ESC	KRAM-ESC
Edm	.442±.125	.521±.141•	.454±.123	.598±.169•	.559±.136	.612±.170	.513±.142	.592±.165•
Flare1	.821±.073	.818±.072	.817±.078	.818±.073	.817±.078	.821±.073	.821±.073	.821±.073
Song	.479±.059	.476±.050	.481±.057	.476±.051	.484±.054	.467±.059	.481±.062	.480±.057
WQplants	.097±.033	.099±.034	.093±.037	.105±.037	.093±.028	.067±.029○	.093±.037	.099±.032
WQanimals	.058±.022	.063±.014	.061±.023	.064±.010	.065±.018	.029±.011○	.064±.024	.059±.014
WaterQuality	.007±.008	.008±.007	.006±.008	.009±.006	.001±.003	.004±.005	.006±.008	.010±.005
Thyroid	.773±.015	.800±.018•	.772±.014	.800±.016•	.773±.014	.802±.015•	.771±.014	.801±.015•
Music	.272±.075	.331±.082•	.346±.079	.343±.078	.343±.076	.341±.073	.350±.078	.345±.084
Image	.394±.028	.459±.033•	.479±.033	.522±.036•	.513±.024	.540±.024•	.499±.025	.529±.038•
Scene	.530±.035	.651±.038•	.649±.035	.708±.026•	.700±.029	.731±.029•	.665±.041	.725±.027•
Yeast	.151±.017	.199±.015•	.207±.014	.252±.014•	.252±.012	.262±.018	.237±.017	.263±.019•

(b) Multi-class classifier: NB

Data Set	BR	KRAM-BR	ECC	KRAM-ECC	ECP	KRAM-ECP	ESC	KRAM-ESC
Edm	.432±.166	.445±.153	.451±.145	.438±.162	.554±.112	.548±.120	.432±.166	.438±.162
Flare1	.774±.099	.756±.095	.774±.087	.771±.088	.790±.081	.777±.084	.780±.093	.768±.086
Song	.238±.054	.224±.050	.228±.036	.219±.043	.311±.053	.317±.051	.274±.047	.304±.054•
WQplants	.001±.003	.036±.026•	.001±.003	.035±.018•	.034±.021	.067±.038•	.001±.003	.040±.025•
WQanimals	.004±.009	.008±.010	.007±.008	.006±.007	.020±.014	.042±.016•	.024±.018	.026±.023
WaterQuality	.000±.000	.000±.000	.000±.000	.000±.000	.008±.009	.004±.007○	.002±.004	.002±.004
Thyroid	.580±.027	.575±.015	.593±.026	.592±.022	.793±.017	.768±.015○	.738±.022	.703±.036○
Music	.206±.043	.218±.058	.230±.058	.221±.065	.249±.078	.281±.073•	.210±.070	.242±.089•
Image	.069±.016	.074±.021•	.069±.019	.074±.020•	.285±.022	.302±.022•	.069±.021	.074±.021
Scene	.177±.023	.198±.022•	.181±.024	.200±.021•	.550±.030	.575±.040•	.541±.024	.528±.046
Yeast	.095±.018	.115±.018•	.102±.016	.125±.024•	.203±.018	.240±.024•	.110±.014	.154±.015•

- *Exact Match*:

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

  The exact match measures the proportion of test examples on which the MDC predictor makes correct classification over all class spaces. Conceptually, exact match serves as a strict metric whose value might be rather low for MDC tasks with large number of class spaces.

- *Sub-Exact Match*:

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

  The sub-exact match corresponds to a relaxed version of exact match, which measures the proportion of test examples on which the MDC predictor makes at most one incorrect classification over all class spaces.

Comparing Approaches KRAM is a meta-strategy to learn from MDC examples, which can be coupled with any off-the-shelf MDC learning algorithm (i.e. $\mathcal{L}$ in Table 1) to improve its generalization performance. In this paper, four well-established MDC approaches (Read, Bielza, and Larrañaga 2014) are used to instantiate KRAM:

- *Binary Relevance* (BR): This approach decomposes the multi-dimensional classification problem into a number of independent multi-class classification problems, one per class space.
- *Ensembles of Classifier Chains* (ECC): This approach transforms the multi-dimensional classification problem into a chain of multi-class classification problems, where subsequent classifiers in the chain are built by treating predictions of preceding ones as extra features. Specifically, an ensemble of classifier chains are built with different random chaining orders.
- *Ensembles of Class Powerset* (ECP): This approach transforms the multi-dimensional classification problem into one multi-class classification problem, where each distinct combination of MDC class variables is treated as a new class. Specifically, an ensemble of class powerset models are built by randomly sampling the MDC training set.

Table 5: Experimental results (mean±std. deviation) of each MDC approach and its KRAM counterpart in terms of *sub-exact match*. In addition, •/○ indicates whether the KRAM counterpart is significantly superior/inferior to the MDC approach on each data set (pairwise t-test at 0.05 significance level).

(a) Multi-class classifier: SVM

Data Set	BR	KRAM-BR	ECC	KRAM-ECC	ECP	KRAM-ECP	ESC	KRAM-ESC
Edm	.935±.061	.947±.076	.935±.069	.940±.058	.883±.074	.915±.075	.883±.074	.909±.070
Flare1	.947±.039	.951±.036	.951±.036	.951±.036	.947±.039	.947±.039	.951±.036	.951±.042
Song	.903±.033	.888±.046	.891±.036	.891±.047	.878±.040	.877±.040	.892±.038	.885±.048
WQplants	.287±.055	.300±.042	.283±.049	.295±.044	.281±.049	.187±.040○	.282±.049	.294±.045
WQanimals	.229±.034	.232±.030	.229±.032	.241±.040	.230±.032	.151±.030○	.232±.032	.241±.032
WaterQuality	.051±.024	.053±.017	.050±.023	.048±.018	.035±.018	.019±.016	.046±.022	.049±.024
Thyroid	.982±.004	.983±.004	.981±.004	.982±.004	.981±.005	.979±.003○	.982±.004	.981±.004
Music	.674±.067	.682±.054	.676±.064	.677±.051	.640±.064	.659±.066	.662±.075	.672±.063
Image	.782±.031	.783±.027	.730±.033	.745±.031	.710±.036	.727±.029•	.738±.032	.740±.036
Scene	.855±.018	.867±.020	.796±.030	.825±.020•	.796±.028	.825±.018•	.799±.032	.823±.024•
Yeast	.269±.029	.307±.020•	.288±.023	.316±.022•	.304±.020	.317±.018	.310±.030	.324±.027•

(b) Multi-class classifier: NB

Data Set	BR	KRAM-BR	ECC	KRAM-ECC	ECP	KRAM-ECP	ESC	KRAM-ESC
Edm	.922±.074	.916±.060	.929±.064	.909±.062	.909±.047	.896±.081	.915±.063	.909±.062
Flare1	.910±.066	.895±.055	.904±.073	.889±.060	.941±.057	.938±.057	.929±.064	.926±.060
Song	.678±.071	.695±.068	.671±.068	.683±.066	.733±.079	.749±.080	.692±.066	.719±.067•
WQplants	.018±.012	.113±.040•	.013±.010	.123±.037•	.175±.043	.258±.056•	.042±.019	.133±.031•
WQanimals	.041±.016	.049±.019	.039±.016	.049±.015•	.143±.054	.221±.049•	.139±.050	.167±.045
WaterQuality	.000±.000	.003±.005	.000±.000	.001±.003	.032±.024	.033±.020	.023±.013	.025±.017
Thyroid	.916±.011	.912±.009	.906±.020	.922±.008•	.974±.005	.973±.005	.970±.007	.966±.006
Music	.552±.057	.591±.050•	.557±.051	.603±.048•	.591±.071	.617±.053	.524±.039	.581±.082•
Image	.255±.028	.279±.034•	.261±.028	.283±.033•	.597±.034	.612±.033•	.289±.032	.315±.029•
Scene	.561±.021	.591±.026•	.569±.027	.595±.031•	.693±.031	.713±.036•	.703±.031	.733±.038•
Yeast	.149±.020	.182±.027•	.163±.020	.193±.027•	.258±.022	.293±.022•	.167±.019	.217±.022•

- *Ensembles of Super Class classifiers* (ESC): This approach works by partitioning the MDC class variables into groups of super-classes, where conditional dependencies among class variables are used to fulfill the partition process. Specifically, an ensemble of super-class models are built by randomly sampling the MDC training set.

Following (Read, Bielza, and Larrañaga 2014), a random cut of 67% examples from the original MDC training set is used to generate the base MDC model and the number of base classifiers is set to be 10 for ensemble approaches ECC, ECP and ESC. Furthermore, predictions of base MDC models are combined via majority voting.

For each MDC approach $\mathcal{A}$ ($\mathcal{A} \in \{$BR, ECC, ECP, ESC$\}$), we use KRAM-$\mathcal{A}$ to denote the instantiation of KRAM with $\mathcal{A}$. In this paper, support vector machine (SVM) (Chang and Lin 2011) and Naïve Bayes (NB) are used as the multi-class classifier to implement each MDC approach. Specifically, Libsvm with linear kernel and NB with Gaussian pdf for continuous feature are used. As shown in Table 1, the only parameter k (number of nearest neighbors considered) is set to be 8 for KRAM.

To show the effectiveness of KRAM, we aim to compare the performance of KRAM-$\mathcal{A}$ against $\mathcal{A}$. On each data set, ten-fold cross-validation is performed where the mean metric value as well as standard deviation are recorded for the comparing approaches.

Experimental Results

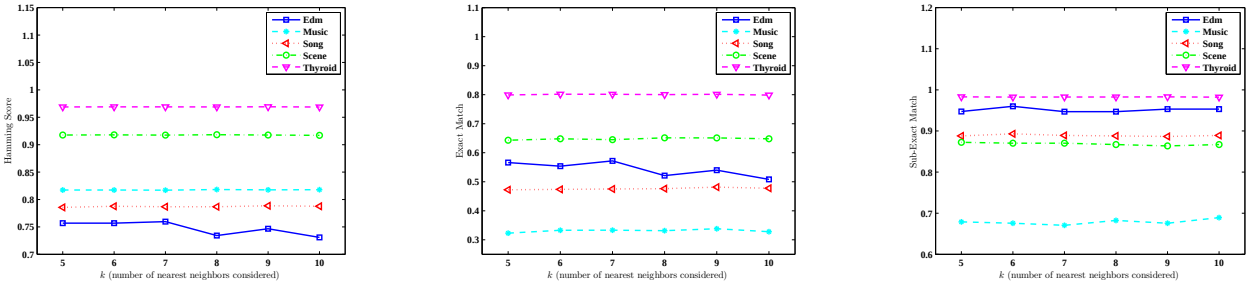
Tables 3 to 5 report the detailed experimental results of each MDC approach and its KRAM counterpart in terms of *hamming score*, *exact match*, and *sub-exact match* respectively. For each data set and multi-class classifier (SVM or NB), pairwise t-test based on ten-fold cross-validation (at 0.05 significance level) is conducted to show whether the performance of KRAM counterpart is significantly different to the MDC approach. Accordingly, Table 6 summarizes the resulting win/tie/loss counts over 11 data sets and 3 evaluation metrics.

Based on the reported experimental results, it is interesting to observe that:

- Across all the 264 configurations (11 data sets × 3 metrics × 4 MDC approaches × 2 multi-class classifiers), the KRAM counterpart achieves superior or at least comparable performance against original MDC approach in 250

Table 6: Win/tie/loss counts of pairwise t-test (at 0.05 significance level) between each MDC approach and its KRAM counterpart in terms of *hamming score* (HScore), *exact match* (EMatch), and *sub-exact match* (SEMatch).

	multi-class classifier: SVM			multi-class classifier: NB			
	HScore	EMatch	SEMatch	HScore	EMatch	SEMatch	**In Total**
KRAM-BR against BR	7/3/1	6/5/0	1/10/0	6/5/0	4/7/0	5/6/0	**29/36/1**
KRAM-ECC against ECC	7/4/0	5/6/0	2/9/0	6/5/0	4/7/0	7/4/0	**31/35/0**
KRAM-ECP against ECP	4/4/3	3/6/2	2/6/3	6/4/1	6/3/2	5/6/0	**26/29/11**
KRAM-ESC against ESC	5/6/0	5/6/0	2/9/0	6/4/1	4/6/1	6/5/0	**28/36/2**



(a) *hamming score* (b) *exact match* (c) *sub-exact match*

Figure 2: Performance of KRAM-BR changes as k ranges from 5 to 10 in terms of each evaluation metric.

configurations.

- BR learns from MDC examples by independent decomposition, where dependencies among class spaces have not been considered in this approach. The prominent advantage of KRAM-BR over BR (with only one loss on HScore with SVM) indicates that the kNN-augmented features generated by KRAM do bring helpful discriminative information in feature space. Specifically, those discriminative information brought into feature space can be regarded as a potential source for dependency modeling when learning the mapping from feature space to output space.
- Both ECC and ESC learn from MDC examples by considering dependencies among class spaces, which are fulfilled by assuming random chaining order over class spaces or partitioning the class spaces into groups. It is impressive to notice that for MDC approaches with inherent dependency modeling mechanism, KRAM can also help improve their generalization ability significantly with kNN-augmented features.
- ECP learns from MDC examples by modeling full-order dependencies, where all possible combinations of class spaces (i.e. class powerset) have been considered in the learning process. ECP generally benefits from the kNN augmented features, while there are 11 cases where the performance of KRAM-ECP is inferior to ECP. Most of the under-performing cases (8 out of 11) for KRAM-ECP occur for *WaterQuality* (including its two divisions *WQplants* and *WQanimals*), where the possible number of CP combinations is high (i.e. 4^{14}).

As shown in Table 1, the only parameter to be set for KRAM is k, which is the number of nearest neighbors considered for generating kNN-augmented features. Figure 2 illustrates how the performance of KRAM (with MDC approach BR) changes as k increases from 5 to 10. In terms of each evaluation metric, KRAM achieves relatively stable performance with varying values of k. Parameter insensitivity is a desirable property for practical use of KRAM, and the value of k is fixed to be 8 in this paper.

Conclusion

The major contributions of our work are two-fold: 1) A new strategy aiming at manipulating feature space for multi-dimensional classification is proposed, which suggests an alternative solution to learn from MDC examples; 2) A simple yet effective approach based on kNN-augmented features is designed to justify the proposed strategy, whose effectiveness is thoroughly validated based on extensive comparative studies. In the future, it is interesting to explore other ways for MDC feature space manipulation. Furthermore, designing feature augmentation techniques customized for specific MDC approach is also worth further investigation.

References

Arias, J.; Gamez, J. A.; Nielsen, T. D.; and Puerta, J. M. 2016. A scalable pairwise class interaction framework for multidimensional classification. *International Journal of Approximate Reasoning* 68:194–210.

Batal, I.; Hong, C.; and Hauskrecht, M. 2013. An efficient probabilistic framework for multi-dimensional classification. In *Proceedings of the 22nd ACM International Conference on Information & Knowledge Management*, 2417–2422.

Benjumeda, M.; Bielza, C.; and Larrañaga, P. 2018. Tractability of most probable explanations in multidimensional bayesian network classifiers. *International Journal of Approximate Reasoning* 93:74–87.

Bielza, C.; Li, G.; and Larrañaga, P. 2011. Multidimensional classification with bayesian networks. *International Journal of Approximate Reasoning* 52(6):705–727.

Bolt, J. H., and van der Gaag, L. C. 2017. Balanced sensitivity functions for tuning multi-dimensional bayesian network classifiers. *International Journal of Approximate Reasoning* 80:361–376.

Borchani, H.; Bielza, C.; Toro, C.; and Larrañaga, P. 2013. Predicting human immunodeficiency virus inhibitors using multi-dimensional bayesian network classifiers. *Artificial Intelligence in Medicine* 57(3):219–229.

Boutell, M. R.; Luo, J.; Shen, X.; and Brown, C. M. 2004. Learning multi-label scene classification. *Pattern Recognition* 37(9):1757–1771.

Chang, C.-C., and Lin, C.-J. 2011. LIBSVM: A library for support vector machines. *ACM Transactions on Intelligent Systems and Technology* 2:27:1–27:27. Software available at `http://www.csie.ntu.edu.tw/~cjlin/libsvm`.

Dheeru, D., and Karra Taniskidou, E. 2017. UCI machine learning repository. `http://archive.ics.uci.edu/ml`.

Džeroski, S.; Demšar, D.; and Grbović, J. 2000. Predicting chemical parameters of river water quality from bioindicator data. *Applied Intelligence* 13(1):7–17.

Elisseeff, A., and Weston, J. 2002. A kernel method for multi-labelled classification. In *Advances in Neural Information Processing Systems*, 681–687.

Gibaja, E., and Ventura, S. 2015. A tutorial on multilabel learning. *ACM Computing Surveys* 47(3):Article 52.

Hernández-González, J.; Inza, I.; and Lozano, J. A. 2015. Multidimensional learning from crowds: Usefulness and application of expertise detection. *International Journal of Intelligent Systems* 30(3):326–354.

Karalič, A., and Bratko, I. 1997. First order regression. *Machine Learning* 26(2-3):147–176.

Kocev, D.; Vens, C.; Struyf, J.; and Džeroski, S. 2007. Ensembles of multi-objective decision trees. In *Lecture Notes in Computer Science 4701*. Berlin: Springer. 624–631.

Ma, Z., and Chen, S. 2018. Multi-dimensional classification via a metric approach. *Neurocomputing* 275:1121–1131.

Read, J.; Pfahringer, B.; Holmes, G.; and Frank, E. 2011. Classifier chains for multi-label classification. *Machine Learning* 85(3):333–359.

Read, J.; Bielza, C.; and Larrañaga, P. 2014. Multidimensional classification with super-classes. *IEEE Transactions on Knowledge and Data Engineering* 26(7):1720–1733.

Read, J.; Martino, L.; and Luengo, D. 2014. Efficient monte carlo methods for multi-dimensional learning with classifier chains. *Pattern Recognition* 47(3):1535–1546.

Rodríguez, J. D.; Pérez, A.; Arteta, D.; Tejedor, D.; and Lozano, J. A. 2012. Using multidimensional bayesian network classifiers to assist the treatment of multiple sclerosis. *IEEE Transactions on Systems, Man, and Cybernetics C Part C: Applications and Reviews* 42(6):1705–1715.

Sagarna, R.; Mendiburu, A.; Inza, I.; and Lozano, J. A. 2014. Assisting in search heuristics selection through multidimensional supervised classification: A case study on software testing. *Information Sciences* 258:122–139.

Serafino, F.; Pio, G.; Ceci, M.; and Malerba, D. 2015. Hierarchical multidimensional classification of web documents with multiwebclass. In *Lecture Notes in Computer Science 9356*. Berlin: Springer. 236–250.

Theeramunkong, T., and Lertnattee, V. 2002. Multidimensional text classification. In *Proceedings of the 19th International Conference on Computational Linguistics-Volume 1*, 1–7. Association for Computational Linguistics.

Zaragoza, J. H.; Sucar, L. E.; Morales, E. F.; Bielza, C.; and Larrañaga, P. 2011. Bayesian chain classifiers for multidimensional classification. In *Proceedings of the 22nd International Joint Conference on Artificial Intelligence*, volume 11, 2192–2197.

Zhang, M.-L., and Zhou, Z.-H. 2007. ML-KNN: A lazy learning approach to multi-label learning. *Pattern Recognition* 40(7):2038–2048.

Zhang, M.-L., and Zhou, Z.-H. 2014. A review on multi-label learning algorithms. *IEEE Transactions on Knowledge and Data Engineering* 26(8):1819–1837.

Zhu, M.; Liu, S.; and Jiang, J. 2016. A hybrid method for learning multi-dimensional bayesian network classifiers based on an optimization model. *Applied Intelligence* 44(1):123–148.