



End-to-End Feature-aware Label Space Encoding for Multi-label Classification with Many Classes

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Summary of Changes and Responses to Reviews

We appreciate very much the handling editor and all reviewers for their time and efforts devoted to the peer-review of this paper. Their constructive comments have guided us to further improve it.

We have conducted a “minor revision” for the manuscript to address the editor’s and reviewers’ comments. And we believe that all the comments raised in the review report have been carefully accommodated. Below we will firstly list the changes we have made in this revision, and then respond to each comment in turn.

I. SUMMARY OF CHANGES

The main changes made in this revision include:

- 1) In the “Introduction” of the revision, we have stated more clearly about the connection between our work and the community of neural networks and related learning systems, as well as our contributions to the community. Moreover, we have improved the language presentation of our manuscript with the help of a native speaker to make it more clear and easier to follow.
- 2) To make our manuscript more focused on the key points, we have moved the following content to a supplementary material: 1) proofs of Lemma 1 and Lemma 3, 2) overmuch details of the experiment for significance tests, and 3) overmuch details of the experiment for validating the orthonormality assumption in our proposed method. Particularly, for 2) and 3), we mainly present the corresponding experimental results and analysis in the manuscript. And for more details, one can refer to the supplementary material.

II. RESPONSES TO REVIEWS

- 1) **Comment:** The language presentation in this paper needs to be improved. The authors are encouraged to have a native speaker or use a professional editing service (see TNNLS website for more information, section “Professional Editing Services” under “Information for Authors”) to help to improve the language presentation.

Response: Thanks for the suggestion. In the revision, we have invited our colleague, who is a native speaker and familiar with the topic, to help polish our manuscript and improve the language presentation.

- 2) **Comment:** The authors should clearly state the key contributions to the core of neural networks and related learning systems to show a strong connection to the NNLS community. The authors might want to take a look of the recently published papers in TNNLS on this

topic as well.

Response: Thanks for the suggestion. In the “Introduction” of the revision, we have stated more clearly about the connection between our work and the NNLS community, as well as our contributions to the community. Please refer to the first two paragraphs of “Introduction” (Page 1) and the 5th paragraph of Page 2.

Specifically, multi-label classification, especially large-scale multi-label classification, is an important topic for the machine learning community, with many research works like [1]–[7] dedicated to it for tackling challenges. Similar to the previous publications like [3], our work also focuses on tackling the challenge of large label sets in large-scale multi-label classification problems. To do so, we propose an effective method termed E²FE to perform label space dimension reduction (LSDR), which aims to yield acceptable classification performance with substantially lower costs. Extensive experiments show that E²FE gains performance improvements over other state-of-the-art LSDR methods. Moreover, since the predictive model used in E²FE is open for any effective one, including neural networks, E²FE can also be applied with existing predictive models or feature dimension reduction approaches in the community to better handle large-scale multi-label classification problems.

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End-to-End Feature-aware Label Space Encoding for Multi-label Classification with Many Classes

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Abstract—To make the problem of multi-label classification with many classes more tractable, in recent years academia has seen efforts devoted to performing label space dimension reduction (LSDR). Specifically, LSDR encodes high-dimensional label vectors into low-dimensional code vectors lying in a latent space, so as to train predictive models at much lower costs. With respect to the prediction, it performs classification for any unseen instance by recovering a label vector from its predicted code vector via a decoding process. In this paper, we propose a novel method, namely End-to-End Feature-aware label space Encoding (E^2FE), to perform LSDR. Instead of requiring an encoding function like most previous works, E^2FE directly learns a code matrix formed by code vectors of the training instances in an end-to-end manner. Another distinct property of E^2FE is its feature awareness attributable to the fact that the code matrix is learnt by jointly maximizing the *recoverability* of the label space and the *predictability* of the latent space. Based on the learnt code matrix, E^2FE further trains predictive models to map instance features into code vectors, and also learns a linear decoding matrix for efficiently recovering the label vector of any unseen instance from its predicted code vector. Theoretical analyses show that both the code matrix and the linear decoding matrix in E^2FE can be efficiently learnt. Moreover, similar to previous works, E^2FE can be specified to learn an encoding function. And it can also be extended with kernel tricks to handle non-linear correlations between the feature space and the latent space. Comprehensive experiments conducted on diverse benchmark datasets with many classes show consistent performance gains of E^2FE over the state-of-the-art methods.

Index Terms—End-to-end feature-aware label space encoding, Label space dimension reduction, Multi-label classification.

I. INTRODUCTION

AS a generalized version of multi-class classification [1], [2], where each instance is restricted to having only one class label, multi-label classification [3]–[20] allows an instance to be associated with several class labels to describe its semantic content or attributes more clearly. Multi-label classification methods are increasingly demanded by modern applications, like multi-label text classification [3], music emotion categorization [4], and semantic image annotation [18]–[20]. In addition, many researches on neural networks and

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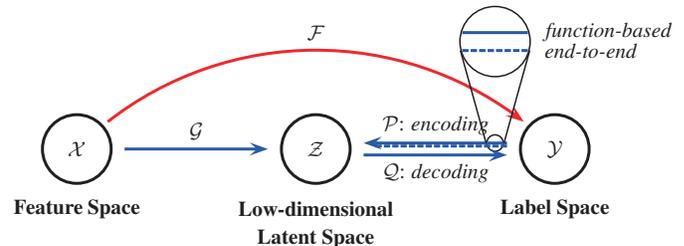


Fig. 1. Illustration of the principles behind traditional multi-label classification methods (red) and those with label space dimension reduction (blue).

other learning approaches are also dedicated to the field, like the tree-structure based method ML-TREE [17], the multiview vector-valued manifold regularization method MV³MR [18], and the label inference method LI-MLC [21], *etc.*

Recently, due to the emergence of web-based applications, multi-label classification problems tend to be large-scale, with new challenges of numerous instances and large label sets (*i.e.* high-dimensional label spaces) coming up. For instance, in the picture sharing community Flickr, there are billions of images and each can be annotated with textual labels selected from millions of candidates. In the community of neural networks and related learning systems, to handle the challenges, some works like [22]–[26] focus on feature dimension reduction or model simplification, while others like LI-MLC [21] focus on shrinking the label space. Here we follow the latter one.

As advocated by Kapoor *et al.* in [5], large label sets cause many existing effective multi-label classification methods [6]–[15] to be infeasible, since generally they need to learn a predictive model for each label independently or with inter-label correlations, and then combine them in a certain manner for prediction. Specifically, for a multi-label classification problem with many classes (*i.e.* a large label set, or a high-dimensional label space), the number of needed predictive models would generally be large, thus making the training costs, if not unaffordable, extremely high. To tackle this issue, researchers have recently proposed to perform label space dimension reduction (LSDR) [5], [27]–[32], which aims to reduce the training costs while maintaining acceptable classification performance. Specifically, for LSDR, as illustrated in Fig. 1, the high-dimensional label vector of any training instance is encoded into a low-dimensional code vector in a latent space. Afterwards, predictive models are trained to map instance features into low-dimensional code vectors, whose quantity is much smaller and thus can significantly reduce the

training costs. As for performing prediction for any unseen instance, a low-dimensional code vector is firstly obtained with the learnt predictive models from its features, and then decoded for recovering its label vector. Generally speaking, if the learnt predictive models and the decoding process are effective and efficient enough, LSDR usually yields acceptable classification performance with much lower costs, making the multi-label classification problem with many classes more tractable.

Prior methods dedicated to LSDR mostly require an encoding function (function-based), *e.g.* a linear one, to map label vectors of training instances into code vectors lying in the latent space. However, due to the following observations, we argue that learning the code vectors of training instances in an end-to-end manner, *i.e.* directly learning them without any encoding functions, can be feasible and even preferable.

- From Fig. 1 it can be seen that, to perform prediction, the encoding process is totally redundant, and thus any encoding function is useless during prediction. Moreover, even for training, it is the encoding result (*i.e.* code vectors of training instances) that will affect the learning of predictive models, no matter whether an encoding function is required or not.
- Defining an encoding function may limit the searching space of the to-be-learnt code vectors of training instances. For example, given the tagging matrix \mathbf{Y} of training instances, using a linear encoding function \mathbf{P} can limit the to-be-learnt code vectors in the space \mathbf{YP} , thereby preventing them from being searched in the whole real space that could potentially minimize the loss of classification performance.
- In some cases, code vectors of training instances are required to have specific properties, like the orthonormality between code dimensions in this paper. Although those property requirements can somehow be transferred to the encoding function, it will inevitably make the objective function much more complex for optimization.

In fact, compared to a function-based encoding, an end-to-end encoding requires no encoding function, and thus can search the whole real space for the optimal to-be-learnt code vectors. Moreover, for an end-to-end encoding, it would be direct to add property requirements for the to-be-learnt code vectors, making the objective function less complex for optimization. To the best of our knowledge, MLC-BMaD [31] is the only previous research that pioneered end-to-end label space encoding via boolean matrix decomposition. However, as will be shown later, its training is not efficient enough and as a result it may not fully accomplish the goal of LSDR. Moreover, MLC-BMaD learns the code vectors of training instances in a *feature-unaware* manner, meaning that the correlations between the latent space and the feature space are not considered. That, as advocated by Chen and Lin [30], can probably make the learnt latent space less predictable and thus degrade the final classification performance. Therefore, further researches on end-to-end label space encoding are highly expected.

In this paper, we propose a novel method termed E²FE

to perform LSDR via **End-to-End Feature-aware** label space **Encoding**. Specifically, E²FE directly learns a code matrix formed by code vectors of training instances via jointly maximizing the *recoverability* of the label space and the *predictability* of the latent space, with the latter considering the correlations between the latent space and the feature space. And thus E²FE is *feature-aware*. Based on the learnt code matrix, predictive models are trained as other LSDR methods, to predict code vectors from instance features. Meanwhile, E²FE further learns a linear decoding matrix that can recover the predicted label vector of any unseen instance from its code vector generated by the trained predictive models.

Since the predictive models in the proposed E²FE are open for any effective ones, including neural networks, E²FE can actually be applied with existing predictive models or feature dimension reduction approaches in the community to better tackle the large-scale multi-label classification problem. Particularly for LSDR, below are three highlighted properties of E²FE, which are in line with our contributions.

- We propose an effective LSDR method termed E²FE for tackling (large-scale) multi-label classification problems with many classes. To the best of our knowledge, it is the first to make LSDR both end-to-end and feature-aware.
- We jointly maximize the *recoverability* of the label space and the *predictability* of the latent space for performing LSDR in E²FE. The objective function *w.r.t* the to-be-learnt code matrix can be transformed to an eigenvalue problem, and is sufficiently flexible in the sense that different optimization strategies can be used depending on the applications for efficient optimization.
- We show that E²FE is a generic approach that covers previous LSDR researches, and it can also be specified to learn an encoding function. Moreover, it can be extended with kernel tricks to handle non-linear correlations between the feature space and the latent space.

This paper is based on our previous work presented in [33], which was termed FaIE, but it substantially extends that work by enhancing the proposed method to be more efficient and effective. Below are the summarized extensions.

- We propose a more efficient optimization method for the proposed method to learn the code matrix in cases where $n \gg d_x + d_y$, with n , d_y , d_x respectively denoting the number of training instances, the dimensionality of the label space and that of the feature space. This is helpful for practical applications, as such cases are quite common. Specifically, the newly proposed optimization method transforms the size of the eigenvalue problem *w.r.t* the objective function of E²FE from $\mathbb{R}^{n \times n}$ to $\mathbb{R}^{(d_x+d_y) \times (d_x+d_y)}$, which can be solved more efficiently and can substantially reduce space costs.
- We further propose π E²FE, π LinearE²FE and *kernel*- π E²FE, to consider the priori knowledge provided by the eigenvalue problem *w.r.t* the to-be-learnt code matrix for learning an enhanced decoding matrix. Experiments comparing π E²FE, π LinearE²FE, *kernel*- π E²FE with their corresponding counterparts, *i.e.* E²FE, LinearE²FE and *kernel*-E²FE, show that enhancing the decoding matrix

with such priori knowledge can help to gain significant performance improvements (on average 48.1% for *label-based macroF1* and 33.9% for *example-based Accuracy*).

- In this paper, we provide a thorough discussion and experimental validation for that the orthonormality assumption for columns of the to-be-learned code matrix in E²FE is reasonable. We also make error analyses for the proposed E²FE, and derive its error bound. Additionally, more theoretical analyses, like those regarding time complexity and parameter settings, are also presented here.
- To better validate the effectiveness of E²FE, we utilize more widely-used benchmark datasets for experiments. We also conduct the experiments on the full datasets instead of the sampled ones in [33], so as to demonstrate the applicability of E²FE for handling larger datasets. More experimental results are also reported, like the significance tests for the improvements gained by E²FE over compared baselines, and the comparison of computational costs between the newly proposed optimization method here and that presented in [33].

The remainder of this paper is organized as follows. Section II gives an overview of related works. Section III elaborates on the proposed E²FE. Section IV shows the proposed optimization methods and its corresponding theoretical analyses. Section V describes details about enhancing the linear decoding matrix with priori knowledge. Then Section VI presents the extensions of E²FE, and analyses its relations to previous works. Experimental settings, results and analyses are given in Section VII. Finally we present discussions regarding E²FE in Section VIII and conclude the paper in Section IX.

II. RELATED WORK

With the explosion of label spaces in real-world applications, many remarkable effective multi-label classification methods tend to be infeasible due to the high training costs. To tackle such multi-label classification problems with many classes, a lot of effective methods were proposed, like constructing a hierarchy of multi-label classifiers [34], refining the output of heuristic efficient classifiers [35], performing label selection to recover the vocabulary with only a subset [36], or using label inference method based on the use of association rules to discover label dependencies [21], *etc.* Recently, LSDR was also proposed and is attracting more and more attention.

To the best of our knowledge, Hsu *et al.* [27] are the first to propose LSDR. Specifically, Hsu *et al.* exploited the sparsity of the label space, and proposed to linearly encode it to a low-dimensional latent space as compressed sensing (CS) and then train linear regression models *w.r.t* the derived codes. As for performing classification for an unseen instance, a code vector is firstly obtained with the learnt regression models from its features and then decoded with standard recovery algorithms like CoSaMP [37] to derive the predicted label vector. Kapoor *et al.* [5] further considered both label space compression and predictive model learning in a single probabilistic model, and derived a Bayesian framework termed BML-CS for multi-label classification via jointly optimizing over both.

Apart from compressed sensing based methods, Tai and Lin [28] proposed to perform principle label space transformation

TABLE I
CATEGORIZATION OF EXISTING LSDR METHODS AND E²FE

	feature-unaware	feature-aware
function-based	CS [27], PLST [28], CL [29], ML-CSSP [32]	BML-CS [5], CPLST [30]
end-to-end	MLC-BMaD [31]	E ² FE

(PLST) for seeking important correlations between labels, which is essentially PCA [38] for the label space. Chen and Lin [30] further enhanced it by proposing feature-aware conditional principal label space transformation (CPLST), which actually integrates orthogonally constrained canonical correlation analysis into the framework of PLST for considering the *predictability* of the latent space. Both PLST and CPLST performed LSDR via linear encoding and linear decoding. Zhou *et al.* [29] proposed another method termed ‘‘Compressed Labelling (CL)’’, which takes the signs of the linear Gaussian random projection results on the original label vectors as the derived code vectors and utilizes a series of Kullback-Leibler divergence based hypothesis tests for decoding. Alternatively, Wicker *et al.* [31] proposed MLC-BMaD for LSDR via boolean matrix decomposition on the binary tagging matrix, factorizing it as the product of a binary code matrix and a binary linear decoding matrix. Bi and Kwok [32] presented an efficient randomized sampling procedure termed ML-CSSP for selecting a column subset of the tagging matrix that can well span it, which is a special case of linear encoding.

Actually, the majority of existing methods perform LSDR in a function-based manner and require an encoding function. Such approaches, as analysed in section I, carry several drawbacks. To avoid those, performing LSDR in an end-to-end manner with no need for any encoding function is highly desired. MLC-BMaD seems to be the only existing LSDR method that supports end-to-end label space encoding via boolean matrix factorization. However, MLC-BMaD is feature-unaware, and thus the learnt latent space could be less predictable, which can result in performance deterioration. Therefore, in this paper we propose E²FE, which performs LSDR in an end-to-end manner and is also feature-aware.

To sum up, Table I categorizes the remarkable existing LSDR methods and the proposed E²FE into different combinations of {function-based, end-to-end} and {feature-unaware, feature-aware}, which well highlights the distinctness of E²FE.

III. PROPOSED APPROACH

A. Preliminaries

Generally in the case of multi-label classification, the features of an instance are represented as a d_x -dimensional feature vector \mathbf{x} in the feature space \mathcal{X} , *i.e.* $\mathbf{x} \in \mathcal{X} \subset \mathbb{R}^{d_x}$, and its labels are represented as a d_y -dimensional binary label vector \mathbf{y} in the label space \mathcal{Y} , *i.e.* $\mathbf{y} \in \mathcal{Y} \subset \{0, 1\}^{d_y}$. Here the i th entry of the label vector \mathbf{y} is set as 1 if the instance is associated with the i th label and 0 otherwise. Suppose that we are given n labelled instances for training, denoted as $\{(\mathbf{x}^{(i)}, \mathbf{y}^{(i)})\}_{i=1}^n$, with $\mathbf{x}^{(i)}$ and $\mathbf{y}^{(i)}$ being the feature vector and the label vector of the i th training instance.

Multi-label classification will utilize them to learn the mapping $\mathcal{F} : \mathcal{X} \rightarrow \mathcal{Y}$ from the feature space \mathcal{X} to the label space \mathcal{Y} , as illustrated in Fig. 1, and then utilize \mathcal{F} for predicting the label vector of any unseen instance based on its feature vector.

As mentioned before, to derive the mapping \mathcal{F} , many existing effective multi-label classification methods will learn a predictive model for each label independently or with inter-label correlations, and then combine them in a certain manner for prediction. In that case, the number of the to-be-learned predictive models will be at least d_y , and even much larger for methods using label powerset [39]. Then for a multi-label classification problem with many classes, d_y will become quite large and the training costs of the to-be-learned predictive models will be extremely high and even unaffordable. To tackle such a challenge, LSDR was recently proposed and is attracting more and more attention. With LSDR, the training process to learn \mathcal{F} is transformed into a two-step learning process. That is, firstly the label vectors of training instances are encoded into low-dimensional code vectors in a latent space $\mathcal{Z} \subset \mathbb{R}^{d_z}$ with an encoding process $\mathcal{P} : \mathcal{Y} \mapsto \mathcal{Z}$, and then a mapping $\mathcal{G} : \mathcal{X} \mapsto \mathcal{Z}$ *w.r.t* the code vectors is learnt. Here d_z is the dimensionality of the latent space \mathcal{Z} , and generally $d_z \ll d_y$. Moreover, as illustrated in Fig. 1, \mathcal{P} can be performed in a function-based manner (*e.g.* linear encoding function) or an end-to-end manner (*e.g.* matrix decomposition). Similar to learning \mathcal{F} , learning \mathcal{G} can be based on training d_z predictive models, one for a dimension of \mathcal{Z} . As for predicting the labels of any unseen instance, a d_z -dimensional code vector in \mathcal{Z} will firstly be derived using the learnt \mathcal{G} with its feature vector, and then a d_y -dimensional predicted label vector will be recovered through a decoding process $\mathcal{Q} : \mathcal{Z} \mapsto \mathcal{Y}$. For LSDR methods, with $d_z \ll d_y$, the number of the to-be-learned predictive models is generally much smaller and thus the training costs are substantially lowered, making the multi-label classification problem with many classes more tractable. Meanwhile, if the mapping \mathcal{G} and the decoding process \mathcal{Q} are effective enough, the classification performance using LSDR is expected to be acceptable.

It should be noticed that for LSDR, the latent space \mathcal{Z} is supposed to be derived from the label space \mathcal{Y} rather than the feature space \mathcal{X} , even though \mathcal{X} can sometimes be considered for increasing the *predictability* of \mathcal{Z} . And thus the dimensionality of the latent space (*i.e.* d_z) can either be higher or lower than that of the feature space (*i.e.* d_x), but will always be lower than that of the label space (*i.e.* d_y). Moreover, for LSDR methods, the mapping \mathcal{G} from \mathcal{X} to \mathcal{Z} is open for any effective mapping algorithm after \mathcal{Z} is derived. Meanwhile, the decoding process \mathcal{Q} generally needs to be specified before deriving \mathcal{Z} , which, from the perspective of efficiency in prediction, is preferred to be linear, like those in PLST, CPLST, MLC-BMad and ML-CSSP.

B. End-to-End Feature-aware Label Space Encoding

Before elaborating on the proposed E²FE, to make it more clear, Table II summarizes the important symbols in this paper.

As mentioned previously, E²FE performs LSDR in an end-to-end manner and directly learns a code matrix $\mathbf{Z} \in \mathbb{R}^{n \times d_z}$

TABLE II
IMPORTANT SYMBOLS IN THE PROPOSED E²FE.

n	the number of training instances
d_x	the dimensionality of the feature space \mathcal{X}
d_y	the dimensionality of the label space \mathcal{Y}
d_z	the dimensionality of the latent space \mathcal{Z} , $d_z \ll d_y$
\mathbf{X}	the feature matrix of training instances, $\mathbf{X} \in \mathbb{R}^{n \times d_x}$
\mathbf{Y}	the tagging matrix of training instances, $\mathbf{Y} \in \{0, 1\}^{n \times d_y}$
\mathbf{Z}	the code matrix of training instances, $\mathbf{Z} \in \mathbb{R}^{n \times d_z}$
\mathbf{Q}	the linear decoding matrix, $\mathbf{Q} \in \mathbb{R}^{d_z \times d_y}$
\mathbf{H}	notation for $\mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T$, $\mathbf{H} \in \mathbb{R}^{n \times n}$
$M_{\cdot, i}$	the i th column of a matrix \mathbf{M}

formed by code vectors of training instances. Generally, the classification performance of LSDR methods depends on both the predictive mapping \mathcal{G} and the decoding process \mathcal{Q} . Therefore, it is crucial for code vectors to be predictable, having a strong correlation with instance features, as revealed in [40]. Meanwhile, the label vectors should also be highly recoverable via decoding the corresponding code vectors. Therefore, to learn \mathbf{Z} , E²FE jointly maximizes the *recoverability* of the label space and the *predictability* of the latent space. The former is denoted as $\Psi_1(\mathbf{Y}, \mathbf{Z})$ and the latter as $\Psi_2(\mathbf{X}, \mathbf{Z})$, where $\mathbf{Y} \in \{0, 1\}^{n \times d_y}$ is the tagging matrix of training instances formed by their label vectors row by row and $\mathbf{X} \in \mathbb{R}^{n \times d_x}$ is the feature matrix formed by their feature vectors in the same way. Then the objective function *w.r.t* \mathbf{Z} is as follows.

$$\Psi = \max_{\mathbf{Z}} \Psi_1(\mathbf{Y}, \mathbf{Z}) + \alpha \Psi_2(\mathbf{X}, \mathbf{Z}) \quad (1)$$

where $\alpha \geq 0$ is a parameter for balancing *recoverability* and *predictability*. When $\alpha = 0$, \mathbf{Z} will be derived via merely maximizing *recoverability*, implying that \mathbf{Z} is just dependent on \mathbf{Y} . On the contrary, when $\alpha > 0$, correlations between instance features and code vectors will be further considered for making \mathbf{Z} feature-aware and more predictable.

1) *Recoverability of Label Space*: To improve the *recoverability* of the label space, the difference between the tagging matrix \mathbf{Y} and the recovered one, which is based on the to-be-learned code matrix \mathbf{Z} , is expected to be minimized. Here we denote the difference as \mathcal{L} . As mentioned previously, for efficient decoding, the proposed E²FE learns a linear decoding matrix $\mathbf{Q} \in \mathbb{R}^{d_z \times d_y}$ to recover label vectors from code vectors, following PLST, CPLST, MLC-BMad and ML-CSSP. Then \mathcal{L} is formulated as follows.

$$\mathcal{L} = \min \|\mathbf{Y} - \mathbf{Z}\mathbf{Q}\|_{fro}^2 \quad (2)$$

where $\|\cdot\|_{fro}$ is the *Frobenius* norm of a matrix. Given \mathbf{Z} , the optimal \mathbf{Q} to minimize \mathcal{L} can be derived as the following closed-form expression by solving $\frac{\partial \mathcal{L}}{\partial \mathbf{Q}} = \mathbf{0}$.

$$\mathbf{Q} = (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}^T \mathbf{Y} \quad (3)$$

To mitigate redundant information in the latent space and then encode the label space more compactly, we assume that the dimensions of the latent space are uncorrelated and thus the columns of \mathbf{Z} are orthonormal, as shown in formula (4).

$$\mathbf{Z}^T \mathbf{Z} = \mathbf{I} \quad (4)$$

where $\mathbf{I} \in \mathbb{R}^{d_z \times d_z}$ is an identity matrix. Actually, as analysed later, although such an orthonormality assumption may seem to be strong, it is still reasonable and important for E²FE. With formula (4), the optimal \mathbf{Q} can be simplified as $\mathbf{Q} = \mathbf{Z}^T \mathbf{Y}$, and then formula (2) can be reformulated as follows.

$$\mathcal{L} = \text{Tr}[\mathbf{Y}^T \mathbf{Y} - \mathbf{Y}^T \mathbf{Z} \mathbf{Z}^T \mathbf{Y}] \quad (5)$$

where $\text{Tr}[\cdot]$ refers to the *trace* of a matrix. With $\text{Tr}[\mathbf{Y}^T \mathbf{Y}]$ being a constant, minimizing \mathcal{L} is identical to maximizing $\text{Tr}[\mathbf{Y}^T \mathbf{Z} \mathbf{Z}^T \mathbf{Y}]$, which can be seen as an expression of the *recoverability* of the label space, *i.e.* $\Psi_1(\mathbf{Y}, \mathbf{Z})$. We can thus derive the following formula.

$$\begin{aligned} \Psi_1(\mathbf{Y}, \mathbf{Z}) &= \text{Tr}[\mathbf{Y}^T \mathbf{Z} \mathbf{Z}^T \mathbf{Y}] = \text{Tr}[\mathbf{Z}^T \mathbf{Y} \mathbf{Y}^T \mathbf{Z}] \\ \text{s.t. } \mathbf{Z}^T \mathbf{Z} &= \mathbf{I} \end{aligned} \quad (6)$$

2) *Predictability of Latent Space*: As advocated in [40], to improve the *predictability* of the latent space, the code matrix \mathbf{Z} is supposed to be strongly correlated with the instance features. Here we firstly consider linear correlations, and will later handle non-linear ones with kernel tricks. Considering a linear projection \mathbf{w} for the feature space and a dimension \mathbf{z} of the latent space, *i.e.* a column of \mathbf{Z} , the correlation between features and \mathbf{z} , denoted as $r(\mathbf{X}, \mathbf{z})$, can be defined as follows.

$$r(\mathbf{X}, \mathbf{z}) = \frac{(\mathbf{X}\mathbf{w})^T \mathbf{z}}{\sqrt{(\mathbf{X}\mathbf{w})^T (\mathbf{X}\mathbf{w})} \sqrt{\mathbf{z}^T \mathbf{z}}} \quad (7)$$

Due to the orthonormality assumption for \mathbf{Z} , *i.e.* formula (4), $\mathbf{z}^T \mathbf{z} = 1$ will hold for any column of \mathbf{Z} . Moreover, linearly rescaling \mathbf{w} by a non-zero multiplier will not change $r(\mathbf{X}, \mathbf{z})$. Then maximizing $r(\mathbf{X}, \mathbf{z})$ equals the following formula.

$$\max (\mathbf{X}\mathbf{w})^T \mathbf{z} \quad \text{s.t.} \quad (\mathbf{X}\mathbf{w})^T \mathbf{X}\mathbf{w} = 1 \quad (8)$$

Given a dimension \mathbf{z} of the latent space, the maximal $r(\mathbf{X}, \mathbf{z})$ reflects its potential maximal correlation with the feature space, and thus the maximal $r(\mathbf{X}, \mathbf{z})$ can be seen as an expression of the *predictability* of \mathbf{z} . Specifically, with \mathbf{z} fixed, the optimal \mathbf{w} for formula (8), denoted as \mathbf{w}^* , can be derived as follows with the method of Lagrange multipliers.

$$\mathbf{w}^* = \frac{(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{z}}{\sqrt{\mathbf{z}^T \mathbf{X} (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{z}}} \quad (9)$$

Note that following CPLST, here we assume $\mathbf{A} = \mathbf{X}^T \mathbf{X}$ to be invertible. Actually, this assumption usually holds when $n > d_x$, but it will fail in cases with $n < d_x$, as \mathbf{A} will not be full-rank then. To handle the latter cases, we propose to ensure \mathbf{A} to be invertible via: 1) performing dimensionality reduction for the feature space via PCA or alternative methods to make d_x small enough for obtaining a full-rank $\mathbf{X}^T \mathbf{X}$, or 2) adding a tiny value to the entries on the diagonal of $\mathbf{X}^T \mathbf{X}$, *i.e.* $\mathbf{A} = \mathbf{X}^T \mathbf{X} + \varepsilon \mathbf{I}_1$ with $\mathbf{I}_1 \in \mathbb{R}^{d_x \times d_x}$ being an identity matrix and ε being a tiny value, *e.g.* 10^{-6} .

By substituting \mathbf{w}^* into formula (7), the *predictability* of \mathbf{z} , denoted as $\psi_2(\mathbf{X}, \mathbf{z})$, can be derived as follows.

$$\psi_2(\mathbf{X}, \mathbf{z}) = \frac{(\mathbf{X}\mathbf{w}^*)^T \mathbf{z}}{\sqrt{(\mathbf{X}\mathbf{w}^*)^T (\mathbf{X}\mathbf{w}^*)} \sqrt{\mathbf{z}^T \mathbf{z}}} = (\mathbf{X}\mathbf{w}^*)^T \mathbf{z} = \sqrt{\mathbf{z}^T \mathbf{H} \mathbf{z}} \quad (10)$$

Algorithm 1 Overview of E²FE

Input: Feature matrix \mathbf{X}_{tr} and tagging matrix \mathbf{Y}_{tr} of the training instances, feature matrix \mathbf{X}_{ts} of the test instances, predefined model parameter α , and latent space dimensionality d_z

Output: Predicted binary tagging matrix \mathbf{Y}_{ts} of the test instances

Training Process:

1: derive code matrix \mathbf{Z}_{tr} via optimizing formula (12)

2: learn predictive models: $\mathcal{G}(\mathbf{X}_{tr}) \rightarrow \mathbf{Z}_{tr}$

3: derive linear decoding matrix: $\mathbf{Q} = \mathbf{Z}_{tr}^T \mathbf{Y}_{tr}$

Predicting Process:

4: predict code vectors of test instances: $\mathbf{Z}_{ts} = \mathcal{G}(\mathbf{X}_{ts})$

5: recover the predicted tagging matrix: $\mathbf{Y}_{ts} = \text{round}(\mathbf{Z}_{ts} \mathbf{Q})$

where $\mathbf{H} = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \in \mathbb{R}^{n \times n}$. To improve the *predictability* of the latent space, each column \mathbf{z} of the code matrix \mathbf{Z} is supposed to maximize $\psi_2(\mathbf{X}, \mathbf{z})$. As maximizing $\psi_2(\mathbf{X}, \mathbf{z})$ can be guaranteed by maximizing $\mathbf{z}^T \mathbf{H} \mathbf{z}$, the overall *predictability* of \mathbf{Z} can be formulated as follows.

$$\Psi_2(\mathbf{X}, \mathbf{Z}) = \sum_{i=1}^{d_z} \mathbf{z}_{:,i}^T \mathbf{H} \mathbf{z}_{:,i} = \text{Tr}[\mathbf{Z}^T \mathbf{H} \mathbf{Z}] \quad (11)$$

$$\text{s.t. } \mathbf{Z}^T \mathbf{Z} = \mathbf{I}$$

where $\mathbf{z}_{:,i} (i \in \{1, 2, \dots, d_z\})$ denotes the i th column of \mathbf{Z} .

3) *Detailed Objective Function*: With $\Psi_1(\mathbf{Z}, \mathbf{Y})$ and $\Psi_2(\mathbf{X}, \mathbf{Z})$ derived, the objective function *w.r.t* the to-be-learned code matrix \mathbf{Z} , *i.e.* formula (1), can be detailed as follows.

$$\begin{aligned} \Psi &= \max_{\mathbf{Z}} \text{Tr}[\mathbf{Z}^T \mathbf{Y} \mathbf{Y}^T \mathbf{Z}] + \alpha \text{Tr}[\mathbf{Z}^T \mathbf{H} \mathbf{Z}] \\ &= \max_{\mathbf{Z}} \text{Tr}[\mathbf{Z}^T (\mathbf{Y} \mathbf{Y}^T + \alpha \mathbf{H}) \mathbf{Z}] \end{aligned} \quad (12)$$

$$\text{s.t. } \mathbf{Z}^T \mathbf{Z} = \mathbf{I}$$

where $\mathbf{H} = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T$. As analysed in section IV, Ψ can be transformed to an eigenvalue problem *w.r.t* $\mathbf{Y} \mathbf{Y}^T + \alpha \mathbf{H}$, and \mathbf{Z} is derived by concatenating the normalized eigenvectors corresponding to the top d_z largest eigenvalues column by column. With the code matrix \mathbf{Z} derived, predictive models can be trained for mapping instance features into code vectors.

4) *Deriving Linear Decoding Matrix*: According to formula (2) and (3), given \mathbf{Z} with $\mathbf{Z}^T \mathbf{Z} = \mathbf{I}$, the optimal linear decoding matrix \mathbf{Q} can be derived as follows.

$$\mathbf{Q} = (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}^T \mathbf{Y} = \mathbf{Z}^T \mathbf{Y} \quad (13)$$

And its computational complexity is $\mathcal{O}(nd_y d_z)$.

An overview of E²FE is given in Algorithm 1.

C. Error Analysis

As shown in Algorithm 1, following PLST, CPLST and ML-CSSP, the proposed E²FE *rounds* each entry of the decoding results into its nearest 0 and 1, so as to derive binary label vectors. Considering that, we proceed to analyse the root mean square error (RMSE) of E²FE on the training instances.

Specifically, RMSE is defined as follows.

$$RMSE = \frac{1}{\sqrt{n}} \|\text{round}(\mathcal{G}(\mathbf{X}) \mathbf{Q}) - \mathbf{Y}\|_{fro} \quad (14)$$

where \mathcal{G} denotes the learnt predictive models for mapping instance features into code vectors, and $\text{round}(\mathcal{G}(\mathbf{X}) \mathbf{Q})$ denotes

the recovered binary tagging matrix. Then we can derive the following lemma regarding the error bound of E²FE.

Lemma 1. *For E²FE, its RMSE is bounded by*

$$RMSE \leq \frac{2}{\sqrt{n}} \left(\sqrt{d_z} \|\mathbf{Y}\|_{fro} \|\mathbf{Z} - \mathcal{G}(\mathbf{X})\|_{fro} + \|\mathbf{Y} - \mathbf{Z}\mathbf{Q}\|_{fro} \right)$$

For a detailed proof, one can refer to the supplementary material. Actually, the error bound for E²FE is similar to those of PLST and ML-CSSP. Namely, it also consists of two parts. The first part, *i.e.* $\sqrt{d_z} \|\mathbf{Y}\|_{fro} \|\mathbf{Z} - \mathcal{G}(\mathbf{X})\|_{fro}$ denotes the weighted training error of predictive models, and the second part, *i.e.* $\|\mathbf{Y} - \mathbf{Z}\mathbf{Q}\|_{fro}$, denotes the loss of encoding label vectors into low-dimensional code vectors.

IV. OPTIMIZATION METHODS

For optimizing the objective function Ψ *w.r.t* the to-be-learned code matrix \mathbf{Z} , any column $\mathbf{Z}_{:,i}$ ($i \in \{1, 2, \dots, d_z\}$) can be derived with the following optimization sub-problem.

$$\begin{aligned} \Psi^{(i)} &= \max_{\mathbf{Z}_{:,i}} \mathbf{Z}_{:,i}^T (\mathbf{Y}\mathbf{Y}^T + \alpha\mathbf{H}) \mathbf{Z}_{:,i} \\ \text{s.t. } & \mathbf{Z}_{:,i}^T \mathbf{Z}_{:,i} = 1, \mathbf{Z}_{:,j}^T \mathbf{Z}_{:,i} = 0 \ (\forall j < i) \end{aligned} \quad (15)$$

With the method of Lagrange multipliers, the optimal $\mathbf{Z}_{:,i}$ should satisfy the following optimality condition.

$$(\mathbf{Y}\mathbf{Y}^T + \alpha\mathbf{H}) \mathbf{Z}_{:,i} = \lambda_i \mathbf{Z}_{:,i} \quad (16)$$

where λ_i is the introduced Lagrange multiplier and will also be the optimal value of the sub-problem. It can be seen that the optimization for \mathbf{Z} can be transformed to an eigenvalue problem. Then by normalizing the eigenvectors of $\mathbf{U} = \mathbf{Y}\mathbf{Y}^T + \alpha\mathbf{H}$ that correspond to the top d_z largest eigenvalues, we can derive the optimal code matrix \mathbf{Z} formed of these eigenvectors column by column, which satisfies $\mathbf{Z}^T \mathbf{Z} = \mathbf{I}$.

As described in our previous work [33], we can directly calculate \mathbf{U} and then utilize effective methods to derive its eigenvectors. However, considering that $\mathbf{U} \in \mathbb{R}^{n \times n}$, for cases with $n \gg d_x + d_y$, which are common in practical applications, calculating \mathbf{U} will result in high space costs. To avoid that, we derive the following lemma and further propose a more efficient optimization method for such cases.

Lemma 2. *Given $\mathbf{H} = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T$, the matrix $\mathbf{U} = \mathbf{Y}\mathbf{Y}^T + \alpha\mathbf{H}$ can be decomposed as $\mathbf{U} = \mathbf{V}\mathbf{V}^T$ with $\mathbf{V} \in \mathbb{R}^{n \times (d_y + d_x)}$. Also, the eigenvectors of \mathbf{U} can be derived from those of $\mathbf{V}^T \mathbf{V}$, meaning that the size of the eigenvalue problem *w.r.t* \mathbf{U} can be transformed from $\mathbb{R}^{n \times n}$ to $\mathbb{R}^{(d_x + d_y) \times (d_x + d_y)}$.*

Proof. Suppose $\mathbf{A} = \mathbf{X}^T \mathbf{X}$ is invertible. Since $\mathbf{A} \in \mathbb{R}^{d_x \times d_x}$ is a real symmetric and positive-semidefinite matrix, \mathbf{A}^{-1} will be real symmetric and positive semi-definite, and thus \mathbf{A}^{-1} is diagonalizable by orthogonal matrices [41]. Namely, $\mathbf{A}^{-1} = \mathbf{B}\mathbf{A}\mathbf{B}^T$, with \mathbf{A} being a diagonal matrix having non-negative diagonal entries and \mathbf{B} being an orthonormal matrix. Then $\mathbf{A}^{-1} = \mathbf{B}\mathbf{A}^{\frac{1}{2}}\mathbf{A}^{\frac{1}{2}}\mathbf{B}^T = \left(\mathbf{B}\mathbf{A}^{\frac{1}{2}}\right)\left(\mathbf{B}\mathbf{A}^{\frac{1}{2}}\right)^T$, where $\mathbf{A}^{\frac{1}{2}}$ is a diagonal matrix with each diagonal entry being the square root of the corresponding diagonal entry in \mathbf{A} . Furthermore, with $\mathbf{G} = \mathbf{X}\mathbf{B}\mathbf{A}^{\frac{1}{2}} \in \mathbb{R}^{n \times d_x}$, $\mathbf{H} = \mathbf{G}\mathbf{G}^T$. Finally, $\mathbf{U} = \mathbf{Y}\mathbf{Y}^T +$

Algorithm 2 Optimization for E²FE

Input: Feature matrix $\mathbf{X}_{tr} \in \mathbb{R}^{n \times d_x}$ and tagging matrix $\mathbf{Y}_{tr} \in \mathbb{R}^{n \times d_y}$ of training instances, predefined model parameter α , latent space dimensionality d_z

Output: Learned code matrix \mathbf{Z}_{tr} of training instances

- 1: **if** $\mathbf{X}_{tr}^T \mathbf{X}_{tr}$ is NOT invertible **then**
- 2: Option 1: {dimension reduction for feature space}
- 3: $\mathbf{X}_{tr} = \text{DimReduce}(\mathbf{X}_{tr})$
- 4: Option 2: {adding a tiny value to diagonal entries}
- 5: $\mathbf{X}_{tr}^T \mathbf{X}_{tr} = \mathbf{X}_{tr}^T \mathbf{X}_{tr} + \varepsilon \mathbf{I}_1$
- 6: **end if**
- 7: **if** $n \gg d_y + d_x$ **then**
- 8: $\mathbf{A} = \mathbf{X}_{tr}^T \mathbf{X}_{tr}$
- 9: $[\mathbf{B}, \mathbf{A}] = \text{diagonalize}(\mathbf{A}^{-1})$ { $\mathbf{A}^{-1} = \mathbf{B}\mathbf{A}\mathbf{B}^T$ }
- 10: $\mathbf{G} = \mathbf{X}_{tr}\mathbf{B}\mathbf{A}^{\frac{1}{2}}$
- 11: $\mathbf{V} = [\mathbf{Y}_{tr}, \sqrt{\alpha}\mathbf{G}]$
- 12: $\mathbf{E} = \text{eigenvector}(\mathbf{V}^T \mathbf{V}, d_z)$ {eigenvectors of $\mathbf{V}^T \mathbf{V}$ corresponding to the top d_z largest eigenvalues}
- 13: $\mathbf{Z}_{tr} = \text{normalize}(\mathbf{V}\mathbf{E})$ {normalizing each column of $\mathbf{V}\mathbf{E}$ into a unit vector}
- 14: **else**
- 15: $\mathbf{H} = \mathbf{X}_{tr}(\mathbf{X}_{tr}^T \mathbf{X}_{tr})^{-1} \mathbf{X}_{tr}^T$
- 16: $\mathbf{U} = \mathbf{Y}_{tr}\mathbf{Y}_{tr}^T + \alpha\mathbf{H}$
- 17: $\tilde{\mathbf{E}} = \text{eigenvector}(\mathbf{U}, d_z)$ {eigenvectors of \mathbf{U} corresponding to the top d_z largest eigenvalues}
- 18: $\mathbf{Z}_{tr} = \text{normalize}(\tilde{\mathbf{E}})$ {normalizing each column of $\tilde{\mathbf{E}}$ into a unit vector}
- 19: **end if**

$$\alpha\mathbf{H} = \mathbf{Y}\mathbf{Y}^T + (\sqrt{\alpha}\mathbf{G})(\sqrt{\alpha}\mathbf{G})^T = [\mathbf{Y}, \sqrt{\alpha}\mathbf{G}][\mathbf{Y}, \sqrt{\alpha}\mathbf{G}]^T = \mathbf{V}\mathbf{V}^T, \text{ with } \mathbf{V} = [\mathbf{Y}, \sqrt{\alpha}\mathbf{G}] \in \mathbb{R}^{n \times (d_y + d_x)}.$$

Suppose $\{\lambda, \mathbf{p}\}$ and $\{\sigma, \mathbf{q}\}$ are respectively the paired eigenvalue/eigenvector of $\mathbf{V}\mathbf{V}^T$ and $\mathbf{V}^T \mathbf{V}$. According to 1) $\mathbf{V}\mathbf{V}^T \mathbf{p} = \lambda \mathbf{p} \rightarrow (\mathbf{V}^T \mathbf{V})\mathbf{V}^T \mathbf{p} = \mathbf{V}^T (\mathbf{V}\mathbf{V}^T \mathbf{p}) = \lambda \mathbf{V}^T \mathbf{p}$ and 2) $\mathbf{V}^T \mathbf{V} \mathbf{q} = \sigma \mathbf{q} \rightarrow (\mathbf{V}\mathbf{V}^T)\mathbf{V} \mathbf{q} = \mathbf{V} (\mathbf{V}^T \mathbf{V} \mathbf{q}) = \sigma \mathbf{V} \mathbf{q}$, we can see that $\mathbf{V}\mathbf{V}^T$ and $\mathbf{V}^T \mathbf{V}$ share identical eigenvalues, and the eigenvectors of $\mathbf{U} = \mathbf{V}\mathbf{V}^T$ can be derived from those of $\mathbf{V}^T \mathbf{V}$ based on the second derivation above. Considering $\mathbf{V}^T \mathbf{V} \in \mathbb{R}^{(d_x + d_y) \times (d_x + d_y)}$, the size of the eigenvalue problem *w.r.t* \mathbf{U} can be transformed from $\mathbb{R}^{n \times n}$ to $\mathbb{R}^{(d_x + d_y) \times (d_x + d_y)}$. \square

With Lemma 2, in different cases we can utilize different optimization methods to obtain the eigenvectors of $\mathbf{U} = \mathbf{Y}\mathbf{Y}^T + \alpha\mathbf{H}$ and then derive the code matrix \mathbf{Z} , as summarized below and illustrated in Algorithm 2.

- 1) If $n \gg d_y + d_x$, it is preferable to firstly derive the matrix \mathbf{V} satisfying $\mathbf{U} = \mathbf{V}\mathbf{V}^T$, then calculate the eigenvectors of $\mathbf{V}^T \mathbf{V}$ corresponding to the top d_z largest eigenvalues, and finally utilize them to derive the eigenvectors of \mathbf{U} . Since $d_z \ll d_y$ and $\mathbf{V}^T \mathbf{V}$ is a real symmetric matrix, the eigenvalue problem *w.r.t* $\mathbf{V}^T \mathbf{V}$ can be solved efficiently using iterative methods like Arnoldi iteration [42], which can achieve an optimal computational complexity of $\mathcal{O}(d_x d_z^2 + d_y d_z^2)$. Here the computational complexity of deriving \mathbf{V} is $\mathcal{O}(n d_x^2)$, while that of calculating $\mathbf{V}^T \mathbf{V}$ and deriving the eigenvectors of \mathbf{U} from those of $\mathbf{V}^T \mathbf{V}$ is $\mathcal{O}(n(d_x + d_y)^2)$.
- 2) Otherwise, it is preferable to directly calculate \mathbf{U} and then perform an eigenvalue decomposition on it. The computational complexity for calculating \mathbf{U} is at most

$\mathcal{O}(\min\{n^2d_x, nd_x^2\}) + \mathcal{O}(n^2d_x + n^2d_y)$. Considering that generally $d_z \ll n$ and \mathbf{U} is a real symmetric matrix, the eigenvalue problem *w.r.t* \mathbf{U} can also be solved efficiently using Arnoldi iteration with an optimal computational complexity of $\mathcal{O}(nd_z^2)$.

V. $\pi\text{E}^2\text{FE}$: ENHANCING LINEAR DECODING MATRIX WITH PRIORI KNOWLEDGE

As analysed in formula (16), each column of the code matrix \mathbf{Z} corresponds to an eigenvalue of $\mathbf{U} = \mathbf{Y}\mathbf{Y}^T + \alpha\mathbf{H}$, which is also the optimal value for its corresponding optimization sub-problem (*i.e.* formula (15)). Knowing that each column denotes one dimension of the latent space, for each column, the eigenvalue *w.r.t* it actually reflects 1) how predictable its corresponding dimension of the latent space is and 2) from the dimension how recoverable the label space is. Specifically, a higher eigenvalue *w.r.t* a column of \mathbf{Z} means that its corresponding dimension of the latent space is more predictable and the label space is more recoverable from the dimension.

Here we propose to consider such priori knowledge to derive an enhanced linear decoding matrix for E^2FE . We denote it as $\pi\text{E}^2\text{FE}$. Essentially, for a linear decoding matrix \mathbf{Q} , its i th column $\mathbf{Q}_{\cdot,i}$ ($i \in \{1, 2, \dots, d_y\}$) acts as a weighting vector to linearly combine dimensions of the latent space for recovering the i th dimension of the label space. Then for dimensions of the latent space that are more predictable and make the label space more recoverable, *i.e.* with higher corresponding eigenvalues, they are expected to be assigned with higher weights in the decoding process. Therefore, we derive the objective function for $\mathbf{Q}_{\cdot,i}$ as follows.

$$\tilde{\mathcal{L}}^{(i)} = \min_{\mathbf{Q}_{\cdot,i}} \|\mathbf{Y}_{\cdot,i} - \mathbf{Z}\mathbf{Q}_{\cdot,i}\|_{fro}^2 - \eta \sum_{j=1}^{d_z} \lambda_j \mathbf{Q}_{j,i}^2 \quad (17)$$

where $\mathbf{Y}_{\cdot,i}$ is the i th column of the tagging matrix \mathbf{Y} , λ_j is the eigenvalue corresponding to the j th column of \mathbf{Z} and η is a non-negative weighting factor. It can be seen that, by considering the priori knowledge as a regularizer in $\tilde{\mathcal{L}}^{(i)}$, a larger λ_j can help to lead $\mathbf{Q}_{j,i}^2$ to be larger, meaning that as expected the j th dimension of the latent space is assigned with a higher weight for decoding. For model simplicity, here η is shared by all $\mathbf{Q}_{\cdot,i}$ ($i \in \{1, 2, \dots, d_y\}$). Then the objective function for deriving the linear decoding matrix \mathbf{Q} of $\pi\text{E}^2\text{FE}$ can be formulated as follows with matrix notations.

$$\tilde{\mathcal{L}} = \min_{\mathbf{Q}} \|\mathbf{Y} - \mathbf{Z}\mathbf{Q}\|_{fro}^2 - \eta \text{Tr}[\mathbf{Q}^T \tilde{\mathbf{\Lambda}} \mathbf{Q}] \quad (18)$$

where $\tilde{\mathbf{\Lambda}}$ is a diagonal matrix with $\tilde{\mathbf{\Lambda}}_{j,j} = \lambda_j$. If η is properly set to make $\tilde{\mathcal{L}}$ non-trivial, as discussed later, the optimal decoding matrix for $\pi\text{E}^2\text{FE}$ can be derived as follows.

$$\mathbf{Q} = (\mathbf{I} - \eta \tilde{\mathbf{\Lambda}})^{-1} \mathbf{Z}^T \mathbf{Y} \quad (19)$$

where $(\mathbf{I} - \eta \tilde{\mathbf{\Lambda}})$ is a diagonal matrix and thus its inverse can be efficiently calculated. Actually, as $d_z \ll d_y$, the computational complexity of deriving \mathbf{Q} in $\pi\text{E}^2\text{FE}$ is also $\mathcal{O}(nd_y d_z)$.

Note that in formula (18), a large η can lead $\tilde{\mathcal{L}}$ to become trivial and achieve an optimum of negative infinity. To cope

with that, we derive the following lemma for properly setting η , where $\vec{\lambda} = [\lambda_1, \lambda_2, \dots, \lambda_{d_z}]$.

Lemma 3. For any $\eta \in [0, \frac{1}{\max(\vec{\lambda})}]$ with $\max(\vec{\lambda})$ being the maximal value of $\vec{\lambda}$, $\tilde{\mathcal{L}}$ will be non-trivial for optimization.

For a detailed proof, one can refer to the supplementary material.

VI. EXTENSIONS AND ANALYSES

A. Function-based Encoding: a Linear Encoding Case

Though the proposed E^2FE requires no encoding function, it can still be specified to learn an encoding function as most previous works, given that the encoding function can be optimized, *e.g.* a linear one, as described below.

Following PLST and CPLST, we use an encoding matrix $\mathbf{P} \in \mathbb{R}^{d_y \times d_z}$ to denote the linear encoding function. Then the code matrix \mathbf{Z} can be expressed as $\mathbf{Z} = \mathbf{Y}\mathbf{P}$. Substituting \mathbf{Z} with $\mathbf{Y}\mathbf{P}$ in the objective function of E^2FE , *i.e.* formula (12), we can derive the following objective function for \mathbf{P} .

$$\begin{aligned} \Psi &= \max_{\mathbf{P}} \text{Tr} [\mathbf{P}^T (\mathbf{Y}^T \mathbf{Y} \mathbf{Y}^T \mathbf{Y} + \alpha \mathbf{Y}^T \mathbf{H} \mathbf{Y}) \mathbf{P}] \\ \text{s.t. } & \mathbf{P}^T \mathbf{Y}^T \mathbf{Y} \mathbf{P} = \mathbf{I} \end{aligned} \quad (20)$$

Similarly, we use the method of Lagrange multipliers and decompose Ψ into d_z optimization sub-problems *w.r.t* each column $\mathbf{P}_{\cdot,i}$ of the to-be-learned \mathbf{P} . Then we derive that $\mathbf{P}_{\cdot,i}$ should satisfy the following optimality condition.

$$(\mathbf{Y}^T \mathbf{Y} \mathbf{Y}^T \mathbf{Y} + \alpha \mathbf{Y}^T \mathbf{H} \mathbf{Y}) \mathbf{P}_{\cdot,i} = \lambda_i (\mathbf{Y}^T \mathbf{Y}) \mathbf{P}_{\cdot,i} \quad (21)$$

where λ_i is a Lagrange multiplier and will be the optimal value of the optimization sub-problem *w.r.t* $\mathbf{P}_{\cdot,i}$. It can be seen that the optimization of \mathbf{P} is essentially a general eigenvalue problem. And the normalized eigenvectors corresponding to the top d_z largest eigenvalues will form the optimal \mathbf{P} .

Denoting this case of linear function-based encoding as Linear E^2FE , the linear decoding matrix \mathbf{Q} without considering priori knowledge is $\mathbf{Q} = (\mathbf{Y}\mathbf{P})^T \mathbf{Y}$. Meanwhile, for the case of utilizing the eigenvalues *w.r.t* \mathbf{P} as priori knowledge, $\mathbf{Q} = (\mathbf{I} - \eta \tilde{\mathbf{\Lambda}})^{-1} (\mathbf{Y}\mathbf{P})^T \mathbf{Y}$ with $\tilde{\mathbf{\Lambda}}$ being a diagonal matrix consisting of the eigenvalues, which is termed $\pi\text{LinearE}^2\text{FE}$.

B. Kernel Version

The proposed E^2FE , thanks to kernel tricks, can be extended to deal with non-linear correlations between the feature space and the latent space, which is termed *kernel-E}^2\text{FE}.*

In *kernel-E}^2\text{FE}, each feature vector $\mathbf{x}^{(i)}$ is mapped to the Reproducing Kernel Hilbert Space (RKHS) as $\phi(\mathbf{x}^{(i)})$. In RKHS, the inner product between $\phi(\mathbf{x}^{(i)})$ and $\phi(\mathbf{x}^{(j)})$ is equal to $\kappa(\mathbf{x}^{(i)}, \mathbf{x}^{(j)})$, where $\kappa(\cdot, \cdot)$ is the introduced kernel function. Using a non-linear $\kappa(\cdot, \cdot)$, the linear correlations between the RKHS and the latent space actually reflect the non-linear correlations between the original feature space and the latent space. Similar to formula (7), we measure the correlation $r(\Phi, \mathbf{z})$ by considering a linear projection \mathbf{w}_1 for kernel features in RKHS and a column \mathbf{z} of the code matrix. Following [43], here \mathbf{w}_1 is assumed to be in the span of*

sampled kernel feature vectors, *i.e.* $\mathbf{w}_1 = \Phi_*^T \tilde{\mathbf{w}}$ where Φ_* is a matrix built by the sampled kernel feature vectors row by row and $\tilde{\mathbf{w}}$ is an s -dimensional weighting vector with s being the sampling size. Then $r(\Phi, \mathbf{z})$ can be measured as follows.

$$r(\Phi, \mathbf{z}) = \frac{(\Phi \Phi_*^T \tilde{\mathbf{w}})^T \mathbf{z}}{\sqrt{(\Phi \Phi_*^T \tilde{\mathbf{w}})^T (\Phi \Phi_*^T \tilde{\mathbf{w}}) \sqrt{\mathbf{z}^T \mathbf{z}}}} \quad (22)$$

$$= \frac{(\mathbf{K} \tilde{\mathbf{w}})^T \mathbf{z}}{\sqrt{(\mathbf{K} \tilde{\mathbf{w}})^T (\mathbf{K} \tilde{\mathbf{w}}) \sqrt{\mathbf{z}^T \mathbf{z}}}}$$

where $\mathbf{K} = \Phi \Phi_*^T \in \mathbb{R}^{n \times s}$ is a kernel matrix and can be efficiently derived using the kernel function with the original feature vectors. Similar to subsection III-B2, the *predictability* of \mathbf{z} based on non-linear correlations can be derived from the maximal $r(\Phi, \mathbf{z})$ and measured as $\psi_2(\Phi, \mathbf{z}) = \sqrt{\mathbf{z}^T \tilde{\mathbf{H}} \mathbf{z}}$ with $\tilde{\mathbf{H}} = \mathbf{K}(\mathbf{K}^T \mathbf{K})^{-1} \mathbf{K}^T$. Then the objective function of *kernel*-E²FE is as follows, which can also be transformed to an eigenvalue problem.

$$\Psi = \max_{\mathbf{Z}} \text{Tr}[\mathbf{Z}^T (\mathbf{Y} \mathbf{Y}^T + \alpha \tilde{\mathbf{H}}) \mathbf{Z}] \quad \text{s.t.} \quad \mathbf{Z}^T \mathbf{Z} = \mathbf{I} \quad (23)$$

Like E²FE, the linear decoding matrix \mathbf{Q} for *kernel*-E²FE is $\mathbf{Q} = \mathbf{Z}^T \mathbf{Y}$. Meanwhile, when eigenvalues *w.r.t* \mathbf{Z} are considered as priori knowledge, $\mathbf{Q} = (\mathbf{I} - \eta \tilde{\Lambda})^{-1} \mathbf{Z}^T \mathbf{Y}$, where $\tilde{\Lambda}$ is a diagonal matrix consisting of eigenvalues. Here we denote this case as *kernel*- π E²FE.

C. Relations to Previous Works

If the mean values of the label vectors are shifted as zeros, the proposed E²FE will degenerate to PLST [28] when only the *recoverability* of the label space is considered (*i.e.* $\alpha = 0$ in formula (12)). Here, we denote this case as R-E²FE and its corresponding objective function is given as follows.

$$\Psi = \max_{\mathbf{Z}} \text{Tr}[\mathbf{Z}^T \mathbf{Y} \mathbf{Y}^T \mathbf{Z}], \quad \text{s.t.} \quad \mathbf{Z}^T \mathbf{Z} = \mathbf{I} \quad (24)$$

The code matrix \mathbf{Z} consists of the normalized eigenvectors of $\mathbf{Y} \mathbf{Y}^T$ corresponding to the top d_z largest eigenvalues, and the linear decoding matrix without considering priori knowledge is $\mathbf{Z}^T \mathbf{Y}$. Meanwhile, the linear encoding matrix \mathbf{P} of PLST is formed with normalized eigenvectors of $\mathbf{Y}^T \mathbf{Y}$ corresponding to the top d_z largest eigenvalues, with the derived code matrix being $\mathbf{Y} \mathbf{P}$ and the linear decoding matrix being \mathbf{P}^T . As in the proof of Lemma 2, we can derive that $\mathbf{Y} \mathbf{Y}^T$ and $\mathbf{Y}^T \mathbf{Y}$ are positive semi-definite and share the same positive eigenvalues. Specifically, provided that λ_i is the i th largest eigenvalue, we can derive that: 1) $\mathbf{Y}^T \mathbf{Y} \mathbf{P}_{:,i} = \lambda_i \mathbf{P}_{:,i}$; 2) $\mathbf{Y} \mathbf{Y}^T \mathbf{Z}_{:,i} = \lambda_i \mathbf{Z}_{:,i}$; 3) $(\mathbf{Y} \mathbf{Y}^T) [\mathbf{Y} \mathbf{P}]_{:,i} = \mathbf{Y} (\mathbf{Y}^T \mathbf{Y} \mathbf{P}_{:,i}) = \lambda_i [\mathbf{Y} \mathbf{P}]_{:,i}$; 4) $(\mathbf{Y}^T \mathbf{Y}) [\mathbf{Y}^T \mathbf{Z}]_{:,i} = \mathbf{Y}^T (\mathbf{Y} \mathbf{Y}^T \mathbf{Z}_{:,i}) = \lambda_i [\mathbf{Y}^T \mathbf{Z}]_{:,i}$. Then for R-E²FE and PLST, we can find one-to-one correspondences between the i th columns of their encoding results (*i.e.* $\mathbf{Z}_{:,i} = \frac{[\mathbf{Y} \mathbf{P}]_{:,i}}{\sqrt{\lambda_i}}$), and between the i th rows of their linear decoding matrices (*i.e.* $[\mathbf{Z}^T \mathbf{Y}]_{i,\cdot} = \sqrt{\lambda_i} [\mathbf{P}^T]_{i,\cdot}$). Therefore, R-E²FE is equivalent to PLST, with $\mathbf{Z}(\mathbf{Z}^T \mathbf{Y}) = (\mathbf{Y} \mathbf{P}) \mathbf{P}^T$. However, when $\alpha > 0$, the code matrix \mathbf{Z} in E²FE will be associated to instance features and will then differ from PLST.

When coping with linear function-based encoding, *i.e.* formula (20), given the mean values of label vectors and those of feature vectors shifted as zeros, E²FE is closely connected

to CPLST [30] if only the *predictability* of the latent space is considered. We denote this case as P-LinearE²FE, with its corresponding objective function defined as follows.

$$\Psi = \max_{\mathbf{P}} \text{Tr}[\mathbf{P}^T \mathbf{Y}^T \mathbf{H} \mathbf{Y} \mathbf{P}], \quad \text{s.t.} \quad \mathbf{P}^T \mathbf{Y}^T \mathbf{Y} \mathbf{P} = \mathbf{I} \quad (25)$$

Meanwhile, the objective function of CPLST is as follows.

$$\tilde{\Psi} = \max_{\mathbf{P}} \text{Tr}[\mathbf{P}^T \mathbf{Y}^T \mathbf{H} \mathbf{Y} \mathbf{P}], \quad \text{s.t.} \quad \mathbf{P}^T \mathbf{P} = \mathbf{I} \quad (26)$$

It can be seen that P-LinearE²FE and CPLST share an identical objective function but with different constraints. Namely, the former requires dimensions of the code matrix (*i.e.* $\mathbf{Y} \mathbf{P}$) to be orthonormal while the latter requires dimensions of the linear encoding matrix (*i.e.* \mathbf{P}) to be orthonormal.

Another useful observation *w.r.t* E²FE is that E²FE actually performs dimensionality reduction for both the label space and the feature space when the *predictability* of the latent space is over-emphasized with an assumption that the code matrix can be directly expressed by the feature matrix, *i.e.* $\mathbf{Z} = \mathbf{X} \mathbf{W}$ where $\mathbf{W} \in \mathbb{R}^{d_x \times d_z}$ is a regression matrix. This case is termed OP-E²FE. As the *predictability* of the latent space is constant in OP-E²FE, its objective function is formulated as follows.

$$\Psi = \max_{\mathbf{W}} \text{Tr}[\mathbf{W}^T \mathbf{X}^T \mathbf{Y} \mathbf{Y}^T \mathbf{X} \mathbf{W}] \quad (27)$$

$$\text{s.t.} \quad \mathbf{W}^T \mathbf{X}^T \mathbf{X} \mathbf{W} = \mathbf{I}$$

The optimization for \mathbf{W} can again be interpreted as a general eigenvalue problem, *i.e.* $(\mathbf{X}^T \mathbf{Y} \mathbf{Y}^T \mathbf{X}) \mathbf{W}_{:,i} = \lambda_i (\mathbf{X}^T \mathbf{X}) \mathbf{W}_{:,i}$, but it requires $d_z \leq d_x$. Here \mathbf{Z} can be seen as the dimensionality reduction result learnt from the label space in an end-to-end manner, or the linear dimensionality reduction result from the feature space with \mathbf{W} . However, for OP-E²FE, we can observe the following weak points. 1) The dimensionality of the to-be-learned latent space cannot be larger than the dimensionality of the feature space, which can sometimes be too small to keep enough information of the label space, especially when $d_x \ll d_y$. 2) The predictive models from the feature space to the latent space are limited to be linear regression whereas for LSDR they are expected to be open for any effective model.

VII. EXPERIMENTS

A. Experimental Settings

To validate the proposed E²FE, we use in our experiments five widely-used benchmark datasets with relatively large vocabularies from Mulan [44], *i.e.* *delicious*, *CAL500*, *mediamill*, *bibtex* and *bookmarks*. They belong to one of the following domains: text, music and video. Moreover, following CS [27], we also conduct experiments on the image dataset *ESPGame* [45], and take those tags appearing at least 20 times in the dataset to form a large vocabulary, which almost doubles the size of that used in the experiments of CS. Each instance in *ESPGame* is represented by a 516-D feature vector¹ extracted with Lire [46], and it is removed if no tags are associated. The original statistics of the datasets are given in Table III.

For performance comparison, we select Binary Relevance (BR) [47], CS [27], PLST [28], CPLST and *kernel*-CPLST

¹516-D feature vector: 60-D Gabor, 192-D FCTH, 80-D Edge Histogram, 120-D Color Layout and 64-D RGB Color Histogram

TABLE III
STATISTICS OF DATASETS

	domain	instances	labels	features
<i>delicious</i>	text	16,105	983	500
<i>CAL500</i>	music	502	174	68
<i>mediamill</i>	video	43,907	101	120
<i>ESPGame</i>	image	65,065	1,718	516
<i>bibtex</i>	text	7,395	159	1,836
<i>bookmarks</i>	text	87,856	208	2,150

[30], MLC-BMaD [31] and ML-CSSP [32] as baselines, where BR is a widely-used multi-label classification method that trains a separate binary relevance model for each label. In our experiments, we use both linear SVM (L-SVM) [48] and linear ridge regression (L-RR) for BR. And for the latter, we use 0.5 as a threshold to decide the binary (0 or 1) classification results. To reduce the computational costs of L-SVM on *bibtex* and *bookmarks*, we perform feature dimensionality reduction for both datasets via PCA. We also follow the reported preprocessing steps of baselines, like shifting the mean values of feature vectors to be zeros, *etc.* Note that BR in fact does not perform LSDR and thus its performance is a reference for other algorithms. BML-CS [5] is not included since it is sophisticated with numerous parameters to tune.

For E²FE, we evaluate the following variants. 1) R-E²FE: considering only the *recoverability* of the label space (*i.e.* formula (24)), theoretically equivalent to PLST; 2) P-LinearE²FE: considering only the *predictability* of the latent space for linear function-based encoding (*i.e.* formula (25)), similar to CPLST; 3) OP-E²FE: over-emphasizing the *predictability* of the latent space (*i.e.* formula (27)); 4) LinearE²FE: linear function-based encoding (*i.e.* formula (20)); 5) π LinearE²FE: identical to LinearE²FE except that the linear decoding matrix is learnt with priori knowledge; 6) E²FE: end-to-end feature-aware label space encoding (*i.e.* formula (12)); 7) π E²FE: identical to E²FE except that the linear decoding matrix is learnt with priori knowledge; 8) *kernel*-E²FE: kernel version of E²FE (*i.e.* formula (23)); 9) *kernel*- π E²FE: identical to *kernel*-E²FE except that the linear decoding matrix is learnt with priori knowledge.

In our experiments, each dataset is evenly and randomly divided into 5 parts. Five runs of each algorithm are then performed on the dataset, taking each time one part for testing and the rest for training without duplication. Experimental results are measured with widely-used metrics in the field of multi-label classification, *i.e.* *label-based macroF1* and *example-based Accuracy* [49], and then averaged over the 5 runs. Higher *label-based macroF1* and *example-based Accuracy* means better performance. Specifically, for each run, *label-based macroF1* is calculated as follows.

$$\begin{aligned} \text{macroF1} &= \frac{1}{d_y} \sum_{i=1}^{d_y} \frac{2p_i r_i}{p_i + r_i} \\ \text{s.t. } p_i &= \frac{|G_i \cap P_i|}{|P_i|}, r_i = \frac{|G_i \cap P_i|}{|G_i|} \end{aligned} \quad (28)$$

where d_y is the number of all labels, G_i and P_i are respectively the sets of the ground-truth and the predicted positive instances for the i th label, and \cap , \cup are operations of intersection and

union between two sets. Meanwhile, *example-based Accuracy* is given by the following formula.

$$\text{Accuracy} = \frac{1}{n_t} \sum_{j=1}^{n_t} \frac{|G'_j \cap P'_j|}{|G'_j \cup P'_j|} \quad (29)$$

where n_t is the test set size, G'_j and P'_j are respectively the ground-truth and the predicted label set of the j th test instance.

Moreover, for each run of any algorithm, we conduct 5-fold cross-validation on the training set for selecting model parameters via grid search in predefined value ranges. Specifically, α in the proposed E²FE and its variants is selected from $\{10^{-1}, 10^0, \dots, 10^4\}$, τ for MLC-BMaD is chosen from $\{0.1, 0.2, \dots, 1.0\}$, and the predefined sparsity level in CS is selected from $\{1, 2, \dots, M\}$ with M being the maximal number of labels in an instance, *etc.* Additionally, for η in π E²FE/ π LinearE²FE/*kernel*- π E²FE, we set $\eta = \xi \frac{1}{\max(\lambda)}$ for each dataset and select ξ from $\{0, 2^{-10}, 2^{-9}, \dots, 2^{-1}, 1\}$ via cross-validation. Following most previous works, like [5], [28], [30], [32], we utilize linear ridge regression as predictive models to learn the mappings from instance features to code vectors. As for *kernel*-CPLST, *kernel*-E²FE and *kernel*- π E²FE, we empirically utilize the Gaussian kernel function and set the smoothing parameter σ as twice the mean Euclidean distance between feature vectors for each dataset. Accordingly, we utilize kernel ridge regression as predictive models for them to learn the non-linear mappings from instance features to code vectors. Moreover, following PLST, CPLST and ML-CSSP, we round each continuous entry of the decoding results into its nearest 0 or 1 to get the binary label vectors for test instances.

B. Experimental Results of LSDR

We run all algorithms on the six datasets with different values of d_z/d_y (mostly from 10% to 50%) where d_z and d_y are respectively the dimensionality of the latent space and that of the label space. Particularly, for *ESPGame*, d_z/d_y is varied from 5% to 25%, as it has a much larger vocabulary.

1) *Performance Comparison with Baselines*: The experimental results of compared baselines and variants of the proposed E²FE are reported in Table IV and V.

A close look at the achieved results reveals: 1) The proposed E²FE as well as its linear function-based variant LinearE²FE generally outperform the compared baselines on each dataset, which clearly demonstrates their effectiveness. 2) E²FE outperforms LinearE²FE on all datasets, reflecting the superiority of learning code vectors in an end-to-end manner rather than a function-based manner. 3) E²FE outperforms R-E²FE and LinearE²FE outperforms P-LinearE²FE, which implies that jointly considering *predictability* and *recoverability* will obtain better performance. 4) OP-E²FE yields inferior performance to E²FE and cannot even perform LSDR on *CAL500* when $d_z/d_y \geq 40\%$, as the dimensionality of the feature space will be smaller than d_z . That points out the weakness of OP-E²FE and further validates the superiority of keeping a good trade-off between *predictability* and *recoverability*. 5) R-E²FE yields nearly the same performance as PLST, as predicted by our theoretical analyses about their equivalence. 6) With an identical objective function but different orthogonality constraints, P-LinearE²FE seems to be slightly superior to

TABLE IV
EXPERIMENTAL RESULTS: *label-based macroF1* ON *delicious*, *CAL500*, *mediamill*, *ESPGame*, *bibtex* AND *bookmarks*, WITH VARYING d_z/d_y

Datasets		<i>delicious</i>					<i>CAL500</i>					<i>mediamill</i>				
d_z/d_y		10%	20%	30%	40%	50%	10%	20%	30%	40%	50%	10%	20%	30%	40%	50%
BR [47]	L-SVM	0.0951					0.1397					0.0866				
	L-RR	0.0377					0.0569					0.0447				
CS [27]		0.0063	0.0208	0.0422	0.0466	0.0415	0.0677	0.0820	0.0906	0.0976	0.1142	0.0052	0.0144	0.0138	0.0319	0.0304
PLST [28]		0.0234	0.0256	0.0271	0.0278	0.0284	0.0604	0.0605	0.0606	0.0609	0.0608	0.0422	0.0439	0.0448	0.0447	0.0447
CPLST [30]		0.0339	0.0341	0.0341	0.0341	0.0341	0.0640	0.0643	0.0644	0.0645	0.0645	0.0432	0.0446	0.0447	0.0447	0.0447
MLC-BMaD [31]		0.0238	0.0259	0.0297	0.0344	0.0347	0.0485	0.0444	0.0420	0.0472	0.0468	0.0398	0.0408	0.0408	0.0408	0.0408
ML-CSSP [32]		0.0160	0.0216	0.0277	0.0324	0.0319	0.0453	0.0498	0.0507	0.0528	0.0543	0.0354	0.0395	0.0426	0.0433	0.0427
R-E ² FE (~PLST)		0.0234	0.0257	0.0271	0.0278	0.0285	0.0592	0.0590	0.0592	0.0593	0.0593	0.0422	0.0439	0.0448	0.0447	0.0447
P-LinearE ² FE (~CPLST)		0.0391	0.0398	0.0399	0.0399	0.0400	0.0795	0.0954	0.1008	0.1003	0.1003	0.0420	0.0437	0.0446	0.0446	0.0447
OP-E ² FE		0.0449	0.0470	0.0476	0.0478	0.0475	0.1034	0.1080	0.1088	-	-	0.0433	0.0447	0.0448	0.0449	0.0448
LinearE ² FE		0.0413	0.0417	0.0416	0.0416	0.0416	0.1061	0.1115	0.1110	0.1101	0.1101	0.0440	0.0449	0.0451	0.0449	0.0448
E ² FE		0.0530	0.0569	0.0577	0.0578	0.0578	0.1198	0.1247	0.1263	0.1258	0.1256	0.0549	0.0575	0.0577	0.0577	0.0577
kernel-CPLST [30]		0.0354	0.0377	0.0383	0.0389	0.0393	0.0754	0.0774	0.0774	0.0774	0.0774	0.0594	0.0688	0.0720	0.0751	0.0756
kernel-E ² FE		0.0500	0.0569	0.0591	0.0599	0.0599	0.1160	0.1208	0.1215	0.1272	0.1307	0.0692	0.0814	0.0945	0.0997	0.1003

Datasets		<i>ESPGame</i>					<i>bibtex</i>					<i>bookmarks</i>				
d_z/d_y		5%	10%	15%	20%	25%	10%	20%	30%	40%	50%	10%	20%	30%	40%	50%
BR [47]	L-SVM	0.0688					0.3023					0.1860				
	L-RR	0.0017					0.0613					0.0415				
CS [27]		0.0005	0.0011	0.0014	0.0022	0.0022	0.0170	0.0377	0.0916	0.1010	0.1017	0.0090	0.0248	0.0271	0.0582	0.0611
PLST [28]		0.0017	0.0017	0.0017	0.0017	0.0017	0.0365	0.0503	0.0540	0.0553	0.0557	0.0248	0.0357	0.0397	0.0403	0.0406
CPLST [30]		0.0017	0.0017	0.0017	0.0017	0.0017	0.0443	0.0560	0.0581	0.0588	0.0588	0.0384	0.0400	0.0401	0.0402	0.0403
MLC-BMaD [31]		0.0017	0.0017	0.0017	0.0017	0.0017	0.0341	0.0505	0.0524	0.0550	0.0582	0.0325	0.0354	0.0385	0.0416	0.0415
ML-CSSP [32]		0.0011	0.0016	0.0014	0.0014	0.0015	0.0281	0.0330	0.0439	0.0480	0.0471	0.0184	0.0292	0.0300	0.0302	0.0339
R-E ² FE (~PLST)		0.0017	0.0017	0.0017	0.0017	0.0017	0.0358	0.0498	0.0538	0.0552	0.0556	0.0249	0.0358	0.0398	0.0404	0.0407
P-LinearE ² FE (~CPLST)		0.0017	0.0017	0.0017	0.0017	0.0017	0.0443	0.0548	0.0574	0.0593	0.0601	0.0389	0.0404	0.0417	0.0421	0.0422
OP-E ² FE		0.0021	0.0021	0.0021	0.0021	0.0024	0.0536	0.0810	0.0906	0.0958	0.0981	0.0400	0.0434	0.0451	0.0454	0.0459
LinearE ² FE		0.0018	0.0017	0.0017	0.0017	0.0017	0.0440	0.0564	0.0604	0.0602	0.0601	0.0397	0.0419	0.0423	0.0424	0.0425
E ² FE		0.0026	0.0025	0.0025	0.0025	0.0025	0.0595	0.0888	0.1169	0.1286	0.1369	0.0472	0.0706	0.0752	0.0764	0.0775
kernel-CPLST [30]		0.0019	0.0019	0.0019	0.0019	0.0019	0.0503	0.0698	0.0728	0.0742	0.0744	0.0410	0.0448	0.0462	0.0472	0.0477
kernel-E ² FE		0.0040	0.0043	0.0043	0.0044	0.0045	0.0629	0.0930	0.1247	0.1396	0.1472	0.0492	0.0699	0.0738	0.0756	0.0770

TABLE V
EXPERIMENTAL RESULTS: *example-based Accuracy* ON *delicious*, *CAL500*, *mediamill*, *ESPGame*, *bibtex* AND *bookmarks*, WITH VARYING d_z/d_y

Datasets		<i>delicious</i>					<i>CAL500</i>					<i>mediamill</i>				
d_z/d_y		10%	20%	30%	40%	50%	10%	20%	30%	40%	50%	10%	20%	30%	40%	50%
BR [47]	L-SVM	0.1500					0.2436					0.3621				
	L-RR	0.0958					0.1995					0.4188				
CS [27]		0.0254	0.0540	0.0890	0.0974	0.0964	0.1130	0.1299	0.1626	0.1904	0.1835	0.0115	0.0304	0.0352	0.1425	0.1426
PLST [28]		0.0870	0.0898	0.0907	0.0911	0.0912	0.2099	0.2103	0.2103	0.2106	0.2104	0.4160	0.4184	0.4187	0.4188	0.4187
CPLST [30]		0.0954	0.0955	0.0955	0.0955	0.0955	0.2003	0.2007	0.2009	0.2010	0.2010	0.4167	0.4187	0.4187	0.4188	0.4187
MLC-BMaD [31]		0.0593	0.0700	0.0855	0.0873	0.0875	0.1286	0.1215	0.1194	0.1244	0.1255	0.3989	0.3995	0.3995	0.3995	0.3995
ML-CSSP [32]		0.0684	0.0785	0.0851	0.0893	0.0904	0.1806	0.1880	0.1913	0.1958	0.1966	0.3466	0.4053	0.4073	0.4140	0.4081
R-E ² FE (~PLST)		0.0870	0.0898	0.0908	0.0911	0.0913	0.2100	0.2098	0.2099	0.2101	0.2100	0.4159	0.4183	0.4188	0.4188	0.4187
P-LinearE ² FE (~CPLST)		0.0984	0.1007	0.1011	0.1011	0.1011	0.2084	0.2189	0.2226	0.2223	0.2223	0.4137	0.4162	0.4182	0.4182	0.4186
OP-E ² FE		0.1085	0.1091	0.1093	0.1094	0.1073	0.2283	0.2262	0.2251	-	-	0.4172	0.4186	0.4189	0.4189	0.4189
LinearE ² FE		0.1068	0.1055	0.1049	0.1048	0.1048	0.2318	0.2301	0.2291	0.2281	0.2281	0.4182	0.4190	0.4191	0.4190	0.4189
E ² FE		0.1187	0.1196	0.1197	0.1196	0.1184	0.2405	0.2411	0.2421	0.2396	0.2392	0.4353	0.4379	0.4378	0.4378	0.4378
kernel-CPLST [30]		0.1116	0.1162	0.1175	0.1181	0.1186	0.2139	0.2148	0.2148	0.2148	0.2148	0.4489	0.4561	0.4572	0.4579	0.4580
kernel-E ² FE		0.1281	0.1291	0.1311	0.1312	0.1293	0.2421	0.2414	0.2397	0.2399	0.2398	0.4606	0.4647	0.4681	0.4685	0.4686

Datasets		<i>ESPGame</i>					<i>bibtex</i>					<i>bookmarks</i>				
d_z/d_y		5%	10%	15%	20%	25%	10%	20%	30%	40%	50%	10%	20%	30%	40%	50%
BR [47]	L-SVM	0.0628					0.2827					0.1679				
	L-RR	0.0572					0.1816					0.1597				
CS [27]		0.0053	0.0057	0.0048	0.0107	0.0106	0.0771	0.0964	0.1435	0.1520	0.1553	0.0155	0.0629	0.0643	0.0940	0.0963
PLST [28]		0.0576	0.0576	0.0576	0.0576	0.0576	0.1434	0.1657	0.1760	0.1768	0.1772	0.1472	0.1530	0.1572	0.1575	0.1578
CPLST [30]		0.0578	0.0578	0.0578	0.0578	0.0578	0.1639	0.1768	0.1793	0.1802	0.1800	0.1542	0.1570	0.1572	0.1572	0.1573
MLC-BMaD [31]		0.0574	0.0573	0.0573	0.0575	0.0573	0.1365	0.1757	0.1767	0.1746	0.1799	0.1494	0.1538	0.1576	0.1597	0.1596
ML-CSSP [32]		0.0409	0.0548	0.0478	0.0541	0.0499	0.1212	0.1205	0.1433	0.1563	0.1573	0.1053	0.1493	0.1249	0.1063	0.1438
R-E ² FE (~PLST)		0.0575	0.0575	0.0575	0.0575	0.0575	0.1429	0.1653	0.1756	0.1766	0.1769	0.1473	0.1532	0.1574	0.1577	0.1580
P-LinearE ² FE (~CPLST)		0.0574	0.0577	0.0578	0.0578	0.0579	0.1598	0.1726	0.1756	0.1783	0.1792	0.1552	0.1574	0.1582	0.1588	0.1590
OP-E ² FE		0.0622	0.0621	0.0621	0.0621	0.0694	0.1751	0.2041	0.2126	0.2167	0.2181	0.1565	0.1616	0.1623	0.1625	0.1626
LinearE ² FE		0.0597	0.0593	0.0588	0.0586	0.0584	0.1618	0.1768	0.1820	0.1816	0.1813	0.1559	0.1592	0.1591	0.1590	0.1589
E ² FE		0.0701	0.0701	0.0700	0.0701	0.0701	0.1835	0.2149	0.2356	0.2440	0.2493	0.1659	0.1913	0.1933	0.1937	0.1939
kernel-CPLST [30]		0.0646	0.0645	0.0645	0.0645	0.0645	0.1739	0.1976	0.2005	0.2006	0.2011	0.1588	0.1638	0.1641	0.1643	0.1645
kernel-E ² FE		0.0832	0.0834	0.0834	0.0834	0.0834	0.1910	0.2232	0.2485	0.2596	0.2640	0.1685	0.1937	0.1952	0.1958	0.1961

CPLST, which validates the reasonableness of assuming the columns of the code matrix to be orthonormal. 7) *kernel-E²FE* outperforms *E²FE*

TABLE VI

PERFORMANCE COMPARISONS BETWEEN LINEARE²FE, E²FE, *kernel*-E²FE AND π LINEARE²FE, π E²FE, *kernel*- π E²FE ON *delicious*, *CAL500*, *mediamill*, *ESPGame*, *bibtex* AND *bookmarks* WITH VARYING d_z/d_y , IN TERMS OF *label-based macroF1*

Datasets	<i>delicious</i>					<i>CAL500</i>					<i>mediamill</i>					
	d_z/d_y	10%	20%	30%	40%	50%	10%	20%	30%	40%	50%	10%	20%	30%	40%	50%
LinearE ² FE	0.0413	0.0417	0.0416	0.0416	0.0416	0.1061	0.1115	0.1110	0.1101	0.1101	0.1101	0.0440	0.0449	0.0451	0.0449	0.0448
π LinearE ² FE	0.0590	0.0595	0.0594	0.0593	0.0593	0.1415	0.1457	0.1479	0.1477	0.1478	0.0580	0.0605	0.0607	0.0604	0.0603	
Relative Improvement	43.0%	42.7%	42.5%	42.6%	42.6%	33.3%	30.8%	33.2%	34.1%	34.1%	31.8%	34.7%	34.7%	34.7%	34.7%	
E ² FE	0.0530	0.0569	0.0577	0.0578	0.0578	0.1198	0.1247	0.1263	0.1258	0.1256	0.0549	0.0575	0.0577	0.0577	0.0577	
π E ² FE	0.0698	0.0727	0.0735	0.0738	0.0717	0.1841	0.1874	0.1883	0.1925	0.1923	0.0685	0.0718	0.0720	0.0721	0.0721	
Relative Improvement	31.8%	27.8%	27.5%	27.8%	24.0%	53.7%	50.3%	49.0%	53.0%	53.1%	24.9%	24.8%	24.8%	24.9%	24.8%	
<i>kernel</i> -E ² FE	0.0500	0.0569	0.0591	0.0599	0.0599	0.1160	0.1208	0.1215	0.1272	0.1307	0.0692	0.0814	0.0945	0.0997	0.1003	
<i>kernel</i> - π E ² FE	0.0768	0.0820	0.0834	0.0838	0.0843	0.1827	0.1864	0.1927	0.2000	0.2024	0.0838	0.0975	0.1117	0.1172	0.1177	
Relative Improvement	53.4%	44.0%	41.1%	39.8%	40.6%	57.4%	54.3%	58.6%	57.3%	54.9%	21.1%	19.8%	18.2%	17.5%	17.3%	

Datasets	<i>ESPGame</i>					<i>bibtex</i>					<i>bookmarks</i>				
	d_z/d_y	5%	10%	15%	20%	25%	10%	20%	30%	40%	50%	10%	20%	30%	40%
LinearE ² FE	0.0018	0.0017	0.0017	0.0017	0.0017	0.0440	0.0564	0.0604	0.0602	0.0601	0.0397	0.0419	0.0423	0.0424	0.0425
π LinearE ² FE	0.0029	0.0028	0.0028	0.0028	0.0028	0.0801	0.1076	0.1186	0.1217	0.1216	0.0518	0.0569	0.0582	0.0593	0.0592
Relative Improvement	64.4%	63.5%	64.0%	64.0%	64.0%	81.9%	90.9%	96.4%	102.2%	102.3%	30.4%	35.8%	37.6%	39.9%	39.4%
E ² FE	0.0026	0.0025	0.0025	0.0025	0.0025	0.0595	0.0888	0.1169	0.1286	0.1369	0.0472	0.0706	0.0752	0.0764	0.0775
π E ² FE	0.0037	0.0037	0.0038	0.0038	0.0038	0.1204	0.1874	0.2264	0.2458	0.2583	0.0751	0.0883	0.0948	0.0976	0.0989
Relative Improvement	43.5%	46.5%	48.3%	48.2%	48.0%	102.1%	111.0%	93.7%	91.2%	88.7%	59.1%	25.1%	26.0%	27.7%	27.6%
<i>kernel</i> -E ² FE	0.0040	0.0043	0.0043	0.0044	0.0045	0.0629	0.0930	0.1247	0.1396	0.1472	0.0492	0.0699	0.0738	0.0756	0.0770
<i>kernel</i> - π E ² FE	0.0054	0.0057	0.0058	0.0059	0.0060	0.1252	0.1936	0.2346	0.2575	0.2740	0.0764	0.0876	0.0936	0.0974	0.0990
Relative Improvement	36.4%	33.8%	34.4%	33.6%	33.6%	99.0%	108.2%	88.2%	84.5%	86.1%	55.4%	25.5%	26.9%	28.7%	28.6%

TABLE VII

PERFORMANCE COMPARISONS BETWEEN LINEARE²FE, E²FE, *kernel*-E²FE AND π LINEARE²FE, π E²FE, *kernel*- π E²FE ON *delicious*, *CAL500*, *mediamill*, *ESPGame*, *bibtex* AND *bookmarks* WITH VARYING d_z/d_y , IN TERMS OF *example-based Accuracy*

Datasets	<i>delicious</i>					<i>CAL500</i>					<i>mediamill</i>				
	d_z/d_y	10%	20%	30%	40%	50%	10%	20%	30%	40%	50%	10%	20%	30%	40%
LinearE ² FE	0.1068	0.1055	0.1049	0.1048	0.1048	0.2318	0.2301	0.2291	0.2281	0.2281	0.4182	0.4190	0.4191	0.4190	0.4189
π LinearE ² FE	0.1465	0.1457	0.1453	0.1453	0.1453	0.2555	0.2495	0.2500	0.2497	0.2497	0.4256	0.4278	0.4277	0.4275	0.4274
Relative Improvement	37.2%	38.0%	38.6%	38.6%	38.6%	10.2%	8.4%	9.1%	9.5%	9.5%	1.8%	2.1%	2.0%	2.0%	2.0%
E ² FE	0.1187	0.1196	0.1197	0.1196	0.1184	0.2405	0.2411	0.2421	0.2396	0.2392	0.4353	0.4379	0.4378	0.4378	0.4378
π E ² FE	0.1971	0.1975	0.1974	0.1974	0.1980	0.3121	0.3044	0.3039	0.3042	0.3040	0.4280	0.4303	0.4304	0.4305	0.4305
Relative Improvement	66.0%	65.1%	64.9%	65.0%	67.2%	29.8%	26.2%	25.5%	27.0%	27.1%	-1.7%	-1.7%	-1.7%	-1.6%	-1.7%
<i>kernel</i> -E ² FE	0.1281	0.1291	0.1311	0.1312	0.1293	0.2421	0.2414	0.2397	0.2399	0.2398	0.4606	0.4647	0.4681	0.4685	0.4686
<i>kernel</i> - π E ² FE	0.2230	0.2244	0.2246	0.2246	0.2247	0.3221	0.3187	0.3166	0.3103	0.3050	0.4533	0.4605	0.4629	0.4633	0.4632
Relative Improvement	74.1%	73.8%	71.3%	71.2%	73.7%	33.1%	32.0%	32.1%	29.3%	27.2%	-1.6%	-0.9%	-1.1%	-1.1%	-1.1%

Datasets	<i>ESPGame</i>					<i>bibtex</i>					<i>bookmarks</i>				
	d_z/d_y	5%	10%	15%	20%	25%	10%	20%	30%	40%	50%	10%	20%	30%	40%
LinearE ² FE	0.0597	0.0593	0.0588	0.0586	0.0584	0.1618	0.1768	0.1820	0.1816	0.1813	0.1559	0.1592	0.1591	0.1590	0.1589
π LinearE ² FE	0.1024	0.1018	0.1015	0.1013	0.1012	0.2000	0.2276	0.2358	0.2399	0.2407	0.1756	0.1833	0.1835	0.1835	0.1832
Relative Improvement	71.4%	71.7%	72.5%	72.8%	73.2%	23.6%	28.7%	29.5%	32.1%	32.8%	12.6%	15.1%	15.3%	15.4%	15.3%
E ² FE	0.0701	0.0701	0.0700	0.0701	0.0701	0.1835	0.2149	0.2356	0.2440	0.2493	0.1659	0.1913	0.1933	0.1937	0.1939
π E ² FE	0.1223	0.1303	0.1303	0.1303	0.1302	0.2449	0.2973	0.3219	0.3296	0.3333	0.2089	0.2256	0.2285	0.2294	0.2295
Relative Improvement	74.4%	86.0%	86.0%	85.9%	85.8%	33.4%	38.4%	36.6%	35.1%	33.7%	26.0%	18.0%	18.2%	18.4%	18.3%
<i>kernel</i> -E ² FE	0.0832	0.0834	0.0834	0.0834	0.0834	0.1910	0.2232	0.2485	0.2596	0.2640	0.1685	0.1937	0.1952	0.1958	0.1961
<i>kernel</i> - π E ² FE	0.1334	0.1335	0.1336	0.1336	0.1336	0.2490	0.3045	0.3296	0.3398	0.3463	0.2138	0.2273	0.2296	0.2308	0.2311
Relative Improvement	60.4%	60.1%	60.3%	60.2%	60.2%	30.4%	36.4%	32.6%	30.9%	31.2%	26.9%	17.3%	17.6%	17.9%	17.9%

the feature space and the latent space. Moreover, *kernel*-E²FE achieves superior performance to *kernel*-CPLST, which outperforms CPLST. 8) On all datasets, as d_z/d_y increases, the performance of E²FE does not vary dramatically due to the orthonormality constraint in formula (4), which leads E²FE to compactly encode the label space with a smaller d_z . Similar phenomenon occurs when applying PLST and CPLST, because both are also orthogonally constrained. Actually, we find that this phenomenon still remains when $d_z/d_y > 50\%$.

Actually, to evaluate the significance of the performance improvements gained by E²FE over the baselines, we also perform *paired-sample t-test* [50] for both *label-based macroF1* and *example-based Accuracy* on all datasets with varying

d_z/d_y . Experimental results show that nearly all *P-values* in significance tests are less than the typical significance level 0.01, and thus the performance improvements gained by E²FE over baselines are statistically significant. For details about the experiments of significance tests, one can refer to the supplementary material.

2) *Experimental Validation for Enhancing Decoding Matrix with Prior Knowledge* : Here on each dataset we compare LinearE²FE, E²FE, *kernel*-E²FE with their counterparts that learn the linear decoding matrix with priori knowledge, *i.e.* π LinearE²FE, π E²FE and *kernel*- π E²FE, as presented in Table VI and VII. Note that in all pairwise comparisons, we also present the relative performance improvements gained by

TABLE VIII

AVERAGE TRAINING COSTS (IN SECONDS) OF COMPARED ALGORITHMS (“PERFORMING LSDR + TRAINING PREDICTIVE MODELS”) WITH $d_z/d_y = 10\%$.

		<i>delicious</i>		<i>ESPGame</i>		<i>bookmarks</i>	
BR [47]	L-SVM	187.400	(0.000 + 187.400)	20,487.185	(0.000 + 20,487.185)	24,809.120	(0.000 + 24,809.120)
	L-RR	15.428	(0.000 + 15.428)	54.666	(0.000 + 54.666)	13.310	(0.000 + 13.310)
CS [27]		1.782	(0.150 + 1.632)	7.235	(1.229 + 6.006)	2.316	(0.169 + 2.147)
PLST [28]		2.271	(0.637 + 1.635)	11.341	(5.310 + 6.031)	2.360	(0.190 + 2.170)
CPLST [30]		2.799	(1.033 + 1.766)	11.594	(5.563 + 6.031)	3.570	(1.426 + 2.143)
MLC-BMaD [31]		68.625	(66.937 + 1.688)	585.494	(579.388 + 6.106)	14.475	(12.344 + 2.131)
ML-CSSP [32]		2.574	(0.780 + 1.794)	11.074	(5.061 + 6.013)	2.328	(0.188 + 2.140)
E ² FE		3.787	(1.984 + 1.803)	16.936	(10.877 + 6.059)	7.039	(4.877 + 2.162)

TABLE IX

TIME COMPLEXITY OF COMPARED ALGORITHMS TO PERFORM LSDR

	Time Complexity
CS [27]	$\mathcal{O}(nd_y d_z)$
PLST [28]	$\mathcal{O}(nd_y d_z)$
CPLST [30]	$\mathcal{O}(\min\{n^2 d_x, nd_x^2\}) + \mathcal{O}(2nd_x d_y + d_x d_y^2) + \mathcal{O}(d_y^2)$
MLC-BMaD [31]	$\mathcal{O}(nd_x^2 d_z)$
ML-CSSP [32]	$\mathcal{O}(nd_y d_z) + \mathcal{O}(d_z \log d_z)$
E ² FE	$\min\{\mathcal{O}(nd_x^2) + \mathcal{O}(n(d_x + d_y)^2) + \mathcal{O}(d_x d_z^2 + d_y d_z^2), \mathcal{O}(\min\{n^2 d_x, nd_x^2\}) + \mathcal{O}(n^2 d_x + n^2 d_y) + \mathcal{O}(nd_z^2)\}$

TABLE X

AVERAGE TIME COSTS (IN SECONDS) FOR THE NEWLY PROPOSED OPTIMIZATION METHOD (E²FE) AND THAT PRESENTED IN OUR PREVIOUS CONFERENCE PAPER (FaIE) TO PERFORM LSDR WITH $d_z/d_y = 10\%$.

	<i>delicious</i> [®]	<i>ESPGame</i> [®]	<i>bookmarks</i> [®]
E ² FE	1.077	2.646	0.683
FaIE [33]	3.869	7.800	2.153

 π LinearE²FE/ π E²FE/*kernel*- π E²FE.

From the comparisons, we can see that in nearly all cases, π LinearE²FE outperforms LinearE²FE, π E²FE outperforms E²FE, and *kernel*- π E²FE outperforms *kernel*-E²FE. Specifically, on average, considering priori knowledge for learning the decoding matrix can achieve a relative improvement of 48.1% for *label-based macroF1* and 33.9% for *example-based Accuracy*. Meanwhile, the maximal gained relative improvement for the former is 111.0%, and that for the latter is 86.0%. Such significant performance improvements well demonstrate the effectiveness of our proposal to further consider the eigenvalues corresponding to each column of the code matrix as priori knowledge to enhance the linear decoding matrix in E²FE and its variants.

C. Analyses of Training Costs

1) *Comparison with Baselines*: For E²FE and compared baselines, apart from classification performance, here we also compare their training costs theoretically and experimentally.

Considering that the training costs of all algorithms mainly differ in those of performing LSDR, *i.e.* learning the code vectors of training instances and the decoding process, here we summarize the time complexity of each algorithm, as presented in Table IX. From the time complexity analysis, it can be seen that MLC-BMaD has the highest time complexity, while CS, PLST and ML-CSSP have the lowest.

Moreover, in Table VIII we also report the average time costs for E²FE and the compared baselines on performing LSDR and training predictive models over 5 runs on *delicious*, *ESPGame* and *bookmarks*, which have the largest label sets, with $d_z/d_y = 10\%$. As a reference, the time costs of BR are also provided. All algorithms are conducted with Matlab R2013a on a server with two Intel Xeon E5-2430 CPUs and 64G RAM, except that BR with L-SVM is conducted using LIBLINEAR [48]. Looking at the results of this comparison,

we can draw the following conclusions. 1) Compared with BR, nearly all LSDR methods can help to reduce the total training costs. 2) For performing LSDR, E²FE generally needs slightly higher costs than CS, PLST, CPLST and ML-CSSP, though with superior classification performance. Also, its training cost is much lower than MLC-BMaD. 3) Like the previous theoretical analysis, the training cost of MLC-BMaD is the highest while those of CS, PLST and ML-CSSP are the lowest.

2) *Evaluation of the Newly Proposed Optimization Method*: To evaluate the optimization method proposed in this paper for efficiently learning the code matrix in cases with $n \gg d_x + d_y$, we also conduct experiments on *delicious*, *ESPGame* and *bookmarks* to compare its efficiency with that of the optimization method presented in our conference paper [33]. Here we respectively denote the former as E²FE and the latter as FaIE.

Considering that FaIE needs to calculate the matrix $\mathbf{U} \in \mathbb{R}^{n \times n}$ and thus needs much memory space for large datasets, to avoid biases brought by high memory space costs, here we follow the experimental settings in [33] and sample 5,000 training instances for evaluating the time costs of both optimization methods to perform LSDR. Note that here $n \gg d_x + d_y$ is still ensured for the sampled training instances. Experimental results on the three datasets with $d_z/d_y = 10\%$ are reported in Table X. It can be seen that the time costs of the newly proposed optimization method are significantly lower than those of the one presented in [33]. That clearly demonstrates the effectiveness of the newly proposed optimization method for cases with $n \gg d_x + d_y$.

D. Parameter Sensitivity Analyses

For a more detailed view, we also conduct experiments to see the effects of α (*i.e.* formula (12)) on the performance of the proposed E²FE. Fig. 2 presents how the performance of E²FE changes as α varies in $\{10^{-2}, 10^{-1}, \dots, 10^4, 10^5\}$ in a run on the largest *delicious*, *ESPGame* and *bookmarks* with $d_z/d_y = 10\%$. It can be seen that on these three datasets the performance of E²FE, in terms of *label-based macroF1* and

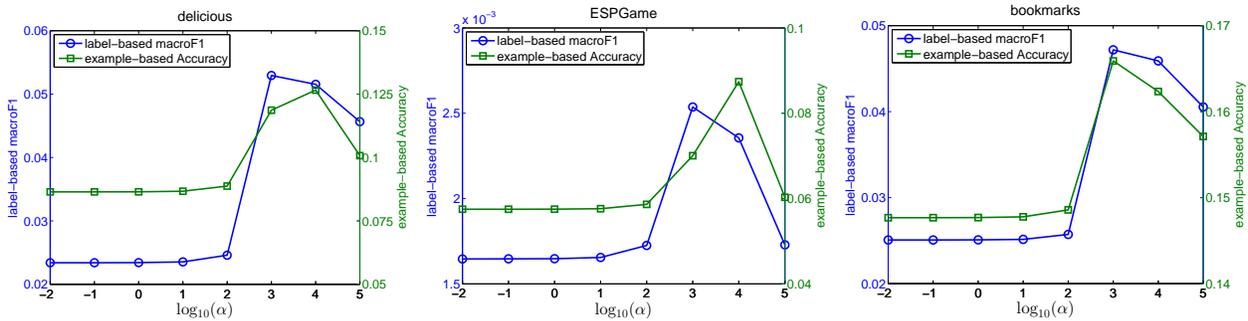


Fig. 2. Effects of α on the performance of E^2FE on *delicious* (left), *ESPGame* (middle) and *bookmarks* (right), with $d_z/d_y = 10\%$.

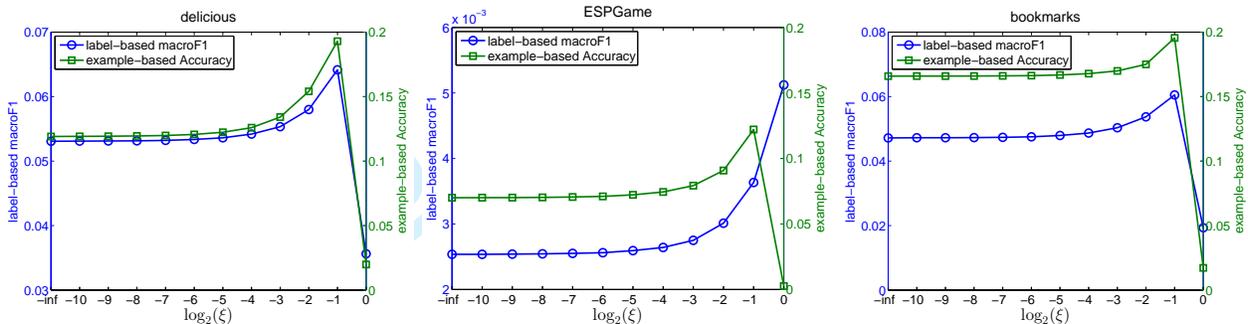


Fig. 3. Effects of $\eta = \xi \frac{1}{\max(\lambda)}$ on the performance of πE^2FE on *delicious* (left), *ESPGame* (middle) and *bookmarks* (right), with $d_z/d_y = 10\%$.

example-based Accuracy, firstly increases and then decreases as α increases from 10^{-2} to 10^5 . That further demonstrates the reasonableness of jointly considering the *recoverability* of the label space and the *predictability* of the latent space, as a good trade-off between both yields superior performance. Moreover, we can observe that for these three datasets the optimal α for E^2FE is near $[10^3, 10^4]$.

By fixing $\alpha = 10^3$, we further analyse the effects of η (i.e. formula (18)) on the performance of πE^2FE . Specifically, on the largest *delicious*, *ESPGame* and *bookmarks* with $d_z/d_y = 10\%$, we rewrite $\eta = \xi \frac{1}{\max(\lambda)}$ and vary ξ in $\{0, 2^{-10}, 2^{-9}, \dots, 2^{-1}, 1\}$ based on Lemma 3 to see how the corresponding learnt linear decoding matrix affects the performance of πE^2FE , as shown in Fig. 3. It can be seen that on the three datasets, as η increases from 0 (i.e. $\xi = 2^{-inf} = 0$) to $\frac{1}{\max(\lambda)}$ (i.e. $\xi = 2^0 = 1$), the performance of πE^2FE , in terms of *label-based macroF1* and *example-based Accuracy*, tends to firstly increase and then decrease in most cases, with the optimal η being near $\frac{0.5}{\max(\lambda)}$ (i.e. $\xi = 2^{-1}$). Actually, $\eta = 0$ makes πE^2FE degenerate to E^2FE , and it generally yields inferior performance than $\eta > 0$, which further demonstrates the reasonableness of considering the eigenvalues *w.r.t* columns of the code matrix as priori knowledge to learn an enhanced linear decoding matrix.

VIII. DISCUSSIONS

The proposed E^2FE assumes that columns of the to-be-learned code matrix \mathbf{Z} are orthonormal. Though this assumption seems to be strong, it is still reasonable and brings useful properties to E^2FE . 1) As each column of \mathbf{Z} denotes one dimension

of the latent space, adding an orthonormality assumption, similar to PLST and CPLST, allows us to mitigate the redundant information among dimensions of the latent space and then enable E^2FE to encode the label space more compactly. 2) As can be seen in formula (2) - (6), adding the orthonormality assumption can simplify the objective function of E^2FE and enable it to be transformed into an eigenvalue problem for efficient optimization. 3) By enabling the objective function to be transformed into an eigenvalue problem, from formula (15) and (16) we can see that adding the orthonormality assumption actually helps to ensure E^2FE obtaining global optima.

Here we also try dropping the orthonormality assumption from the objective function of E^2FE and conduct experiments on all datasets to evaluate it. We denote it as E^2FE_{NoOrth} , with its objective function given as follows.

$$\begin{aligned} \Psi &= \max_{\mathbf{Z}, \mathbf{Q}} -\|\mathbf{Y} - \mathbf{Z}\mathbf{Q}\|_{fro}^2 + \alpha \text{Tr}[\mathbf{Z}^T \mathbf{H} \mathbf{Z}] \\ &= \min_{\mathbf{Z}, \mathbf{Q}} \|\mathbf{Y} - \mathbf{Z}\mathbf{Q}\|_{fro}^2 - \alpha \text{Tr}[\mathbf{Z}^T \mathbf{H} \mathbf{Z}] \\ \text{s.t. } &\forall i \in \{1, 2, \dots, d_z\}, \quad \mathbf{Z}_{:,i}^T \mathbf{Z}_{:,i} = 1 \end{aligned} \quad (30)$$

Note that $\mathbf{Z}_{:,i}^T \mathbf{Z}_{:,i} = 1$ is still required due to formula (7). Like other matrix factorization methods [51], we can derive the code matrix \mathbf{Z} and the linear decoding matrix \mathbf{Q} by using gradient descent methods to iteratively and alternatively optimize one while keeping the other fixed until convergence. For more details, one can refer to the supplementary material.

The performance of E^2FE_{NoOrth} on all datasets, using random initial values for \mathbf{Z} and \mathbf{Q} to perform optimization, is presented in Table XI. It can be seen that E^2FE_{NoOrth} is inferior to E^2FE . In fact, even using the derived \mathbf{Z} and \mathbf{Q} of E^2FE as initial values, E^2FE_{NoOrth} can hardly gain performance improvement over E^2FE . It is mainly attributed

TABLE XI
PERFORMANCE COMPARISONS BETWEEN E^2FE AND E^2FE_{NoOrth} ON ALL DATASETS, WITH $p = 5$ FOR *ESPGame* AND $p = 10$ FOR OTHERS.

	d_z/d_y	$p\%$	$2p\%$	$3p\%$	$4p\%$	$5p\%$	
label-based macroF1	<i>delicious</i>	E^2FE	0.0530	0.0569	0.0577	0.0578	0.0578
		E^2FE_{NoOrth}	0.0336	0.0401	0.0444	0.0462	0.0438
	<i>CAL500</i>	E^2FE	0.1198	0.1247	0.1263	0.1258	0.1256
		E^2FE_{NoOrth}	0.0966	0.1086	0.1074	0.1122	0.1120
	<i>mediamill</i>	E^2FE	0.0549	0.0575	0.0577	0.0577	0.0577
		E^2FE_{NoOrth}	0.0436	0.0448	0.0459	0.0451	0.0453
	<i>ESPGame</i>	E^2FE	0.0026	0.0025	0.0025	0.0025	0.0025
		E^2FE_{NoOrth}	0.0018	0.0018	0.0017	0.0018	0.0018
	<i>bibtex</i>	E^2FE	0.0595	0.0888	0.1169	0.1286	0.1369
		E^2FE_{NoOrth}	0.0420	0.0727	0.0847	0.0929	0.1000
	<i>bookmarks</i>	E^2FE	0.0472	0.0706	0.0752	0.0764	0.0775
		E^2FE_{NoOrth}	0.0298	0.0455	0.0459	0.0471	0.0488
example-based Accuracy	<i>delicious</i>	E^2FE	0.1187	0.1196	0.1197	0.1196	0.1184
		E^2FE_{NoOrth}	0.1037	0.1073	0.1082	0.1093	0.1045
	<i>CAL500</i>	E^2FE	0.2405	0.2411	0.2421	0.2396	0.2392
		E^2FE_{NoOrth}	0.2261	0.2294	0.2256	0.2267	0.2250
	<i>mediamill</i>	E^2FE	0.4353	0.4379	0.4378	0.4378	0.4378
		E^2FE_{NoOrth}	0.4192	0.4201	0.4204	0.4192	0.4199
	<i>ESPGame</i>	E^2FE	0.0701	0.0701	0.0700	0.0701	0.0701
		E^2FE_{NoOrth}	0.0613	0.0635	0.0605	0.0585	0.0590
	<i>bibtex</i>	E^2FE	0.1835	0.2149	0.2356	0.2440	0.2493
		E^2FE_{NoOrth}	0.1501	0.2018	0.2121	0.2167	0.2233
	<i>bookmarks</i>	E^2FE	0.1659	0.1913	0.1933	0.1937	0.1939
		E^2FE_{NoOrth}	0.1521	0.1627	0.1636	0.1645	0.1660

TABLE XII
AVERAGE TIME COSTS (IN SECONDS) FOR PERFORMING LSDR IN E^2FE AND E^2FE_{NoOrth} WITH $d_z/d_y = 10\%$.

	<i>delicious</i>	<i>ESPGame</i>	<i>bookmarks</i>
E^2FE	1.984	10.877	4.877
E^2FE_{NoOrth}	145.253	215.199	41.434

to that, without the orthonormality assumption, 1) more redundant information rather than complementary information exists between dimensions of the latent space, and 2) global optima cannot be ensured for Z .

Moreover, we also evaluate the time costs for E^2FE_{NoOrth} to perform LSDR on the largest *delicious*, *ESPGame* and *bookmarks* with $d_z/d_y = 10\%$, as reported in Table XII. We can see that E^2FE_{NoOrth} costs much more time than E^2FE , because its objective function is more complex for optimization. Its time costs are even higher than those of the binary relevance model L-RR (Table VIII).

Therefore, dropping the orthonormality assumption does not bring substantial performance improvements and instead will increase the time costs for optimization. On the contrary, keeping the orthonormality assumption gains a good trade-off between efficiency and effectiveness for LSDR.

IX. CONCLUSION

Aiming to address the multi-label classification problem with many classes, in this paper we have proposed an effective method termed E^2FE to perform LSDR via end-to-end feature-aware label space encoding. In contrast to most previous works, E^2FE requires no encoding functions, and it directly learns a feature-aware code matrix via jointly maximizing the recoverability of the label space and the predictability of the latent space. Subsequently, a linear decoding matrix is further learnt for efficiently recovering the predicted label vectors of unseen instances from their corresponding code vectors

generated by trained predictive models. The proposed E^2FE has close connections to several previous works. It can also be specified to learn an encoding function as previous works, or extended with kernel tricks to handle non-linear correlations between the feature space and the latent space.

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Supplementary Material for “End-to-End Feature-aware Label Space Encoding for Multi-label Classification with Many Classes”

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I. PROOFS FOR LEMMA 1 AND LEMMA 3

Lemma 1. For E^2FE , its RMSE is bounded by

$$RMSE \leq \frac{2}{\sqrt{n}} \left(\sqrt{d_z} \|\mathbf{Y}\|_{fro} \|\mathbf{Z} - \mathcal{G}(\mathbf{X})\|_{fro} + \|\mathbf{Y} - \mathbf{ZQ}\|_{fro} \right) \quad \square$$

Proof. RMSE for E^2FE is defined as follows.

$$RMSE = \frac{1}{\sqrt{n}} \|\text{round}(\mathcal{G}(\mathbf{X})\mathbf{Q}) - \mathbf{Y}\|_{fro} \quad (1)$$

where \mathcal{G} denotes the learnt predictive models for mapping instance features into code vectors, and $\text{round}(\mathcal{G}(\mathbf{X})\mathbf{Q})$ denotes the recovered binary tagging matrix.

For clarification, we introduce a matrix \mathbf{R} defined as follows.

$$\mathbf{R} = \text{round}(\mathcal{G}(\mathbf{X})\mathbf{Q}) - \mathbf{Y} \quad (2)$$

Then for any entry $\mathbf{R}_{i,j}$, we have $\mathbf{R}_{i,j} \in \{-1, 0, 1\}$ and thus $\mathbf{R}_{i,j}^2 \in \{0, 1\}$.

According to the $\text{round}(\cdot)$ operation, there are two cases making $\mathbf{R}_{i,j}^2 = 1$, i.e. 1) $(\mathcal{G}(\mathbf{X})\mathbf{Q})_{i,j} \geq \frac{1}{2}$ while $\mathbf{Y}_{i,j} = 0$, and 2) $(\mathcal{G}(\mathbf{X})\mathbf{Q})_{i,j} < \frac{1}{2}$ while $\mathbf{Y}_{i,j} = 1$. In both cases, we have the following inequality.

$$\left((\mathcal{G}(\mathbf{X})\mathbf{Q})_{i,j} - \mathbf{Y}_{i,j} \right)^2 \geq \left(\frac{1}{2} \right)^2 = \frac{1}{4} \mathbf{R}_{i,j}^2 \quad (3)$$

Actually, when $\mathbf{R}_{i,j}^2 = 0$, the inequality above still holds.

Then, we have $\sum_{i,j} \mathbf{R}_{i,j}^2 \leq 4 \sum_{i,j} \left((\mathcal{G}(\mathbf{X})\mathbf{Q})_{i,j} - \mathbf{Y}_{i,j} \right)^2$. With matrix notations, we can further derive:

$$\|\mathbf{R}\|_{fro} \leq 2 \|\mathcal{G}(\mathbf{X})\mathbf{Q} - \mathbf{Y}\|_{fro} \quad (4)$$

With the triangle inequality and the Cauchy Schwarz inequality, we can derive that: 1) $\forall \mathbf{A}, \mathbf{B}, \|\mathbf{A} + \mathbf{B}\|_{fro} \leq \|\mathbf{A}\|_{fro} + \|\mathbf{B}\|_{fro}$, and 2) $\forall \mathbf{A}, \mathbf{B}, \|\mathbf{AB}\|_{fro} \leq \|\mathbf{A}\|_{fro} \|\mathbf{B}\|_{fro}$. Moreover, with $\mathbf{Z}^T \mathbf{Z} = \mathbf{I}$, we have $\|\mathbf{Z}\|_{fro} = \sqrt{d_z}$. Then we can utilize them with $\mathbf{Q} = \mathbf{Z}^T \mathbf{Y}$ to have the following derivations.

$$\begin{aligned} & \|\mathcal{G}(\mathbf{X})\mathbf{Q} - \mathbf{Y}\|_{fro} \\ &= \|(\mathcal{G}(\mathbf{X})\mathbf{Q} - \mathbf{ZQ}) + (\mathbf{ZQ} - \mathbf{Y})\|_{fro} \\ &\leq \|\mathcal{G}(\mathbf{X})\mathbf{Q} - \mathbf{ZQ}\|_{fro} + \|\mathbf{ZQ} - \mathbf{Y}\|_{fro} \\ &\leq \|\mathcal{G}(\mathbf{X}) - \mathbf{Z}\|_{fro} \|\mathbf{Q}\|_{fro} + \|\mathbf{ZQ} - \mathbf{Y}\|_{fro} \\ &= \|\mathbf{Z} - \mathcal{G}(\mathbf{X})\|_{fro} \|\mathbf{Z}^T \mathbf{Y}\|_{fro} + \|\mathbf{Y} - \mathbf{ZQ}\|_{fro} \\ &\leq \|\mathbf{Z} - \mathcal{G}(\mathbf{X})\|_{fro} \|\mathbf{Z}\|_{fro} \|\mathbf{Y}\|_{fro} + \|\mathbf{Y} - \mathbf{ZQ}\|_{fro} \\ &= \sqrt{d_z} \|\mathbf{Y}\|_{fro} \|\mathbf{Z} - \mathcal{G}(\mathbf{X})\|_{fro} + \|\mathbf{Y} - \mathbf{ZQ}\|_{fro} \end{aligned} \quad (5)$$

Combining formula (1), (2), (4) and (5), we can derive:

$$RMSE \leq \frac{2}{\sqrt{n}} \left(\sqrt{d_z} \|\mathbf{Y}\|_{fro} \|\mathbf{Z} - \mathcal{G}(\mathbf{X})\|_{fro} + \|\mathbf{Y} - \mathbf{ZQ}\|_{fro} \right) \quad \square$$

Lemma 3. For any $\eta \in [0, \frac{1}{\max(\vec{\lambda})}]$ with $\max(\vec{\lambda})$ being the maximal value of $\vec{\lambda}$, $\tilde{\mathcal{L}}$ will be non-trivial for optimization.

Proof. In πE^2FE , the objective function for the enhanced linear decoding matrix \mathbf{Q} is defined as follows.

$$\tilde{\mathcal{L}} = \min_{\mathbf{Q}} \|\mathbf{Y} - \mathbf{ZQ}\|_{fro}^2 - \eta \text{Tr}[\mathbf{Q}^T \tilde{\mathbf{\Lambda}} \mathbf{Q}] \quad (6)$$

where $\tilde{\mathbf{\Lambda}}$ is a diagonal matrix with $\tilde{\Lambda}_{j,j} = \lambda_j$, and λ_j is the eigenvalue corresponding to the j th column of the code matrix \mathbf{Z} . Moreover, here $\vec{\lambda} = [\lambda_1, \lambda_2, \dots, \lambda_{d_z}]$.

Then $\tilde{\mathcal{L}}$ can be rewritten as the following Quadratic Programming form.

$$\begin{aligned} \tilde{\mathcal{L}} &= \min_{\mathbf{Q}} \text{Tr}[\mathbf{Q}^T (\mathbf{Z}^T \mathbf{Z} - \eta \tilde{\mathbf{\Lambda}}) \mathbf{Q} - 2\mathbf{Y}^T \mathbf{ZQ}] \\ &= \min_{\mathbf{Q}} \text{Tr}[\mathbf{Q}^T (\mathbf{I} - \eta \tilde{\mathbf{\Lambda}}) \mathbf{Q} - 2\mathbf{Y}^T \mathbf{ZQ}] \end{aligned} \quad (7)$$

where \mathbf{I} is an identity matrix. To make $\tilde{\mathcal{L}}$ non-trivial for optimization, $(\mathbf{I} - \eta \tilde{\mathbf{\Lambda}})$ needs to be positive semi-definite. Knowing that $\tilde{\mathbf{\Lambda}}$ is a diagonal matrix with its diagonal entries being $\vec{\lambda}$, $(\mathbf{I} - \eta \tilde{\mathbf{\Lambda}})$ is also diagonal, and all its diagonal entries are non-negative when $\eta \in [0, \frac{1}{\max(\vec{\lambda})}]$ with $\max(\vec{\lambda})$ being the maximal value of $\vec{\lambda}$. In that case $(\mathbf{I} - \eta \tilde{\mathbf{\Lambda}})$ is positive semi-definite, making $\tilde{\mathcal{L}}$ non-trivial for optimization. \square

II. SUPPLEMENTARY EXPERIMENTAL RESULTS

A. Statistical Significance of the Superiority of E^2FE

As mentioned in the paper (section VII-B1), to evaluate the significance of the performance improvements gained by E^2FE over the baselines, we further perform *paired-sample t-test* [1] for both *label-based macroF1* and *example-based Accuracy* on all datasets with varying d_z/d_y .

For *label-based macroF1*, we take the corresponding *F1* values (i.e. $\frac{2p_i r_i}{p_i + r_i}$ in formula (28)) of all labels for each algorithm as the samples from its *F1* distribution. Meanwhile, for *example-based Accuracy*, we take the corresponding *accuracy* values (i.e. $\frac{|G'_i \cap P'_j|}{|G'_i \cup P'_j|}$ in formula (29)) of all test instances for each algorithm as the samples from its *accuracy* distribution. Then for each performance metric, we compare the samples of

TABLE I
RESULTS OF SIGNIFICANCE TEST (*i.e.* P -value) FOR *label-based macroF1* BETWEEN E^2FE AND THE COMPARED BASELINES ON ALL DATASETS WITH VARYING d_z/d_y

Datasets	<i>delicious</i>					<i>CAL500</i>					<i>mediamill</i>					
	d_z/d_y	10%	20%	30%	40%	50%	10%	20%	30%	40%	50%	10%	20%	30%	40%	50%
CS	€	€	€	€	€	€	€	€	3.57e-08	4.19e-08	2.25e-06	1.73e-10	2.11e-08	8.27e-09	6.87e-05	1.76e-05
PLST	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€
CPLST	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€
MLC-BMaD	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€
ML-CSSP	€	€	€	€	€	€	€	€	€	€	€	2.61e-09	6.16e-10	€	€	€

Datasets	<i>ESPGame</i>					<i>bibtex</i>					<i>bookmarks</i>					
	d_z/d_y	5%	10%	15%	20%	25%	10%	20%	30%	40%	50%	10%	20%	30%	40%	50%
CS	€	3.41e-05	0.0015	0.206	0.181	€	€	9.1e-05	4.16e-05	4.65e-07	€	€	€	€	0.000371	0.00152
PLST	€	€	€	€	€	1.19e-10	€	€	€	€	€	€	€	€	€	€
CPLST	€	€	€	€	€	€	€	€	€	€	€	4.3e-05	€	€	€	€
MLC-BMaD	€	€	€	€	€	1.87e-09	€	€	€	€	€	€	€	€	€	€
ML-CSSP	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€

TABLE II
RESULTS OF SIGNIFICANCE TEST (*i.e.* P -value) FOR *example-based Accuracy* BETWEEN E^2FE AND THE COMPARED BASELINES ON ALL DATASETS WITH VARYING d_z/d_y

Datasets	<i>delicious</i>					<i>CAL500</i>					<i>mediamill</i>					
	d_z/d_y	10%	20%	30%	40%	50%	10%	20%	30%	40%	50%	10%	20%	30%	40%	50%
CS	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€
PLST	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€
CPLST	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€
MLC-BMaD	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€
ML-CSSP	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€

Datasets	<i>ESPGame</i>					<i>bibtex</i>					<i>bookmarks</i>					
	d_z/d_y	5%	10%	15%	20%	25%	10%	20%	30%	40%	50%	10%	20%	30%	40%	50%
CS	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€
PLST	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€
CPLST	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€
MLC-BMaD	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€
ML-CSSP	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€	€

the proposed method against those of any compared baseline, and calculate the differences between pairwise samples for significance tests. The *null hypothesis* H_0 here is that the mean value of such differences equals zero, and the *alternative hypothesis* H_α is that the mean value of such differences does not equal zero and the mean value of the *F1/accuracy* values yielded by E^2FE is larger than that yielded by the compared baseline. We set the significance level as a typical value 0.01. Then if a P -value generated by the significance test satisfies that P -value ≤ 0.01 , the *null hypothesis* H_0 will be rejected and the *alternative hypothesis* H_α is considered to be statistically significant.

Here Table I and II report all the P -values of the significance tests between E^2FE and each baseline for both *label-based macroF1* and *example-based Accuracy* on all datasets with varying d_z/d_y . For clarity, here a P -value less than 10^{-10} is denoted as a tiny value ϵ . From the results of significance tests, we can find that: 1) for *label-based macroF1*, except the cases where E^2FE is compared against CS with $d_z/d_y \in \{20\%, 25\%\}$ on *ESPGame*, the maximal P -value in all significance tests between E^2FE and the compared baselines is around 1.5×10^{-3} , 2) for *example-based Accuracy*, all P -values in significance tests are less than 10^{-10} . Therefore, considering that nearly all P -values in the significance tests are less than the significance level, *i.e.* 0.01, the performance improvements gained by E^2FE over the compared baselines are statistically significant.

B. Experimental Validation for the Orthonormality Assumption in E^2FE

As mentioned in the paper (section VIII), to further demonstrate the reasonableness of introducing the orthonormality assumption into the proposed E^2FE , we also try dropping it from the objective function and conduct experiments to see how it affects the classification performance and the computational costs of E^2FE . We denote this case as E^2FE_{NoOrth} . Specifically, without the orthonormality assumption, the objective function of E^2FE_{NoOrth} will be as follows.

$$\begin{aligned} \Psi &= \max_{\mathbf{Z}, \mathbf{Q}} -\|\mathbf{Y} - \mathbf{Z}\mathbf{Q}\|_{fro}^2 + \alpha \text{Tr}[\mathbf{Z}^T \mathbf{H} \mathbf{Z}] \\ &= \min_{\mathbf{Z}, \mathbf{Q}} \|\mathbf{Y} - \mathbf{Z}\mathbf{Q}\|_{fro}^2 - \alpha \text{Tr}[\mathbf{Z}^T \mathbf{H} \mathbf{Z}] \quad (8) \\ \text{s.t. } &\forall i \in \{1, 2, \dots, d_z\}, \mathbf{Z}_{:,i}^T \mathbf{Z}_{:,i} = 1 \end{aligned}$$

where \mathbf{Y} is the tagging matrix of training instances, \mathbf{Z} and \mathbf{Q} are respectively the to-be-learned code matrix and the linear decoding matrix, and $\mathbf{H} = \mathbf{X}(\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T$ with \mathbf{X} being the feature matrix of training instances. Note that $\mathbf{Z}_{:,i}^T \mathbf{Z}_{:,i} = 1$ is still required here as it is the precondition for $\text{Tr}[\mathbf{Z}^T \mathbf{H} \mathbf{Z}]$ being an expression of predictability, as described in section III-B2. Like other matrix factorization methods [2], [3], we can derive the code matrix \mathbf{Z} and the linear decoding matrix \mathbf{Q} via iteratively and alternatively optimizing one with the other fixed, though that cannot ensure to obtain the global optima. Specifically, with \mathbf{Z} fixed, \mathbf{Q} can be optimized as $\mathbf{Q} = (\mathbf{Z}^T \mathbf{Z})^{-1} \mathbf{Z}^T \mathbf{Y}$. Meanwhile, with \mathbf{Q} fixed, the gradient *w.r.t* \mathbf{Z} can be calculated as $\frac{\partial \Psi}{\partial \mathbf{Z}} = -2(\mathbf{Y} - \mathbf{Z}\mathbf{Q})\mathbf{Q}^T - 2\alpha \mathbf{H}\mathbf{Z}$. Considering the constraints for each column of \mathbf{Z} , it is infea-

TABLE III
PERFORMANCE COMPARISONS BETWEEN E^2FE AND E^2FE_{NoOrth} ON ALL DATASETS, WITH $p = 5$ FOR *ESPGame* AND $p = 10$ FOR OTHERS.

		d_z/d_y	p%	2p%	3p%	4p%	5p%
label-based macroF1	<i>delicious</i>	E^2FE	0.0530	0.0569	0.0577	0.0578	0.0578
		E^2FE_{NoOrth}	0.0336	0.0401	0.0444	0.0462	0.0438
	<i>CAL500</i>	E^2FE	0.1198	0.1247	0.1263	0.1258	0.1256
		E^2FE_{NoOrth}	0.0966	0.1086	0.1074	0.1122	0.1120
	<i>mediamill</i>	E^2FE	0.0549	0.0575	0.0577	0.0577	0.0577
		E^2FE_{NoOrth}	0.0436	0.0448	0.0459	0.0451	0.0453
	<i>ESPGame</i>	E^2FE	0.0026	0.0025	0.0025	0.0025	0.0025
		E^2FE_{NoOrth}	0.0018	0.0018	0.0017	0.0018	0.0018
	<i>bibtex</i>	E^2FE	0.0595	0.0888	0.1169	0.1286	0.1369
		E^2FE_{NoOrth}	0.0420	0.0727	0.0847	0.0929	0.1000
	<i>bookmarks</i>	E^2FE	0.0472	0.0706	0.0752	0.0764	0.0775
		E^2FE_{NoOrth}	0.0298	0.0455	0.0459	0.0471	0.0488
example-based Accuracy	<i>delicious</i>	E^2FE	0.1187	0.1196	0.1197	0.1196	0.1184
		E^2FE_{NoOrth}	0.1037	0.1073	0.1082	0.1093	0.1045
	<i>CAL500</i>	E^2FE	0.2405	0.2411	0.2421	0.2396	0.2392
		E^2FE_{NoOrth}	0.2261	0.2294	0.2256	0.2267	0.2250
	<i>mediamill</i>	E^2FE	0.4353	0.4379	0.4378	0.4378	0.4378
		E^2FE_{NoOrth}	0.4192	0.4201	0.4204	0.4192	0.4199
	<i>ESPGame</i>	E^2FE	0.0701	0.0701	0.0700	0.0701	0.0701
		E^2FE_{NoOrth}	0.0613	0.0635	0.0605	0.0585	0.0590
	<i>bibtex</i>	E^2FE	0.1835	0.2149	0.2356	0.2440	0.2493
		E^2FE_{NoOrth}	0.1501	0.2018	0.2121	0.2167	0.2233
	<i>bookmarks</i>	E^2FE	0.1659	0.1913	0.1933	0.1937	0.1939
		E^2FE_{NoOrth}	0.1521	0.1627	0.1636	0.1645	0.1660

TABLE IV
AVERAGE TIME COSTS (IN SECONDS) FOR PERFORMING LSDR IN E^2FE AND E^2FE_{NoOrth} WITH $d_z/d_y = 10\%$.

	<i>delicious</i>	<i>ESPGame</i>	<i>bookmarks</i>
E^2FE	1.984	10.877	4.877
E^2FE_{NoOrth}	145.253	215.199	41.434

sible to derive a closed-form solution for the optimal \mathbf{Z} . And thus in our experiments we utilize a gradient descent based method for optimizing \mathbf{Z} , which always takes one appropriate step to make the objective function decrease while keeping the constraints satisfied. By iteratively optimizing \mathbf{Z} and \mathbf{Q} until convergence (*i.e.* the relative change of the objective function is less than 0.1% in our experiments), we utilize them to train predictive models and then perform classification for unseen instances.

The performance of E^2FE_{NoOrth} on all datasets, using random initial values for \mathbf{Z} and \mathbf{Q} to perform optimization, is presented in Table III. It can be seen that E^2FE_{NoOrth} is inferior to E^2FE . In fact, even using the derived \mathbf{Z} and \mathbf{Q} of E^2FE as initial values, E^2FE_{NoOrth} can hardly gain performance improvement over E^2FE . It is mainly attributed to that, without the orthonormality assumption, 1) more redundant information rather than complementary information exists between dimensions of the latent space, and 2) global optima cannot be ensured for \mathbf{Z} .

Moreover, we also evaluate the time costs for E^2FE_{NoOrth} to perform LSDR on the largest *delicious*, *ESPGame* and *bookmarks* with $d_z/d_y = 10\%$, as reported in Table IV. We can see that E^2FE_{NoOrth} costs much more time than E^2FE , because its objective function is more complex for optimization. Its time costs are even higher than those of the binary relevance model L-RR (see Table VIII in the paper), which means that E^2FE_{NoOrth} may be unsuitable for LSDR.

Therefore, dropping the orthonormality assumption does

not bring substantial performance improvements and instead will increase the time costs for optimization. On the contrary, keeping the orthonormality assumption gains a good trade-off between efficiency and effectiveness for LSDR.

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