LTSA-LE: A Local Tangent Space Alignment Label Enhancement Algorithm

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Abstract: According to smoothness assumption, local topological structure can be shared between feature and label manifolds. This study proposes a new algorithm based on Local Tangent Space Alignment (LTSA) to implement the label enhancement process. In general, we first establish a learning model for feature extraction in label space and use a feature extraction method of LTSA to guide the reconstruction of label manifolds. Then, we establish an unconstrained optimization model based on the optimal theory presented in this paper. The model is suitable for solving problems with a large number of sample points. Finally, the experiment results show that the algorithm can effectively improve the training speed and multilabel dataset prediction accuracy.

Key words: smoothness assumption; feature manifold; label manifold; unconstrained optimization

1 Introduction

Multi-Label Learning (MLL) is a major topic in recent machine learning and pattern recognition studies. In an MLL framework, each instance is represented by a feature vector that can belong to multiple labels. MLL deals with the case where an instance is associated with multiple labels, and its goal is to learn a multilabel predictor that maps an instance to a relevant label set. With the introduction of MLL, many scholars have conducted extensive research on this basis and proposed many effective algorithms.

This learning process works by mapping an instance and then assigning a label. However, with the increase in the number of labels, the standard MLL methods that work in the original label space become impractical easily when training multilabel classifiers.

Some researchers have considered low-dimensional embedded label space and proposed many label space reduction methods. For example, Tai and Lin attempted to reduce the amount of computation by seeking a major correlation between labels, especially for the datasets with numerous labels. Sun et al. mapped the feature space and label space into the new space, where the correlation between the mapping of the two spaces is maximized. In these cases, the dimension of the label space is reduced to digest the information between the labels and learn more effectively.

However, some existing methods perform label space embedding without considering feature information, and a few methods can effectively utilize the local structure or label correlation of the feature space. Thus, these methods tend to lose some of the information, thereby seriously affecting the effectiveness of multilabel


2 Related Work on Label Enhancement

2.1 Formulation of label enhancement

First of all, the main notations used in this paper are listed as follows: the instance variable is denoted by \( x \); the particular \( i \)-th instance is denoted by \( x_i \), the label variable is denoted by \( y \), and the particular \( j \)-th label is denoted by \( y_j \). The logical label vector of \( x_i \) is denoted by \( L_i = (l_{i1}, l_{i2}, \ldots, l_{ic}) \), where \( L_i \in \{0, 1\}^c \) and \( c \) is the number of possible labels. The description degree of \( y \) to \( x \) is denoted by \( d^y_i \), where \( d^y_i \in [0, 1] \) and \( \sum_j d^y_{ij} = 1 \). The label distribution of \( x_i \) is denoted by \( D_i = (d_{i1}, d_{i2}, \ldots, d_{ic}) \), where \( D_i \in [0, 1]^c \).

Then, the label distribution learning for label enhancement can be defined as follows: given a training set \( S = \{(x_i, L_i) | 1 \leq i \leq n\} \), the goal of label enhancement is to transform the logical label vector \( L_i \) of \( x_i \) to the label distribution \( D_i \) according to the correlation between labels contained in \( S \), thereby obtaining a Label Distribution Learning (LDL) training set \( \mathcal{E} = \{(x_i, D_i) | 1 \leq i \leq n\} \).

2.2 Label enhancement based on manifold

The label enhancement algorithm based on manifold assumes that the data are distributed in the feature and label manifolds. This algorithm connects the manifolds of the two spaces according to the smoothness assumption, so that the label manifold is reconstructed with the topological structure from the feature manifold and the logical label of this instance is enhanced to the label distribution on this basis.

As many graph-based learning methods do, the topological structure from the feature space of multiple label training set \( S \) can be represented by a graph \( G = (V, E, \hat{W}) \), where \( V \) is the vertex set, \( E \) is the edge set, and \( \hat{W} = (\hat{w}_{ij})_{n \times n} \) is the weight matrix with the edge. First, we assume that the manifold of the instance distribution satisfies local linearity, that is, each instance \( x_i \) can be optimally reconstructed using a linear combination of its \( k \)-nearest neighbors. The reconstructed weight matrix is to induce the minimization of

\[
\Omega(\hat{W}) = \sum_{i=1}^{n} ||x_i - \sum_{i \neq j} \hat{w}_{ij}x_j ||^2
\]

where \( \hat{w}_{ij} = 0 \) unless \( x_j \) is one of \( x_i \)'s \( k \)-nearest neighbors. The constraint is \( \hat{W}^T \hat{W} = 1 \) for translation invariance, where \( \hat{W}^T \) represents the vector consisting of all 1 and \( \hat{w}_{ij} \) is the \( i \)-th row of \( \hat{W} \). According to the smoothness assumption, the instances with similar
features are likely to have similar labels. Thus, one can migrate the topological structure of the feature space into the label space, that is, the feature and the label space share the same local linear reconstruction weight matrix $\hat{W}$. Therefore, the label distribution of the label space can infer to the minimization of

$$\Phi(D) = \sum_{i=1}^{n} \|D_i - \sum_{i \neq j} \hat{w}_{ij}D_j\|^2$$

(2)

where $D_i = (d_i^1, d_i^2, \ldots, d_i^C)$ denotes the distribution of $x_i$. A constraint is added on $d_i$ to introduce logical labels.

$\forall 1 \leq i \leq n, \ 1 \leq l_i \leq c, \ l_i^c d_i^c \geq \lambda (\lambda > 0)$

(3)

To facilitate the construction of the aforementioned constraints, the logical label vector defined in Ref. [8] is $L_i \in \{-1, 1\}^c$, instead of $L_i \in \{0, 1\}^c$, which is commonly used in other methods. However, no difference exists between these two vectors. After solving the preceding quadratic programming problem, we can obtain the label distribution $D_i$ by normalization, and thereafter obtain the label distribution training set $\varepsilon = \{x_i, D_i\} | 1 \leq i \leq n\}.

The manifold-based method reconstructs the feature and space manifolds according to the smoothness assumption that migrates the topological relationship of the feature space into the label space. Then, the method establishes the relationship between the correlation between the instances and the correlation between the labels, thereby establishing the logic. Finally, the logical labels are enhanced to label distribution[11].

### 2.3 Label enhancement for label distribution learning

To solve the Label Enhancement (LE) problem, Xu et al.[10] introduced an existing algorithm that can be used for LE and proposed a new method of label enhancement called label distribution learning. The label distribution is recovered from the logical labels in the training set by utilizing the topology information of the feature space and the correlation between the labels.

### 2.4 Label embedding based on multi-scale locality preservation

Peng et al.[11] proposed a new label distribution learning algorithm by using local sample correlation. Label distribution is learned by leveraging sample correlation locally.

### 2.5 Multi-label learning with label enhancement

Shao et al.[12] proposed an effective MLL method called label-enhanced MLL, which is based on label enhancement. Through this approach, problems were developed by combining numerical label and label-enhanced regression into a unified framework, in which numerical labels and predictive models are learned jointly.

### 3 Proposed Algorithm

#### 3.1 Preprocessing on training set: Establish the correlation between manifolds and label spaces

In this section, we explore multilabel manifold learning. To study the label manifold, we have to extend the label space to the Euclidean space, because the traditional label space is logical and the label vector is a logical label. Here we extend the label vector from logic to real numbers called numerical labels. Hou et al.[8] mentioned that numerical labels carry more semantic information and can describe instances more comprehensively than logical labels. To reconstruct the label manifold, we first preprocess the training set, and then establish the association between the manifold and label spaces. Finally, we extend the feature space to the label space and obtain the numerical label.

Inspired by the LTSA algorithm proposed by Zhang and Zha[13], we approximate the feature manifold by overlapping local linear neighborhoods and obtain the topological structure of the feature space by using LTSA.

To obtain the mapping coordinates of the high-dimensional data set $X$ in the low-dimensional space, we use the LTSA algorithm to determine the global coordinates by applying LTSA. The dataset is denoted by $X = [x_1, \ldots, x_N]$ with $N$ high-dimensional coordinates. We minimize

$$\min_{x, L, \Theta} \|X - (\hat{x}e^T + L\Theta)\|^2$$

(4)

where $X_i = [x_{i1}, \ldots, x_{ik}]$ is a matrix consisting of its $k$-nearest neighbors including $x_i$, in terms of the Euclidean distance, $\hat{x}_i$ is the average of $X_i$, $\Theta = [\theta_1, \ldots, \theta_k]$ is the weight matrix, $L$ is the optimal alignment matrix consisting of $d$-dimensional orthogonal column vectors $L_i$, given by the eigenvectors of $X_i(I - ee^T/k)$ corresponding to $d$ eigenvalues in descending order, $e$ is the $k$-dimensional identity matrix. Thus,

$$X_i = \hat{x}_i + L_i\theta_i + e_i$$

(5)

where $e_i = (I - L_iL_i^T)(x_i - \hat{x}_i)$ is the reconstruction error.
The objective of this study is to recover the low-dimensional coordinate $Y_i$ from the least squares and reconstruct the topological structure of the label manifold from the feature manifold and the existing logical labels. Furthermore, the study aims to determine that a reasonable label distribution $d_i$ can be generated for the instance $x_i$.

Our model is described as follows:

$$Y_i = \frac{1}{k} Y_i ee^T + L_i \Theta^T_i + E_i$$

(6)

where $E_i = [e_i 1, \ldots e_i k]$ is the local reconstruction error matrix. To minimize the reconstruction error, we utilize quadratic programming on the model to obtain the following optimization function,

$$\min_{1 \leq i \leq N} \sum_{i=1}^{N} \left( \|E_i\|_F^2 \right) = \left\| Y_i \left( I_k - \frac{1}{k} ee^T \right) - L_i \Theta^T_i \right\|_F^2$$

(7)

To obtain a unique solution, we express the reconstruction error as

$$\sum_{i=1}^{N} \left\| Y_i \left( I_k - \frac{1}{k} ee^T \right) \left( I_k - \Theta \Theta^T \right) \right\|_F^2 = \text{trace} \left( T \Phi T^T \right)$$

(8)

where $\Theta^T_i$ is the Moor-Penrose generalized inverse of $\Theta_i$, $T$ is a matrix composed by the low-dimensional embeddings, $\Phi = \sum_{i=1}^{N} S_i H_i \Phi^T_i$, $S_i$ is the 0-1 selection matrix, such that $TS_i = T_i$, and $H_i$ is given by

$$H_i = \left( I_k - \frac{1}{k} ee^T \right) \left( I_k - Q_i Q_i^T \right)$$

(9)

The low-dimensional embeddings that minimize the reconstruction error can be solved by the eigenvectors corresponding to the $d$ largest eigenvalues of the matrix $\Phi$.

### 3.2 Unconstrained optimization model

The feature manifold is represented by a graph and approximated by overlapping local linear neighborhood patches. The edge weights in each patch can be calculated by a least squares programming method. The label manifold and transferred local topological reconstructed structure can be reconstructed based on the feature manifold and existing logical labels. The reconstruction can be accomplished through a quadratic method.

As shown in the previous section, in the manifold space, the feature manifold is represented by a graph and approximated by overlapping local linear neighborhoods. An optimization model that can solve the edge weight in each patch is expressed as Eq. (6).

We propose a new LE algorithm called LTSA Label Enhancement (LTSA-LE) in this paper. Given a training set, we construct a feature matrix $X = [x_1, x_2, \ldots, x_N]$ and a logical label matrix $L = [l_1, l_2, \ldots, l_N]$. Our goal is to recover the label distribution matrix $D = [d_1, d_2, \ldots, d_N] \in \mathbb{R}^{c \times N}$ from the logical label matrix $L$. To solve this problem, we consider the model:

$$D_i = W \Theta_i + r$$

(10)

where $W = [w_1, \ldots, w_d] \in \mathbb{R}^{c \times d}$, $\Theta_i \in \mathbb{R}^d$ is the nonlinear transformation of the sample point in the low-dimensional space $\mathbb{R}^d$ and is the optimal solution of Eq. (6), $r \in \mathbb{R}^c$ is the model parameter.

As the information in the label distribution is inherited from the initial logical label, we choose the least squares loss function, which is actually a multiple output regression problem in the case of multiple labels. After determining $d_i$ by solving the quadratic programming problem, the label distribution is obtained by normalization,

$$F(W, r) = \frac{1}{2} \sum_{j=1}^{c} \|w_j\|^2 + C \sum_{i=1}^{N} \text{Loss}(u_i)$$

(11)

where Loss( ) is the loss function and $u_i = y_i - W \Theta_i - r$, $C$ is the model parameter.

Then, $y_i \in \{-1, +1\}^c$ represents a numeric label vector, where we use $-1$ instead of $0$ to indicate that it is independent of the instance. This study explores manifolds in label space and treats labels as numbers. The label set contains additional semantic information, which is beneficial for the learning process.

The multilabel manifold learning algorithm proposed by Hou et al.\cite{8} solves a quadratic programming problem with constraints and obtains the label distribution through optimization. Constraints are utilized to express constraints on problems, such as structural features in the real dataset, local neighborhood relationships, and manifold structure information. However, the solution to the quadratic programming problem with constraints will face limitations in time and memory when the number of samples is large.

Based on the MSVR constrained optimization model, we establish an unconstrained optimization model based on the optimal theory. By introducing the maximum entropy function, we transform the original optimization problem into an unconstrained optimization problem, which solves the difficulty that the MSVR constrained optimization problem seeks the solution from a large number of samples. However, the standard maximum entropy function method may lead to data overflow. In this study, we improve the maximum entropy function and propose an MSVR model based on adaptively adjusting the Shannon entropy function, which ensures
convergence and utilizes the quasi-Newton method to obtain the model. In particular, the model is suitable for problems with a large number of sample points.

### 3.3 Multi-output regression adaptive weighting strategy based on Shannon entropy

The existing multi-output regression algorithm almost defaults to the same premise, that is, the weight parameter of each sample contributes equally to the final classification result. In fact, some sample spaces often have serious spatial overlaps and are inseparable. The suitable treatment should give different degrees of importance according to the divisible characteristics of the sample, so that the classification results can be optimal. However, artificially setting importance weights is unreasonable. Thus, using the Shannon entropy theory\(^\text{[14]}\), we propose an adaptive weighted term with multi-output regression technique, and then introduce the viewing angle weight coefficient \(w_k\). Finally, we reconstructed objective function formula according to the condition \(\sum_{k=1}^{N} \tilde{w}_k = 1\) and \(\tilde{w}_k \geq 0\).

We consider weights as probability distributions expressed with Shannon entropy as

\[
 f(\tilde{w}) = \sum_{j=1}^{c} \tilde{w}_j \ln \tilde{w}_j \quad (12)
\]

According to the definition of the unconstrained optimization model in Section 3.2 and the multi-output regression adaptive weighting strategy, the objective function in this section is reconstructed as follows:

\[
 \Gamma(W, e) = F(W, e) + f(\tilde{w}) \quad (13)
\]

We define the adaptive adjustment Shannon entropy function as an adaptive weighting part based on Shannon entropy theory,

\[
 \Gamma(W, e) = \frac{1}{2} \sum_{j=1}^{c} \|\tilde{w}_j\|^2 + C \sum_{i=1}^{N} \text{Loss}(u_i) + \frac{1}{2} \sum_{j=1}^{c} \alpha \tilde{w}_j \ln \tilde{w}_j \quad (14)
\]

where \(\alpha\) is an adaptive adjustment factor. We use an iterative quasi-Newton method called IRWLS\(^\text{[6,8]}\) to optimize Eq. (14). In terms of convergence, we know that the Newton algorithm is convergent; thus, the entire algorithm has convergence.

The main procedure of the LTSA-LE algorithm is presented in Algorithm 1.

### 4 Experiment

#### 4.1 Experimental setup

##### 4.1.1 Comparing algorithms

We select two well-established MLL algorithms to compare with the performance of LTSA-LE: an MLL algorithm based on a neural network model (called BP-MLL)\(^\text{[15]}\) and multilabel manifold learning (called ML\(^2\))\(^\text{[8]}\). We also selected three types of LDL algorithms: Label Distribution Support Vector Regressor (LDSVR)\(^\text{[16]}\), Conditional Probability Neural Network (CPNN)\(^\text{[17]}\), and Algorithm Adaptation \(k\)-Nearest Neighbors (AA-KNN)\(^\text{[7]}\).

**Algorithm 1 Procedure of LTSA-LE**

**Input:** A training sample matrix \(X = [x_1, \ldots, x_N] \in \mathbb{R}^{d \times N}\), a numeric label vector \(y_i \in \{-1, +1\}^c\), where \(-1\) indicates it is independent of the instance \(x_i\).

**Output:** Label distribution \(D\) for the multilabel sample set \(X\).

1. \(i \leftarrow 1, j \leftarrow 1\).
2. Compute the optimal solution of Eq. (6), and obtain \(\theta_i \in \mathbb{R}^d\), which is the nonlinear transformation of the sample point in the low-dimensional space \(\mathbb{R}^d\).
3. repeat
4. Optimize \(\Gamma(W, e)\) according to Eq. (14).
5. Update \(f(\tilde{w})\) according to Eq. (12).
6. Update Eq. (14) via the Iterative Re-Weighted Least Square (IRWLS) procedure.
7. \(j \leftarrow j + 1, i \leftarrow i + 1\).
8. until convergence is reached.
9. Return \(D\) according to Eq. (10).

| Dataset   | \(S\) | \(T\) | \(\text{dim}(S)\) | \(L(S)\) | \(\text{LCard}(S)\) | \(\text{LDen}(S)\) | \(\text{DL}(S)\) | \(F(S)\) |
|-----------|------|------|----------------|--------|----------------|----------------|--------|--------|
| Emotions  | 415  | 178  | 72            | 6      | 1.869         | 0.311           | 27     | numeric |
| Medical   | 645  | 333  | 1449          | 45     | 1.245         | 0.028           | 94     | nominal |
| Cal500    | 250  | 252  | 68            | 174    | 26.044        | 0.150           | 502    | numeric |
| Birds     | 320  | 325  | 260           | 19     | 1.014         | 0.053           | 133    | numeric |
| Enron     | 1123 | 579  | 1001          | 55     | 3.378         | 0.064           | 753    | nominal |
| Yeast     | 1200 | 1217 | 103           | 14     | 4.237         | 0.303           | 198    | numeric |
| Image     | 1000 | 1000 | 294           | 5      | 1.236         | 0.247           | 20     | numeric |
| Scene     | 1211 | 1196 | 294           | 6      | 1.074         | 0.179           | 15     | numeric |
| Corel5k   | 2500 | 2500 | 499           | 374    | 3.522         | 0.009           | 3175   | nominal |
| Bibtex    | 3700 | 3695 | 1836          | 159    | 2.402         | 0.015           | 2856   | nominal |

**Table 1 Characteristic of multilabel datasets.**
4.1.2 Datasets
To compare our algorithm with the state-of-the-art MLL algorithms, we selected 10 real-world multilabel datasets for performance evaluation. Table 1 summarizes the detailed features of these datasets selected from the Mulan website (http://mulan.sourceforge.net/datasets-mlc.html, 2019-03-01) and sorted in ascending order. $S$ is the number of examples, $T$ is the number of testing samples, $\text{dim}(S)$ denotes the feature dimensions, $L(S)$ represents the number of class labels, and $L\text{Card}(S)$ is the label cardinality. Other multilabel statistics include the label density $L\text{Den}(S)$, distinct label sets $D\text{L}(S)$, and feature type $F(S)$. Half of them are regular-sized and half are large-scale; thus, the dataset covered a wide range of multilabel attributes.

4.1.3 Evaluation metrics
When comparing LTSA-LE to traditional MLL methods, we selected five widely used evaluation metrics for multilabel learning: Hamming loss, one error, coverage, ranking loss, and average precision\[18\]. For average precision, the larger the value, the better the performance. For the other four metrics, the smaller the values, the better the performance.

When comparing LTSA-LE with LDL algorithms\[7, 16, 17\], we used six representative label distribution evaluation indicators\[7\]: Chebyshev distance (Cheb), Clark distance (Clark), Canberra distance (Canber), Kullback-Leibler divergence (KL-div), Cosine coefficient (Cosine), and intersectional similarity (Intersec). The first four are distance measures and the last two are similarity measures.

4.2 Experiment results on MLL
The first part of the experiment compares LTSA-LE with traditional MLL algorithms on 10 real-world multilabel datasets. Half the examples on each dataset were selected randomly as a training set, and the remaining half were used to form a test set. We used 10-fold cross-validation on each dataset, set $\text{C} = 0.5$ and $\alpha = 0.5$. We recorded the average performance of each algorithm on five MLL evaluation metrics in Tables 2, 3, 4, 5, and 6. Table 7 shows the time complexity comparison. The $\downarrow$ after the evaluation index means the smaller the better, and the $\uparrow$ means the larger the better. Bold font indicates the best performance among the algorithms.

### Table 2 Comparison of MLL and multilabel distribution algorithms on Hamming loss $\downarrow$.

| Algorithm | Dataset    | Average rank |
|-----------|------------|--------------|
| BP-MLL    | 0.4500     | 1.0094       |
| ML$^2$    | 0.2267     | 0.0096       |
| LDSVR     | 0.3037     | 0.0145       |
| CPNN      | 0.6964     | 0.1406       |
| AA-KNN    | 0.2297     | 0.1052       |
| LTSA-LE   | 0.1958     | 0.0000       |

### Table 3 Comparison of MLL and multilabel distribution algorithms on ranking loss $\downarrow$.

| Algorithm | Dataset    | Average rank |
|-----------|------------|--------------|
| BP-MLL    | 0.4450     | 0.2695       |
| ML$^2$    | 0.3325     | 0.4764       |
| LDSVR     | 0.4974     | 0.5101       |
| CPNN      | 0.9708     | 0.6954       |
| AA-KNN    | 0.5054     | 0.7416       |
| LTSA-LE   | 0.3244     | 0.1052       |

### Table 4 Comparison of MLL and multilabel distribution algorithms on one error $\downarrow$.

| Algorithm | Dataset    | Average rank |
|-----------|------------|--------------|
| BP-MLL    | 0.7034     | 0.9716       |
| ML$^2$    | 0.4286     | 0.8269       |
| LDSVR     | 0.4286     | 0.9479       |
| CPNN      | 0.0714     | 0.5470       |
| AA-KNN    | 0.4999     | 0.4419       |
| LTSA-LE   | 0.0000     | 0.0000       |
Table 5 Comparison of MLL and multilabel distribution algorithms on coverage ↓.

| Algorithm | Dataset          | Average rank |
|-----------|------------------|--------------|
|           | Yeast            | Emotions     | Medical | Cal500 | Birds | Image | Scene | Enron | Corel5k | Bibtex |          |
| BP-MLL    | 0.8990           | 0.3089       | 0.2955  | 1.3386 | 0.4415| 2.1460| 2.0761| **0.2369**| 0.1980  | 0.7356 | 5.100     |
| ML²       | 0.8950           | 0.1723       | 0.7684  | 0.2313 | 0.3031| 0.9962| 1.0617| 0.5029  | 0.1912  | 0.3513 | 4.200     |
| LDSVR     | 0.8982           | **0.1568**   | 0.2087  | 0.2284 | 0.3014| 0.9608| 1.0843| 0.4936  | 1.5023  | 0.3382 | 3.250     |
| CPNN      | **0.8845**       | 0.1703       | 0.2081  | 0.2316 | **0.2309**| 0.9648| 1.0773| 0.5028  | 1.5023  | 0.3598 | 3.650     |
| AA-KNN    | 0.8794           | 0.1661       | 0.1374  | 0.2315 | 0.2899| 0.9644| 1.0505| 0.4956  | 1.5126  | 0.3585 | 3.300     |
| LTSA-LE   | 0.8846           | 0.1586       | 0.0598  | 0.2275 | 0.2523| 0.9538| 0.1048| 0.4456  | 0.1502  | 0.2596 | 1.500     |

Table 6 Comparison of MLL and multilabel distribution algorithms on average precision ↑.

| Algorithm | Dataset          | Average rank |
|-----------|------------------|--------------|
|           | Yeast            | Emotions     | Medical | Cal500 | Birds | Image | Scene | Enron | Corel5k | Bibtex |          |
| BP-MLL    | 0.4297           | 0.5161       | 0.2081  | 0.4783 | **0.2460**| 0.5111| 0.4200| **0.2057**| 0.2012  | 0.0659 | 2.600     |
| ML²       | 0.4366           | 0.4442       | 0.4683  | 0.1644 | 0.1407| 0.4905| 0.3078| 0.1234  | 0.2930  | 0.3872 | 3.200     |
| LDSVR     | 0.3965           | 0.4900       | 0.1676  | 0.0759 | 0.2729| 0.7859| 0.0747| 0.0141  | 0.0226  | 4.750  | 5.750     |
| CPNN      | 0.3064           | 0.3123       | 0.0467  | 0.1598 | 0.1013| 0.2645| 0.2954| 0.0828  | 0.0141  | 0.1111 | 3.100     |
| AA-KNN    | 0.4779           | 0.4926       | 0.3692  | 0.1705 | 0.1131| 0.5954| 0.7649| 0.1201  | 0.0252  | 0.3678 | 1.600     |
| LTSA-LE   | **0.4825**       | **0.5567**   | **0.5631**| 0.1829 | 0.1602| **0.7105**| **0.7957**| 0.1843  | 0.0278  | 0.3678 | 1.600     |

Table 7 Comparison of MLL and multilabel distribution algorithms on time (s) ↓.

| Algorithm | Dataset          | Average rank |
|-----------|------------------|--------------|
|           | Yeast            | Emotions     | Medical | Cal500 | Birds | Image | Scene | Enron | Corel5k | Bibtex |          |
| BP-MLL    | 4.6563           | 0.7020       | 6.7080  | 10.2337| 1.5625| 1.5288| 1.6380| 13.2757| 218.3234| 122.6948| 5.600     |
| ML²       | 0.4836           | 0.0005       | 0.1716  | 1.404  | 0.0469| 0.2500| 0.3438| 0.1875| 1.5444  | 4.5625  | 3.300     |
| LDSVR     | 0.1406           | **0.0001**   | 0.1872  | 0.0780 | **0.0001**| 0.2496| 0.2652| 0.1716| 1.0156  | 3.5781  | 2.300     |
| CPNN      | 0.1092           | **0.0001**   | 0.5616  | 0.2496 | 0.0468| 0.1404| 0.0780| 0.9048| 15.0385 | 25.6466 | 3.100     |
| AA-KNN    | 3.9936           | 0.2340       | 9.8593  | 0.2184 | 0.5460| 3.9624| 5.7876| 14.7109| 21.4345 | 107.28  | 5.300     |
| LTSA-LE   | **0.0938**       | **0.0001**   | 0.0781  | 0.0469| 0.1404| **0.0938**| **0.0624**| **0.1406**| **0.7969**| **2.9531**| 1.400     |

The experimental results show that on the regular-sized and large-scale datasets, LTSA-LE ranks first in more than half of the evaluation metrics. Particularly on large-scale datasets, these metrics fully validate the effectiveness of LTSA-LE for MLL.

4.3 Time performance comparison

As Table 7 shows, our algorithm LTSA-LE performs effectively among the well-established MLL algorithms, especially on large-scale datasets. Although the accuracy of some algorithms (such as BP-MLL, ML², and AA-KNN) have improved, their time complexity increases rapidly as the sample set size increases. Combined with the recognition accuracy experiments in the previous section, LTSA-LE maintains a good average performance and is remarkably adept in the label manifold learning of a large-scale dataset.

4.4 Friedman test

The Friedman test\(^{[19]}\) is a nonparametric equivalent of repeated measurement ANOVA. The test separately ranks the algorithm for different datasets, and the algorithms with best performances get the first rank, the second rank, and so on, as shown in the average rank in Tables 2, 3, 4, 5, 6, and 7. Let \(r_{ij}\) represents the rank of the \(j\)-th of the \(k\) algorithms on the \(i\)-th of the \(N\) data sets. The Friedman statistic is calculated as follows:

\[
F = \frac{12N}{k(k+1)} \left[ \sum \frac{R_j^2}{k} - \frac{k(k+1)^2}{4} \right]
\]

which obeys the \(F\)-distribution with a freedom degree of \(k - 1\), where \(N\) and \(k\) are large enough (generally \(N \geq 10\) and \(k > 5\)). The exact threshold for a small number of algorithms and data sets has been calculated. Demšar\(^{[19]}\) showed that Friedman estimate of \(F\) is conservative and suggested a better statistic that satisfies the \(F\)-distribution with \(k - 1\) and \((k - 1)(N - 1)\) degrees of freedom.
of freedom as follows:
\[ F_F = \frac{(N - 1) \chi_F^2}{N (k - 1) - \chi_F^2} \quad (16) \]
If the null hypothesis is rejected, then we can proceed with a post-hoc test. The Bonferroni-Dunn test is used in this study. The test method controls the overall error level by dividing \( \alpha \) to one of the original \( k - 1 \) points. Thus, we only need to test whether the new algorithm is better than the existing algorithm. We do not need a two-two pairwise comparison, and we only need to set the new algorithm as the control algorithm. Whenever the performance between an existing algorithm \( i \) and the new algorithm \( j \) is significantly different, we only need to compare whether the difference between their corresponding average ranks (i.e., \( |R_j - R_i| \)) is greater than the significant difference. If greater, the algorithms are considered different; otherwise, they are considered similar.

Table 8 denotes the Friedman statistics \( F_F \) and the corresponding critical value on each evaluation metric.

The significance level \( CD \) is defined as follows:
\[ CD = q_a \sqrt{\frac{k (k + 1)}{6N}} \quad (17) \]
where \( q_a \) is a critical value for post-hoc tests after the Friedman test.

Owing to the existence of 6 algorithms and 10 datasets, \( F_F \) obeys the \( F \)-distribution with degrees of freedom of \( 6 - 1 = 5 \) and \( (6 - 1) \times (10 - 1) = 45 \). \( F(5, 45) = 2.42 \) at \( \alpha = 0.05 \). Thus, we reject the original null hypothesis, i.e., the six algorithms are considered to be significantly different.

Then, we use the Bonferroni-Dunn test with LTSA-LE as the control algorithm to test whether other algorithms are significantly different from LTSA-LE. From Table 9 we can find that when six algorithms exist, \( q_{0.05} = 2.576 \); thus \( CD = 2.576 \sqrt{\frac{6 \times (6 + 1)}{6 \times 10}} = 2.155 \).

In Table 2, the difference between the average ranks between CPNN and LTSA-LE is \( 5.950 - 1.900 = 4.050 > 2.155 \). Thus, we think that CPNN and LTSA-LE are significantly different. The difference between the average ranks of the other four algorithms (BP-MLL, ML\(^2\), LDSVR, and AA-KNN) and LTSA-LE < 2.155, which is not significantly different. Thus, we can approximate an improvement of these algorithms from LTSA-LE.

### 4.5 Experimental results on LDL

We conduct quantitative analysis on the performance of four LDL algorithms on the datasets in Table 10. Tables 10 – 15 provide the comparison results of various types of LDL algorithms on six evaluation metrics: Cheb, Clark, Canber, KL-div, Cosine, and Intersee, respectively. As described in Section 4.1, we calculate the average ranks of the corresponding algorithms based on the six metrics in the last row of each table (bold font indicates the best performance on each dataset). We obtain the rankings of the algorithms on six measures according to their average ranks, LTSA-LE > CPNN ≈ LDSVR > AA-KNN.

As the results show, LTSA-LE performs best on all six measures. The reason might be that applying the kernel technique allows LTSA-LE to solve the problem of higher dimensionality and therefore obtain a

| Evaluation metric | \( F_F \) | Evaluation metric | \( F_F \) |
|-------------------|----------|-------------------|----------|
| Hamming loss      | 9.50     | Coverage          | 6.25     |
| Ranking loss      | 12.29    | Average precision | 16.38%   |
| One error         | 3.91     | Time              | 2.75 s   |

Table 8 Friedman statistics \( F_F \) in terms of each evaluation metric, the critical value is 2.42 when the significance level is 0.05 (the number of comparing algorithms, \( k \) is 6 and the number of datasets, \( N \) is 10).

| Number of classifiers | \( q_{0.05} \) | \( q_{0.10} \) | Number of classifiers | \( q_{0.05} \) | \( q_{0.10} \) |
|----------------------|--------------|--------------|----------------------|--------------|--------------|
| 2                    | 1.960        | 1.645        | 7                    | 2.638        | 2.394        |
| 3                    | 2.241        | 1.960        | 8                    | 2.690        | 2.450        |
| 4                    | 2.394        | 2.128        | 9                    | 2.724        | 2.498        |
| 5                    | 2.498        | 2.241        | 10                   | 2.773        | 2.539        |
| 6                    | 2.576        | 2.326        |                       |              |              |

Table 9 Critical values for post-hoc tests after the Friedman test.

The average rank

| Dataset                | LDSVR | CPNN | AA-KNN | LTSA-LE |
|------------------------|-------|------|--------|---------|
| Yeast-alpha            | 0.0080| 0.0073| 0.0090 | 0.0073  |
| Yeast-cdc              | 0.0141| 0.0138| 0.0229 | 0.0083  |
| Yeast-elu              | 0.0267| 0.0262| 0.0189 | 0.0078  |
| Yeast-diau             | 0.0414| 0.0505| 0.0572 | 0.0194  |
| Yeast-heat             | 0.0481| 0.0504| 0.0669 | 0.0118  |
| Yeast-spo              | 0.1774| 0.1969| 0.1830 | 0.0268  |
| Yeast-cold             | 0.0773| 0.0727| 0.0833 | 0.0172  |
| Yeast-dtt              | 0.0417| 0.0436| 0.0543 | 0.0074  |
| Yeast-spo5             | 0.1722| 0.1751| 0.2006 | 0.0491  |
| Yeast-spoem            | 0.3369| 0.2869| 0.1512 | 0.0125  |
| Human Gene             | 0.0179| 0.0202| 0.0140 | 0.0130  |
| Natural Scene          | 0.4045| 0.1877| 0.2473 | 0.1291  |
| Movie                  | 0.1697| 0.1420| 0.1544 | 0.1359  |
| s-JAFFE                | 0.1300| 0.1416| 0.1183 | 0.0576  |
| s-BU_3DFE              | 0.1790| 0.1745| 0.2229 | 0.0794  |
| Average rank           | 2.97  | 2.77  | 3.23   | 1.03    |
Table 11 Experimental results on real-world datasets measured by the Clark↓.

| Dataset       | LDSVR | CPNN | AA-KNN | LTSA-LE |
|---------------|-------|------|--------|---------|
| Yeast-alpha   | 0.1713| 0.1141| 0.1262 | 0.1021  |
| Yeast-cdc     | 0.2178| 0.2005| 0.2857 | 0.1186  |
| Yeast-eu      | 0.2494| 0.2351| 0.2386 | 0.1024  |
| Yeast-diav    | 0.2890| 0.3287| 0.3393 | 0.0927  |
| Yeast-heat    | 0.2534| 0.2492| 0.3438 | 0.0545  |
| Yeast-spo     | 0.4690| 0.5093| 0.4928 | 0.1204  |
| Yeast-cold    | 0.1979| 0.2077| 0.2392 | 0.0452  |
| Yeast-dtt     | 0.1244| 0.1366| 0.1363 | 0.0181  |
| Yeast-spo5    | 0.4098| 0.4233| 0.4501 | 0.0948  |
| Yeast-spoem   | 0.5671| 0.5117| 0.3180 | 0.0176  |
| Human Gene    | 1.0551| 1.0739| 1.3913 | 0.9660  |
| Natural Scene | 2.3735| 2.1469| 2.1008 | 2.0813  |
| Movie         | 0.7311| 0.6558| 0.5541 | 0.4177  |
| s-JAFFE       | 0.3860| 0.5163| 0.3324 | 0.2401  |
| s-BU_3DFE     | 0.4379| 0.4457| 0.5710 | 0.2573  |

Average rank 2.87 2.93 3.20 1.00

Table 12 Experimental results on real-world datasets measured by the Canber↓.

| Dataset       | LDSVR | CPNN | AA-KNN | LTSA-LE |
|---------------|-------|------|--------|---------|
| Yeast-alpha   | 0.5686| 0.3792| 0.4057 | 0.3315  |
| Yeast-cdc     | 0.7528| 0.6780| 0.9368 | 0.3230  |
| Yeast-eu      | 0.7263| 0.7003| 0.6932 | 0.3064  |
| Yeast-diav    | 0.6489| 0.7181| 0.7262 | 0.1648  |
| Yeast-heat    | 0.5499| 0.5282| 0.7659 | 0.1114  |
| Yeast-spo     | 0.9634| 1.0667| 0.9917 | 0.2340  |
| Yeast-cold    | 0.3574| 0.3990| 0.4401 | 0.0723  |
| Yeast-dtt     | 0.2436| 0.2709| 0.2184 | 0.0296  |
| Yeast-spo5    | 0.5826| 0.5843| 0.6554 | 0.1505  |
| Yeast-spoem   | 0.7600| 0.6749| 0.3972 | 0.0249  |
| Human Gene    | 1.0551| 1.0739| 1.3913 | 0.9660  |
| Natural Scene | 2.3735| 2.1469| 2.1008 | 2.0813  |
| Movie         | 0.7311| 0.6558| 0.5541 | 0.4177  |
| s-JAFFE       | 0.3860| 0.5163| 0.3324 | 0.2401  |
| s-BU_3DFE     | 0.4379| 0.4457| 0.5710 | 0.2573  |

Average rank 2.87 2.93 3.20 1.00

Table 13 Experimental results on real-world datasets measured by KL-div↓.

| Dataset       | LDSVR | CPNN | AA-KNN | LTSA-LE |
|---------------|-------|------|--------|---------|
| Yeast-alpha   | 0.0030| 0.0015| 0.0018 | 0.0012  |
| Yeast-cdc     | 0.0064| 0.0054| 0.0111 | 0.0018  |
| Yeast-eu      | 0.0094| 0.0085| 0.0080 | 0.0015  |
| Yeast-diav    | 0.0198| 0.0258| 0.0273 | 0.0023  |
| Yeast-heat    | 0.0193| 0.0187| 0.0367 | 0.0009  |
| Yeast-spo     | 0.0952| 0.1182| 0.1047 | 0.0048  |
| Yeast-cold    | 0.0201| 0.0219| 0.0290 | 0.0009  |
| Yeast-dtt     | 0.0077| 0.0092| 0.0096 | 0.0001  |
| Yeast-spo5    | 0.0836| 0.0934| 0.1144 | 0.0057  |
| Yeast-spoem   | 0.2484| 0.1858| 0.0538 | 0.0003  |
| Human Gene    | 0.0355| 0.0355| 0.0594 | 0.0285  |
| Natural Scene | 1.4482| 0.6021| 0.6874 | 0.5503  |
| Movie         | 0.0955| 0.1190| 0.0994 | 0.0688  |
| s-JAFFE       | 0.0619| 0.1073| 0.0473 | 0.0206  |
| s-BU_3DFE     | 0.0925| 0.0809| 0.1625 | 0.0252  |

Average rank 2.83 2.83 3.33 1.00

Table 14 Experimental results on real-world datasets measured by the Cosine↑.

| Dataset       | LDSVR | CPNN | AA-KNN | LTSA-LE |
|---------------|-------|------|--------|---------|
| Yeast-alpha   | 0.9971| 0.9985| 0.9981 | 0.9988  |
| Yeast-cdc     | 0.9935| 0.9946| 0.9893 | 0.9982  |
| Yeast-eu      | 0.9904| 0.9913| 0.9921 | 0.9985  |
| Yeast-diav    | 0.9832| 0.9778| 0.9766 | 0.9978  |
| Yeast-heat    | 0.9821| 0.9826| 0.9648 | 0.9990  |
| Yeast-spo     | 0.9032| 0.8815| 0.8944 | 0.9952  |
| Yeast-cold    | 0.9803| 0.9785| 0.9710 | 0.9990  |
| Yeast-dtt     | 0.9925| 0.9909| 0.9903 | 0.9998  |
| Yeast-spo5    | 0.9310| 0.9268| 0.9075 | 0.9945  |
| Yeast-spoem   | 0.8293| 0.8808| 0.9556 | 0.9997  |
| Human Gene    | 0.9647| 0.9639| 0.9420 | 0.9717  |
| Natural Scene | 0.4386| 0.7315| 0.6838 | 0.7690  |
| Movie         | 0.9371| 0.9225| 0.9205 | 0.9364  |
| s-JAFFE       | 0.9360| 0.8879| 0.9482 | 0.9791  |
| s-BU_3DFE     | 0.9018| 0.9147| 0.8432 | 0.9739  |

Average rank 2.73 2.80 3.40 1.07

5 Conclusion

We studied a label-enhanced algorithm based on manifold. According to the optimization theory, we established the unconstrained optimization model of MSVR and provided the adaptively adjusted maximum entropy function to solve the model. The function is based on the characteristics of the original model quadratic programming problem and transforms the original objective function into an unconstrained optimization problem according to the optimization.
principle. To avoid the numerical overflow phenomenon in the standard maximum entropy function, we proposed an MSVR model for adaptively adjusting the Shannon entropy function.

We state the convergence of the model and solve it with the quasi-Newton method, which is particularly suitable for problems with a large number of sample points. Extensive experimental results using real-world multilabel datasets show that the algorithm can effectively improve the training speed and prediction accuracy of multilabel datasets.

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